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A multifluid model extended for strong temperature nonequilibrium

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We present a multifluid model in which the material temperature is strongly affected by the degree of segregation of each material. In order to track temperatures of segregated form and mixed form of the same material, they are defined as different materials with their own energy. This extension makes it necessary to extend multifluid models to the case in which each form is defined as a separate material. Statistical variations associated with the morphology of the mixture have to be simplified. Simplifications introduced include combining all molecularly mixed species into a single composite material, which is treated as another segregated material. Relative motion within the composite material, diffusion, is represented by material velocity of each component in the composite material. Compression work, momentum and energy exchange, virtual mass forces, and dissipation of the unresolved kinetic energy have been generalized to the heterogeneous mixture in temperature nonequilibrium. The present model can be further simplified by combining all mixed forms of materials into a composite material. Molecular diffusion in this case is modeled by the Stefan-Maxwell equations.

I. INTRODUCTION

Imagine mixing of materials A and B. The material A absorbs radiative energy very well (optically thick), while the material B is virtually transparent (optically thin). When radiative heating is present, material A would be selectively heated. Consequently, material A would have much higher temperature when it is pure segregated form than when it is mixed at the molecular level with the material B. When mixed, a large fraction of energy is used for heating the material B, and the mixture temperature will be lower than pure material A. In order to model this situation, it is necessary to represent temperature dependency on the mixture morphology.

Multifluid models [1–3] provide natural framework to include material strength effects, demixing, and inertial effects required in modeling complex fluid instabilities and mixing. They can be categorized as "multicomponent" models in which mixtures are assumed to be mixed at the molecular level [2], and "multiphase" models where mixtures are segregated in small scales [1]. In these models, the pressure force depends on the mixture morphology [4]. When mixture evolves from segregated form to molecular form, it is possible to make a transition of the pressure force in mathematical form [4].

When the mixture temperature depends strongly on the mixture morphology, however, making this transition as in Ref. [3] does not correctly track the energetics of the mixture. In Refs. [1–3], a material temperature is defined as a quantity that does not depend on the morphology. That is, the temperature of material A is the same regardless whether the material is segregated or not, and the temperature dependency on the mixture morphology will not be represented. The natural way to have the necessary features would be defining the mixed material A as a new form of A. That is, material A is subdivided into two materials, pure and mixed parts, with their own energies (temperatures). This way, instead of having one temperature, two temperatures are assigned to the material A. Of course, material B can also be subdivided into two materials.

A question arises. Mixed A and mixed B have the identical temperatures. Therefore, would it be better to represent mixed material as one material instead of two different material? In view of energetics, it would make sense. However, adopting this approach would prohibit further diffusion within the mixed material. That is, homogenization of mixed material by inter-molecular diffusion will not occur. Unless the time scale of the problem of interest is very small, further diffusion should be modeled, and the natural way to include the diffusion in mixture is to represent mixed A and B as separate materials. That is, it is possible to represent the energy and temperatures of mixed material as combined quantities. But their concentration needs to be individually tracked with diffusion.

In this report, we present a multifluid model extended by further dividing mixing materials into pure and mixed forms. This approach eliminates the necessity of using the transition in the pressure force

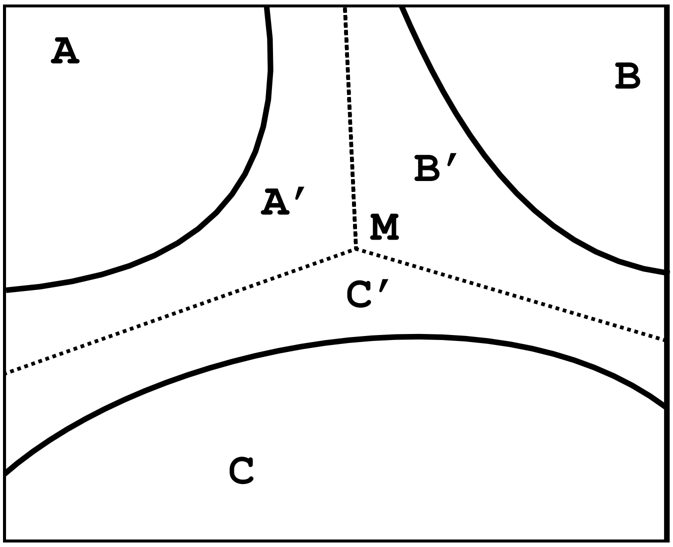

FIG. 1: Simplified mixture morphology.

introduced in Ref. [3]. Appropriate forms of pressure force terms still need to be used depending on the material morphology. Energy conservation of both pure and mixed materials are also presented. We then present a simplified version of the model by combining momentum and energy equations of the mixed forms into the composite momentum and energy equations. Material densities of mixed forms still need to be separately tracked, and diffusion of mixed components is modelled by the Stefan-Maxwell equations.

II. SIMPLIFIED MIXTURE MORPHOLOGY

Mixture morphology usually is very complex, and a complete description would require various statistical information such as distributions of chunk size, velocity, etc. The description of molecular mixtures also requires a variety of additional information, including distributions of compositions and concentrations. It is thus clear that a complete description of such a mixture would be hopelessly complicated and intractable for practical purposes. One is therefore led to seek a simplified description that captures the essential or the most important information in terms of a manageable reduced set of basic variables while neglecting finer details of lesser importance.

We shall conceptually combine all chunks of each pure species into a single region for that species, and all the contents of molecularly mixed regions of all types into a single molecularly mixed region M, as illustrated in Fig. 1 suggested in Ref. [4]. In Fig. 1, there are three materials, A, B, and C. The molecularly mixed portions area denoted as A', B' and C', which are parts of the composite mixture material M. The volume fraction of all segregated pure (chunks) species i (i.e., the volume of chunks of pure species i per unit total volume) will be denoted by α_i^c. Similarly, the volume fraction of the molecularly mixed portion is denoted by α_i^m. (Superscripts c and m respectively represent pure and molecular mixture forms.) Note that $\alpha_i = \alpha_i^c + \alpha_i^m$. The volume fraction of the composite material (i.e., the volume of the molecular mixture per unit total volume) is denoted by $\alpha_M = \sum_i \alpha_i^m$. Since the pure and the composite material fill the total volume, $\sum_i \alpha_i^c + \alpha_M = 1$.

It is also necessary to evaluate the volume effectively occupied by species i within the molecular mixture M. As mentioned above, the volume fraction of species i in an ideal gas mixture (i.e., volume of species i per unit mixture volume) can be identified with the pressure ratio $z_i \equiv p_i/p$ of species i within the mixture [5]. (This interpretation remains valid even in multitemperature mixtures, in which the different species may have different temperatures. When all the species temperatures are equal with the same common value T, z_i reduces to the mole fraction x_i of species i, the interpretation of which as a volume fraction is familiar from Amagat's law.) It follows that α_i^m is simply $\alpha_M z_i^m$, where $z_i^m = p_i^m/p_M$, p_i^m is the partial pressure of species i within the composite material M, and $p_M = \sum_i p_i^m$. Thus the *total* volume fraction of species i (i.e., the volume of all species i present per unit total volume, including both chunks of pure species i and the Amagat's law volume occupied by species i within M) is simply

$$\alpha_i \equiv \alpha_i^c + \alpha_i^m = \alpha_i^c + \alpha_M z_i^m \tag{1}$$

and we see that $\sum_i \alpha_i = 1$ as it should. These relations are valid in the mixture in which each material has its own pressures (pressure nonequilibrium). In this situation, $\tilde{p}_i^c$ represents the pressure of pure material i, not the partial pressure. The average pressure p is then $p = \sum_i \alpha_i^c \tilde{p}_i^c + \sum_i \alpha_i^m \tilde{p}_i^m$, the composite material pressure is given by $\alpha_M p_M = \sum_i \alpha_i^m \tilde{p}_i^m$, and $z_i^m = \alpha_i^m \tilde{p}_i^m / (\alpha_M p_M)$.

Note that there are two material pressures, $\tilde{p}_i^c$ and $\tilde{p}_i^m$. Since we now distinguish the temperatures of pure and mixed components, pressure should also be separately determined for pure and mixed components. Densities, ρ_i^c and ρ_i^m, and energies, e_i^c and e_i^m, are all separately tracked in the present model. Therefore, the system is closed and application of equations of state (EOS) to each component should be possible. In order to reduce computational resources used, EOS can be simplified by combining e_i^c and e_i^m as well as ρ_i^c and ρ_i^m, producing the averaged $\tilde{p}_i = \tilde{p}_i^c = \tilde{p}_i^m$. But this simplification should be used with care.

III. MASS CONSERVATION AND VOLUME FRACTION EVOLUTION

The continuity equations are given by

$$\frac{\partial \left(\alpha_i^c \tilde{\rho}_i^c\right)}{\partial t} + \nabla \cdot \left(\alpha_i^c \tilde{\rho}_i^c \mathbf{u}_i^c\right) \ = \ \dot{M}_i^c \tag{2}$$

$$\frac{\partial \left(\alpha_i^m \tilde{\rho}_i^m\right)}{\partial t} + \nabla \cdot \left(\alpha_i^m \tilde{\rho}_i^m \mathbf{u}_i^m\right) \ = \ \dot{M}_i^m \tag{3}$$

where $\tilde{\rho}_i^c$ is the mass density of pure species i, and $\mathbf{u}_i^c$ and $\mathbf{u}_i^m$ respectively are the mean velocities of species i in pure and molecular mixture forms. $\dot{M}_i^c = -\dot{M}_i^m$ is the mass conversion rate from the pure component to mixed component of material i. ($M_i^c = \alpha_i^c \tilde{\rho}_i^c$ and $M_i^m = \alpha_i^m \tilde{\rho}_i^m$.)

As discussed previously [4], the development of an accurate model for the time evolution of the mixture morphology presents a difficult problem which is out of this report's scope. In this report, this evolution model for $\dot{M}_i^c$ is presumed to be available.

When pressure nonequilibrium is employed, it is required to have an additional set of governing equations to close the system. Otherwise, the system is indeterminate. These additional equations usually take the form of volume fraction evolution [6]. The volume fraction evolution is generalized as

$$\frac{\partial \alpha_i^c}{\partial t} + \nabla \cdot \left(\alpha_i^c \mathbf{u}_i^c\right) \ = \ \alpha_i^c \nabla \cdot \mathbf{u}_v + \alpha_i^c \Delta E_i^c + \dot{\alpha}_i^c \tag{4}$$

$$\frac{\partial \alpha_M}{\partial t} + \nabla \cdot \left(\alpha_M \mathbf{u}_M\right) \ = \ \alpha_M \nabla \cdot \mathbf{u}_v + \alpha_M \Delta E_M + \sum_i \dot{\alpha}_i^m \tag{5}$$

where $\dot{\alpha}_i^c = -\dot{\alpha}_i^m$ is the volume fraction change associated with $\dot{M}_i^c$, ΔE_i^c is the rate of expansion of phase i relative to the overall rate of expansion of the whole mixture, and $\mathbf{u}_v$ is the volume-averaged velocity of the mixture given by

$$\mathbf{u}_v = \sum_i \alpha_i^c \mathbf{u}_i^c + \alpha_M \mathbf{u}_M \tag{6}$$

The mixture average velocity $\mathbf{u}_M$ is given by

$$\mathbf{u}_M = \frac{\sum_i \alpha_i^m \tilde{\rho}_i^m \mathbf{u}_i^m}{\sum_i \alpha_i^m \tilde{\rho}_i^m} \tag{7}$$

α_i^m can be determined by equilibrating $\tilde{p}_i^m$.

We emphasize that Eqs. (4) and (5) are rigorous, since no approximations have been made in their derivations. Simple ΔE models take the form given by [6]

$$\Delta E_i^c = \frac{Ac}{Lp}\alpha_i^c\left(\tilde{p}_i^c - p\right) \tag{8}$$

$$\Delta E_M = \frac{Ac}{Lp}\alpha_M\left(p_M - p\right) \tag{9}$$

where A is a positive dimensionless constant of order unity, L is the length scale representing the mean size of the phase fragments, and c is the mixture speed of sound given by

$$c^2 = \frac{\sum_i Y_i^c\gamma_i^c c_{vi}^c + Y_M\gamma_M c_{vM}}{\rho^2(\sum_i Y_i^c c_{vi}^c + Y_M c_{vM})}\left(\sum_i \frac{Y_i^c\gamma_i^c}{\rho_i^{c2}c_i^{c2}} + \frac{Y_M\gamma_M}{\rho_M^2 c_M^2}\right) \tag{10}$$

where $Y_i = \alpha_i\tilde{\rho}_i/\rho$ is the mass fraction, and $c_{vi} \equiv (\partial e_i/\partial T_i)_{\rho_i}$, γ_i and c_i respectively are the specific heat at constant volume, the specific heat ratio, and speed of sound of material i. Suggested values of L and A can be found in Refs. [3, 6].

Equation (5) and equilibration of $\tilde{p}_i^m$ can be replaced by a set of evolution equations for α_i^m given by

$$\frac{\partial\alpha_i^m}{\partial t} + \nabla\cdot(\alpha_i^m\mathbf{u}_i^m) = \alpha_i^m\nabla\cdot\mathbf{u}_v + \alpha_i^m\Delta E_i^m + \dot{\alpha}_i^m \tag{11}$$

where ΔE_i^m is given by

$$\Delta E_i^m = \frac{Ac}{Lp}\alpha_i^m\left(\tilde{p}_i^m - p\right) \tag{12}$$

Note that the material pressures $\tilde{p}_i^m$ in the composite material are not equilibrated, and thus adequate modeling is highly desirable for ΔE_i^m that provides the equilibration tendency.

IV. DYNAMICS OF HETEROGENEOUS MIXTURES IN PRESSURE NONEQUILIBRIUM

IV.1. Pressure forces

In single-pressure multiphase flow models, the pressure gradient term takes the form $\mathbf{G}_i = -\alpha_i\nabla p$, where $\mathbf{G}_i$ is the stress (force), α_i is the volume fraction of the material i, and p is the total pressure. This form arises as the net result of the terms $-\nabla(\alpha_i p) + p\nabla\alpha_i$, which respectively represent the intraphase pressure force of phase i on itself and the interphase pressure force at the interface exerted on phase i by the other phases [3, 4, 7, 8]. In multicomponent models, the pressure force term is $\mathbf{G}_i = -\nabla p_i$, where p_i is the partial pressure of species i. The partial pressure can be interpreted as $\alpha_i p$, where $\alpha_i = p_i/p$ is the effective volume fraction of species i in the mixture in the sense of Amagat's law. As a mixture evolves from segregated to molecular mixing, the pressure gradient terms should also make a smooth mathematical transition between the forms $\alpha_i\nabla p$ and ∇p_i appropriate to those two limiting cases. A formulation showing such a transition has recently been suggested [4]. However, when segregated and mixed components are treated as separate materials, it is unnecessary to employ the pressure force transition. But it is required to use appropriate pressure force for each component. That is, $\alpha_i\nabla p$ should be used for segregated components, while ∇p_i is used for mixed components.

When pressure nonequilibrium is employed, it becomes necessary to model the pressure at material interfaces [9–13]. Depending on the selection, it becomes necessary to model subzonal internal motion such as the motion of the interface [10, 11]. One obvious way to eliminate the modeling need of the internal motion is to set the interface pressure as the local average pressure p as in Ref. [3]. We adopt this approach in the present model.

The species momentum equations are given by

$$\begin{aligned}\frac{\partial\left(\alpha_i^c\tilde{\rho}_i^c\mathbf{u}_i^c\right)}{\partial t}+\nabla\cdot\left(\alpha_i^c\tilde{\rho}_i^c\mathbf{u}_i^c\mathbf{u}_i^c\right) &= -\nabla\left[\alpha_i^c\left(\tilde{p}_i^c-p\right)\right]-\alpha_i^c\nabla p+\nabla\cdot\left(\alpha_i^c\tilde{\boldsymbol{\tau}}_i\right)+\dot{M}_i^c\mathbf{u}_i^c+\mathbf{V}_i^c+\mathbf{F}_i^c \quad (13)\\ \frac{\partial\left(\alpha_i^m\tilde{\rho}_i^m\mathbf{u}_i^m\right)}{\partial t}+\nabla\cdot\left(\alpha_i^m\tilde{\rho}_i^m\mathbf{u}_i^m\mathbf{u}_i^m\right) &= -\nabla\left[\alpha_i^m\left(\tilde{p}_i^m-p\right)\right]-\alpha_M\nabla\frac{\alpha_i^m}{\alpha_M}p-\dot{M}_i^c\mathbf{u}_i^c+\mathbf{V}_i^m+\mathbf{F}_i^m \quad (14)\end{aligned}$$

where $\mathbf{V}$ is the virtual mass force, $\mathbf{F}$ is the momentum exchange (friction) force, and $\tilde{\boldsymbol{\tau}}_i$ is the deviatoric stress of pure material i. Note that material strength is presumed to disappear in the composite material.

The sum of pressure forces in Eq. (14) becomes $\nabla\alpha_M p_M + p\nabla\alpha_M$, which is the correct pressure force for the whole mixture (M) material. When this term is added to the sum of the pressure forces in Eq. (13), we obtain ∇p, the correct pressure force for the entire mixture. That is, the sum of pressure forces in Eqs. (13) and (14) is ∇p.

It is important to recognize that Eq. (13) provides the framework for handling fluid instabilities, since they retain the inertial differences between materials. Fluid instabilities result from the fact that materials with different density (inertia) responds differently to the acceleration in a mixture. Therefore, retaining the inertial difference is essential in modeling of fluid instabilities. Observe that many mixing models cannot arrive at the correct steady state in which heavy fluid is at the bottom and light fluid at the top with gravity pointing downwards. They usually end up producing uniform mixture due to their inability of simulating demixing.

At the limit of large friction (large momentum exchange coefficients), the inertial difference can be ignored. When it is ignored, Eqs. (14) reduce to the Stefan-Maxwell equations [14] (derivation shown in Sec. VI.2), which are the fundamental equations describing diffusion. That is, Eq. (14) is applicable to the wide range including diffusion, regardless of the magnitude of the frictional forces. Thermal diffusion effects are not included in Eqs. (13) and (14). They can be included in a similar manner as in Ref. [14].

IV.2. Virtual mass forces

Upon inspecting the development in Ref. [3], virtual mass forces are obtained as

$$\begin{aligned}\mathbf{V}_i^c &= \sum_j C_{ij}^V\alpha_i^c\alpha_j^c\left(\frac{D_j^c\mathbf{u}_j^c}{Dt}-\frac{D_i^c\mathbf{u}_i^c}{Dt}\right)+\sum_j C_{ij}^V\alpha_i^c\alpha_j^m\left(\frac{D_j^m\mathbf{u}_j^m}{Dt}-\frac{D_i^c\mathbf{u}_i^c}{Dt}\right) \quad (15)\\ \mathbf{V}_i^m &= \sum_j C_{ij}^V\alpha_i^m\alpha_j^c\left(\frac{D_j^c\mathbf{u}_j^c}{Dt}-\frac{D_i^m\mathbf{u}_i^m}{Dt}\right) \quad (16)\end{aligned}$$

The material derivatives are defined as $D_i^c/Dt = \partial/\partial t + \mathbf{u}_i^c\cdot\nabla$ and $D_i^m/Dt = \partial/\partial t + \mathbf{u}_i^m\cdot\nabla$. The virtual mass coefficient C_{ij}^V is given by

$$C_{ij}^V = \frac{(\tilde{\rho}_i+\tilde{\rho}_j)}{2\pi\mu(1+r)}\frac{\lambda}{|h_{ij}^C|}-\frac{\tilde{\rho}_i\tilde{\rho}_j}{\rho} \quad (17)$$

where the average material density $\tilde{\rho}_i$ is given by

$$\tilde{\rho}_i = \frac{\alpha_i^c\tilde{\rho}_i^c+\alpha_i^m\tilde{\rho}_i^m}{\alpha_i^c+\alpha_i^m} \quad (18)$$

$\mu = 0.5$ is a model coefficient, λ is the perturbation wave length, and r is the density ratio given by [15]

$$r = \min\left[\left(\frac{\max(\tilde{\rho}_i,\tilde{\rho}_j)}{\min(\tilde{\rho}_i,\tilde{\rho}_j)}\right)^{1/3},\frac{1}{2*0.06}\right] \quad (19)$$

The perturbation amplitude h_{ij}^c is given by

$$h_{ij}^c = \frac{|\mathbf{L}_{ij}^c|}{\mu(1+r)} \quad (20)$$

where L_{ij}^c is the mixing length scale given by

$$\frac{D_v \mathbf{L}_{ij}^c}{Dt} = \mathbf{u}_j^c - \mathbf{u}_i^c \tag{21}$$

The material derivative $D_v/Dt = \partial/\partial t + \mathbf{u}_v \cdot \nabla$ is based on the volume-averaged velocity $\mathbf{u}_v = \sum_i (\alpha_i^c \mathbf{u}_i^c + \alpha_i^m \mathbf{u}_i^m)$.

The virtual mass coefficient C_{ij}^V presented above involves simplifying approximations [3]. Note also that by separating pure and mixed components, we no longer need the model parameter n defined in Ref. [3] for controlling the speed of the transition from segregated to molecular mixtures. The presented virtual mass force vanishes appropriately as the segregated mixture evolves to molecular mixture as it should. The virtual mass force also vanishes on a material when it becomes completely mixed at the molecular level.

IV.3. Momentum exchange

The friction forces are given by [2, 3]

$$\mathbf{F}_i^c = \sum_j B_{ij}^c \alpha_i^c \alpha_j^c \left(\mathbf{u}_j^c - \mathbf{u}_i^c\right) + \sum_j B_{ij}^c \alpha_i^c \alpha_j^m \left(\mathbf{u}_j^m - \mathbf{u}_i^c\right) \tag{22}$$

$$\mathbf{F}_i^m = \sum_j B_{ij}^c \alpha_i^m \alpha_j^c \left(\mathbf{u}_j^c - \mathbf{u}_i^m\right) + \sum_j B_{ij}^m \alpha_i^m \alpha_j^m \left(\mathbf{u}_j^m - \mathbf{u}_i^m\right) \tag{23}$$

B_{ij}^c and B_{ij}^m are the coefficients given by

$$B_{ij}^c = C\left(\tilde{\rho}_i + \tilde{\rho}_j\right) \frac{\left|\mathbf{u}_j^c - \mathbf{u}_i^c\right|}{\mu(1+r)\left|\mathbf{L}_{ij}^c\right|} \tag{24}$$

$$B_{ij}^m = \frac{\tilde{\rho}_i \tilde{\rho}_j}{\rho} \frac{C_s}{\lambda_c + \alpha_{ij}\left|\mathbf{L}_{ij}^m\right|} \tag{25}$$

where C_s is the adiabatic speed of the sound of the mixture, λ_c is the mean free path of the mixture, α_{ij} is the model constant, and $\mathbf{L}_{ij}^m$ and $\mathbf{L}_{ij}^c$ are the length scales obtained by

$$\frac{D_v \mathbf{L}_{ij}^m}{Dt} = \mathbf{u}_j^m - \mathbf{u}_i^m \tag{26}$$

$$\frac{D_v \mathbf{L}_{ij}^c}{Dt} = \mathbf{u}_j^c - \mathbf{u}_i^c \tag{27}$$

Note that B_{ij}^c and B_{ij}^m have been simplified using $\tilde{\rho}_i$ in a similar manner as C_{ij}^V. The coefficient C is given by [15]

$$C = \frac{2 - 3\theta}{4\alpha(2-\theta)} \tag{28}$$

where α is the dimensionless coefficient used in the late-time scaling of Rayleigh-Taylor instability, $h = \alpha A a t^2$ (α here should not be confused with the volume fraction which has a subscript representing material), A is the Atwood number, a is the acceleration, and θ is the exponent that appears in the Richtmyer-Meshkov scaling law, $h \sim t^\theta$. Note again that the model coefficient n [3] for controlling the speed of the transition from segregated to molecular mixtures is no longer necessary.

IV.4. Total momentum conservation

It may be intuitively obvious to many that the summation of momentum equations over all species should reduce to the momentum equation of the whole mixture (the single fluid momentum equation) given by

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla \cdot (\rho\mathbf{u}\mathbf{u}) = -\nabla p \tag{29}$$

where $\rho = \sum_i (\alpha_i^c \tilde{\rho}_i^c + \alpha_i^m \tilde{\rho}_i^m)$ is the total mass density, $\mathbf{u} = (1/\rho) \sum_i (\alpha_i^c \tilde{\rho}_i^c \mathbf{u}_i^c + \alpha_i^m \tilde{\rho}_i^m \mathbf{u}_i^m)$ is the mass-averaged mixture velocity. However, the summation reduces to

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \sum_i \left[\nabla (\alpha_i^c \tilde{\rho}_i^c \mathbf{w}_i^c \mathbf{w}_i^c) + \nabla (\alpha_i^m \tilde{\rho}_i^m \mathbf{w}_i^m \mathbf{w}_i^m) \right] \tag{30}$$

where $\mathbf{w}_i = \mathbf{u}_i - \mathbf{u}$ is the drift velocity of the material i. The term involving $\mathbf{w}$ represents the advection of the drift momentum, which can become large when the mixture is virtually stationary but with strong mixing motion. Since this term is not negligible, a question arises: which one is correct?

We need to recognize that the total momentum of many bodies moving at their own velocities is the sum of the individual momentum. That is, the total momentum does not serve as a constraint. It just is a derived quantity that represents the sum of each material momentum in the system. Therefore, Eq. (30), not Eq. (29), should be solved if the total momentum equation needs to be solved.

V. ENERGETICS IN HETEROGENEOUS MIXTURES

The material internal energy equations are given by

$$\begin{aligned} \frac{\partial (\alpha_i^c \tilde{\rho}_i^c e_i^c)}{\partial t} + \nabla \cdot (\alpha_i^c \tilde{\rho}_i^c e_i^c \mathbf{u}_i^c) &= \nabla \cdot \alpha_i^c k_i^c \nabla T_i^c + \dot{M}_i^c e_i^c + W_i^c + Q_i^{Vc} + Q_i^{Fc} + Q_i^{Tc} & (31) \\ \frac{\partial (\alpha_i^m \tilde{\rho}_i^m e_i^m)}{\partial t} + \nabla \cdot (\alpha_i^m \tilde{\rho}_i^m e_i^m \mathbf{u}_i^m) &= \nabla \cdot \alpha_i^m k_i^m \nabla T_i^m - \dot{M}_i^c e_i^c + W_i^m + Q_i^{Vm} + Q_i^{Fm} + Q_i^{Tm} & (32) \end{aligned}$$

where e_i and T_i respectively are the specific energy and temperature of material i. Thermal conductivities k_i^c and k_i^m are evaluated at the temperatures of pure and mixture phases, respectively. Terms represented by W and Q are discussed below. Note that enthalpy diffusion, or diffusion-thermo effect (Dufour effect), has been included in Eqs. (31) and (32) [5].

V.1. Compression work and energy dissipation due to stress

The compression work W_i is given by

$$\begin{aligned} W_i^c &= \alpha_i^c \tilde{\boldsymbol{\tau}}_i : \nabla \mathbf{u}_i^c - p \left[\frac{\partial \alpha_i^c}{\partial t} + \nabla \cdot (\alpha_i^c \mathbf{u}_i^c) \right] & (33) \\ W_i^m &= -\frac{\alpha_i^m}{\alpha_M} p \left[\frac{\partial \alpha_M}{\partial t} + \nabla \cdot (\alpha_M \mathbf{u}_i^m) \right] & (34) \end{aligned}$$

Dissipation by the deviatoric stress $\tilde{\boldsymbol{\tau}}_i$ has been included in Eq. (33). Observe that the present W_i terms reduce to the proper compression work in the limiting cases of multiphase and multicomponent mixtures.

V.2. Dissipation of unresolved kinetic energy

Virtual mass effects induce secondary flows. These secondary flows and the associated kinetic energy are not usually resolved in macroscopic hydrodynamic simulations. (We adopt the term “unresolved kinetic energy” (UKE) suggested in Ref. [16].) UKE is similar to turbulent kinetic energy, as both represent kinetic energy of unresolved fluid motion, not thermal energy. They eventually dissipate into thermal energy via viscous dissipation. Since the dissipation of UKE is not instantaneous, it is strongly desirable to have additional model equation(s) similar to the turbulent kinetic energy equation to properly model generation, advection, and dissipation of UKE. When turbulent kinetic energy equation is a part of the system of equations solved, it could include UKE.

In the absence of an appropriate model, instantaneous dissipation of UKE may be assumed. The thermal energy sources Q_i^V due to dissipation of UKE are given by

$$\begin{aligned}
Q_i^{Vc} &= \sum_j \zeta_{ij}^{cc} Q_{ij}^{Vcc} + \sum_j \zeta_{ij}^{cm} Q_{ij}^{Vcm} && (35)\\
Q_i^{Vm} &= \sum_j \zeta_{ij}^{mc} Q_{ij}^{Vmc} && (36)\\
Q_{ij}^{Vcc} &= C_{ij}^V \alpha_i^c \alpha_j^c \left(\frac{D_j^c \mathbf{u}_j^c}{Dt} - \frac{D_i^c \mathbf{u}_i^c}{Dt} \right) \cdot \left(\mathbf{u}_j^c - \mathbf{u}_i^c \right) && (37)\\
Q_{ij}^{Vcm} &= C_{ij}^V \alpha_i^c \alpha_j^m \left(\frac{D_j^m \mathbf{u}_j^m}{Dt} - \frac{D_i^c \mathbf{u}_i^c}{Dt} \right) \cdot \left(\mathbf{u}_j^m - \mathbf{u}_i^c \right) && (38)\\
Q_{ij}^{Vmc} &= C_{ij}^V \alpha_i^m \alpha_j^c \left(\frac{D_j^c \mathbf{u}_j^c}{Dt} - \frac{D_i^m \mathbf{u}_i^m}{Dt} \right) \cdot \left(\mathbf{u}_j^c - \mathbf{u}_i^m \right) && (39)
\end{aligned}$$

The dissipation between the (i,j) material pair, Q_{ij}^{Vcc}, Q_{ij}^{Vcm}, and Q_{ij}^{Vmc}, need to be divided between species i and j. By assuming that the temperature changes of the thin layers (film) at the contact surfaces due to UKE dissipation are identical for both materials, the fraction of dissipation energy into species i, ζ_{ij}, is given by

$$\begin{aligned}
\zeta_{ij}^{cc} &= \frac{C_{vi}^c}{C_{vi}^c + C_{vj}^c} && (40)\\
\zeta_{ij}^{cm} &= \frac{C_{vi}^c}{C_{vi}^c + C_{vj}^m} && (41)\\
\zeta_{ij}^{mc} &= \frac{C_{vi}^m}{C_{vi}^m + C_{vj}^c} && (42)\\
\zeta_{ij}^{mm} &= \frac{C_{vi}^m}{C_{vi}^m + C_{vj}^m} && (43)
\end{aligned}$$

where C_{pi} and C_{vi} respectively are the constant-pressure and constant-volume specific heats of species i.

V.3. Frictional dissipation

Q_i^F is the dissipation caused by the frictional forces, given by

$$\begin{aligned}
Q_i^{Fc} &= \sum_j \zeta_{ij}^{cc} B_{ij}^c \alpha_i^c \alpha_j^c \left(\mathbf{u}_j^c - \mathbf{u}_i^c \right) \cdot \left(\mathbf{u}_j^c - \mathbf{u}_i^c \right) + \sum_j \zeta_{ij}^{cm} B_{ij}^c \alpha_i^c \alpha_j^m \left(\mathbf{u}_j^m - \mathbf{u}_i^c \right) \cdot \left(\mathbf{u}_j^m - \mathbf{u}_i^c \right) && (44)\\
Q_i^{Fm} &= \sum_j \zeta_{ij}^{mc} B_{ij}^c \alpha_i^m \alpha_j^c \left(\mathbf{u}_j^c - \mathbf{u}_i^m \right) \cdot \left(\mathbf{u}_j^c - \mathbf{u}_i^m \right) + \sum_j \zeta_{ij}^{mm} B_{ij}^m \alpha_i^m \alpha_j^m \left(\mathbf{u}_j^m - \mathbf{u}_i^m \right) \cdot \left(\mathbf{u}_j^m - \mathbf{u}_i^m \right) && (45)
\end{aligned}$$

The distribution factors ζ_{ij} are given by Eqs.(40)–(43).

V.4. Energy exchange due to temperature difference

The subzonal scale inter-material energy exchange in heterogeneous mixture is composed of the energy exchange via molecular collisions in composite material and spatial heat transport between segregated components. This can be represented in a simple manner as [17]

$$\begin{aligned}
Q_i^{Tc} &= \sum_j \alpha_i^c \alpha_j^c E_{ij}^c \left(T_j^c - T_i^c \right) + \sum_j \alpha_i^c \alpha_j^m E_{ij}^c \left(T_j^m - T_i^c \right) && (46)\\
Q_i^{Tm} &= \sum_j \alpha_i^m \alpha_j^c E_{ij}^c \left(T_j^c - T_i^m \right) + \sum_j \alpha_i^m \alpha_j^m R_{ij}^m \left(T_j^m - T_i^m \right) && (47)
\end{aligned}$$

where E_{ij} is the energy exchange coefficient constructed by modeling subzonal heat conduction, and R_{ij} is the energy exchange coefficients via molecular collision processes. Generalized from the recent development presented in Ref. [17], they are given by

$$E^c_{ij} \;=\; \max\left(\frac{S_{ij}k^c_{ij}}{\ell_i+\ell_j}, \frac{3k_B}{m_i+m_j}\frac{B^c_{ij}}{\mathrm{Pr}^c_{ij}}\right) \tag{48}$$

$$R^m_{ij} \;=\; \frac{16k_B}{(m_i+m_j)^2}\tilde{\rho}^m_i\tilde{\rho}^m_j\Omega^{(1)}_{ij}(1, T^m_{ij}) \tag{49}$$

where m_i is the molecular mass of the species i, and k_B is the Boltzmann's constant. The effective pair temperature T^m_{ij} in the composite material is given by [18]

$$T^m_{ij} = \frac{m_iT^m_j + m_jT^m_i}{m_i+m_j} \tag{50}$$

$\Omega^{(1)}_{ij}(n, T)$ is the integral defined as [19]

$$\Omega^{(1)}_{ij}(n, T) = \frac{1}{2\sqrt{\pi}}\left(\frac{\mu_{ij}}{2k_BT}\right)^{(2n+3)/2}\int_0^\infty \exp\left(-\frac{\mu_{ij}v^2}{2k_BT}\right)v^{2n+3}Q^{(1)}_{ij}(v)\,dv \tag{51}$$

where $\mu_{ij} = m_im_j/(m_i+m_j)$ is the reduced mass of the particle pair i and j, T is the dummy temperature variable, and $Q^{(1)}_{ij}(v)$ is the cross-section for relative speed v, which is an integral involving the angle of deflection χ over all impact parameters b given by [19]

$$Q^{(1)}_{ij}(v) = 2\pi\int_0^\infty (1-\cos\chi)b\,db \tag{52}$$

S_{ij} is the characteristic contact surface area between materials i and j, and ℓ_i is the characteristic length scale of material i. The inter-material diffusivity k^r_{ij} between segregated pure materials pair (i,j) can be modeled as

$$\frac{\ell_i+\ell_j}{k^c_{ij}} = \frac{\ell_i}{k^c_i} + \frac{\ell_j}{k^c_j} \tag{53}$$

when ℓ_i are given. In the absence of that information, we can use the simple harmonic mean given by

$$\frac{2}{k^c_{ij}} = \frac{1}{k^c_i} + \frac{1}{k^c_j} \tag{54}$$

Pr^c_{ij} is the Prandtl number at the segregated material interface. When this value is not available, we can use the value of order unity, e.g., 0.7.

Note that B^c_{ij} and E^c_{ij} are not subdivided into B^{cc}_{ij}, B^{cm}_{ij}, B^{mc}_{ij}, etc. That is, momentum and energy exchange between the segregated material and the composite mixture material has been modeled as momentum and energy exchange between segregated materials throughout this report. Inaccuracies resulting from this simplification is expected to be minor.

The energy exchange rate R_{ij} usually is very large, resulting in the much shorter time scale than the time scale of interest. With an appropriate numerical scheme (time implicit scheme), equilibrium results should automatically be produced in the composite material. For plasma-photon mixtures, it is necessary to generalize the energy equations and all the related terms. This generalization can follow the generalization presented in [3, 17], and thus is not presented here. When radiation transport is involved, the fast energy exchange and resulting temperature equilibrium in the composite mixture material can be achieved by solving for the composite material energy when the radiation transport is solved. Details of this approach is summarized in Ref. [20].

Determining the contact surface area S_{ij} and the length scales ℓ_i usually require models for them. The development of those models are outside the scope of this report, and thus is not discussed here. A model for monodisperse spherical particles has been presented in Ref. [21].

VI. COMBINED MOMENTUM AND ENERGY OF MIXED PHASE

Although solving momentum and energy equations for each species in the mixed phase (solving Eqs. (14) and (32)) is a valid approach, this is not necessary in practice. In molecular mixture, the time scale of velocity equilibration would usually be much smaller than the time scale of interest. Therefore, it is possible to combine species momentum and energy equations into the momentum and energy conservation equations for the composit mixture material. In this section, we present this approach.

Note that species conservation, Eq. (3), still needs to be solved. Therefore, it is necessary to determine $\mathbf{u}_i^m$, and they are obtained by the Stefan-Maxwell equations. The solved volume fraction evolution is given by Eq. (5), not Eq. (11). The volume fractions of species in the composite mixture, α_i^m, is obtained by the equilibration of $\tilde{p}_i^m$.

VI.1. Composite momentum equation

In the composite material, friction coefficients B_{ij}^m are large [22]. Due to large friction, large differences in species velocities do not develop, and it becomes a good approximation to ignore inertial differences in the species. That is $D_i^m \mathbf{u}_i^m / Dt \equiv \partial \mathbf{u}_i^m / \partial t + \mathbf{u}_i^m \cdot \nabla \mathbf{u}_i^m$ is replaced by $D_M \mathbf{u}_M / Dt \equiv \partial \mathbf{u}_M / \partial t + \mathbf{u}_M \cdot \nabla \mathbf{u}_M$. The resulting momentum equation for the composite material is then given by

$$\frac{\partial \left(\alpha_M \tilde{\rho}_M \mathbf{u}_M\right)}{\partial t} + \nabla \cdot \left(\alpha_M \tilde{\rho}_M \mathbf{u}_M \mathbf{u}_M\right) = -\nabla \left[\alpha_M \left(p_M - p\right)\right] - \alpha_M \nabla p - \sum_i \dot{M}_i^c \mathbf{u}_i^c + \mathbf{V}_M + \mathbf{F}_M \tag{55}$$

where $\tilde{\rho_M} = \sum_i \alpha_i^m \tilde{\rho}_i^m / \alpha_M$ is the composite material density. Virtual mass forces and friction forces now take the form

$$\begin{aligned}
\mathbf{V}_i^c &= \sum_j C_{ij}^V \alpha_i^c \alpha_j^c \left(\frac{D_j^c \mathbf{u}_j^c}{Dt} - \frac{D_i^c \mathbf{u}_i^c}{Dt}\right) + C_{iM}^V \alpha_i^c \alpha_M \left(\frac{D_M \mathbf{u}_M}{Dt} - \frac{D_i^c \mathbf{u}_i^c}{Dt}\right) && (56)\\
\mathbf{V}_M &= \sum_j C_{Mj}^V \alpha_M \alpha_j^c \left(\frac{D_j^c \mathbf{u}_j^c}{Dt} - \frac{D_M \mathbf{u}_M}{Dt}\right) && (57)\\
\mathbf{F}_i^c &= \sum_j B_{ij}^c \alpha_i^c \alpha_j^c \left(\mathbf{u}_j^c - \mathbf{u}_i^c\right) + B_{iM}^c \alpha_i^c \alpha_M \left(\mathbf{u}_M - \mathbf{u}_i^c\right) && (58)\\
\mathbf{F}_M &= \sum_j B_{Mj}^c \alpha_M \alpha_j^c \left(\mathbf{u}_j^c - \mathbf{u}_M\right) && (59)
\end{aligned}$$

VI.2. Diffusion in composite material

When Eqs. (14) are combined to constitute the composite material momentum conservation, it is implied that the virtual mass and friction forces between the composite material and pure material are distributed to each species in the composite material by the mass ratio $\alpha_i^m \tilde{\rho}_i^m / \alpha_M \tilde{\rho}_M$. That is, these forces act like the body force for each species in the composite material, and these forces do not directly contribute in the diffusion of species within the composite material. (They indirectly contribute. They affect the momentum balance and pressure gradient, which will result in stratification of density and concentration.) Also, it should be noted that the material pressures $\tilde{p}_i^m$ in the composite material are in fact in equilibrium. That is $\tilde{p}_i^m = p_M$. Eqs. (14) and (55) then becomes

$$\begin{aligned}
\alpha_i^m \tilde{\rho}_i^m \frac{D_i^m \mathbf{u}_i^m}{Dt} &= -\nabla \left[\alpha_i^m \left(p_M - p\right)\right] - \alpha_M \nabla \frac{\alpha_i^m}{\alpha_M} p + \sum_j B_{ij}^m \alpha_i^m \alpha_j^m \left(\mathbf{u}_j^m - \mathbf{u}_i^m\right) + \mathbf{G}_i^m && (60)\\
\alpha_M \tilde{\rho}_M \frac{D_M \mathbf{u}_M}{Dt} &= -\nabla \left[\alpha_M \left(p_M - p\right)\right] - \alpha_M \nabla p + \mathbf{G}_M && (61)
\end{aligned}$$

where $\mathbf{G}$ represents the combined virtual mass and friction forces. $\mathbf{G}_i^m = (\alpha_i^m \tilde{\rho}_i^m / \alpha_M \tilde{\rho}_M) \mathbf{G}_M$ as discussed above, Replacing $D_i^m \mathbf{u}_i^m/Dt$ with $D_M \mathbf{u}_M/Dt$, and using Eq. (61), Eq. (60) becomes

$$\sum_j B_{ij}^m \frac{\alpha_i^m \alpha_j^m}{\alpha_M} \left(\mathbf{u}_j^m - \mathbf{u}_i^m \right) = p \nabla z_i^m + (z_i^m - y_i^m) \nabla p_M + (p_M - p)(1 - y_i^m) \frac{\nabla \alpha_M}{\alpha_M} \tag{62}$$

where the pressure fraction $z_i^m \equiv \alpha_i^m \tilde{p}_i^m/(\alpha_M p_M)$ is α_i^m/α_M, since $\tilde{p}_i^m = p_M$ here, and $y_i^m \equiv \alpha_i^m \tilde{\rho}_i^m/(\alpha_M \tilde{\rho}_M)$ is the mass fraction. Equation (62) is the generalized Stefan-Maxwell equations for heterogeneous mixture in pressure nonequilibrium. The term involving ∇z_i^m represents the ordinary diffusion due to concentration gradient, while the term involving $(z_i^m - y_i^m)$ represents the pressure diffusion driving the concentration stratification. (This stratification is in fact caused by the same driving force as the Rayleigh-Taylor instabilities. However, since the inertial difference is ignored, this does not correctly represent the transient Rayleigh-Taylor instabilities. Only the steady-state would be represented.) Note that thermal diffusion is not included in the development of Eq. (62). It can be included in a similar manner as Ref. [14]. When $p = p_M$, Eq. (62) reduces to

$$\sum_j B_{ij}^m \frac{\alpha_i^m \alpha_j^m}{\alpha_M} \left(\mathbf{u}_j^m - \mathbf{u}_i^m \right) = p \nabla z_i^m + (z_i^m - y_i^m) \nabla p_M \tag{63}$$

Observe that Eqs. (62) are not linearly independent, as their sum over species reduces to an identity. Only $N-1$ of them are linearly independent, where N is the number of species in the composite material. The contraint imposed by Eq. (7) provide the additional equation needed. That is, $N-1$ Eqs. (62) and Eq. (7) provide N equations in the N unknowns $\mathbf{u}_i^m$.

When materials are in plasma state, it is necessary to include the ambipolar diffusion effect. In plasmas, free electrons have high mobility, and thus electrons would diffuse away faster than heavy ions. However, electric field would develop, pulling back electrons. As a result, electrons and ions diffuse as pair in the absence of external electric field. (When electric field is exerted, it will cause the electrons to diffuse at a different speed from ions, resulting in electrical current.) The ambipolar effect can be included by adding the electric force term as presented in [14]. Equation (62) becomes

$$\sum_j B_{ij}^m \frac{\alpha_i^m \alpha_j^m}{\alpha_M} \left(\mathbf{u}_j^m - \mathbf{u}_i^m \right) = p \nabla z_i^m + (z_i^m - y_i^m) \nabla p_M + (p_M - p)(1 - y_i^m) \frac{\nabla \alpha_M}{\alpha_M} - \tilde{\rho}_i^m q_i^I \mathbf{E} \tag{64}$$

where q_i^I is the electrical charge of the single ion of species i, and $\mathbf{E}$ is the electrical field. When the electron mass is ignored (this leads to zero electrical resistance, resulting in the ideal magnetohydrodynamics), $\mathbf{E}$ is given by

$$\mathbf{E} = \frac{\nabla p_M^E}{\rho_M^E q^E} \tag{65}$$

where p_M^E is the electron pressure gradient in the composite material, ρ_M^E is the electron mass density in the composite material, and q_E is the electrical charge per unit mass of electron.

When a mix model such as Eq. (25) is used, directly adding the electrical force term as in Eq. (64) is not correct. These models usually represent the turbulence effects, which is often dominated by large scale eddies. Equation (64) would produce enhanced eddy effects, which is incorrect. Instead, modifying λ_c in Eq. (25) is recommended. In the absence of a good approximation, simply multiplying λ_c by $1 + (T^E/T^I)$ can be used, resulting in

$$B_{ij}^m = \frac{\tilde{\rho}_i \tilde{\rho}_j}{\rho} \frac{C_s}{\lambda_c \left[1 + (T^E/T^I) \right] + \alpha_{ij} \left| \mathbf{L}_{ij}^m \right|} \tag{66}$$

where T^E and T^I respectively are electron and ion temperatures. In short, Eqs. (62) and (66) should be used, instead of Eq. (64), in this case.

VI.3. Composite energy equation

The internal energy equation for the composite material is given by

$$\begin{aligned}\frac{\partial\left(\alpha_M\tilde{\rho}_M e_M\right)}{\partial t}+\nabla\cdot\left(\alpha_M\tilde{\rho}_M e_M\mathbf{u}_M\right) &= \sum_i\nabla\cdot\alpha_i^m k_i^m\nabla T_M-\sum_i\nabla\cdot\mathbf{J}_i^m h_i^m-\sum_i\dot{M}_i^c e_i^c\\ &\quad +W_M+Q_M^V+Q_M^F+Q_M^T \qquad (67)\end{aligned}$$

where $e_M\equiv\sum_i\alpha_i^m\tilde{\rho}_i^m e_i^m/(\alpha_M\tilde{\rho}_M)$ is the specific energy of the composite material, $\mathbf{J}_i^m\equiv\alpha_i^m\tilde{\rho}_i^m(\mathbf{u}_i^m-\mathbf{u}_M)$ is the diffusional mass flux of species i in the composite material, and h_i^m is the specific enthalpy of species i. (Diffusion-thermo effect is now explicitely included in Eq. (67).) Compression work W_i^m, dissipation of UKE Q_M^V, frictional dissipation Q_M^F, and energy exchange Q_M^T are given by

$$W_M = -p\left[\frac{\partial\alpha_M}{\partial t}+\nabla\cdot\left(\alpha_M\mathbf{u}_M\right)\right] \qquad (68)$$

$$Q_M^V = \sum_j\zeta_{Mj}^{Mc}C_{Mj}^V\alpha_M\alpha_j^c\left(\frac{D_j^c\mathbf{u}_j^c}{Dt}-\frac{D_M\mathbf{u}_M}{Dt}\right)\cdot\left(\mathbf{u}_j^c-\mathbf{u}_M\right) \qquad (69)$$

$$Q_M^F = \sum_j\zeta_{Mj}^{Mc}B_{Mj}^c\alpha_M\alpha_j^c\left(\mathbf{u}_j^c-\mathbf{u}_M\right)\cdot\left(\mathbf{u}_j^c-\mathbf{u}_M\right) \qquad (70)$$

$$Q_M^T = \sum_j\alpha_M\alpha_j^c E_{Mj}^c\left(T_j^c-T_M\right) \qquad (71)$$

Note that there is no frictional dissipation between molcularly mixed components, since diffusion approximaion is used. Specific heat used in the distribution factor ζ_{Mj}^{Mc} for the composite material is given by

$$C_{vM}=\frac{\sum_i\alpha_i^m\tilde{\rho}_i^m C_{vi}^m}{\alpha_M\tilde{\rho}_M} \qquad (72)$$

Composite material properties needed in E_{Mj}^c can be constructed in a similar manner.

VII. CONCLUDING REMARKS

We have presented an extension of the multifluid model to represent the temperature dependence on the mixture morphology. The present models are based on either $2N$ or $N+1$ materials. In the $N+1$ model, all molecular mixture components are combined as a composite material. Even in the $N+1$ model, $2N$ continuity equations are solved, requiring $2N$ species velocities.

The $N+1$ model described in Sec. VI should require fewer computational resources. However this may not be the case. Equations (62) or (63) are linear equations that need to be solved for all velocity components. $2N$ continuity equations (Eqs. (3)) still need to be solved. Numerous equilibration procedures required may also make the computing more challenging than having dynamically equilibrating tendencies in energy exchange and volume fraction revolution. Furthermore, time steps would be restricted by the diffusion limit, when Stefan-Maxwell equations are used. (When multifluid equations are solved, time step is not restricted by the diffusion limit [23].) Therefore, selection between $2N$ and $N+1$ should be made with care.

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