Numerical stability in multifluid gas dynamics with implicit drag forces

J. D. Ramshaw

*Lawrence Livermore National Laboratory, Livermore, CA 94551, USA
Department of Physics, Portland State University, Portland, OR 97207*

C. H. Chang*

Los Alamos National Laboratory, Los Alamos, NM 87545, USA

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.

Keywords: multifluid, two-fluid, friction, drag, diffusion, diffusional limit, stability, numerical stability, stability analysis

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, 2, 3, 4, 5], multiphase flow [6, 7, 8, 9, 10], and other areas. A particular physical application of timely interest is the quantitative description of material mixing [11, 12, 13, 14, 15, 16, 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, 18, 19, 20, 21, 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

*Corresponding author.

Email addresses: john@ramshaw.org (J. D. Ramshaw), chc@lanl.gov (C. H. Chang)

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 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 Sect. 2. In Sect. 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 Sect. 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 Sect. 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 Sect. 6. This analysis confirms that the diffusional stability condition does indeed reappear in that limit, but is essentially harmless. In Sect. 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]

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

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

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

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 of species m . The partial pressures are given by the ideal gas state equation $p_m = (\rho_m/M_m)RT_m$, where M_m and T_m are respectively the molecular weight and temperature of species m and R is the universal gas constant. These equations must be simultaneously solved for all species in the mixture, the total number of which is denoted by N_s .

The interspecies interaction terms in the equations are as follows:

$$\mathbf{F}_{mn} = -\mathbf{F}_{nm} = \beta_{mn}(\mathbf{u}_n - \mathbf{u}_m) \quad (4)$$

is the drag force per unit volume exerted by species n on species m , $\beta_{mn} = \beta_{nm}$ is the associated drag coefficient,

$$Q_{mn} = -Q_{nm} = K_{mn}(T_n - T_m) \quad (5)$$

is the direct rate of thermal energy transfer from species n to species m per unit volume, $K_{mn} = K_{nm}$ is the associated energy exchange coefficient, and

$$\Phi_{mn} = \beta_{mn}|\mathbf{u}_n - \mathbf{u}_m|^2 > 0 \quad (6)$$

is the volumetric rate at which the kinetic energy of species m and n is dissipated by $\mathbf{F}_{mn}$, which is apportioned between them by the weighting factors $\gamma_{mn} = 1 - \gamma_{nm}$. The total volumetric rate of energy dissipation for the mixture is $\Phi = \frac{1}{2} \sum_{mn} \Phi_{mn}$. The binary diffusivities that emerge in the diffusional limit are given by

$$D_{mn} = \frac{p_m p_n}{p \beta_{mn}} \quad (7)$$

where $p = \sum_m p_m$ is the total pressure of the mixture. From a macroscopic perspective, the quantities β_{mn} , K_{mn} , and γ_{mn} are phenomenological coefficients to be obtained from experiments, models, or microscopic theories. However, when binary molecular collisions are the dominant transport mechanism their values can be derived from the kinetic theory of gases, which yields the relations [2] $K_{mn} = 3R\beta_{mn}/(M_m + M_n)$ and $\gamma_{mn} = M_n/(M_m + M_n)$.

3. The linearized two-fluid differential equations

The above equations must be greatly simplified to make analytical stability analyses tractable. To this end, we restrict attention to binary mixtures in one space dimension, and we linearize the equations about a quiescent steady state in which the unperturbed fluid velocities vanish. This effectively removes the convection terms, so the analysis will not reveal the associated convective stability conditions, which are not the focus of the present investigation but must of course be observed in practical calculations. The dissipation rates Φ_{mn} are quadratic in the velocities and are consequently removed by the linearization, and we shall further restrict attention to situations in which the two species share the same temperature, which removes the terms Q_{mn} as well. The energy equations then become isentropic, so that the pressures can be obtained from the isentropic state equation for an ideal gas. The energy equations then decouple from the continuity and momentum equations, which then reduce to the following closed system of four equations ($m = 1, 2$):

$$\frac{\partial \rho_m}{\partial t} = -\rho_m^0 \frac{\partial u_m}{\partial x} \quad (8)$$

$$\rho_m^0 \frac{\partial u_m}{\partial t} = -c_m^2 \frac{\partial \rho_m}{\partial x} - \beta(u_m - u_{3-m}) \quad (9)$$

where ρ_m^0 and c_m are the mass density and isentropic sound speed, respectively, of species m in the unperturbed quiescent fluid mixture. We further restrict attention to the case in which the two species have the same sound speeds; i.e., $c_1 = c_2 = c$.

It is advantageous to transform from the variables ρ_m and u_m to the variables

$$\rho = \rho_1 + \rho_2 \quad (10)$$

$$u = \rho_0^{-1}(\rho_1^0 u_1 + \rho_2^0 u_2) \quad (11)$$

$$\sigma = \sigma_0 \left(\frac{\rho_2}{\rho_2^0} - \frac{\rho_1}{\rho_1^0} \right) \quad (12)$$

$$v = u_2 - u_1 \quad (13)$$

where $\rho_0 = \rho_1^0 + \rho_2^0$ and $1/\sigma_0 = 1/\rho_1^0 + 1/\rho_2^0$. Combining Eqs. (8)–(13), we obtain

$$\frac{\partial \rho}{\partial t} = -\rho_0 \frac{\partial u}{\partial x} \quad (14)$$

$$\rho_0 \frac{\partial u}{\partial t} = -c^2 \frac{\partial \rho}{\partial x} \quad (15)$$

$$\frac{\partial \sigma}{\partial t} = -\sigma_0 \frac{\partial v}{\partial x} \quad (16)$$

$$\sigma_0 \frac{\partial v}{\partial t} = -c^2 \frac{\partial \sigma}{\partial x} - \beta v \quad (17)$$

We now observe that Eqs. (14) and (15) are a closed subsystem of two equations in the two unknowns ρ and u , while Eqs. (16) and (17) are a closed subsystem of two equations in the two unknowns σ and v . Equations (14)

and (15) will be referred to as Subsystem 1, while Eqs. (16) and (17) are referred to as Subsystem 2. We see that Subsystem 1 looks formally the same as the linearized equations for a single fluid with density ρ and velocity u and no drag forces, while Subsystem 2 looks formally the same as the linearized equations for a single fluid with density σ and velocity v subject to a volumetric drag force $-\beta v$. We further note that Subsystems 1 and 2 are identical in mathematical form except for the drag term in Subsystem 2, so that Subsystem 1 may be regarded as a special case of Subsystem 2 obtained by setting $\beta = 0$ and replacing (σ_0, σ, v) therein by (ρ_0, ρ, u) .

It is of interest to examine the behavior of Subsystem 2 in the diffusional limit when β becomes large. In this case, inspection of Eq. (17) shows that v rapidly decays, on a time scale $\tau = \sigma_0/\beta$, to the value

$$v = -\frac{c^2}{\beta} \frac{\partial \sigma}{\partial x} \quad (18)$$

which combines with Eq. (16) to yield

$$\frac{\partial \sigma}{\partial t} = D \frac{\partial^2 \sigma}{\partial x^2} \quad (19)$$

where $D = \sigma_0 c^2 / \beta = c^2 \tau$. Equation (19) is of course a standard diffusion equation with diffusion coefficient D . This confirms that the equations become diffusional in character when the drag coefficient is large, which is a general feature of the multifluid equations [5, 17, 18, 19, 20, 21, 22].

4. The finite-difference scheme

As discussed above, Subsystem 1 may be regarded as a special case of Subsystem 2, so it suffices to restrict our attention and analysis to the latter. The results can then readily be specialized to the former as discussed above. Equations (16) and (17) will be approximated by means of a widely used standard finite-difference numerical scheme for the solution of compressible flow problems [23, 24]. The scheme is explicit except that the drag term is treated implicitly to avoid the corresponding explicit stability condition [24, 25], which becomes onerous when β is large. This scheme is defined by

$$\frac{\sigma_j^{v+1} - \sigma_j^v}{\Delta t} = -\sigma_0 \frac{v_{j+1/2}^v - v_{j-1/2}^v}{\Delta x} \quad (20)$$

$$\sigma_0 \frac{v_{j+1/2}^{v+1} - v_{j+1/2}^v}{\Delta t} = -c^2 \frac{\sigma_{j+1}^{v+1} - \sigma_j^{v+1}}{\Delta x} - \beta v_{j+1/2}^{v+1} \quad (21)$$

where the time level v is denoted by a superscript, j is the spatial index, and spatial derivatives have been approximated by central differences in a conventional staggered mesh [23, 24]. Numerical schemes of this type, in which stiff terms with short time scales are treated implicitly while terms with longer time scales are treated explicitly, have been widely used for decades on an informal intuitive basis, and have received more systematic study in recent years under the rubric of asymptotic-preserving (AP) implicit-explicit (IMEX) schemes [28, 29, 30]. In the present context, the asymptotic behavior being preserved is the diffusional limit for large β .

In spite of the appearance of Eq. (21), this scheme is actually explicit when $\beta = 0$, because Eqs. (20) and (21) can be solved sequentially, so that Eq. (20) can explicitly be solved for σ_j^{v+1} , which is then available for use in Eq. (21) [23, 24]. By the same token, Eq. (21) can easily be solved algebraically for $v_{j+1/2}^{v+1}$ even when $\beta \neq 0$, by virtue of the fact that the drag term does not involve spatial derivatives, and therefore does not introduce coupling between the values of v^{v+1} at neighboring mesh points. The present scheme consequently corresponds to an explicit diffusional scheme for large β , as can be seen by noting that v and σ are evaluated at the same time level in the right member of Eq. (21), while v is evaluated at time level v in Eq. (20), so that an explicit diffusional term results when the two are combined. In contrast, an implicit diffusional scheme would entail coupling between all N mesh points, which would then require the numerical solution of an $N \times N$ linear system.

5. Stability analysis for the two-fluid equations

The stability behavior of Eqs. (20) and (21) is analyzed by means of a standard Fourier stability analysis [23, 24], in which the dependence of σ and v on the spatial and time indices j and ν has the form of a single Fourier mode with amplitudes $\hat{\sigma}$ and $\hat{v}$, respectively, and a wavelength $\lambda = 2\pi/k$; i.e.,

$$\sigma_j^\nu = \hat{\sigma} \xi^\nu \exp(ikj\Delta x) \quad (22)$$

$$v_j^\nu = \hat{v} \xi^\nu \exp(ikj\Delta x) \quad (23)$$

where ξ is the growth factor, which can be real or complex. The stability condition is that $|\xi| \leq 1$ for all allowed values of k . The shortest wavelength that can be supported by the mesh is $2\Delta x$, so k varies in the range $0 \leq k \leq \pi/\Delta x$.

Substituting Eqs. (22) and (23) into Eqs. (20) and (21), we obtain a homogeneous linear system of two equations in the two unknown quantities $\hat{\sigma}$ and $\hat{v}$. In order for a nontrivial solution to exist, the determinant of the coefficient matrix must vanish. This condition reduces, after a little algebra, to the quadratic equation

$$A\xi^2 + B\xi + 1 = 0 \quad (24)$$

where

$$A = 1 + \Delta t/\tau \quad (25)$$

$$B = 4Q^2S^2 - (A + 1) \quad (26)$$

in which $Q = c\Delta t/\Delta x$ is the Courant number based on sound speed, and $S = \sin(k\Delta x/2)$, which varies between zero and unity as k varies from zero to $\pi/\Delta x$. The two solutions of Eq. (24) are of course

$$\xi = \frac{1}{2A}(-B \pm \sqrt{B^2 - 4A}) \quad (27)$$

We now proceed to determine the stability restriction on Δt that must be satisfied to ensure that $|\xi| \leq 1$ for all S in the range $0 \leq S \leq 1$. The analysis requires separate consideration of the following three cases, which encompass all possibilities:

$$(a) \quad -2\sqrt{A} < B < 2\sqrt{A}$$

$$(b) \quad B \leq -2\sqrt{A}$$

$$(c) \quad B \geq 2\sqrt{A}$$

In case (a), $B^2 - 4A < 0$, so that Eq. (27) becomes

$$\xi = \frac{1}{2A}(-B \pm i\sqrt{4A - B^2}) \quad (28)$$

from which it follows at once that

$$|\xi|^2 = \frac{1}{4A^2}(B^2 + 4A - B^2) = \frac{1}{A} \leq 1 \quad (29)$$

The scheme is therefore always stable in case (a).

In case (b), $B^2 - 4A \geq 0$, and since B is negative the value of ξ largest in magnitude is obtained by taking the upper sign in Eq. (27). We thereby obtain

$$\xi = \frac{1}{2A}(-B + \sqrt{B^2 - 4A}) \quad (30)$$

which is never negative, so stability in this case requires $\xi \leq 1$. Equation (26) implies that $B + A + 1 \geq 0$, from which it readily follows that $B^2 + 4AB + 4A^2 = (B + 2A)^2 \geq B^2 - 4A$, so that

$$\sqrt{B^2 - 4A} \leq B + 2A \quad (31)$$

Combining Eqs. (30) and (31), we obtain

$$\xi \leq \frac{1}{2A}(-B + B + 2A) = 1 \quad (32)$$

so that the scheme is always stable in case (b) as well.

Thus we see that the only possibility for instability occurs in case (c). This suggests that we reverse the usual logic and derive the restriction on Δt that must be satisfied to ensure that the scheme is *unstable* for a given value of S . This condition can be derived by restricting attention entirely to case (c). The resulting instability condition, however, is no longer restricted to case (c) but encompasses all three cases, since instability cannot occur in cases (a) and (b). The general condition for that particular value of S to be stable in all three cases is then obtained simply by requiring the general instability condition to be violated. The final stability condition is then obtained by requiring the stability condition for a given value of S to be satisfied for all allowed values of S ; i.e., $0 \leq S \leq 1$.

In case (c), the value of ξ largest in magnitude is obtained by taking the lower sign in Eq. (27), so that

$$|\xi| = \frac{1}{2A}(B + \sqrt{B^2 - 4A}) \quad (33)$$

The condition for instability is $|\xi| > 1$, or

$$B + \sqrt{B^2 - 4A} > 2A \quad (34)$$

This immediately implies $B^2 - 4A > (2A - B)^2$, which reduces to

$$B > 1 + A \quad (35)$$

Equation (35) combines with Eq. (26) to yield $2Q^2S^2 > (1 + A)$, or

$$QS > \sqrt{\frac{1 + A}{2}} \quad (36)$$

At the same time, we must also require that we are actually in case (c) for this result to apply. That is to say, we must verify that we are in the regime where instability can occur. This requires $B \geq 2\sqrt{A}$, which combines with Eq. (26) to yield

$$4Q^2S^2 \geq 1 + 2\sqrt{A} + A = (1 + \sqrt{A})^2 \quad (37)$$

or

$$QS \geq \frac{1 + \sqrt{A}}{2} \quad (38)$$

Instability therefore requires that both Eqs. (36) and (38) be simultaneously satisfied. However, $(\sqrt{A} - 1)^2 = A - 2\sqrt{A} + 1 \geq 0$, which implies $1 + A \geq 2\sqrt{A}$ and $2(1 + A) \geq 1 + 2\sqrt{A} + A = (1 + \sqrt{A})^2$. It follows that

$$\sqrt{\frac{1 + A}{2}} \geq \frac{1 + \sqrt{A}}{2} \quad (39)$$

so that Eq. (36) implies Eq. (38). Equation (36) is therefore the condition for the scheme to be unstable for any particular value of S .

The condition for the scheme to be *stable* for a particular value of S is simply the negation or complement of Eq. (36), which is

$$QS \leq \sqrt{\frac{1 + A}{2}} \quad (40)$$

This condition is most restrictive for the maximum allowed value of S , namely $S = 1$, so the condition that must be imposed for all allowed wavelengths to be stable is simply

$$Q \leq \sqrt{\frac{1 + A}{2}} \quad (41)$$

All that remains is to express Eq. (41) as an explicit restriction on the time step Δt . Squaring Eq. (41), we obtain

$$\left(\frac{c\Delta t}{\Delta x}\right)^2 - \left(\frac{\Delta t}{2\tau}\right) - 1 \leq 0 \quad (42)$$

The left member of Eq. (42) is a quadratic in Δt , the roots of which are

$$\Delta t_{\pm} = \frac{\Delta x^2}{4c^2\tau} \left[1 \pm \sqrt{1 + (4c\tau/\Delta x)^2} \right] \quad (43)$$

Clearly $\Delta t_+ > 0$ and $\Delta t_- < 0$. For Eq. (42) to be satisfied, we must have $\Delta t_- \leq \Delta t \leq \Delta t_+$. The left inequality is always satisfied, so the right inequality provides the final numerical stability condition for Subsystem 2 in the form

$$\Delta t \leq \Delta t_2 \equiv \frac{\Delta x^2}{4c^2\tau} \left[1 + \sqrt{1 + (4c\tau/\Delta x)^2} \right] \quad (44)$$

When the drag coefficient β is small, the relaxation time τ is large and Eq. (44) reduces to

$$\Delta t \leq \Delta x/c \equiv \Delta t_c \quad (45)$$

which is the usual sound-speed stability limit. In the opposite limit of large β , τ becomes very small and Eq. (44) reduces to

$$\Delta t \leq \frac{\Delta x^2}{2c^2\tau} = \frac{\Delta x^2}{2D} \equiv \Delta t_D \quad (46)$$

which is the usual explicit diffusional stability limit. Note that in the former case the diffusional stability condition no longer applies, as one would intuitively expect, but conversely in the latter case the sound-speed stability condition no longer applies, which is perhaps less intuitive.

It is instructive to reexpress the stability condition of Eq. (44) in terms of Δt_c and Δt_D . The result is readily found to be

$$\Delta t \leq \Delta t_2 = \frac{1}{2} \left[\Delta t_D + \sqrt{\Delta t_D^2 + 4\Delta t_c^2} \right] \quad (47)$$

This form clearly shows the reduction to the limiting cases discussed above, and also shows that in the general case Δt_2 is in fact *larger* than either Δt_c or Δt_D ; i.e., $\Delta t_2 \geq \max(\Delta t_c, \Delta t_D)$. The stability condition for Subsystem 2 therefore permits the use of a larger time step than either the sound-speed or diffusional restrictions would allow.

As previously discussed, the stability condition for Subsystem 1 can be obtained from that for Subsystem 2 simply by setting $\beta = 0$ in the latter, which corresponds to taking the limit as $\tau = \sigma_0/\beta \rightarrow \infty$. Equation (44) then reduces to

$$\Delta t \leq \Delta t_1 \equiv \Delta x/c = \Delta t_c \quad (48)$$

which is just the Courant sound-speed stability condition. The complete solution of the multifluid equations requires the simultaneous solution of Subsystems 1 and 2, which in turn requires their respective stability conditions, namely Eqs. (48) and (47), to be simultaneously satisfied; i.e., $\Delta t \leq \min(\Delta t_1, \Delta t_2) = \min(\Delta t_c, \Delta t_2)$. Equation (47) clearly shows that $\Delta t_2 \geq \Delta t_c$, so the overall stability condition for solving the multifluid equations by the present numerical scheme is therefore simply the usual Courant condition of Eq. (48), regardless of the value of β , D , or Δt_D . Thus the present scheme is not subject to a diffusional stability limit for any values of β , D , and/or Δx , no matter how large or small they might be.

A similar but somewhat simpler analysis shows that the corresponding fully implicit scheme, in which the superscripts ν in the right member of Eq. (20) are replaced by $\nu + 1$, is unconditionally stable. The implicitness removes the Courant condition, just as one would intuitively expect [24], and there is no diffusional stability condition either.

6. Stability analysis for the diffusional equations

In the diffusional limit, the two-fluid equations reduce to a single-fluid description in which the relative velocity v is determined by Eq. (18) rather than Eq. (17). Equation (21) is then replaced by

$$\beta v^{\nu+1} = -c^2 \frac{\sigma_+^{\nu+1} - \sigma_-^{\nu+1}}{\Delta x} \quad (49)$$

In contrast to the analysis of the previous section, the Fourier stability analysis of Eqs. (20) and (49) is trivial, and the growth factor ξ is easily found to be

$$\xi = 1 - \frac{4c^2\tau\Delta t}{\Delta x^2} S^2 \quad (50)$$

The stability condition is therefore simply $\xi \geq -1$, or

$$\frac{4c^2\tau\Delta t}{\Delta x^2}S^2 \leq 2 \quad (51)$$

As before, this condition is most restrictive when $S = 1$, when it reduces to

$$\Delta t \leq \Delta t_2 \equiv \frac{\Delta x^2}{2c^2\tau} = \frac{\Delta x^2}{2D} = \Delta t_D \quad (52)$$

which is therefore the stability condition for Subsystem 2 in the diffusional limit. The stability condition for Subsystem 1 is unchanged in that limit, and remains Eq. (48). Stability of the complete calculation requires that both Eqs. (48) and (52) be simultaneously satisfied, so that the overall stability condition is

$$\Delta t \leq \min(\Delta t_1, \Delta t_2) = \min(\Delta t_c, \Delta t_D) \quad (53)$$

Thus, in contrast to the numerical solution of the two-fluid equations, the numerical solution of the single-fluid equations to which they reduce in the diffusional limit is subject to *both* the Courant and diffusional stability limits, just as one would intuitively respect. Since Δt_c is linear in Δx while Δt_D is quadratic, the latter always dominates for sufficiently small Δx . What is remarkable is that the same situation does not obtain for the two-fluid equations, which remain immune from the diffusional limit for any values of the parameters β , D , and Δx in spite of the fact that they reduce to the diffusional equations for large β .

As is well known, the explicit diffusional stability condition is eliminated by the use of a fully implicit difference scheme [24]. One might therefore wonder whether the implicit treatment of the drag term in Eq. (21) is effectively equivalent to the use of a fully implicit difference scheme in the diffusional limit, for if that were the case it would explain why the numerical solution of the multifluid equations is not subject to a diffusional stability condition. However, the above analysis shows clearly that no such equivalence exists, because the drag term in Eq. (49) is treated implicitly just as it was in Eq. (21), and yet the diffusional stability condition nevertheless reappears in Eq. (53). This is not surprising, since as previously remarked implicit diffusional schemes involve coupling between all N cells in the computational region, and thereby require the numerical solution of a large linear system of order N , whereas the implicit treatment of the drag and energy exchange terms merely requires the algebraic solution of a small linear system at each of the N mesh points.

7. Numerical computations

The preceding analytical stability results were derived under highly restrictive conditions which are unlikely ever to obtain in problems of practical interest. In order to empirically investigate whether the absence of a diffusional stability restriction is a more general feature, we computed numerical solutions of the full multifluid equations of Sect. 2 for binary and ternary monatomic gas mixtures with unequal sound speeds in one space dimension, using a standard explicit numerical scheme for compressible flow [23, 24, 31] from which the scheme of Eqs. (20) and (21) was extracted. The computer code used for this purpose was obtained by modifying the code used to generate the numerical results in Ref. [31]. The required modifications were straightforward, and mainly consisted of adding the species index m , introducing linearly implicit approximations to the interspecies coupling terms in Eqs. (2) and (3), and disabling the damped artificial compressibility method for accelerating the approach to steady state.

Calculations were performed for a binary mixture of He and Ar, and a ternary mixture of He, Ne, and Ar. Both calculations were performed in a computational region of length $L = 10$ cm subdivided into a grid of 1000 cells with cell size $\Delta x = 0.01$ cm, and were run out to a final time of $t = 50 \mu\text{s}$. The initial conditions for both calculations were $p_i = x_m p$ and $T_m = 1000$ K, where $p = 0.1$ atm and the initial mole fractions x_m were defined by $x_{\text{Ar}} = 1 - x_{\text{He}} = x/L$ in the binary mixture, and by $x_{\text{Ne}} = 1/3$ and $x_{\text{Ar}} = 2/3 - x_{\text{He}} = (2/3)x/L$ in the ternary mixture. The drag coefficients β_{mn} were obtained from the turbulent mixing model of Scannapieco and Cheng [15, 16], and have the form

$$\beta_{mn} = \frac{\bar{c}}{\lambda + \alpha\ell} \frac{\rho_m \rho_n}{\rho} \quad (54)$$

Figure 1: Courant, diffusional, and actual time steps for He-Ar mixture.

where $\rho = \sum_m \rho_m$, $\bar{c} = \sqrt{(5/3)p/\rho}$ is the mixture sound speed, and the remaining parameters were set to the values $\lambda = 0$, $\alpha = 0.1$, and $\ell = 3$ cm. The resulting values of β_{mn} are roughly three orders of magnitude smaller than those obtained from kinetic theory of gases [22], so that the corresponding diffusion coefficients given by Eq. (7) are roughly three orders of magnitude larger than the corresponding molecular values. The resulting diffusional stability condition is then much more restrictive than the Courant condition, which makes it easy to see whether or not the calculations are subject to it. The energy exchange coefficients K_{mn} were taken from the kinetic theory of gases [2]. The species sound speeds c_m are unequal in these calculations, and the Courant condition was computed based on the largest one; i.e., $\max\{c_m\}$. The diffusional stability condition was similarly computed based on the largest of the binary diffusion coefficients defined by Eq. (7).

Both calculations were performed using the largest time steps for which they remained stable, as empirically determined by numerical experiments to within a tolerance of 1%. Figure 1 shows the Courant and diffusional time step limits as functions of time during the calculation for the binary mixture, as well as the actual time step at which the calculation was performed, which exceeds the diffusional limit by roughly a factor of 100. Figure 2 shows the same information for the ternary mixture, for which the results are entirely similar. It is clear that neither calculation is subject to the diffusional stability limit. Together with the preceding analytical stability analysis, these results strongly suggest that numerical solutions of the multifluid equations are immune from diffusional stability conditions involving the diffusion coefficients D_{mn} given by Eq. (7). However, they will not of course be immune to diffusional stability conditions arising from other diffusional terms in the equations, such as those associated with viscosity and thermal diffusivity.

8. Concluding remarks

The relation $\Delta t_2 \geq \max(\Delta t_c, \Delta t_D)$ may seem odd, since simultaneous stability restrictions typically involve minima, as in Eq. (53), rather than maxima. However, this can be intuitively understood on the following basis. Subsystems 1 and 2 both contain sound waves, so they are both subject to stability restrictions that involve the sound speed. The fact that $\Delta t_2 \geq \Delta t_c$ simply reflects the fact that the implicit drag term introduces additional damping into the system, thereby enhancing the stability and enlarging the stable region relative to what it would be for sound waves alone. The fact that $\Delta t_2 \geq \Delta t_D$ as well reflects the fact that in spite of the notation, the parameter D only has the significance of a diffusivity when β is large, and does not otherwise restrict the time step as much as a diffusivity would. As previously

Figure 2: Courant, diffusional, and actual time steps for He-Ne-Ar mixture.

noted, Δt_D will always become smaller than Δt_c for sufficiently small Δx , but in that case the stability limit does not require $\Delta t \leq \Delta t_D$. Indeed, Eq. (47) shows that the latter condition only obtains when $\Delta t_D \gg \Delta t_c$.

Why then does the diffusional stability limit reappear when we first simplify the differential equations to the diffusional limit prior to approximating them by difference equations? The reason is because that simplification removes the sound waves from Subsystem 2 and renders it purely diffusional in character for all values of D . However, the resulting diffusional equations are not unconditionally valid for all values of D , but rather only when τ is much shorter than the other physical time scales in the problem. When the latter condition is violated, the diffusional equations can still be solved, of course, but they no longer accurately approximate the multifluid equations.

In the present context, the shortest physical time scale present is L/c , where L is the size of the smallest flow feature of interest. The condition for the diffusional description to be physically valid is therefore $\tau \ll L/c$, which can be rewritten as

$$\Delta t_D \gg \frac{\Delta x}{2L} \Delta t_c \quad (55)$$

Equation (55) is roughly equivalent to the condition $\Delta t_D > \Delta t_c$, and the stability condition of Eq. (47) then becomes roughly equivalent to $\Delta t < \Delta t_c$, so that Δt_D does not significantly restrict the time step. Conversely, when $\Delta t_D < \Delta t_c$ so that the time step is controlled by the diffusional stability limit, the diffusional formulation no longer accurately approximates the multifluid equations and the calculation becomes pointless.

The question naturally arises as to whether the absence of an explicit diffusional limit is a general feature common to a wider class of numerical schemes that employ similar IMEX temporal differencing to solve the multifluid equations. We intuitively suspect that such is the case, but the present results do not provide a definitive answer to this question, since no other schemes of this general type have yet been subjected to a similar analysis. It is hoped that those who employ such schemes will further elucidate this question by reporting their observed stability properties in due course.

Acknowledgments

Portions of this work were performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore and Los Alamos National Laboratories under Contracts DE-AC52-07NA27344 and DE-AC52-06NA25396. We are grateful to L. D. Cloutman and the anonymous reviewers for their thoughtful and detailed comments and suggestions, which significantly improved the manuscript.

References

- [1] E. H. Holt, R. E. Haskell, Foundation of Plasma Dynamics, Macmillan, New York, 1965.
- [2] J. M. Burgers, Flow Equations for Composite Gases, Academic, New York, 1969.
- [3] N. A. Krall, A. W. Trivelpiece, Principles of Plasma Physics, McGraw-Hill, New York, 1973.
- [4] F. F. Chen, Introduction to Plasma Physics, Plenum, New York, 1974.
- [5] J. D. Ramshaw, C. H. Chang, Phys. Rev. E 53 (1996) 6382–6388.
- [6] G. B. Wallis, One-Dimensional Two-Phase Flow, McGraw-Hill, New York, 1969.
- [7] J. R. Travis, F. H. Harlow, A. A. Amsden, Nucl. Sci. Eng. 61 (1976) 1–10.
- [8] J. D. Ramshaw, J. A. Trapp, Nucl. Sci. Eng. 66 (1978) 93–102.
- [9] J. D. Ramshaw, Theoret. Comput. Fluid Dynamics 14 (2000) 195–202.
- [10] M. Ishii, T. Hibiki, Thermo-Fluid Dynamics of Two-Phase Flow, 2nd Edition, Springer, New York, 2011.
- [11] D. B. Spalding, Int. J. Num. Meths. Eng. 24 (1987) 1–23.
- [12] N. Freed, D. Ofer, D. Shvarts, S. A. Orszag, Phys. Fluids A 3 (1991) 912–918.
- [13] D. L. Youngs, Laser and Particle Beams 12 (1994) 725–750.
- [14] D. Saltz, W. Lee, T.-R. Hsiang, Phys. Fluids 12 (2000) 2461–2477.
- [15] A. J. Scannapieco, B. Cheng, Phys. Lett. A 299 (2002) 49–64.
- [16] C. H. Chang, A. K. Stagg, J. Comput. Phys. 231 (2012) 4279–4294.
- [17] J. D. Ramshaw, Phys. Fluids 24 (2012) 093301-1–13.
- [18] W. H. Furry, Am. J. Phys. 16 (1948) 63–78.
- [19] F. A. Williams, Am. J. Phys. 26 (1958) 467–469.
- [20] F. A. Williams, Combustion Theory, 2nd Edition, Benjamin/Cummings, Menlo Park, CA, 1985, pp. 631–633.
- [21] C. Truesdell, J. Chem. Phys. 37 (1962) 2336–2344.
- [22] J. D. Ramshaw, J. Non-Equilib. Thermodyn. 18 (1993) 121–134.
- [23] R. D. Richtmyer, K. W. Morton, Difference Methods for Initial-Value Problems, 2nd Edition, Wiley/Interscience, New York, 1967.
- [24] J. D. Ramshaw, Elements of Computational Fluid Dynamics, Imperial College Press/World Scientific, London/Singapore, 2011.
- [25] J. D. Ramshaw, J. Non-Equilib. Thermodyn. 23 (1998) 135–140.
- [26] C. H. Chang, J. D. Ramshaw, Theor. Comput. Fluid Dyn. 19 (2005) 253–260.
- [27] J. D. Ramshaw, Am. J. Phys. 70 (2002) 508–512.
- [28] U. M. Ascher, S. J. Ruuth, B. T. R. Wetton, SIAM J. Num. Anal. 32 (1995) 797–823.
- [29] L. Pareschi, G. Russo, J. Sci. Comput. 25 (2005) 129–155.
- [30] S. Jin, Riv. Mat. Univ. Parma 3 (2012) 177–216.
- [31] J. D. Ramshaw, V. A. Mousseau, Computers & Fluids 20 (1991) 177–186.