Compressible two-phase flow modelling based on thermodynamically compatible systems of hyperbolic conservation laws

E. Romenski[*,†,‡] and D. Drikakis

Aerospace Science Department, Fluid Mechanics and Computational Science Group, Cranfield University, Cranfield MK43 0AL, U.K.

SUMMARY

This paper outlines the development of a two-phase flow model based on the theory of thermodynamically compatible systems of hyperbolic conservation laws. The conservative hyperbolic governing equations are numerically implemented in conjunction with the second-order MUSCL method and the GFORCE flux, while for the reduced isentropic model the first-order Godunov method is also derived. Results are presented for the water–air shock tube and water-faucet test problems. Copyright © 2007 John Wiley & Sons, Ltd.

1. INTRODUCTION

The development of accurate computational models for compressible multi-phase flows is of interest in relation to a number of scientific and engineering disciplines. In the last few decades, several models and associated numerical algorithms for two-phase flows have been developed [1–3], but none of these models has been universally accepted as a complete formulation for modelling two- and multi-phase flows.

Here, a new multi-phase modelling approach based on the thermodynamically compatible systems of hyperbolic conservation laws [4–6] is outlined for the development of single temperature two-phase flow model. The mixture with equal phase temperatures is considered as a continuum

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[*]Correspondence to: E. Romenski, Aerospace Science Department, Cranfield University, Cranfield MK43 0AL, U.K.
[†]E-mail: evrom@math.nsc.ru, e.romenskiy@cranfield.ac.uk
[‡]On leave from Sobolev Institute of Mathematics, Russian Academy of Sciences, Novosibirsk, Russia.

medium with the governing equations casted in hyperbolic conservation form. Owing to the complexity of the governing equations, the solution of the Riemann problem cannot be easily obtained. Therefore, a centred method for computing the numerical fluxes, called GFORCE, has been employed [7]. The linearized Riemann solver has been derived for the reduced isentropic model using eigenstructure analysis [8]. The two-phase flow model has been applied to water–air shock tube [2] and water-faucet [2, 9] problems.

2. DEVELOPMENT OF CONSERVATIVE MODEL FOR TWO-PHASE FLOW

The compressible two-phase flow model presented here concerns different phase velocities and pressures, and equal phase temperatures. The development of the model consists of several closely inter-related steps:

- Introduction of new physical variables, in addition to the classical variables (velocity, density, entropy), characterizing a two-phase flow.
- Formulation of new conservation laws for the new variables in addition to the classical mass, momentum and energy conservation laws.
- Introduction of source terms for modelling phase interaction and dissipative processes.
- Formulation of closures for the mixture, such as equation of state, and dependencies of the source terms on the state parameters.

2.1. Parameters of state for two-phase flow with equal phase temperatures

A two-phase model that represents a simplification of the general model for a flow with different phase velocities, pressures and temperatures [6] is presented in this paper. A continuum two-phase medium with phase volume concentrations α_1 and α_2 and the saturation constraint $\alpha_1 + \alpha_2 = 1$ being held is considered. The phases (denoted by the indices $n = 1, 2$) are characterized by the velocities u_n^i, $i = 1, 2$ and 3, for the three velocities, respectively, and densities ρ_n. The phase temperatures are assumed to be the same ($T_1 = T_2 = T$), that is valid for processes with characteristic time much greater than the time required for equilibration of phase temperatures. The model can then be derived from [6] for relaxation time of phase temperatures difference tending to zero.

The above variables along with an equation of state for each phase, defining the dependence of internal energy on its density and entropy $e_n(\rho_n, s_n)$, provide a full description of two-phase compressible flows. The total density of the mixture is defined as $\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2$. By introducing a mixture entropy $s = c_1 s_1 + c_2 s_2$, where $c_n = \alpha_n \rho_n / \rho$ is the mass concentration of nth phase, additional flow parameters, such as phase entropies s_n, pressures p_n, etc., can be defined. The phase entropies $s_n = s_n(\alpha_1, \rho_1, \rho_2, s), n = 1, 2$, can be calculated as functions of volume fraction α_1, phase densities ρ_1, ρ_2, and mixture entropy s by solving the system:

$$c_1 s_1 + c_2 s_2 = s, \quad \frac{\partial e_n(\rho_n, s_n)}{\partial s_n} = T_n = T, \quad n = 1, 2$$

Further we consider the one-dimensional flow along the x-axis with the basic set of parameters of state for the governing equations $\alpha_1, \rho_1, \rho_2, u_1, u_2, s$, and any other parameter of state can be obtained by these ones.

2.2. Thermodynamically compatible system of conservation laws and derivation of two-phase flow equations

A general thermodynamically compatible system of conservation laws is fully defined by a potential L depending on variables q_k, which can be scalars, vectors or tensors. All conserved variables are identical to $\partial L/\partial q_k$, and the fluxes are expressed via q_k and $\partial L/\partial q_k$. The convexity of L provides the hyperbolicity of the resulting system. Details of the transformation of the system to symmetric form as well as derivation of energy conservation law for compatibility of the governing equations can be found in [5]. Once the subsystem of the general thermodynamically compatible system for modelling two-phase flows has been selected, the governing equations can be obtained by identifying the physical and generating variables. A set of physical conserved variables is given by the derivatives $\partial L/\partial q_i$. The constitutive relation, which is necessary for closing the system, is the equation of state for the mixture. It is obtained by the sum of averaged phase equations of state and kinetic energy of the phase relative motion: $E(\alpha_1, \rho_1, \rho_2, s, w) = c_1 e_1(\rho_1, s_1) + c_2 e_2(\rho_2, s_2) + c_1 c_2 (u_1 - u_2)^2/2$, where $s_n = s_n(\alpha_1, \rho_1, \rho_2, s)$ is the entropy of nth phase. The source terms introduced in the governing equations concern the modelling of pressure relaxation for reaching the equilibrium state with equal phase pressures and interfacial friction (drag). The above are defined according to the second law of thermodynamics, namely providing positiveness of entropy production. The final system is expressed in conservation form in terms of the parameters of state:

$$\frac{\partial \rho \alpha_1}{\partial t} + \frac{\partial u \rho \alpha_1}{\partial x} = -\chi(p_2 - p_1)$$

$$\frac{\partial(\alpha_1 \rho_1 u_1 + \alpha_2 \rho_2 u_2)}{\partial t} + \frac{\partial(\alpha_1 \rho_1 u_1^2 + \alpha_2 \rho_2 u_2^2 + \alpha_1 p_1 + \alpha_2 p_2)}{\partial x} = 0$$

$$\frac{\partial \alpha_n \rho_n}{\partial t} + \frac{\partial \alpha_n \rho_n u_n}{\partial x} = 0, \quad n = 1, 2$$

$$\frac{\partial(u_1 - u_2)}{\partial t} + \frac{\partial}{\partial x}\left(e_1 + \frac{p_1}{\rho_1} + \frac{u_1^2}{2} - e_2 - \frac{p_2}{\rho_2} - \frac{u_2^2}{2} - (s_1 - s_2)T\right) = -\lambda(u_1 - u_2) \quad (1)$$

$$\frac{\partial}{\partial t}\left(\alpha_1 \rho_1 \left(e_1 + \frac{u_1^2}{2}\right) + \alpha_2 \rho_2 \left(e_2 + \frac{u_2^2}{2}\right)\right) + \frac{\partial}{\partial x}\left(\alpha_1 \rho_1 u_1 \left(e_1 + \frac{u_1^2}{2} + \frac{p_1}{\rho_1}\right)\right.$$

$$\left. + \alpha_2 \rho_2 u_2 \left(e_2 + \frac{u_2^2}{2} + \frac{p_2}{\rho_2}\right) - \rho c_1 c_2 (u_1 - u_2)(s_1 - s_2)T\right) = 0$$

where $p_1 = \rho_1^2 \partial e_1/\partial \rho_1$, $p_2 = \rho_2^2 \partial e_2/\partial \rho_2$, $T = \partial e_1/\partial s_1 = \partial e_2/\partial s_2$, and the coefficients χ and λ characterize the rate of pressure relaxation and velocity relaxation (drag force). The equations of the above system represent balance laws for volume fraction, mixture total momentum, phase mass, relative velocity and mixture total energy. All the above equations are known in the two-phase flow theory except the equation for the relative velocity $u_1 - u_2$. The latter is obtained by using the thermodynamically compatible systems theory. In fact, the classical thermodynamics uses the equality of phase chemical potentials $e_1 + p_1/\rho_1 - s_1 T_1 = e_2 + p_2/\rho_2 - s_2 T_2$ as a condition for phase thermodynamic equilibrium in reactive media. Similarly, a kinematic equilibrium for zero gradient of phase chemical potentials difference is provided by the relative velocity balance law.

System (1) is solved by the MUSCL scheme in conjunction with the GFORCE (Generalized FORCE) method [7], the *minmod* limiter and the third-order TVD Runge–Kutta scheme for the time integration [10, 11]. For the water-faucet problem, a reduced isentropic model has been considered, which is solved also by a first-order Godunov method.

3. NUMERICAL TESTS

3.1. Water–air shock tube problem

The first test case is the one-dimensional water–air shock tube problem [2, 12] consisting of a moving interface between water and air. In the numerical framework, the initial condition consists of a small amount of air added to the water and *vice versa* because the governing equations are de-generated for volume fractions of 0 or 1 for each phase, respectively. Both the pressure and relative velocity relaxation are assumed to be instantaneous ($\chi = \infty, \lambda = \infty$). Note that the numerical realization of instantaneous relaxations consists of two steps. First, Equations (1) are solved by the numerical method mentioned in the previous section, assuming zero source terms. Second, a solution correction in each grid cell is applied by assuming $u_1 = u_2$ and solving the algebraic equation $p_1(m_1/\alpha_1, s_1) = p_2(m_2/\alpha_2, s_2)$ with respect to α_1 using computed phase entropies s_1, s_2 and known values $m_1 = \alpha_1 \rho_1$, $m_2 = \alpha_2 \rho_2$. The perfect and stiffened gas equations of state are employed for air and water, respectively [2]. The computational domain is $x \in [0, 1]$ (in metres), and the domain consists of two sections $[0, 0.7)$ and $(0.7, 1]$ for air and water. Transmissive boundary conditions are applied at $x = 0$ and 1. The indices 1 and 2 are assigned to the variables for water and air, respectively. The initial data for the left and right states are ($\varepsilon = 10^{-7}$)

Left: $\alpha_1 = 1.0 - \varepsilon, \alpha_2 = \varepsilon, u_1 = u_2 = 0\,\text{m/s}, p_1 = p_2 = 10^9\,\text{Pa}, \rho_1 = 10^3\,\text{kg/m}^3$;
Right: $\alpha_1 = \varepsilon, \alpha_2 = 1 - \varepsilon, u_1 = u_2 = 0\,\text{m/s}, p_1 = p_2 = 10^6\,\text{Pa}, \rho_2 = 50\,\text{kg/m}^3$.

Other parameters such as phase entropies, temperatures, air and water densities can be computed using the corresponding equations of state. In this study, the initial data for temperature are different than that of [2] because the single temperature model is employed. In Figure 1 the pressure, density, velocity and volume fraction of the mixture are shown at $t = 2.2 \times 10^{-4}\,\text{s}$, for 200 (dashed line) and 800 grid points (thick solid line), and also compared with the exact solution (thin solid line). The exact solution is obtained by solving the Riemann problem for the Euler equations. The results reveal a very good agreement between the computational (800 grid points) and exact solution.

3.2. Water-faucet test problem

The water-faucet test problem is a classical test case in two-phase flow modelling [2, 9, 12]. An isentropic simplification of (1), which can be obtained by neglecting phase entropies ($s_1 = s_2 = 0$) and assuming $e_1 = e_1(\rho_1)$, $e_2 = e_2(\rho_2)$, has been employed. The above approximations are valid because the temperature variations are negligibly small at low Mach water-faucet flow. The flow consists of a homogeneous water column in a gas annulus in a tube, which due to gravitational acceleration results in the water column getting thinner. The gravity force must be taken into account in the second (momentum) equation of (1) as the source term $f = -\rho g$, where $g = 9.81\,\text{m/s}^2$. The tube has length 12 m and the flow is initialized with $p_1^0 = p_2^0 = 10^5\,\text{Pa}$, water and air volume fractions $\alpha_1^0 = 0.8, \alpha_2^0 = 0.2$, water and air velocities $u_1^0 = 10\,\text{m/s}$ and $u_2^0 = 0$. The boundary conditions at the
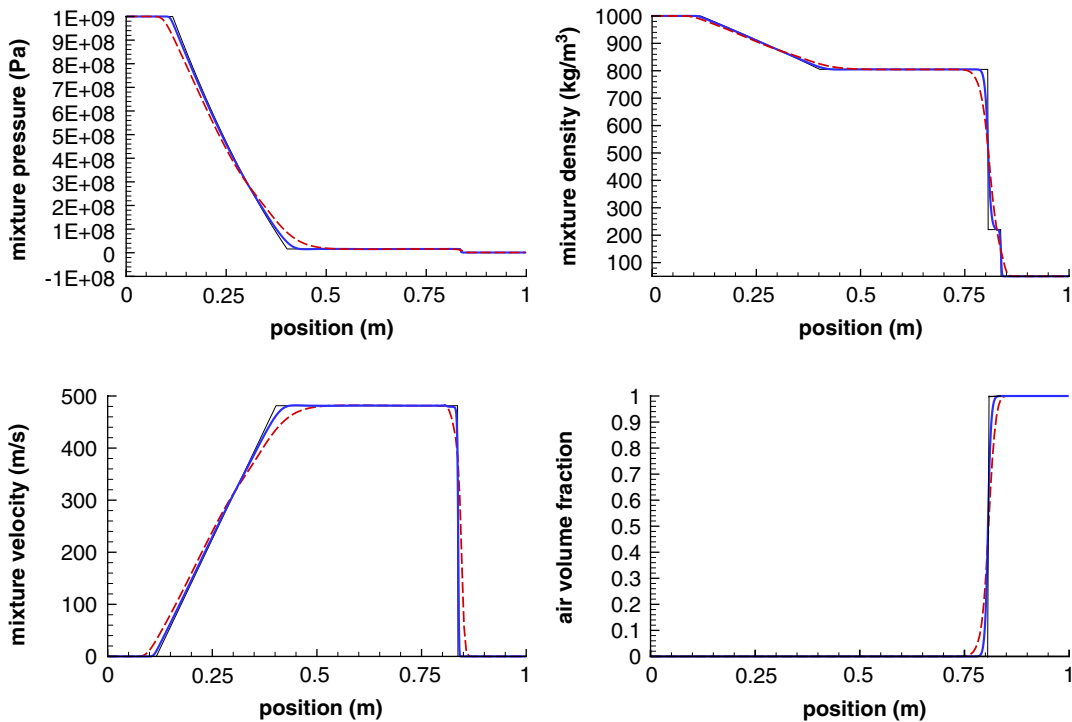
Figure 1. Mixture pressure (top left) and density (top right), velocity (bottom left) and air volume fraction (bottom right) at $t = 2.2 \times 10^{-4}$ s for 200 (dashed line) and 800 grid points (thick solid line), respectively, and comparison with the exact solution (thin solid line).

tube inlet are air volume fraction $\alpha_2 = 0.2$, and water and air velocities $u_1 = 10$ m/s and $u_2 = 0$. At the tube outlet the pressure remains unchanged as $p = 10^5$ Pa.

The analytical solution can be derived by neglecting pressure gradients [9]:

$$\alpha_2(t, x) = \begin{cases} 1 - \dfrac{\alpha_1^0 u_1^0}{\sqrt{(u_1^0)^2 + 2gx}} & \text{if } x < \dfrac{gt^2}{2} + u_1^0 t \\[2ex] 1 - \alpha_0^1 & \text{otherwise} \end{cases}$$

Computations have been conducted by assuming instantaneous pressure relaxation, $\chi = \infty$, and ignoring the interfacial friction, i.e. $\lambda = 0$. Two numerical methods have been employed: the first-order Godunov method in conjunction with a linearized Riemann solver and the second-order MUSCL method in conjunction with the GFORCE flux and linear reconstruction. The linearized Riemann solver has been derived using eigenstructure analysis [8]. The isentropic perfect gas and stiffened gas equations of state have been employed for air and water, respectively. The material constants are for air $\rho_2 = 1$ kg/m^3, $c_2 = 374$ m/s, $\gamma_2 = 1.4$ and for water $\rho_1 = 1000$ kg/m^3, $c_1 = 1543$ m/s, $\gamma = 2.8$. Figure 2 shows the computed air volume fraction, α_2, for the GFORCE method and the first-order Godunov scheme at $t = 0.5$ s; the Courant–Friedrichs–Lewy number used in the
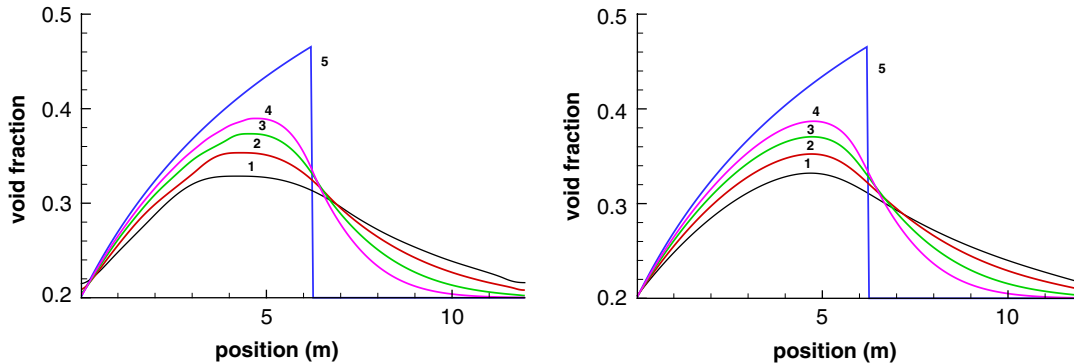
Figure 2. Air volume fraction at $t = 0.5\,$s for $200, 400, 800$ and 1600 grid points, curves $1, 2, 3$ and 4, respectively. The results have been obtained using the GFORCE flux (left) and linearized Riemann solver (right). The analytic solution is labelled as curve 5.

computations is 0.5. Both numerical schemes provide very similar results. The results labelled as 'curve 5' correspond to the exact solution, while curves 1–4 correspond to computations using $N = 200, 400, 800$ and 1600 grid points, respectively. Similar to previous studies [12], which used the Baer–Nunziato-type model and different Riemann solvers, slow rates of convergence were also observed in this study.

4. CONCLUDING OVERVIEW

A new model for two-phase flows based on hyperbolic conservation laws for non-equilibrium thermodynamics is proposed. The model has been implemented in conjunction with two numerical methods and applied to two test problems for which analytical solutions are available. Comparison with the analytic solutions shows that the new model provides promising results. Future work will concern extension of the model to complex two-phase flows compressible turbulent mixing and instabilities such as Richtmyer–Meshkov and Rayleigh–Taylor.

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