

A Numerical Study of Compressible Two-Phase Flows Shock and Expansion Tube Problems

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ABSTRACT

A compressible and multiphase flows solver has been developed for the study of one-dimensional shock and expansion tube problems. This solver has a structure similar to those of the one-fluid Euler solvers, differing from them by the presence of a void ratio transport-equation. The model and the system of equations to be simulated are presented. Results are displayed for shock and expansion tube problems. Close agreement with reference solutions, obtained from explicit finite volume approaches, is demonstrated for all of the examples. Different numerical methods are additionally displayed to provide comparable and improved computational efficiency to the model and the system of equations. The overall procedure is therefore very well suited for use in general two-phase fluid flow simulations.

Keywords: Two-phase flows, shock and expansion tube problems, homogeneous model, Riemann problem, finite volume, inviscid simulation

Introduction

Theoretical and numerical modeling of two-phase fluid flow problems is of practical importance in many areas of industry such as thermal power generation plants and other interesting phenomena occurring in environmental applications. Despite their relevance in industrial and environmental applications, compressible two-phase flow investigations have remained complex and challenging areas of applied mathematics and computational methods. The most widely used modeling approach is based on averaged two-phase fluid flow model such as the one-fluid formulation. Within such averaged model, there are different approaches according to the physical assumptions of interest made on the local mechanical and thermodynamical equilibrium and to the slip condition between phases. This has resulted in the development of diverse models and system of equations ranging from seven to three equations only. There also have been a number of significant contributions in different areas and applications relevant to two-phase flows. These are very well acknowledged in the scientific literature for which we refer the reader to [2, 5, 9, 19] for further details.

A critical aspect for two-phase simulations concerns the numerical methods of interest and their accuracy problems. The hyperbolic nature of such flows and their characteristic analysis makes the simulation very stiff and challenging. In addition to that, the volume fraction variation across acoustic waves causes difficulties for the Riemann problem resolution particularly in the derivation of approximate Riemann solvers. This is due to the occurrence of the large discontinuities of thermodynamic variables and equations of state involved at material interfaces. As a result, numerical instabilities and spurious oscillations appear through the complete wave structure [1]. The reason for such unusual behavior lies in the numerical dissipation of the methods which reproduce a thermodynamic path that is not correct. This also implies computational failure for Godunov methods which is due to the large decrease of the pressure up to vacuum ghost.

In the present paper, modeling and computer simulations are performed on the basis of Navier-Stokes applications. A four-equation model of the two-fluid model type is considered for the current purpose. The set of equations includes three conservation laws for mixture quantities along with a void ratio transport-equation [6, 7]. This set of equations is solved by means of explicit finite volume techniques based on Jameson, Rusanov, AUSM-type, VF Roe and HLLC Riemann solvers methods. This is followed by computational simulations on one-dimensional inviscid problems to study the behavior of the performed numerical methods. Computational results are then displayed for shock tube and rarefaction problems, including problems of large depression. These test cases establish the ability, accuracy and efficiency of our computational treatment.

Models and Methods

The homogeneous mixture approach is used to model two-phase flows. In addition, the phases are assumed to be in thermal and mechanical equilibrium, that is, both phases share the same temperature T and the same pressure P . The evolution of the two-phase flow can be described by the conservation laws that employ the representative flow properties as unknowns just as in a single-phase problem.

A four-equation model

We consider a reduction form of the five-equation Kapila model [9] under thermal equilibrium between phases. We also assume that the liquid phase is in a saturation state. The model consists of three conservation laws for mixture quantities and an additional equation for the void ratio. The governing equations under consideration are then governed by the following set of partial differential equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \quad (1)$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + P)}{\partial x} = 0 \quad (2)$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho u H)}{\partial x} = 0 \quad (3)$$

$$\frac{\partial \alpha}{\partial t} + u \frac{\partial \alpha}{\partial x} = \underbrace{\left(\frac{\rho_l c_l^2 - \rho_v c_v^2}{\frac{\rho_l c_l^2}{1-\alpha} + \frac{\rho_v c_v^2}{\alpha}} \right)}_{=K} \frac{\partial u}{\partial x} \quad (4)$$

The individual variables are ρ mixture density, u velocity, P pressure, α void fraction, E and H are total energy and enthalpy of the two-phase flow. The source term K involves the speed of sound, c_k , and densities, ρ_k , of pure phases, $k = l, v$. The subscripts v and l indicate the vapor and the liquid phase, respectively. The four equations model form a system of conservation laws having a hyperbolic nature. The eigenvalues of the system are found to be:

$$\lambda_1 = u - c_{wallis}, \quad \lambda_2 = u = \lambda_3, \quad \lambda_4 = u + c_{wallis} \quad (5)$$

where c_{wallis} is the the propagation of acoustic waves without mass and heat transfer [17]. This speed of sound is expressed as a weighted harmonic mean of speeds of sound of each phase:

$$\frac{1}{\rho c_{wallis}^2} = \frac{\alpha}{\rho_v c_v^2} + \frac{1-\alpha}{\rho_l c_l^2} \quad (6)$$

Equation of state

To close the system, an equation of state (EOS) is necessary to link the pressure and the temperature to the internal energy and density. For the pure phases, we have employed the convex stiffened gas EOS. An expression for the pressure and the temperature can be deduced from the thermal and mechanical equilibrium assumption (see [13], and references therein, for details).

Numerical methods

In this short paper, the finite volume techniques are performed on the basis of the Riemann problem. In one-dimensional space, the conservative part of the four-equation model can be represented in a matrix form as:

$$\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} = 0 \quad (7)$$

$$\frac{\partial \alpha}{\partial t} + u \frac{\partial \alpha}{\partial x} = S(W) \quad (8)$$

Here W is the vector of conserved variables, F and S are the convective flux and the source term that includes the void ratio equation given in (4). These vectors are defined by

$$W = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix} \quad \text{and} \quad F = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho u H \end{pmatrix}$$

Based on finite volume techniques, the computational cells involve the discretization of the spatial domain x into regular meshes of length Δx and the temporal domain t into intervals of duration Δt . A discrete form of equations (7) and (8) can be written as:

$$\Delta x \frac{W_i^{n+1} - W_i^n}{\Delta t} + F_{i+1/2}^n - F_{i-1/2}^n = S_i^n \Delta x \quad (9)$$

where the time step should fulfill the CFL condition in order to guarantee stability requirement and $F_{i+1/2}^n$ is the numerical flux through the cell interface. This numerical flux can be computed using the solution of the Riemann problem or any other numerical method of interest where the resolution of the Riemann problem is fully numerical.

Various formulations of numerical flux have been proposed to solve multiphase compressible flows. See for instance [18] or [14], and references therein, for such formulations and extensions. In the present study, we have tested and compared five documented formulations, namely, the Jameson-Schmidt-Turkel scheme [8], an AUSM-type scheme [4], the Rusanov scheme [12], the HLLC scheme [16] and a VF Roe non-conservative scheme [3].

Computational Results on One-Dimensional Two-Phase Flow Problems

In this section we exhibit the ability of the current four-equation model, convergence and computational performance of the proposed numerical methods on two groups of two-phase flow problems. In the first group, we considered two shock tube problems to validate the current numerical tool. A comparison with solutions provided with a seven-equation model using the Discrete Equations Method (DEM) is proposed [15]. In DEM approach, the pure fluids are first integrated at the microscopic level and then the discrete formulae are averaged. The obtained continuous model of multiphase flow is equivalent to the Baer-Nunziato model. The infinite rate relaxation procedures are used to correctly treat the full system. The second group tests the expansion tube, double rarefaction, problems which are very stiff cases for numerical methods. Results of the expansion tube problems are validated with other models as we shall see later.

Water-gas mixture shock tube

This test case is proposed in [10], computed with five- and seven-equation models. A one meter shock tube involves a discontinuity of the volume fraction. For $x < 0.7$ the gas volume fraction is 0.2, while it is 0.8 otherwise. The fluids are governed by the stiffened gas EOS and are initially at rest. The left chamber contains high pressure fluids (10^9 Pa) while the right one contains low pressure fluids (10^5 Pa). The parameters of EOS are:

$$\begin{pmatrix} \gamma \\ P_\infty \\ \rho \end{pmatrix}_{Liq} = \begin{pmatrix} 4.4 \\ 6.10^8 \\ 1000 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \gamma \\ P_\infty \\ \rho \end{pmatrix}_{Gas} = \begin{pmatrix} 1.4 \\ 0 \\ 1 \end{pmatrix}$$

Computations have been performed with a mesh of 1000 cells and with a time step of 10^{-7} s. Results are shown at time $0.2 \mu s$ in Fig. 1 for all numerical methods. Profiles of void ratio and pressure. Near discontinuities, the Jameson scheme produced small oscillations of the solution. For the void ratio profile, we observe a small discrepancy in the post-shock area around $x = 0.85$ m. The solution obtained with the Rusanov and AUSM methods present a small variation, not captured by other methods.

In comparison with the seven-equation model, the pressure curve is quite similar. Yet, we notice some differences between the solutions in the volume fraction profile. In particular, the post-shock values of the void ratio are not the same and the seven-equation model shows an oscillation near the contact discontinuity zone. This behaviour was also noted in simulations presented in [10].

Epoxy-spinel mixture shock tube

In [11] a one meter tube contains two chambers separated at $x = 0.6$ m. A mixture of epoxy and spinel fills both chambers. The initial volume fraction of epoxy is 0.5954 everywhere. The left chamber pressure is $2 \cdot 10^{11}$ Pa, while the right chamber is at atmospheric pressure. The fluids are initially at rest. The parameters of EOS are:

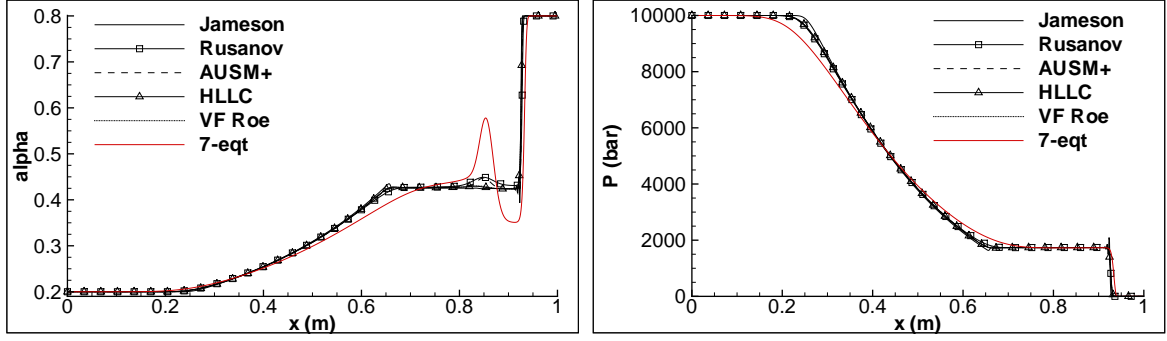


Figure 1. Water-gas shock tube problem. Comparison of different numerical methods comparison on a mesh of 1000 cells at a time of $t = 0.2$ ms. Void ratio and pressure profiles.

$$\begin{pmatrix} \gamma \\ P_\infty \\ \rho \end{pmatrix}_{Epoxy} = \begin{pmatrix} 2.43 \\ 5.3 \cdot 10^9 \\ 1185 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \gamma \\ P_\infty \\ \rho \end{pmatrix}_{Spinel} = \begin{pmatrix} 1.62 \\ 141 \cdot 10^9 \\ 3622 \end{pmatrix}$$

Computations have been performed with a mesh of 1000 cells and with a time step of 10^{-7} s. Numerical solutions computed with the 4-equation model at time $t = 29 \mu s$ are shown in Figure 2. The analytical solution of the equilibrium model proposed in [11] is incorporated for the sake of comparison and validation. Differences between solutions are weak. For the void ratio profiles, the plateau after the shock is less intense with the Rusanov scheme. As previously indicated, the solution computed with the Jameson scheme presents small oscillations near discontinuities. For all methods, the pressure profiles are in close agreement with the analytical solution. Discrepancies appear on the void ratio jump at shock front, which is underestimated by all models, especially the seven-equation model.

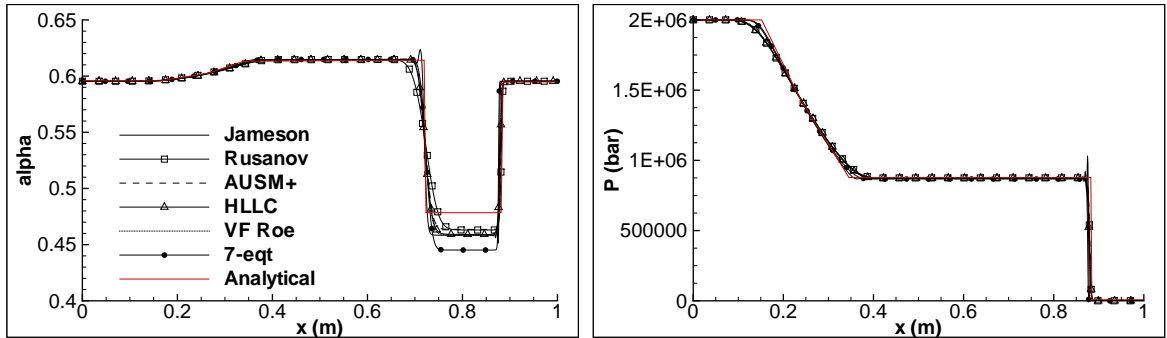


Figure 2. Epoxy-spinel shock tube problem. Different numerical methods comparison on a mesh 1000 cells at time $t = 0.29 \mu s$. Void ratio and pressure profiles.

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

An expansion tube problem is considered with an initial velocity discontinuity located at the middle of the tube. This test consists in a one meter long tube filled with liquid water at atmospheric pressure and with density $\rho_l = 1150 \text{ kg/m}^3$. A weak volume fraction of vapor $\alpha = 0.01$ is initially added to the liquid. The initial discontinuity is set at 0.5 m, the left velocity is -2 m/s and the right velocity is 2 m/s. The solution involves two expansion waves. As gas is present, the pressure cannot become negative. To maintain positive pressure, the gas volume fraction increases due to the gas mechanical expansion and creates a pocket [13].

In Figure 3, the solution obtained is presented at time $t = 3.2$ ms. The mesh contains 1000 cells. The time step is set to 10^{-7} s. The pressure evolution marks large discrepancies. Solutions provided by the Jameson, Rusanov and AUSM+ methods are in close agreement with the two-fluid solution computed in [20]. With the approximate Riemann solvers, the rarefaction waves are badly predicted. A CPU time of 14h was necessary for the two-fluid simulation. With our 4-equation model, using the Rusanov or Jameson scheme, the CPU time is less than five minutes.

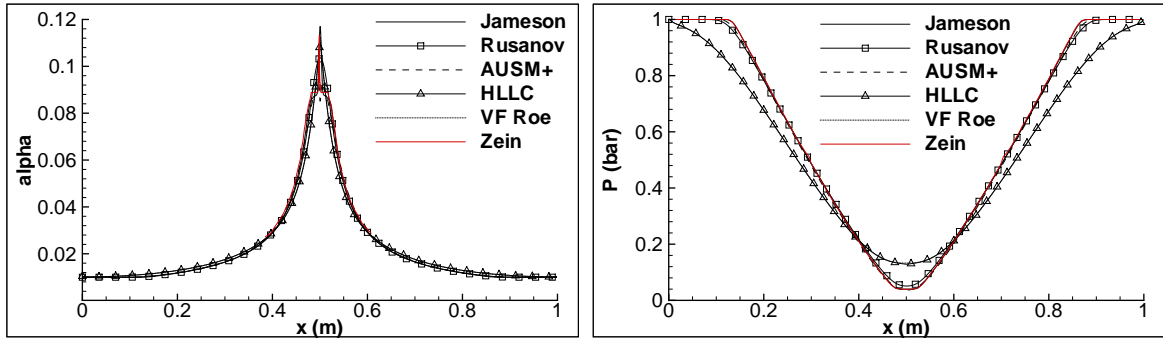


Figure 3. Water-gas expansion tube $|u| = 2$ m/s. Different numerical methods comparison on a mesh of 1000 cells at time $t = 3.2 \mu\text{s}$. Void ratio and pressure profiles.

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

In [13], an expansion tube, double rarefaction, test is considered. A one meter tube filled with pure water is at atmospheric pressure. The density for water is 1000 kg/m^3 . An initial velocity discontinuity is located at $x = 0.5$ m. The velocity of the right part is set as 100 m/s , and the left part as -100 m/s . The EOS parameters are similar to those used for the previous test case. A small volume fraction of gas (1 kg/m^3) is initially present in the water. This case is stiffer than the previous one because of the high value of the initial velocity. Computations are performed on a 1000-cell mesh with a time step set to 10^{-7} s. The approximate Riemann solvers (HLLC and VF Roe) were not able to provide a solution. An anti-diffusive term can be added to the HLLC dissipation to improve the scheme. It has been not tested in the present study.

Figure 4 presents results obtained with the 4-equation model at time $t = 1.85$ ms. The pressure evolution given by the AUSM scheme is not correct. With a grid refinement, the solver leads to divergence. We observe also oscillations on the velocity profiles near the initial discontinuity position. On the contrary, the solutions provided by both the Jameson and Rusanov scheme are in very good agreement with solutions presented in [13].

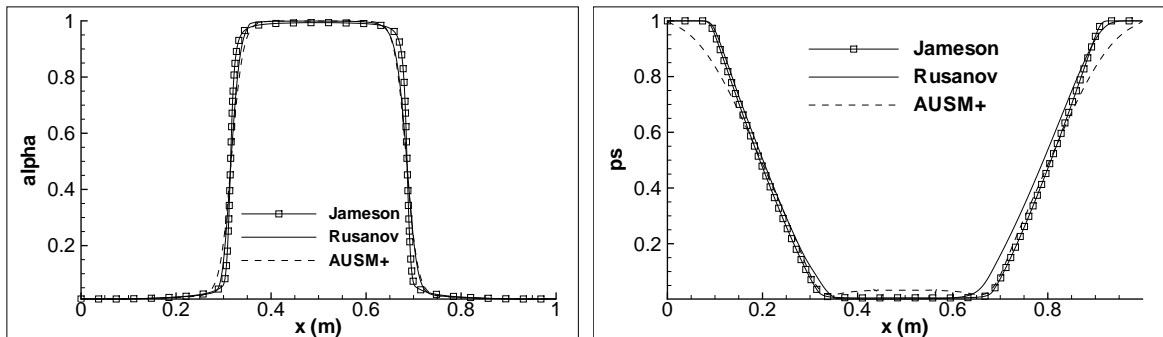


Figure 4. Water-gas expansion tube $|u| = 100$ m/s, numerical methods comparison, mesh 1000 cells, $t = 1.85 \mu\text{s}$. Void ratio and pressure profiles.

Concluding Remarks

This paper provides a comparison of various numerical methods for compressible two-phase flow four-equation model. In its present form, these methods include the AUSM-family, approximate Riemann solvers (VF Roe, HLLC), a simple Godunov approach (Rusanov) and a space-centered scheme with artificial dissipation (Jameson). We then extensively investigated the proposed methods in the existing system of equations on the basis of shock and expansion tube problems. The simulation results suggest the rarefaction waves near the vacuum apparition is more than hard situation for both the approximate Riemann solvers and the AUSM scheme. More specifically, it is not possible to obtain a resolution using these methods. Only the Jameson and Rusanov methods facilitated the simulation of large rarefaction cases.

The presented computational results give considerable confidence in our four-equation model and methods for use as a robust and reliable approach in shock and expansion tube problems of two-phase flows. Room is still available for further work on such problems. For instance, investigation of anti-diffusive terms is needed towards homogeneous and

non-equilibrium two-phase flows.

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