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Numerical stability in multifluid gas dynamics with implicit drag forces

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ABSTRACT

The numerical stability of a conventional explicit numerical scheme for solving the inviscid multifluid dynamical equations describing a multicomponent gas mixture is investigated both analytically and computationally. Although these equations do not explicitly contain diffusion terms, it is well known that they reduce to a single-fluid diffusional description when the drag coefficients in the species momentum equations are large. The question then arises as to whether their numerical solution is subject to a diffusional stability restriction on the time step in addition to the usual Courant sound-speed stability condition. An analytical stability analysis is performed for the special case of a quiescent binary gas mixture with equal sound speeds and temperatures. It is found that the Courant condition is always sufficient to ensure stability, so that no additional diffusional stability restriction arises for any value of the drag coefficient, however large. This result is confirmed by one-dimensional computational results for binary and ternary mixtures with unequal sound speeds, which remain stable even when the time step exceeds the usual diffusional limit by factors of order 100.

1. Introduction and summary

The dynamics of fluid mixtures is often described by means of multifluid equations in which each component, species, or material in the mixture satisfies its own continuity, momentum, and energy equations. These equations contain interspecies interaction terms that represent the pairwise exchange of mass, momentum, and energy between the species. Equations of this type are widely used in plasma physics [1–5], multiphase flow [6–10], and other areas. A particular physical application of timely interest is the quantitative description of material mixing [11–17], which is important in combustion, inertial confinement fusion, and certain astrophysical problems, *inter alia*.

Mixing (or demixing) inherently involves relative motion of the species; i.e., unequal species velocities. Those velocities are determined by the individual species momentum equations, which normally contain drag terms representing the pairwise exchange of momentum between species due to frictional forces. When the drag coefficients are large, the differences between the species velocities correspondingly become small. As is well (but perhaps not widely) known, the relative motion of the species then becomes diffusional rather than inertial in character [5,17–22]. In this regime, which we refer to as the diffusional or large-friction limit, the multifluid momentum equations reduce to a single momentum equation for the mixture together with diffusional expressions for the species velocities. The binary diffusion coefficients in those expressions are inversely proportional to the drag coefficients. The resulting diffusion equations determine the mass fluxes in the species continuity equations, and when they are treated explicitly in numerical calculations they of course give rise to the usual familiar diffusional stability restrictions on the time step Δt [23,24].

However, the multifluid equations remain valid and can still be solved in their general form even when the drag coefficients are large, provided the drag terms are treated implicitly to avoid the unacceptably restrictive explicit stability condition that would otherwise be incurred [16,24,25]. As will be seen, however, the implicit treatment of the drag terms actually results in an *explicit* treatment of the corresponding diffusion terms in the large-friction limit, and therefore would not be expected to remove or alleviate the associated diffusional stability condition. Nevertheless, the full multifluid equations themselves contain no explicit mass diffusion

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terms, so one might not at first expect their numerical solution to be subject to a corresponding diffusional stability condition. On the other hand, their known diffusional behavior for large drag suggests that a diffusional stability condition should somehow arise in that limit, but it is not immediately apparent whether, and if so how, this occurs.

Our purpose here is to ascertain whether or not the numerical solution of the multifluid momentum equations is subject to a diffusional stability limit. To this end, we perform a Fourier stability analysis of a standard numerical scheme for solving a simplified linearized system of multifluid equations for a binary gas mixture. The scheme is explicit except for the drag terms, which are treated implicitly as discussed above. One would therefore expect it to be subject to the usual Courant sound-speed stability condition [23,24], in addition to whatever diffusional stability condition might also arise. The value of the drag coefficient β is left arbitrary, so the results encompass the opposite limiting cases of large and small drag as well as all intermediate cases.

In order to derive analytical results, we find it necessary to restrict attention to the case in which the temperatures and sound speeds of the two species are equal. Even so, the stability analysis is somewhat intricate, and it constitutes the bulk of the paper. The analysis shows that the usual explicit diffusional stability condition does indeed arise in the limit of large β, but in that limit it is actually much *less* restrictive than the Courant condition and consequently drops out of the overall stability condition for the scheme as a whole. In the general case of arbitrary β, the stability condition for the scheme as a whole is found to be simply the usual Courant sound-speed condition, independently of β. The numerical scheme is therefore not subject to a diffusional stability condition for *any* value of β, however large (or small). These results may seem counterintuitive if not paradoxical, so they are discussed in sufficient detail to resolve the apparent paradox.

In contrast, the numerical solution of the single-fluid diffusional equations to which the multifluid equations reduce for large β *is* subject to the usual explicit diffusional stability condition, just as one would intuitively expect. Since the latter condition is quadratic in the cell size Δx, whereas the Courant condition is linear, the diffusional condition always becomes the more restrictive for sufficiently small Δx. In that case, however, we further show that the diffusional stability restriction only comes into play in situations where the diffusional equations no longer accurately approximate the multifluid equations, so it is an essentially harmless disadvantage.

As mentioned, these analytical results are based on rather draconian simplifications, so one has no assurance that they are more generally applicable. To obtain more general, albeit empirical, evidence, we also used a standard finite-difference scheme for compressible flow to compute numerical solutions of the one-dimensional multifluid equations for binary and ternary mixtures with unequal sound speeds, to which the analytical results do not apply. The calculations were found to remain stable even when the time step exceeds the diffusional limit by factors of order 100. This behavior is consistent with previous computational experience [16] and strongly suggests that the present analytical stability results are more general than their derivation, and that numerical schemes of this type are not subject to diffusional stability conditions, in spite of the fact that the equations become diffusional in form and character for large β.

The present investigation is restricted to multicomponent mixtures in which the different components are intimately mixed together on the atomic or molecular level. The multifluid equations describing multiphase mixtures are generally similar in form except for the pressure gradient terms [9,26], but those differences profoundly affect the stability properties of the differential equations. The multiphase differential equations inherently contain a physical instability analogous to the classical Kelvin–Helmholtz instability [8], which does not occur in the multicomponent equations. This instability disappears in the diffusional limit, in which the multiphase equations reduce to a single-fluid diffusional description just as the multicomponent equations do [17]. It seems likely that numerical schemes for solving the multifluid equations for multiphase mixtures are likewise immune from any corresponding diffusional stability conditions, since there is no obvious reason to suspect otherwise. However, this would be more difficult to confirm analytically because the numerical stability analysis is complicated by the presence of the physical instability.

The remainder of the paper is organized as follows. The inviscid multifluid equations for a multicomponent ideal gas mixture are summarized in Section 2. In Section 3 the equations are specialized to a binary gas mixture and are linearized about a quiescent steady solution. The resulting linear equations are further specialized to the case in which the two species have the same temperatures and sound speeds, which allows the resulting system of four equations to be decomposed into two decoupled subsystems of two equations each. This greatly simplifies the subsequent numerical stability analysis because the stability of each subsystem can be analyzed separately, and the resulting equations for the growth factors are quadratic rather than quartic.

In Section 4 we present the finite-difference equations that define the numerical scheme used to solve these two subsystems. The overall numerical scheme consists of finite-difference approximations to the equations in each subsystem. The numerical scheme we consider is explicit except for the drag terms, which occur only in Subsystem 2 and are treated implicitly. The numerical stability conditions for Subsystems 1 and 2 are derived in Section 5 by means of a conventional Fourier stability analysis. The two subsystems are of the same mathematical form except for the drag term in Subsystem 2. A single stability analysis of Subsystem 2 thereby also applies to Subsystem 1 as a special case. The stability condition for the scheme as a whole is then simply the more restrictive of the stability conditions for Subsystems 1 and 2, and one thereby obtains the results described above.

The stability analysis for the single-fluid equations that result in the diffusional limit is given in Section 6. This analysis confirms that the diffusional stability condition does indeed reappear in that limit, but is essentially harmless. In Section 7 we present the results of the aforementioned numerical calculations for more general binary and ternary mixtures. Section 8 contains a few concluding remarks.

2. The multifluid differential equations

The multifluid equations for an ideal gas mixture are essentially just the usual governing equations for each individual component or species in the mixture, with the addition of coupling terms representing the exchange of mass, momentum, and energy between the species. For simplicity we neglect the effects of viscosity, thermal conductivity, and chemical reactions. The equations then take the form [2,19,20,22,27]

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}_m) = 0 \tag{1}$$

$$\frac{\partial (\rho_m \mathbf{u}_m)}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}_m \mathbf{u}_m) = -\nabla p_m + \sum_{n \neq m} \mathbf{F}_{mn} \tag{2}$$

$$\begin{aligned} \frac{\partial (\rho_m e_m)}{\partial t} + \nabla \cdot (\rho_m e_m \mathbf{u}_m) \; &= \; -p_m \nabla \cdot \mathbf{u}_m \\ &\quad + \sum_{n \neq m} (Q_{mn} + \gamma_{mn} \Phi_{mn}) \end{aligned} \tag{3}$$

where ρ_m, $\mathbf{u}_m$, p_m, and e_m are respectively the partial mass density, mean velocity, partial pressure, and thermal internal energy