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Consistent numerical diffusion terms for simulating compressible multicomponent flows

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ABSTRACT

An interface-capturing method using a high-order central difference scheme is presented for simulations of compressible multicomponent flows. The present method adds consistent numerical diffusion terms to robustly capture interface discontinuities, while maintaining the velocity, pressure, and temperature equilibriums at interfaces. Analysis of the numerical errors generated at the interfaces leads to a proposal of new consistent numerical diffusion terms. The method solves a fully conservative form of the total mass, momentum, total energy, and species-mass, and an additional advection form of the specific heats ratio to preserve the pressure oscillation-free property at the interfaces. Several one- and two-dimensional problems are used to verify the proposed method.

1. Introduction

For simulations of interfaces in compressible multicomponent flows, such as in the case of the thermodynamic state where the specific heats ratio is different between two fluids, it is well known that spurious pressure and velocity oscillations are generated at the interfaces. Abgrall [1] addressed this unphysical oscillation problem and solved it by introducing an advection form of the transport equation of the specific heats ratio under the ideal gas law (commonly called the quasi-conservative form). It was later extended to the use of mass fraction by Shyue [2], and for more complicated equations of state by Shyue [3] and Saurel and Abgrall [4]. Karni [5] introduced a non-conservative model using primitive variables to avoid the pressure oscillations, which was later modified to capture strong shock waves using the pressure evolution equation [6]. A successful application of Karni's method to a bubble-shock interaction problem [7] has now become the benchmark for compressible multicomponent flow algorithms. Saurel and Abgrall [8] constructed a two-phase flow model without assuming pressure equilibrium to circumvent some of the restrictions of Abgrall's and their original method, such as limitation of the equation of state and difficulty in including other physical effects such as mass transfer and surface tension at the interface. Allaire et al. [9] developed five-equation models with general equations of state, including tabulated laws, extending the method of Abgrall. Some recent studies have used the quasi-conservative form in the development of numerical methods for the purpose of sharply capturing interfaces, for example, by coupling an interface compression method [10] or using a Lagrange–Remap solver [11]. A drawback of using the quasi-conservative form is its poor species-mass conservation property. Another issue is the spatial accuracy; the most simulations of compressible multicomponent flows have been limited to low-order accuracy using conventional upwind-biased schemes.

With regard to high-order methods in compressible multicomponent flows, using the quasi-conservative form, Johnsen and Colonius [12] attempted to apply higher-order methods using weighted essentially non-oscillatory (WENO) schemes. They demonstrated that the primitive variables must be reconstructed in the characteristic interpolation to preserve the oscillation-free property at the interfaces. Nonomura et al. [13] implemented a weighted compact nonlinear scheme (WCNS) with the oscillation-free property, showing the effects of the choice of fully conservative or quasi-conservative forms and the choice of characteristic interpolation of conservative or primitive variables. Johnsen and Ham [14] recently addressed the two drawbacks in the quasi-conservative form: the species-mass conservation error and temperature spikes problems, and proposed a solution using modified WENO weights for the transport equation of mass fraction in the conservative form.

On the other hand, Marquina and Mulet [15] directly solved the conservation form of the governing equations using a flux-split algorithm with WENO5 flux reconstruction, assuming that the pressure fluctuations at interfaces are small and do not disturb interface physics. Cook [16] used the conservative form of the

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Navier–Stokes equations for compressible multicomponent flow simulations with a sixth-order compact differencing scheme, where pressure and temperature equilibrations are achieved in a computational cell by introducing the partial density and internal energy with an iterative procedure. Kawai and Terashima [17] applied a sixth-order compact differencing scheme in the conservation form, where the pressure and velocity oscillations were alleviated by introducing the localized artificial diffusivity (LAD) method, while avoiding initial start-up errors (by not using one-point jump initial conditions). Although the use of the conservative form is promising, it introduces spurious oscillations which have the potential to induce severe computational instabilities and harm flow fields, such as acoustics and turbulence, especially when high-order schemes are applied.

Thus, while high-order upwind-biased schemes (finite volume WENO [12,14] and finite differencing WCNS [13]) have been successfully applied to compressible multicomponent flow simulations with the oscillation-free property, the use and possibility of other high-order schemes, i.e., central-differencing-based schemes, have not been discussed. In case of central-differencing-based scheme, explicit numerical diffusion terms added for capturing numerical discontinuities may deteriorate the oscillation-free property, if they are inconsistently introduced. To the best of our knowledge, there is no central-differencing-based method proposed which satisfies the oscillation-free property. Further, some recent studies of single component fluids [18] have shown that the numerical dissipation introduced by high-order upwind-biased schemes overwhelms a wide range of flow scales, even if the formal order of accuracy is high, illustrating that the upwind-biased high-order schemes may be too dissipative for resolving the broad range of flow scales. In contrast, central-difference-based schemes perform better for accurately resolving small scales due to their low dissipation characteristic (e.g., see the comparisons between high-order WENO schemes and central/upwind hybrid schemes [18,19] or the LAD method [18,20]).

In this paper, we propose consistent numerical diffusion terms that can be coupled with high-order central difference schemes for the simulation of compressible multicomponent flows, in which the velocity, pressure, and temperature equilibriums, and the conservation of total mass, momentum, total energy, and species mass are all satisfied. The key lies in the consistent construction of numerical diffusion terms introduced to robustly capture interfaces while maintaining the interface equilibriums. We first analytically derive the consistent numerical diffusion terms that satisfy the velocity, pressure, and temperature equilibriums at interfaces, and then test the proposed method on one- and two-dimensional compressible multicomponent problems.

2. Numerical method

2.1. Governing equations

The Euler equations for multicomponent gases are written as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0, \tag{1}$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + p\boldsymbol{\delta}) = 0, \tag{2}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot ((E+p)\boldsymbol{u}) = 0, \tag{3}$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \boldsymbol{u}) = 0, \tag{4}$$

where ρ is the density, $\boldsymbol{u}$ is the velocity vector, p is the pressure, $E = \rho e + \frac{1}{2}\rho \boldsymbol{u} \cdot \boldsymbol{u}$ is the total energy, Y_i is the mass fraction of a component i, and $\boldsymbol{\delta}$ is the unit tensor. e is the internal energy per unit mass. In this study, a calorically perfect gas is assumed with the ideal gas equation of state:

$$p = \rho RT = \rho \frac{R_u}{W} T = (\gamma - 1)\rho e, \tag{5}$$

where R is the specific gas constant, R_u is the universal gas constant, W is the molar weight of the mixture, T is the temperature, and γ is the ratio of the specific heat of the mixture.

2.2. Mixing rule

Since an artificial diffuse zone is generated near interfaces in interface-capturing schemes, mixing rules are required to define variables in the diffuse zone. The mean molar weight of the mixture W is given using mass fractions by:

$$\frac{1}{W} = \sum_i \frac{Y_i}{W_i}. \tag{6}$$

The mean specific heat ratio of the mixture is defined using the heat capacities of the mixture C_p and C_v as:

$$\gamma = \frac{C_p}{C_v} = \frac{\sum_i C_{p,i} Y_i}{\sum_i C_{v,i} Y_i}, \tag{7}$$

where the heat capacities are defined in mass values (i.e., $C_{p,i} = C_{v,i} + R_u/W_i$).

2.3. Discretization of the governing equations

Discretization of Eqs. (1)–(4) at node j and time n can be written in a one-dimensional form as:

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} D_j[\rho u], \tag{8}$$

$$(\rho u)_j^{n+1} = (\rho u)_j^n - \frac{\Delta t}{\Delta x} D_j[\rho u u + p], \tag{9}$$

$$E_j^{n+1} = E_j^n - \frac{\Delta t}{\Delta x} D_j[(E+p)u], \tag{10}$$

$$(\rho Y_i)_j^{n+1} = (\rho Y_i)_j^n - \frac{\Delta t}{\Delta x} D_j[\rho u Y_i], \tag{11}$$

where $D_j[\cdot]$ represents a discretization operator. Δx and Δt are the grid spacing and time step sizes, respectively. Then, considering that generally any numerical scheme including upwind schemes can be recast into a form that consists of a central difference discretization plus a numerical diffusion term, i.e., $D_j[f] = D_j^c[f - A_\cdot]$, where $D_j^c[\cdot]$ denotes a central discretization operator (e.g., $D_j^c[f] = (f_{j+1} - f_{j-1})/2$) and $D_j^c[A_\cdot]$ represents a numerical diffusion term, Eqs. (8)–(11) can be rewritten as:

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} D_j^c[\rho u - A_\rho], \tag{12}$$

$$(\rho u)_j^{n+1} = (\rho u)_j^n - \frac{\Delta t}{\Delta x}\left(D_j^c[\rho u u - A_{\rho u}] + D_j^c[p]\right), \tag{13}$$

$$E_j^{n+1} = E_j^n - \frac{\Delta t}{\Delta x} D_j^c[(E+p)u - A_E], \tag{14}$$

$$(\rho Y_i)_j^{n+1} = (\rho Y_i)_j^n - \frac{\Delta t}{\Delta x} D_j^c[\rho u Y_i - A_{\rho Y_i}], \tag{15}$$

where A_E consists of two terms, $A_E = A_{\rho e} + A_{ke}$, in which $A_{\rho e}$ and A_{ke} are the numerical diffusion terms for the internal energy and kinetic energy, respectively. Note that the pressure is split from the momentum in Eq. (13), for which numerical diffusion is not added.

2.4. Numerical diffusion term for mass equations

In the case of multicomponent flow simulations, Eq. (12) must be recovered when Eq. (15) is summed over all the components i. Eqs. (12), (15), and $\sum_i Y_i = 1$ therefore give: