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Two-phase flow numerical simulation with real-gas effects and occurrence of rarefaction shock waves

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HIGHLIGHTS

- A reduced five equation model is used and discretized through the Discrete Equations Method (DEM), assuming no mass and heat transfer.
- The system is coupled with a mixture equation of state (EOS), formulated for a general EOS, thus permitting real EOS-SG based mixture.
- We assess the importance of using a complex EOS for temperature estimation in a two-phase flow.
- Occurrence of a rarefaction shock wave (RSW) in a two-phase flow is assessed for the first time in the literature.
- We study the sensitivity of the RSW with respect to the initial conditions and to the thermodynamic model.

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ABSTRACT

A discrete equation method (DEM) for the simulation of compressible multiphase flows including real-gas effects is illustrated. A reduced five equation model is obtained starting from the semi-discrete numerical approximation of the two-phase model. A simple procedure is then proposed for using a more complex equation of state, thus improving the quality of the numerical prediction. Classical test-cases well-known in literature are performed featuring a strong importance of thermodynamic complexity for a good prediction of temperature evolution. Finally, a computational study on the occurrence of rarefaction shock waves (RSW) in a two-phase shock tube is presented, with dense vapors of complex organic fluids. Since previous studies have shown that a RSW is relatively weak in a single-phase (vapor) configuration, its occurrence and intensity are investigated considering the influence of the initial volume fraction, initial conditions and the thermodynamic model.

1. Introduction

In many engineering applications, the working fluid is made of two or more non-mixable fluids, thus the modeling of multiphase flows is of primary importance. A major issue remains how to model the interface between two fluids with different thermodynamic properties. Inaccurate physical models, in particular from a thermodynamic point of view, can degrade the accuracy of the numerical simulation. Actually, in many works of interface problems, very simple equations of state (EOSs) are used for both phases.

Several methods have been proposed in the literature for solving multiphase flows, *i.e. Lagrangian methods*, *Arbitrary Lagrangian–Eulerian methods (ALE)*, the *Level set method*, *etc.*, see for example [1–3]. Another class of method is known as *diffusive interface models* [4–7]. They consist in hyperbolic systems of partial differential equations, where each phase is governed by their own equations of state in order to determine their thermodynamic behavior in time. In many cases, in particular when the interface between the phases is not isolated, the system, after the modelization step, cannot be written in conservation form. From a physical point of view, this is a problem because the particular form of these non-conserved terms is very *model closure* dependent. From the mathematical point of view, this is also a problem because the numerical discretization becomes very dependent on the structure of the numerical dissipation, as shown among others by [8].

The discrete equation method (DEM) allows a clear treatment of non-conservative terms because it mimics all the modelization steps, starting from first principle as the Godunov method [9], applying averages procedures (here statistical ones), and a modelization step which is similar to what is done in standard finite volume schemes. With the DEM, each phase is compressible and behaves according to a convex EOS. The *Stiffened Gas* (SG) EOS is usually used [6,10–12]. The reason, as explained in [13,14], is that this EOS allows an explicit mathematical calculations of important flow relation. Moreover, in mass transfer problems it assures the positivity of speed of sound in the two-phase region, under the saturation curve.

When complex fluids are considered, such as cryogenic, molecularly complex ones, the use of simple EOS can produce imprecise estimation of the thermodynamic properties, thus leading to the deterioration of the accuracy of the prediction. Increasing the complexity of the model and calibrating the additional parameters with

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respect to the available experimental data are certainly valid options for improving the model prediction. Nevertheless, this is very challenging because of the numerical difficulties for the implementation of more complex mathematical model and because of the large uncertainties that generally affect the experimental data.

The aim of this paper is twofold: (i) to show how the numerical solver based on a DEM formulation can be modified to include more complex equations of state for the vapor region, (ii) to apply the proposed procedure to a particular application: the simulation of a rarefaction shock wave (RSW) in a multiphase flow. In a forthcoming paper, we will study the coupling of this method with Uncertainty Quantification tools, in order to have a better understanding of the effect of not knowing very accurately the EOS coefficients on the structure of the solutions.

The method used in this paper is the DEM (see [6]) for the resolution of a reduced five equation model with the assumption of pressure and velocity equilibrium [15], without mass and heat transfer. This formulation is obtained by an asymptotic development of the scheme for the resolution of a seven equation model, relaxing the phase pressure and velocity, in order to obtain the dynamic equilibrium, *i.e.* the single mixture pressure and velocity. This development is able to deal with non-thermodynamic equilibrium between the phases and to consider two completely different states [6,15,16].

In this paper, three thermodynamic models are considered: the SG EOS, the Peng–Robinson (PRSV) EOS, and the Span–Wagner (SW) EOS. While SG allows to preserve the hyperbolicity of the system also in the spinodal zone, real-gas effects can be taken into account by using more complex equations (such as PRSV or SW). In this paper, no mass transfer effect is taken into account, thus PRSV and SW equations can be used only to describe the vapor behavior, while the SG model is used for describing the liquid. In the five equations model, the main challenge of the EOS coupling is the mixture pressure formulation that must be modified in order to take into account the contribution of both phase pressures weighted with respect to the phase volume fraction.

After validating the proposed procedure, we focus on a particular application: we are interested in using the simulation of two-phase flows for providing a numerical evidence of non-classical gas-dynamic effects in flows of mixtures of liquid/dense vapors [17–19]. Phenomena such as rarefaction shock waves and compression fans are theoretically admissible for transonic flows of dense vapors of substances formed by complex organic molecules. Fluids that might exhibit non-classical gas-dynamic phenomena are called BZT fluids from the name of the three scientists, Bethe–Zel'dovich–Thompson, who first theorized their existence [17–19]. These anomalous gas-dynamic behaviors are predicted provided that the flow encompasses fluid thermodynamic states for which the fundamental derivative of gas-dynamics $\Gamma = 1 + \frac{\rho}{a}\left(\frac{\partial a}{\partial \rho}\right)_s$ [1] is negative. Several suitable fluid thermodynamic models predict Γ to be negative in the superheated vapor region close to saturation and to the vapor–liquid critical point of complex organic molecules, see, e.g., [20]. Such a region is often referred to as the *inversion zone* and the $\Gamma = 0$ contour is called the *transition line*. Non-classical gas-dynamic effects could be exploited to considerably increase the efficiency of supersonic turbines for small-capacity Organic Rankine Cycle power systems [21].

An attempt to experimentally prove for the first time the existence of non-classical gas-dynamics is underway at the Delft University of Technology. A newly realized shock tube [22] will be used to generate a rarefaction shock wave (RSW) in the dense vapor of a siloxane fluid at high reduced temperature and pressure. A major problem emerged from several studies [23–26]:

1. if non-classical gas-dynamic effects do exist, they are relatively weak, compared, for instance, to compression shock waves,
2. they can occur only if the experimental conditions are controlled within a relatively small range of pressures and temperatures.

A recent study [27] has dealt with the quantification of uncertainties in the results of simulations of the TU Delft dense gas shock tube experiments in order to correctly determine the level of accuracy needed to set the initial experimental conditions. The objective was therefore the maximization of the probability of actually observing the expected non-classical RSW. In this work, unfortunately, the requirements on the experimental uncertainties seemed hardly achievable, thus demanding a stronger effort for controlling the experiment.

For these reasons, the idea explored in this work is to estimate the reproducibility of the rarefaction shock wave in a two-phase flows, since it could represent a valid alternative option for setting up another experience. To the best of our knowledge, it is the first attempt to verify the numerical evidence of a RSW in a multiphase flow.

This paper is organized as follows. In Section 2, a description of the reduced five equation model is illustrated. We derive the DEM approximation of the seven equation model and then, the asymptotic expansion is proposed to obtain a semi-discrete approximation for a reduced five-equation model as in [15]. Then, in Section 2.3, we describe the SG, PRSV and SW EOS for the pure fluid, thus deriving the thermodynamic properties of mixture, assuming SG EOS for all phases and PRSV and SW EOS only for the vapor phase. The Section 3 presents several results. First, the implementation of the complex equation of state is validated by reproducing a quasi-single-fluid shock tube, *i.e.* considering a very reduced liquid fraction. Secondly, the code is validated against some well-known two-phase test-cases in the literature. Moreover, the influence of using a more complex equation of state is analyzed by considering several operating conditions close to the saturation curve. Finally, the numerical evidence of a rarefaction shock wave in a two-phase flow is demonstrated, displaying also the sensitivity with respect to the volume fraction and the thermodynamic model.

2. Problem statement

The computations presented in this work rely on a five-equation model with pressure and velocity equilibrium. A discrete equations method (DEM) is used for its discretization [6,15].

We recall the main lines of the scheme. First, we illustrate how to obtain the reduced model. Then, the final numerical scheme with the thermodynamic closure is presented step by step.

2.1. From seven to five-equation model

Let us introduce the two-phase model without heat and mass transfer in one-dimension. It can be written as follows:

$$\begin{cases} \dfrac{\partial}{\partial t}\alpha_k + v_I \dfrac{\partial}{\partial x}\alpha_k = \mu(P_k - P_{k^*}) \\ \dfrac{\partial}{\partial t}(\alpha_k\rho_k) + \dfrac{\partial}{\partial x}(\alpha_k\rho_k v_k) = 0 \\ \dfrac{\partial}{\partial t}(\alpha_k\rho_k v_k) + \dfrac{\partial}{\partial x}(\alpha_k\rho_k v_k^2 + \alpha_k P_k) \\ \quad = P_I \dfrac{\partial}{\partial x}\alpha_k + \lambda(v_{k^*} - v_k) \\ \dfrac{\partial}{\partial t}(\alpha_k\rho_k E_k) + \dfrac{\partial}{\partial x}(\alpha_k(\rho_k E_k + P_k)v_k) \\ \quad = P_I v_I \dfrac{\partial}{\partial x}\alpha_k + \lambda v_I(v_{k^*} - v_k) + \mu P_I(P_k - P_{k^*}), \end{cases} \quad (1)$$

[1] With ρ the fluid density, a the sound speed and s the entropy.