Numerical errors generated by shock-capturing schemes in compressible multicomponent flows

By E. Johnsen, F. Ham AND J. Larsson

1. Motivation and objectives

For decades, high-order accurate shock-capturing schemes have been used to simulate inviscid compressible flows with shocks for a single-component fluid in a stable and accurate fashion. However, when applying such schemes to problems with multiple fluids, specifically when the ratio of specific heats is different in each fluid, numerical errors are typically generated, *e.g.*, spurious pressure oscillations, temperature spikes and species conservation errors, depending on the treatment of the interface.

When multiple fluids are present, an additional transport equation must be solved to determine the fluid composition. Mulder *et al.* (1992) solved the transport equation in conservative form and coupled it to the Euler equations. However, spurious pressure oscillations were generated at interfaces; these oscillations propagate in the flow field and may interact with other flow features. Abgrall (1996) proposed to overcome this drawback by solving the transport equation in advection form for a specific function of the ratio of specific heats. Shyue (1998) extended this idea to solving the transport equation for the mass fraction in advection form as well. Johnsen & Colonius (2006) extended the work of Abgrall (1996) to high-order accurate weighted essentially non-oscillatory (WENO) schemes in which average primitive variables are reconstructed. Though these last three schemes conserve the total mass, momentum and energy of the system and do not generate pressure oscillations, they do not discretely conserve the mass of each species. Furthermore, spikes in the temperature may be generated at interfaces. These three types of errors (spurious pressure oscillations, temperature spikes, species conservation errors) depend on the form of the transport equation and on the treatment of the convective terms.

The numerical schemes of Abgrall (1996), Shyue (1998) and Johnsen & Colonius (2006) are interface-capturing, in that interfaces separating fluids of different composition are smeared over a few grid points, in analogy to shock capturing. The present work focuses on the capturing framework, which is particularly well-suited to problems in which physical diffusion is present (i.e. compressible Navier-Stokes equations with heat and mass transfer). If physical diffusion is included, the errors generated at interfaces may be damped to some extent. However, an accurate representation of the temperature and mass of each species (i.e. through the mass fraction) is imperative, because errors in these quantities will generate further numerical errors due to the diffusion terms.

Thus, the goal of the present work is to provide a deeper understanding of errors generated in multifluid calculations (pressure oscillations, temperature spikes, species conservation errors) and devise a scheme to prevent them. The focus is on the treatment of the convective terms (i.e. Euler equations), with particular care to ensuring that temperature and mass fraction are accurate, so that more complicated calculations with simultaneous heat and mass diffusion can be carried out. This work generalizes that of Johnsen (2008) to flow discontinuities across which the pressure and velocity are constant.

2. Numerical framework

2.1. *Governing equations*

The errors generated by shock-capturing schemes applied to multicomponent flows depend on how the transport equation and the convective terms are treated. For simplicity, the present analysis focuses on the one-dimensional multicomponent Euler equations for two (different) gases:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0, \tag{2.1a}$$

$$\frac{\partial (\rho z)}{\partial t} + \frac{\partial}{\partial x}(\rho u z) = 0, \tag{2.1b}$$

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial}{\partial x}\left(\rho u^2 + p\right) = 0, \tag{2.1c}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}[u(E+p)] = 0, \tag{2.1d}$$

where ρ is the density, u is the velocity vector, z is the mass fraction, $E = \rho(e + u^2/2)$ is the total energy, e is the internal energy and p is the pressure. The system is closed by the following equation of state

$$\frac{p}{\gamma - 1} = \rho e, \tag{2.2}$$

where $\gamma = c_p/c_v$ is the ratio of specific heats, which is a function of the mass fraction. Equation (2.2) is equivalent to the ideal gas law,

$$p = \rho R T, \tag{2.3}$$

where T is the temperature and R is the gas constant, given the relationship between the temperature and the internal energy,

$$e = c_v T, \tag{2.4}$$

where c_v is the specific heat at constant volume. The gas constant and specific heats of a mixture depend on the mass fraction. The mixture molecular mass is given by

$$\frac{1}{M} = \frac{z}{M^\alpha} + \frac{1-z}{M^\beta}, \tag{2.5}$$

where the superscripts α and β denote the different gases. The gas constant is therefore given by

$$R = \frac{R_u}{M} = R^\alpha z + R^\beta (1 - z), \tag{2.6}$$

where R_u is the universal gas constant, and the specific heat at constant volume is given by

$$c_v = c_v^\alpha z + c_v^\beta (1 - z). \tag{2.7}$$

An additional expression of interest is the following:

$$\frac{1}{\gamma - 1} = \frac{z}{\gamma^\alpha - 1}\frac{M}{M^\alpha} + \frac{1-z}{\gamma^\beta - 1}\frac{M}{M^\beta}. \tag{2.8}$$

2.2. *Numerical method*

In the present work, a high-order accurate finite volume discretization is used. For a conservation law of the type

$$q_t + [f(q)]_x = 0, \tag{2.9}$$

TABLE 1. Different schemes considered in the present study.

Scheme	Transport variables	Model for γ	WENO variables
1. Fully conservative	ρz	Physical	$(\rho, \rho u, E, \rho z)$
2. $1/(\gamma-1)$	$1/(\gamma-1)$	Physical	$(\rho, u, p, 1/(\gamma-1))$
3. z	z	Shyue	(ρ, u, p, z)
4. ρz	ρz	Physical	$(\rho, u, T, \rho z^*)$
5. $1/(\gamma-1)$ & ρz	ρz and $1/(\gamma-1)$	Physical	$(\rho, u, p, \rho z^*, 1/(\gamma-1))$

the finite volume discretization yields the following semi-discrete form:

$$\frac{d}{dt}\bar{q}_i = -\frac{f_{i+1/2} - f_{i-1/2}}{\Delta x}, \tag{2.10}$$

where the overbar refers to the cell-average value and $f_{i+1/2}$ is the numerical flux. A typical algorithm for finite volume shock-capturing methods is as follows: given the cell average values, $\bar{q}_i$, reconstruct the pointwise left and right values at the cell edges, $q^L_{i+1/2}$ and $q^R_{i+1/2}$; then, compute the numerical flux, using an approximate Riemann solver, h, with $f_{i+1/2} = h(q^L_{i+1/2}, q^R_{i+1/2})$. The solution is then marched forward in time.

In the present work, a fifth-order accurate WENO reconstruction is used in physical space with a Harte-Lax-van Leer (HLL) approximate Riemann solver for the spatial discretization. For the time marching, a third-order accurate total variation diminishing (TVD) Runge-Kutta scheme is used, with $\Delta t/\Delta x = 0.5$ and $\Delta x = 0.02$.

For convenience, the schemes used in the next section are summarized in Table 1. Detailed information on each scheme is provided in Section 3. The transport variables (ρz or $1/(\gamma-1)$ or both) are first listed. If the variable is ρz, the transport equation is solved in conservative form; if the variable is $1/(\gamma-1)$ or z, the transport equation is solved in advection form. The model for γ is either the physical model (2.8) or that of Shyue (1998); as described in Section 3.1, $M^\alpha = M^\beta$ is implied in the latter. Finally, the variables reconstructed in the WENO procedure are listed; the asterisk denotes the fact that the WENO weights from ρ are used for ρz as well. The first scheme is the simplest possible way to couple a transport equation to the Euler equations. The second and third schemes are that of Abgrall (1996) and that of Shyue (1998) extended to higher-order accurate WENO by Johnsen & Colonius (2006). The last two schemes are proposed in the present work, with the latter being the preferred scheme for multifluid calculations. The first scheme listed in Table 1 is as follows:

SCHEME 1 (FULLY CONSERVATIVE). *In addition to the conservative variables, $(\rho, \rho u, E)$, the transport variable, ρz, is reconstructed and the Riemann solver is applied directly to the transport equation in conservative form to compute the flux.*

Though this scheme is fully conservative, spurious oscillations and temperature errors are generated when multiple fluids are present.

3. Results

Historically, shock-capturing schemes were designed to provide stable solutions to flows with shocks specifically. In the present section, the performance of high-order accurate shock-capturing schemes for the treatment of contact discontinuities and material interfaces is investigated. In both of these problems, the velocity and pressure are continuous, but the density is not. There are three possible cases:

(a) Contact discontinuity in a single-component fluid,
(b) Material interface,
(c) Contact discontinuity separating different fluids.

In flows in which shock waves interact with interfaces, all three phenomena are present. Since the first case is trivial, only the latter two cases are considered in the following sections. A one-dimensional discontinuity between helium and nitrogen moves at a constant velocity (equal to the sound speed in helium) with uniform pressure. The variables are non-dimensionalized by the density, ρ_{He}, and sound speed, c_{He}, of helium, and the domain length, L. The final time is $t_f c_{He}/L = 4.0$ (i.e. the solution is plotted after the interface has traveled two periods). The initial conditions are as follows:

$$\begin{aligned} \rho/\rho_{He} &= \frac{p_a/RT}{p_a/R_{He}T_a}, \\ u/c_{He} &= 1, \\ p/\rho_{He}c_{He}^2 &= 1/\gamma_{He}, \end{aligned} \tag{3.1}$$

where R is given by equation (2.6) z and T are defined as follows:

- Material interface: $T/T_o = 1$ and

$$z_{He} = \begin{cases} 0, & \text{if } -0.5 \le x \le 0.5, \\ 1, & \text{otherwise.} \end{cases} \tag{3.2}$$

- Contact discontinuity separating different fluids:

$$T/T_o = \begin{cases} 2, & \text{if } -0.5 \le x \le 0.5, \\ 1, & \text{otherwise,} \end{cases} \qquad z_{He} = \begin{cases} 0, & \text{if } -0.5 \le x \le 0.5, \\ 1, & \text{otherwise.} \end{cases} \tag{3.3}$$

Since the Euler equations are considered, the temperature only enters the problem through the initial conditions. The initial discontinuity (in ρ and ρz) consists of a one-point jump. Both u and p are supposed to remain constant.

For simplicity, a difference operator, $D(\cdot)$, is assumed to have the following properties: $D(ab+c) = aD(b) + D(c)$ for a constant, b and c not constant; thus, the chain rule does not apply discretely: $D(bc) \neq bD(c) + cD(b)$. Note that WENO schemes typically do not satisfy this property, but can be modified accordingly. The underlying numerical method is conservative for the mass, momentum and energy equations, in that $f_{i+1/2} = f_{i+1-1/2}$.

Assuming the discontinuity is located in cell i, the mass, momentum and energy conservation equations can be marched forward by one time step or substep:

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\Delta x} D(\rho u), \tag{3.4a}$$

$$(\rho u)_i^{n+1} = \rho u_i^n - \frac{\Delta t}{\Delta x} \left[D(\rho u^2) + D(p) \right], \tag{3.4b}$$

$$\left(\rho e + \rho \frac{u^2}{2} \right)_i^{n+1} = \left(\rho e + \rho \frac{u^2}{2} \right)_i^n - \frac{\Delta t}{\Delta x} \left[D(\rho u e) + D\left(\rho \frac{u^3}{2} \right) + D(up) \right]. \tag{3.4c}$$

For constant u and p, equations (3.4) reduce to

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\Delta x} u D(\rho), \tag{3.5a}$$

$$(\rho u)_i^{n+1} = \rho u_i^n - \frac{\Delta t}{\Delta x} u^2 D(\rho), \tag{3.5b}$$

$$\left(\rho e + \rho \frac{u^2}{2}\right)_i^{n+1} = \left(\rho e + \rho \frac{u^2}{2}\right)_i^n - \frac{\Delta t}{\Delta x} u \left[D(\rho e) + \frac{u^3}{2} D(\rho)\right]. \tag{3.5c}$$

The mass and momentum equations can be combined to yield

$$u_i^{n+1} = u_i^n = u, \tag{3.6}$$

and the energy equation can be written

$$(\rho e)_i^{n+1} = (\rho e)_i^n - \frac{\Delta t}{\Delta x} u D(\rho e). \tag{3.7}$$

Again, it is emphasized that this equation holds only if $D(p) = 0$ and $D(u) = 0$.

The goal now is to determine how the transport equation must be solved in order to prevent numerical errors in pressure, temperature and mass fraction. Two different directions may be followed: using either equation (2.2) relating the pressure to the internal energy (pressure viewpoint), or using equation (2.4) to relate the temperature to the internal energy (temperature viewpoint). These two viewpoints are different and will lead to different results.

3.1. *Advection of a material interface*

The advection of a material interface (between two different fluids) is considered. In this case, u, p, and T are constant; z, and therefore ρ, are not.

- *Pressure viewpoint*

Substituting the relationship between pressure and internal energy (2.2) into the equation for the internal energy (3.7) yields

$$\left(\frac{p}{\gamma - 1}\right)_i^{n+1} = \left(\frac{p}{\gamma - 1}\right)^n - \frac{\Delta t}{\Delta x} u D\left(\frac{p}{\gamma - 1}\right). \tag{3.8}$$

Thus, in order to maintain a constant pressure at time $n+1$, the following must hold:

$$p_i^{n+1} = p \quad \Leftrightarrow \quad \left(\frac{1}{\gamma - 1}\right)_i^{n+1} = \left(\frac{1}{\gamma - 1}\right)_i^n - \frac{\Delta t}{\Delta x} u D\left(\frac{1}{\gamma - 1}\right). \tag{3.9}$$

In other words, a transport equation for $1/(\gamma - 1)$ in advection form must hold in order to preserve the pressure equilibrium. Abgrall (1996) proposes to solve the transport equation directly for $1/(\gamma - 1)$, which is the basis for scheme 2, as follows:

Scheme 2 ($1/(\gamma - 1)$). *In order to preserve velocity and pressure equilibria, the average primitive variables, (ρ, u, p), and the transport variable, $1/(\gamma - 1)$, are reconstructed. The Riemann solver must be modified to solve the transport equation in advection form.*

There are several drawbacks to this scheme. First, the transport equation is solved in advection form, so that species conservation does not hold discretely. Furthermore, an additional transport equation must be solved if the two gases (of different molecular

weight) have the same γ. Finally, small temperature errors may be generated.

If equation (3.9) does not hold, an error will be generated in the pressure at time $n+1$ and this error will propagate in the flow field. It should be noted that since $\gamma = \gamma(z)$ and z obeys the advection equation, any function of γ obeys the advection equation as well. However, the discrete relationship between $1/(\gamma-1)$ and z must be linear; otherwise, equation (3.9) cannot be recovered. Shyue (1998) proposes to solve an advection equation for z,

$$z_i^{n+1} = z_i^n - \frac{\Delta t}{\Delta x} uD(z), \tag{3.10}$$

instead of equation (2.8), along with the following relationship between $1/(\gamma-1)$ and z:

$$\frac{1}{\gamma-1} = \frac{z}{\gamma^\alpha - 1} + \frac{1-z}{\gamma^\beta - 1}. \tag{3.11}$$

Thus, equation (3.9) holds. However, this equation introduces a modeling error, in that it implicitly assumes that $M^\alpha = M^\beta$ in equation (2.8). Thus, the scheme of Shyue (1998) is the following:

SCHEME 3 (z). *In order to preserve velocity and pressure equilibria, the average primitive variables, (ρ, u, p), and the transport variable, z, are reconstructed. The Riemann solver must be modified to solve the transport equation in advection form. Furthermore, the relationship between z and $1/(\gamma-1)$ must be linear.*

This scheme has several drawbacks. Similarly to the previous scheme, the transport equation is not solved in conservative form. Furthermore, a modeling error, which does not vanish as the grid is refined, is introduced. Finally, as shown later, a large temperature spike is generated.

The temperature is given by the ideal gas law (2.3). Following scheme 2 (z):

$$\begin{aligned} T_i^{n+1} &= \frac{p}{\rho^{n+1}\left[z^{n+1}R^\alpha + (1-z^{n+1})R^\beta\right]} \\ &= \frac{p}{\left[\rho^n - \frac{\Delta t}{\Delta x} uD(\rho)\right]\left(R^\alpha - R^\beta\right)\left[z^n - \frac{\Delta t}{\Delta x} uD(z)\right]} \\ &\neq \frac{p}{(\rho R)^{n+1}} = T^n. \end{aligned} \tag{3.12}$$

Thus, a temperature error is generated. However, because the temperature does not enter the problem, this issue is not relevant to the Euler equations. In practice, a spike forms at interfaces and is advected by the flow. Scheme 3 ($1/(\gamma-1)$) also leads to (smaller) temperature errors.

- *Temperature viewpoint*

Substituting the relationship between temperature and internal energy (2.4) into the equation for the internal energy (3.7) yields

$$(\rho c_v T)^{n+1} = (\rho c_v T)^n - \frac{\Delta t}{\Delta x} uD(\rho c_v T). \tag{3.13}$$

Thus, in order to maintain a constant temperature, the following must hold:

$$T_i^{n+1} = T \quad \Leftrightarrow \quad (\rho c_v)_i^{n+1} = (\rho c_v)_i^n - \frac{\Delta t}{\Delta x} uD(\rho c_v). \tag{3.14}$$

This equation can be re-arranged into the following form:

$$\begin{aligned}\left[(c_v^\alpha - c_v^\beta)(\rho z)^{n+1} + c_v^\beta \rho^{n+1}\right] = \left[(c_v^\alpha - c_v^\beta)(\rho z)^n + c_v^\beta \rho^n\right] \\ - \frac{\Delta t}{\Delta x} u \left[(c_v^\alpha - c_v^\beta) D(\rho z) + c_v^\beta D(\rho)\right],\end{aligned} \tag{3.15}$$

provided D acting on ρz and on ρ is the same. This condition is not trivial for general reconstructions; for WENO, a sufficient condition to meet this criterion is that the non-linear weights for ρ and ρz be the same, *e.g.*, using the weights of ρ for ρz. If this is the case, the pressure equilibrium is maintained:

$$\begin{aligned}p^{n+1} &= \left[(R^\alpha - R^\beta)(\rho z)^{n+1} + R^\beta \rho^{n+1}\right] T \\ &= \left[(R^\alpha - R^\beta)\rho z_i^n + R^\beta \rho_i^n\right] T - \frac{\Delta t}{\Delta x} u D \left[(R^\alpha - R^\beta)\rho z + R^\beta \rho\right] T = p,\end{aligned} \tag{3.16}$$

since the pressure is uniform initially. In order to maintain the temperature equilibrium, p, and ρR must both be constant at every stage of the process. A significant advantage over schemes 2 and 3 is that the transport equation is solved in conservative form, so that the mass of each species is conserved. Based on the temperature viewpoint, scheme 4 is proposed:

SCHEME 4 (ρz). *In order to preserve velocity and temperature equilibria, the average primitive variables, (ρ, u, T), and the transport variable, ρz, are reconstructed using the WENO-weights of ρ for the calculation of ρz. This scheme further maintains the pressure equilibrium.*

As will be shown later, though this scheme preserves velocity, pressure and temperature equilibria for a material interface and is fully conservative, it generates errors for contact discontinuities.

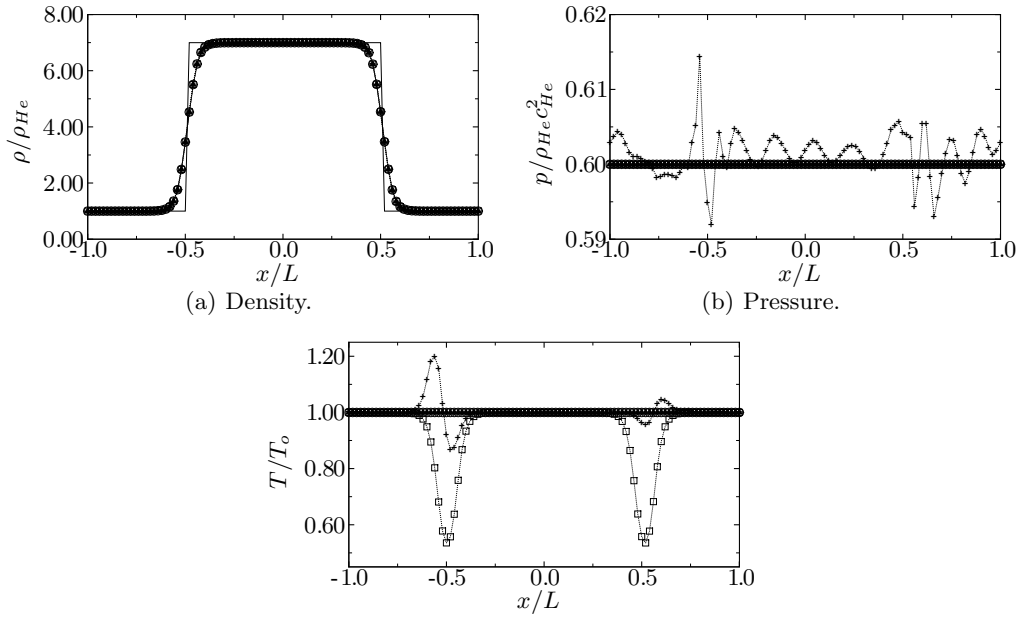
Figures 1 and 2 show the density, pressure and temperature profiles at the final time and the time history of the maximum pressure and temperature errors, as well as the mass of helium for the advection of a material interface. The errors in the pressure when using the standard fully conservative scheme are approximately 5%; the decrease of these errors as the grid is refined is not very rapid (Johnsen 2008). Temperature errors are observed in all the schemes except for scheme 5 ($1/(\gamma-1)$ & ρz); the errors generated by scheme 2 ($1/(\gamma-1)$) are quite small. When using scheme 3 (z), these errors may be up to 50%. Furthermore, the error in the mass of helium increases significantly with time when using scheme 3 (z). This error decreases smoothly as the grid is refined (Johnsen 2008). Scheme 2 ($1/(\gamma-1)$) does not generate significant errors in the mass of helium. Results from scheme 4 (ρz) are not included because they are almost identical to those of scheme 5 for this problem.

3.2. *Advection of a contact discontinuity separating different fluids*

The advection of a contact discontinuity between two different fluids is considered. In this case, u and p are constant; z and T, and therefore ρ, are not.

- *Pressure viewpoint*

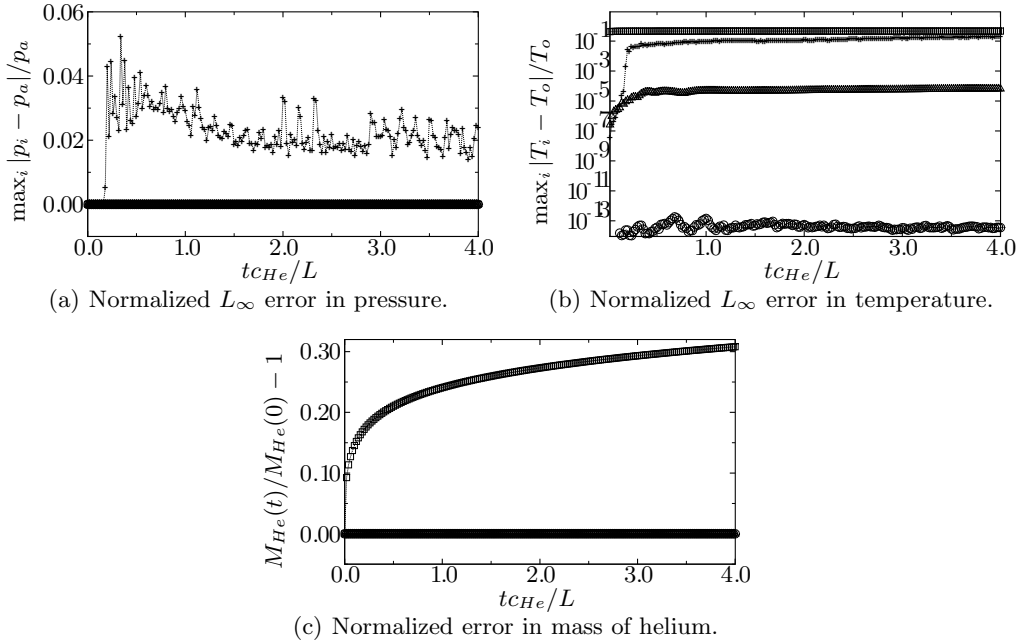
The same condition as for the material interface problem holds in order to maintain the pressure equilibrium: the transport equation for $1/(\gamma-1)$ must be solved in advection



(a) Density. (b) Pressure.

(c) Temperature.

FIGURE 1. Profiles at $tc_{He}/L = 4$ for the advection of a material interface between helium and nitrogen. Solid line: exact solution; pluses: scheme 1 (fully conservative); open triangles: scheme 2 ($1/(\gamma-1)$); open squares: scheme 3 (z); open circles: scheme 5 ($1/(\gamma-1)$ & ρz).



(a) Normalized L_∞ error in pressure. (b) Normalized L_∞ error in temperature.

(c) Normalized error in mass of helium.

FIGURE 2. Time histories for the advection of a material interface between helium and nitrogen. Pluses: scheme 1 (fully conservative); open squares: scheme 2 ($1/(\gamma-1)$); open triangles: scheme 3 (z); open circles: scheme 5 ($1/(\gamma-1)$ & ρz).

form.

- *Temperature viewpoint*

Substituting the relationship between temperature and internal energy (2.4) into the equation for the internal energy (3.7) yields

$$\begin{aligned}\left[(c_v^\alpha - c_v^\beta)(\rho z T)^{n+1} + c_v^\beta(\rho T)^{n+1}\right] &= \left[(c_v^\alpha - c_v^\beta)(\rho z T)^{n} + c_v^\beta(\rho T)^{n}\right] \\ &\quad - \frac{\Delta t}{\Delta x} u\left[(c_v^\alpha - c_v^\beta) D(\rho z T) + c_v^\beta D(\rho T)\right].\end{aligned} \tag{3.17}$$

This equation can be re-organized as follows:

$$(c_v^\alpha - c_v^\beta)\left[(\rho z T)^{n+1} - (\rho z T)^n + \frac{\Delta t}{\Delta x} u D(\rho z T)\right] + c_v^\beta\left[(\rho T)^{n+1} - (\rho T)^n + \frac{\Delta t}{\Delta x} u D(\rho T)\right] = 0. \tag{3.18}$$

Thus, if the following two equations are solved

$$\begin{aligned}(\rho z T)_i^{n+1} &= (\rho z T)_i^n - \frac{\Delta t}{\Delta x} u \Delta(\rho z T), \\ (\rho T)_i^{n+1} &= (\rho T)_i^n - \frac{\Delta t}{\Delta x} u \Delta(\rho T),\end{aligned} \tag{3.19}$$

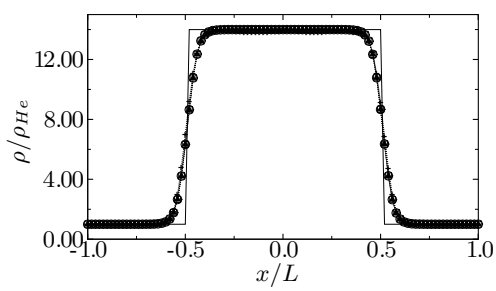
the pressure at the next time step is given by

$$\begin{aligned}p_i^{n+1} &= (\rho z T)^{n+1}(R^\alpha - R^\beta) + R_2(\rho T)^{n+1} \\ &= (R^\alpha - R^\beta)(\rho z T)_i^n + R^\beta(\rho T)_i^n - \frac{\Delta t}{\Delta x} u\left[(R^\alpha - R^\beta)\Delta(\rho z T) + R^\beta \Delta(\rho T)\right] \\ &= p - \frac{\Delta t}{\Delta x} u\left[\Delta\left((R^\alpha - R^\beta)(\rho z T) + R^\beta \rho T\right)\right] = p.\end{aligned} \tag{3.20}$$

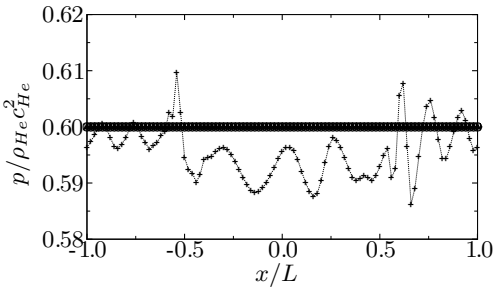
However, equations (3.19) are not very useful because they imply that the continuity equation be replaced by an equation for ρT and the transport equation be replaced by an equation for $\rho z T$, and that both equations be solved consistently. A further difficulty is that the density can no longer be computed from the conserved variables, so that an additional equation for the density must be solved.

In order to overcome these drawbacks, the advantages of the pressure and temperature viewpoints can be combined. Using the pressure viewpoint, it was found that solving a transport equation for $1/(\gamma - 1)$ is sufficient to maintain the pressure equilibrium; furthermore, this formulation does not introduce a modeling error. The drawback is that the transport equation is solved in advection form, and a relationship between $1/(\gamma - 1)$ and z must be provided if z is required. On the other hand, the temperature viewpoint is expected to lead to a monotonic temperature profile if the equations for ρ and ρz are solved consistently; however, pressure oscillations may be generated in this case.

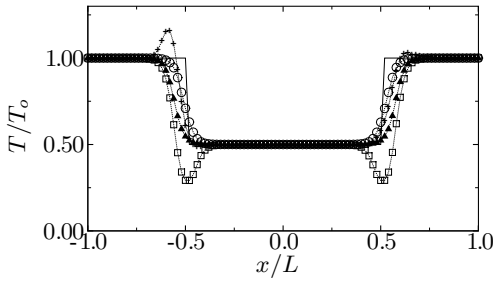
Thus, the following scheme is proposed: the Euler equations are solved along with two transport equations, one in conservative form for ρz, which is used to compute the temperature and mass fraction, and one in advection form for $1/(\gamma - 1)$, which is used to compute the pressure in the convective terms only. This latter equation can be viewed as an equation for a pressure correction that maintains pressure equilibrium when needed. This framework will conserve the mass of each species and preserve pressure equilibrium (and temperature equilibrium in the case of a material interface). Furthermore, no



(a) Density profile at $tc_{He}/L = 4$.



(b) Pressure profile at $tc_{He}/L = 4$.



(c) Temperature profile at $tc_{He}/L = 4$.

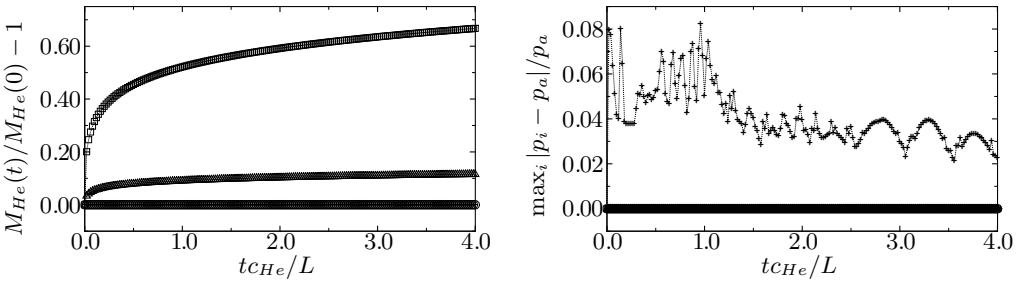
FIGURE 3. Profiles for the advection of a contact discontinuity between helium and nitrogen. Solid line: exact solution; pluses: scheme 1 (fully conservative); open triangles: scheme 2 ($1/(\gamma-1)$); open squares: scheme 3 (z); open circles: scheme 5 ($1/(\gamma-1)$).

modeling error is introduced. The only caveat is that a discrepancy may exist between $1/(\gamma-1)$, which is calculated from the advection equation for $1/(\gamma-1)$, and from z, which is calculated from the advection equation for ρz; however, this discrepancy is expected to diminish as the grid is sufficiently fine. These observations lead to the following scheme:

SCHEME 5 ($1/(\gamma-1)$ AND ρz). *In order to preserve velocity and pressure equilibria and prevent errors in the calculation of the temperature, the average primitive variables, (ρ, u, p), are reconstructed, and two transport equations are solved, one for ρz and one for $1/(\gamma-1)$. Both ρz and $1/(\gamma-1)$ are reconstructed; ρz is used to compute the temperature and $1/(\gamma-1)$ is used to compute the pressure only. The Riemann solver is applied directly to the transport equation in conservative form for ρz but must be modified to solve the transport equation for $1/(\gamma-1)$ in advection form.*

This scheme is effectively an extension of scheme 2 ($1/(\gamma-1)$), in which care is taken to prevent temperature errors through scheme 4 (ρz). Since the transport equation for mass fraction is solved in conservative form, the mass of each species is discretely conserved.

Figures 3 and 4 show the density, pressure and temperature profiles at the final time and the time history of the maximum pressure errors and of the mass of helium for the advection of a contact discontinuity between two different gases. The errors in the pressure when using the standard fully conservative scheme grow up to approximately 8%; the decrease of these errors as the grid is refined is not very rapid (Johnsen 2008). Temperature errors are present again. Scheme 5 is the only one that prevents pressure, temperature and species conservation errors.



(a) History of the normalized error in mass of helium.

(b) History of the normalized L_∞ error in pressure.

FIGURE 4. Time histories for the advection of a contact discontinuity between helium and nitrogen. Pluses: scheme 1 (fully conservative); open triangles: scheme 2 $(1/(\gamma-1))$; open squares: scheme 3 (z); open circles: scheme 5 $(1/(\gamma-1))$.

TABLE 2. Summary of the findings for the different problems.

Scheme	1 (fully conservative)	2 $(1/(\gamma-1))$	3 (z)	4 (ρz)	5 $(1/(\gamma-1)$ & $\rho z)$
Species conservation	yes	no	no	yes	yes
Contact (gas1/gas1)					
Pressure errors	oscillations	–	–	oscillations	–
Temperature errors	–	–	–	–	–
Material interface					
Pressure errors	oscillations	–	–	–	–
Temperature errors	spike	oscillations	spike	–	–
Contact (gas1/gas2)					
Pressure errors	oscillations	–	–	oscillations	–
Temperature errors	spike/oscillations	–	spike	–	–

4. Conclusions and future work

Accurate numerical simulations of compressible multicomponent flows are challenging, as errors in the pressure, temperature and mass of each species may be generated. Previous schemes have been developed to overcome pressure oscillations at interfaces. However, this methodology was not extended to prevent temperature and species conservation errors. In the present work, these three types of errors are examined and quantified, and a new scheme is proposed to overcome them for isolated material interfaces and contact discontinuities. Table 2 provides a summary of the findings.

Preventing errors in the pressure are key to ensure that the solution is stable and that other flow quantities are not affected, even for the Euler equations. Furthermore, preventing temperature and species conservation errors is imperative when the compressible Navier-Stokes equations with heat and mass transfer are considered. If numerical errors due to the convective terms lead to errors in the temperature and mass fraction, the diffusive terms will generate further numerical errors.

Acknowledgements

The author is grateful for the comments by Dr. M. Raessi on the manuscript and for discussions with Dr. V. Terrapon and Dr. C. Liang. This work was supported by DOE-SciDAC2 (Grant DE-FC02-06-ER25787).

REFERENCES

Abgrall, R. 1996 How to prevent pressure oscillations in multicomponent flow calculations: a quasi conservative approach. *J. Comp. Phys.* **125** (1), 150–160.

Johnsen, E. 2008 Spurious oscillations and conservation errors in interface-capturing schemes. *CTR Ann. Res. Briefs*, 115–126.

Johnsen, E. & Colonius, T. 2006 Implementation of WENO schemes in compressible multicomponent flows. *J. Comp. Phys.* **219** (2), 715–732.

Mulder, W., Osher, S., & Sethian, J. A. 1992 Computing interface motion in compressible gas dynamics. *J. Comp. Phys.* **100** (2), 209–228.

Shyue, K. M. 1998 An efficient shock-capturing algorithm for compressible multicomponent problems. *J. Comp. Phys.* **142** (1), 208–242.