Non-Equilibrium Two-Phase Flow Computations by a Mixture Model

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ABSTRACT

This work presents an assessment of the capabilities of mixture processes to solve two-phase flows developing shocks and discontinuities. The mixture equations are based on a two-phase flow model with full non-equilibrium processes expressed in conservative form. This mixture model is computed by using Godunov-type finite volume methods. A four shock waves test problem is simulated to highlight the performance of the proposed mixture model for one-dimensional compressible two-phase flows. The results from the simulations appear to be qualitatively in agreement with those available in literature.

Keywords: Gas-liquid, Non-equilibrium, Mixture equations, Shock waves, Simulation

Introduction and Equations

The demand for two-phase fluid flow computations and their understanding is growing because of their attractive challenges in both basic research and engineering applications. Two-phase flows investigations have relied comprehensively on either the two-fluid model or homogeneous mixture model types. However, both types are always expensive due to their theoretical and physical nature in addition to their own difficulties [1, 2]. Alternatively, two-phase flows such as gas and liquid can be formulated in terms of mixture parameters of state. In this approach, mixture models are based on non-linear partial differential equations and are able to describe dynamically the evolution of non-equilibrium behaviour between the different phases. See [3, 4] and references therein. These models assume knowledge of several parameters, for instance, the relative motion between phases, and compressibility for all phases can be taken into account. These models also are practical because they contain more information about both the different phases and their combination, i.e., the mixture flow. In this framework, the mixture model consists of equations for the conservation of mixture mass (ρ), conservation of mixture momentum (ρu), conservation of mixture energy (ρE) and a gas void fraction equation $(\rho\alpha)$, a gas mass fraction equation (ρc) and a relative velocity (u_r) between the gas and liquid. These are written in a compact vector form as [5]:

$$\frac{\partial \mathbb{U}}{\partial t} + \frac{\partial \mathbb{F}(\mathbb{U})}{\partial x} = \mathbb{S}, \quad t > 0, \quad x \in \mathbb{R}. \tag{1}$$

where

$$\mathbb{U} = \begin{pmatrix} \rho \\ \rho\alpha \\ \rho u \\ \rho c \\ u_r \\ \rho E \end{pmatrix} \quad \text{and} \quad \mathbb{F}(\mathbb{U}) = \begin{pmatrix} \rho u \\ \rho u\alpha \\ \rho u^2 + P + \rho c(1-c)u_r^2 \\ \rho uc + \rho c(1-c)u_r \\ uu_r + \frac{1-2c}{2}u_r^2 + \psi(P) \\ \rho uE + Pu + \rho c(1-c)u_r\Big(uu_r + \frac{1-2c}{2}u_r^2 + \psi(P)\Big) \end{pmatrix}. \quad (2)$$

In the above, $\mathbb{U}$ is the vector of conservation variables; $\mathbb{F}$ and $\mathbb{S}$ are the mathematical flux function in the x-direction and the vector of source terms assumed to be at this time, respectively. Other notations denote ρ = mixture density, u = mixture velocity, u_r = relative velocity, E = mixture energy, P = mixture pressure, c = gas mass fraction and α = gas void fraction which satisfies $\alpha + (1-\alpha) = 1$. The term ψ links the two phases through the relative velocity equation. The above system has the common form of a conservation law and fulfill an addition conservation law [6, 7]:

$$\frac{\partial}{\partial t}(\rho S) + \frac{\partial}{\partial x}(\rho S u) = Q, \quad (3)$$

which is the conservation of mixture entropy and Q is the entropy introduction. Furthermore, each phase has its own thermodynamics properties described through different equations of state. An often employed equation of state in simulating realistic two-phase problems is the stiffened equations of state (EoS) [8]. This is due to its simplicity and ability to capture strong and weak shock-waves in addition to its resemblance to other equations of state. Thus, the EoS is given by:

$$P_j = K_j\left(\frac{\rho_j}{\bar{\rho}_j}\right)^{\gamma_j} \exp\left(\frac{S_j}{c_{j,v}}\right) - \bar{P}_j,$$

where $\gamma_j, K_j, c_{j,v}, \bar{\rho}_j$ and $\bar{P}_j$ are characteristic constants of the thermodynamic behaviour of each phase and S_j is the entropy of the different phases [6, 7]. This equation becomes the EoS for the gas phase if $\bar{P}$ is set to zero. It is worth noting that the above mixture model is different from the homogeneous relaxation model and the homogeneous equilibrium model. Certainly, the model in hand processes advantages, for instance, the well-posedness and conservativity natures makes of interest to different applications.

Computations and Results

The model equations (1)- (3) constitute a non-linear hyperbolic system written in a conservation form which can be solved by any numerical method of interest. These equations are solved by means of Godunov-type approach where the hyperbolic conservative left hand side is integrated using finite volume, high-resolution, shock-capturing methods. In a finite volume Godunov-type approach, there are mainly central and upwind intercell flux computations which are carried out by a discretization of a spatial computational domain and time computational domain of interest, respectively. In the context of Godunov-type centred methods, this discretization in processes without relaxation takes the following form [9]:

$$\mathbb{U}_i^{n+1} = \mathbb{U}_i^n - \frac{\Delta t}{\Delta x}\Big(\mathbb{F}^n_{i+\frac{1}{2}} - \mathbb{F}^n_{i-\frac{1}{2}}\Big), \quad (4)$$

where $\mathbb{U}_i^n$ denotes the integral average of the solution $\mathbb{U}$ and $\mathbb{F}$ is the numerical flux function which is a scheme-dependent function of the conservative variables. This is the Slope-Limited Centered (SLIC) scheme where the solution of the Riemann problem is fully numerical rather than analytical as in upwind methods. The SLIC scheme is a second-order in time and space and Total Variation Diminishing (TVD) using any limiter of interest. For further work on the SLIC scheme for fluid flow problems see, for example, [9]. To illustrate the type of outputs which the model equations produces for two-phase flow problems, a benchmark test is considered from the literature on the basis of the Riemann problem. Further, the SLIC scheme is employed for the resolution of shock waves problem presented in [7]. For this test problem, CFL $= 0.9$, SUPERBEE limiter along with transmissive boundary conditions are considered in the computational domain of $[-10, 10]$. Finally, simulation results are evaluated by comparing them with other numerical methods that do not depend on the structure of the Riemann problem. Numerical results are presented in figures 1. The results are displayed for three different numerical methods, namely, the Lax-Friedrichs which avoids solving the Riemann problem at every cell interface, First-Order Centered (FORCE) and Total Variation Diminishing (TVD) SLIC methods with 100 coarse grid cells and compared with the reference solution which is provided on a very fine mesh of 5000 cells. Clearly, the results agree well with the reference solutions and with those presented earlier in [7]. It is worth nothing that the relative velocity and different EoS have strong effect on the complete wave structure of this shock waves problem. Finally, the mixture equations together with the mixture entropy provided similar wave structure by the different numerical methods without any source terms effects.

Concluding Remarks

A non-equilibrium fully compressible mixture model is presented and simulated with Riemann problem based methods. Four shock waves problem is tested with liquid water and vapour using real and ideal equations of state. Simulation results show that the mixture formulations together with the mixture entropy can accurately resolve the left and right shocks as well as contact discontinuities. It is observed that the model in hand agree well with the calculus of the eigenstructure of the system by providing six waves. This demonstrate the capabilities of mixture formulations to resolve two-phase flow discontinuities when using the mixture entropy equation. Ongoing and future research will include the simulation of rarefaction wave propagation using a temperature gradient.

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References

[1] Ishii M and Hibiki T, *Thermo-fluid Dynamics of Two-Phase Flow*, Springer, 2011.

[2] Yadigaroglu G, Hewitt GF, Introduction to Multiphase Flow: Basic Concepts, Applications and Modelling, Zurich Lectures on Multiphase Flow, Springer; 2018.

[3] Godunov SK and Romenski E, *Elements of Continuum Mechanics and Conservation Laws*, Kluwer Academic/Plenum Publishers, 2003.

[4] Baer M, Nunziato JW. A two-phase mixture theory for the deflagration-to-detonation transition (DDT) in reactive granular materials. Int J Multiphase Flows 1986; 12: 861-889.

[5] Zeidan D, Romenski E, Slaouti A, Toro EF. Numerical study of wave propagation in compressible

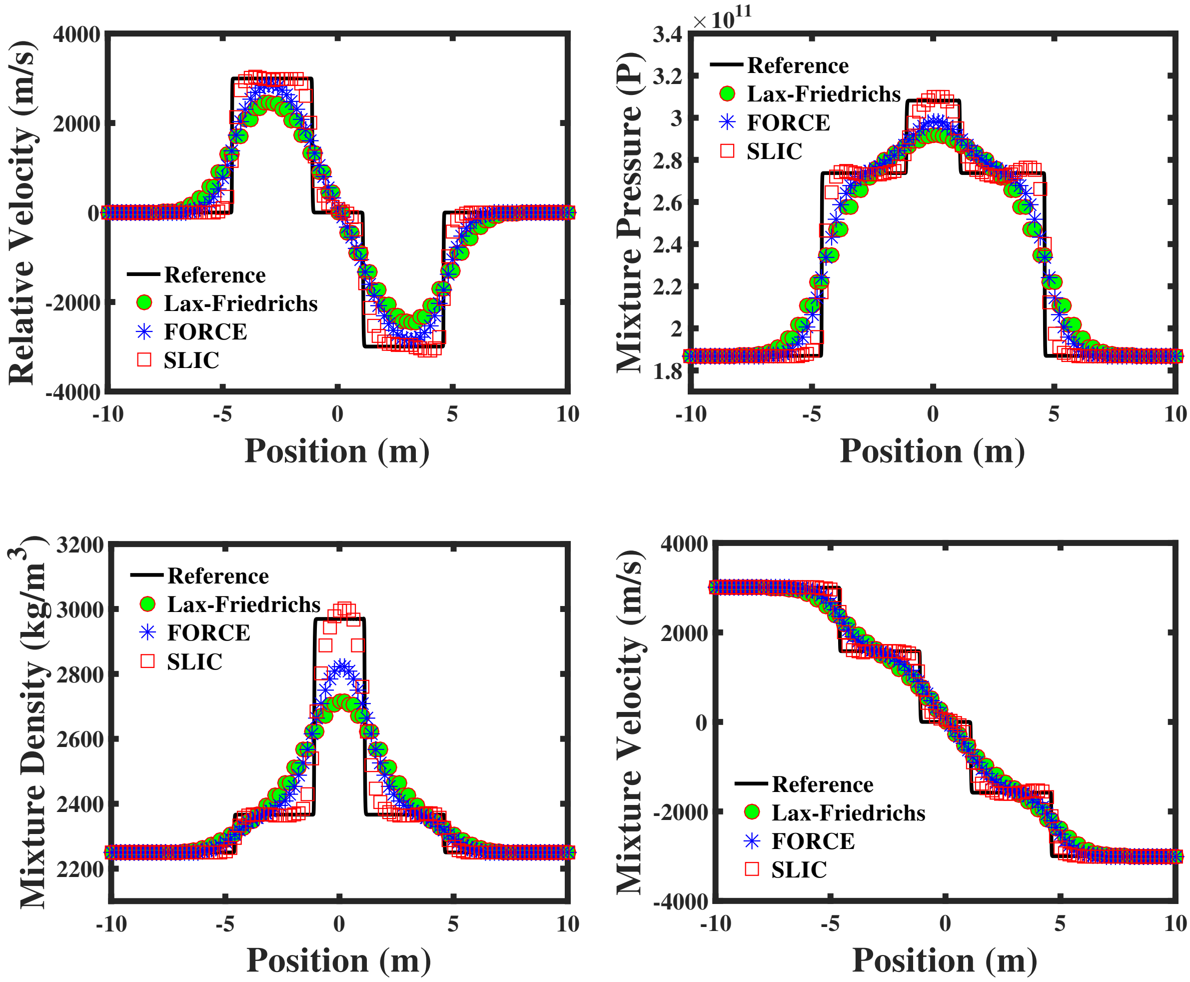

Figure 1: Shock-tube problem of [7] at time $t = 9.0 \times 10^{-5}s$ ms. The TVD SLIC, FORCE and Lax-Friedrichs methods are compared with the reference solution results. Coarse meshes, symbols, are provided on 100 cells and very fine meshes of 5000 cells for the solid lines. The waves seen from left to right, two left shock and two right shock waves separated by a multiple contact discontinuity for the mixture velocity u.

two-phase flow. Int J Numer Meth Fluids 2007; 54 (4): 393-417.

[6] Romenski E, Resnyansky AD, Toro EF. Conservative hyperbolic formulation for compressible two-phase flow with different phase pressures and temperatures. Quart Appl Math 2007; 65: 259-279.

[7] La Spina G, de'Michieli Vitturi M. High-Resolution Finite Volume Central Schemes for a Compressible Two-Phase Model. SIAM J Sci Comput 2012; 34(6), B861-B880.

[8] Cowperthwaite M. Relationships between incomplete equations of state. J.Franklin Inst 1969; 285: 379-387.

[9] Toro EF. *Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction*, Springer, 2009.