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Abstract. Two diffuse interface models for compressible two-phase flows including phase transfer are presented. The first one is based on conservation laws for mixture variables with an additional equation for the void ratio in which the mass transfer appears explicitly in the source term. The second one is fully conservative and a relaxation model is built to introduce the mass transfer between phases. The stiffened-gas equation of state is used for calculating thermodynamic properties. Simulation results from expansion tube cases with cavitation are presented.

INTRODUCTION

The simulation and the accurate prediction of cavitation hold paramount significance in the efficient design and performance enhancement of various engineering applications, including fuel injectors, propellers, and turbomachinery. Modelling these complex flows for simulation purposes presents a challenge due to the intricate interplay between the two phases and the mass transfer phenomena involved. Furthermore, the presence of non-equilibrium thermodynamic effects and the potential emergence of metastable states, such as superheated liquid, during the mass transfer process, underscores the criticality of accurately modelling phase transitions.
To address these complexities, various physical and numerical models have been developed to investigate cavitating flows within the framework of averaged models. The choice of approach depends on the underlying assumptions, from two-fluid to one-fluid models. Within this modelling hierarchy, the number of equations employed can vary widely, ranging from the seven-equation model capturing full non-equilibrium effects to a simplified three-equation model known as the homogeneous equilibrium model (HEM).
In the present paper, we compare two formulations for the mass transfer between phases based on four-equation models. The first one consists in three conservation laws for mixture mass, mixture momentum and total energy with a supplementary equation for the void ratio. To account for mass transfer, which explicitly appears in the source term, it is assumed to be proportional to the divergence of the mixture velocity [1, 2]. The second one is based on two mass balance equations, mixture momentum and total energy. A relaxation model is derived to drive the system to thermodynamic equilibrium to include the effects of mass transfer due to phase transition. We implemented an algebraic relaxation system as outlined by Pelanti and Shyue [5] on their six-equation system. For both PDE systems, a mixture of stiffened gas is considered for the equation of state (EOS) in the mixture. Viscous effects are non considered and the nature of systems is fully hyperbolic.

MODELS AND EQUATIONS

The numerical simulations are carried out using a two-phase code solving various compressible inviscid systems. We aim for a model which incorporates phase transfer as simple as possible and different assumptions are done:

1. Phases have equal velocities, i.e. a homogeneous flow model,
2. Phases are in thermal equilibrium, i.e. one-temperature model,
3. Phases are in mechanical equilibrium, i.e. one-pressure model.

Surface tension effects are dominated by inertia and are thus neglected.

The first model consists in three conservation laws for mixture quantities (mass, momentum and total energy) and an additional equation for the void fraction

$$\frac{\partial \rho}{\partial t} + \text{div}(\vec{V}) = 0 \tag{1}$$

$$\frac{\partial (\rho \vec{V})}{\partial t} + \text{div}(\rho \vec{V} \otimes \vec{V} + P I_{\text{d}}) = 0 \tag{2}$$

$$\frac{\partial (\rho E)}{\partial t} + \text{div}(\rho \vec{V} H) = 0 \tag{3}$$

$$\frac{\partial \alpha}{\partial t} + \vec{V}.\text{grad}(\alpha) = \underbrace{\left(\frac{\rho_l c_l^2 - \rho_v c_v^2}{\frac{\rho_l c_l^2}{1-\alpha} + \frac{\rho_v c_v^2}{\alpha}} \right)}_{=K} \text{div}\, \vec{V} + \underbrace{\left(\frac{\frac{c_v^2}{\alpha} + \frac{c_l^2}{1-\alpha}}{\frac{\rho_l c_l^2}{1-\alpha} + \frac{\rho_v c_v^2}{\alpha}} \right)}_{= 1/\rho_I \, the \, interfacial \, density} \dot{m} \tag{4}$$

where $\vec{V} = (u, v)$ is the center of mass velocity vector, $E = e + V^2/2$ the mixture total energy and $H = h + V^2/2$ the total enthalpy. Subscripts 'l' and 'v' denote liquid and vapor, respectively. The term K involves the speed of sound of pure phases c_k and it reflects the effects of changes in volume of each phase. The mass transfer $\dot{m}$ is closed assuming its proportionality to the divergence of the velocity [1, 2]

$$\dot{m} = \frac{\rho_l \rho_v}{\rho_l - \rho_v} \left(1 - \frac{c_{EOS}^2}{c_{Wallis}^2} \right) \text{div}(\vec{V}) \qquad \text{with} \qquad \frac{1}{\rho c_{Wallis}^2} = \frac{\alpha}{\rho_v c_v^2} + \frac{1-\alpha}{\rho_l c_l^2} \tag{5}$$

where c_{EOS} is the mixture speed of sound given by the EOS activated when the local pressure P is smaller than the saturation pressure $P_{sat}(T)$ and c_{Wallis} is the speed of sound without mass transfer. In the following, this model will be denoted as 4-equation-alpha model.

The second model consists of two mass balance equations and conservation equations for the momentum and total energy. It will be denoted 4-equation-relax model in the following.

$$\frac{\partial (1-\alpha)\rho_l}{\partial t} + \text{div}((1-\alpha)\rho_l \vec{V}) = \dot{m} \tag{6}$$

$$\frac{\partial \alpha \rho_v}{\partial t} + \text{div}(\alpha \rho_v \vec{V}) = -\dot{m} \tag{7}$$

$$\frac{\partial (\rho \vec{V})}{\partial t} + \text{div}(\rho \vec{V} \otimes \vec{V} + P I_{\text{d}}) = 0 \tag{8}$$

$$\frac{\partial (\rho E)}{\partial t} + \text{div}(\rho \vec{V} H) = 0 \tag{9}$$

Physically, differences in the chemical potentials of the two phases, represented by the Gibbs free energy $g = h - Ts$, induce a mass flow from one phase to another, following the gradient of diminishing chemical potential. Consequently, we aim to incorporate a phase transfer term in the following form:

$$\dot{m} = \lambda (g_l - g_v) \tag{10}$$

When the parameter $\lambda \to \infty$, we reach an equilibrium model wherein phase transfer occurs instantaneously, meaning the phases share the same chemical potential. In this limit, the model (6)–(9) can be expressed as the four-equation system without source term.
The system is solved is two steps: firstly we solve the system without mass transfer to obtain variables $(\alpha, \rho, u, P, T)^0$ and then the system including the source term is solved assuming the total energy and momentum conservation during the relaxation process. The system can be simplified to solve a single equation involving one variable, such as the equilibrium pressure denoted as P^*. The determination of the saturation temperature T_{sat} involves solving the non-linear $P - T$ saturation curve, which is obtained by applying the equilibrium condition to the Gibbs free energy $g_l = g_v$ (see [5]).

The PDE systems are discretized through the finite-volume method. Numerical fluxes are computed with a HLLC scheme combined with the Hancock-MUSCL approach in order to obtain the second-order in both time and space. More details can be found in [2].

NUMERICAL TESTS

CO2 depressurisation without mass transfer

We consider the case of the depressurisation of a pipe of length $L = 80$ m containing CO_2 as proposed by Lundt and Aursand [4]. Initially, the left part of the pipe ($x < 50$ m) contains liquid at pressure $P = 60$ bar, while the right part is filled of gas at pressure $P = 10$ bar. The initial temperature is $T_0 = 273$ K and the fluid is at rest ($u = 0$ m/s).
During the process, a rarefaction wave will travel in the leftward direction starting from $x = 50$ m, while a shock wave will propagate towards the right. Figure 1 shows the results (in logarithmic scale) at time $t = 80$ ms compared with the exact solution. The five-equation model derived from the works of Kapila et al. [3] is added for the comparison. All results are in close agreement with the analytical solution.

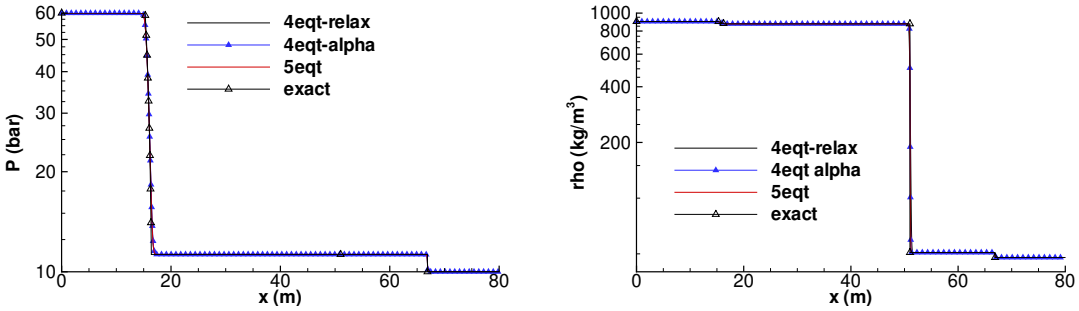

FIGURE 1. CO_2 depressurisation without mass transfer, models comparison, $t = 80$ ms. Pressure and density profiles.

Water-gas mixture expansion tube with cavitation, $|u| = 2$ m/s

We consider the case of the double expansion tube problem for which an initial velocity discontinuity is located at the middle of the tube. The tube is filled of water at the reference temperature $T = 354.78$ K. A small volume fraction of vapor α =0.01 is initially added to the liquid. The vapour pressure at the reference temperature is $P_{sat} = 51000$ Pa. This case was computed by different authors to validate mass transfer models [6, 7]. The mesh contains 4000 cells. The time step is set to 10^{-7} s. Liquid water undergoes expansion until it reaches the saturation pressure, leading to evaporation with the formation of a small amount of vapor. This phase-transition process involves a total of four expansion waves, with the additional two expansion waves specifically corresponding to the evaporation fronts.

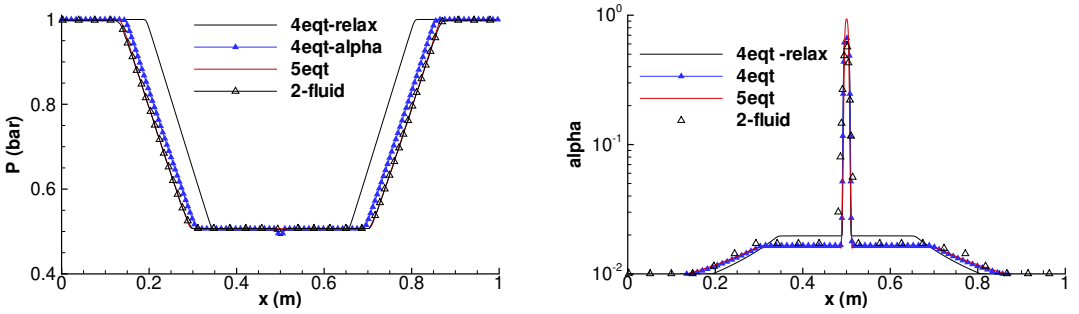

FIGURE 2. Water-gas double rarefaction with cavitation, $|u| = 2$ m/s, models comparison, $t = 3.2$ ms. Pressure and void ratio profiles.

Solutions are shown in Figure 2 at time t =3.2 ms. The pressure profiles are in very close agreement with the two-fluid solution of Zein et al. [7] except for the 4-equation-relax model where the position of the expansion waves are shifted, certainly due to small differences in the speed of sound in the mixture. The void ratio profiles are plotted with a logarithmic scale. We clearly observe that the two evaporation fronts are well captured by all models. Small discrepancies appear on the maximum value of the void fraction at mid-tube.

Water-gas mixture expansion tube with cavitation, $| u |= 100$ m/s

The same conditions are considered except regarding velocities which are set to $| u |= 100$ m/s leading to a more intense evaporation process. A large cavitation pocket containing a mixture at thermodynamic equilibrium is generating in the middle of the tube. The mesh contains 4000 cells and the time step is set to 10^{-7} s. The saturation pressure is assuming to vary linearly with the temperature for the 4-equation-alpha model.

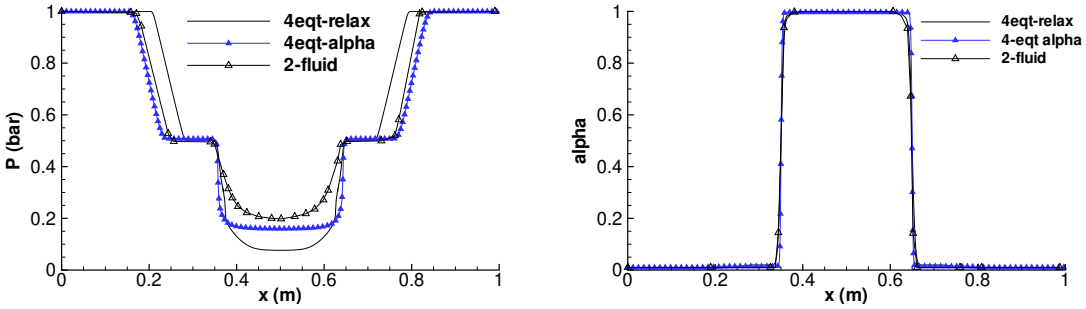

FIGURE 3. Water-gas double rarefaction with cavitation, $|u| = 100$ m/s, models comparison, $t = 1.5$ ms. Pressure and void fraction profiles.

Models are compared in Figure 3, at time $t = 1.5$ ms. As observed previously, the position of the expansion waves is shifted using the 4-equation-relax model. The evaporation fronts are well predicted by both models. Yet, discrepancies are noticed for the pressure decrease inside the cavitation pocket, the evolution being more abrupt using the 4-equation models. The void ratio profiles are in close agreement with the 2-fluid solution for both models.

CONCLUSION AND PERSPECTIVES

Two formulations of mass transfer between phases are compared through test-cases based on rarefaction waves leading to a phase transition. An empirical formulation assuming that the mass transfer is proportional to the divergence of the velocity and a relaxation model with an infinite rate are integrated in a finite volume solver. Both models are able to well predict the evaporation fronts. Yet, a small gap appears on the expansion waves position certainly due to differences on the mixture speed of sound.

ACKNOWLEDGMENTS

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