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Intended for: Report

Issued: 2016-08-19

LA-UR-16-????? August 9, 2016

A modeling approach for heat conduction and radiation diffusion in plasma-photon mixture in temperature nonequilibrium

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We present a simple approach for determining ion, electron, and radiation temperatures of heterogeneous plasma-photon mixtures, in which temperatures depend on both material type and morphology of the mixture. The solution technique is composed of solving ion, electron, and radiation energy equations for both mixed and pure phases of each material in zones containing random mixture and solving pure material energy equations in subdivided zones using interface reconstruction. Application of interface reconstruction is determined by the material configuration in the surrounding zones. In subdivided zones, subzonal inter-material energy exchanges are calculated by heat fluxes across the material interfaces. Inter-material energy exchange in zones with random mixtures is modeled using the length scale and contact surface area models. In those zones, inter-zonal heat flux in each material is determined using the volume fractions.

I. INTRODUCTION

It is possible that each component in a mixture can have different temperatures (temperature nonequilibrium). In fact, it is exceptional when all materials have identical temperatures. Modeling of heat transport through mixtures in temperature nonequilibrium needs to include the local heat transfer between materials (energy exchange) as well as the spatial heat conduction. When thermal radiation becomes important, local energy exchange and spatial radiation transport also need to be determined in the nonequilibrium mixture, adding complexity.

It is rather obvious that the material configuration, or mixture morphology, would critically affect the modeling approach. For example, when materials are segregated in large scale, resolution of contact interfaces would help determining heat transport. Heat flux through interfaces could of course be calculated using discretized heat conduction between subdivided zones. If a component in the mixture is dispersed, i.e., segregated in small scales, local energy exchange is often modeled as subzonal energy exchange between materials present in the zone, and typically takes the form of source or sink terms, while spatial heat conduction and radiation diffusion is modeled by discretized conduction and diffusion terms. Since inter-material energy exchange in fact is conduction/diffusion in this case, the source/sink terms should be based on conduction and diffusion. On the other hand, when materials are mixed at the molecular level, inter-material energy exchange should take the form of collisional energy exchange.

Very little is usually known about the mixture morphology, and a reliable model for morphology modeling is not currently available. Nonetheless, it is possible to adopt a relatively simple approach to circumvent the lack of mixture morphology information, and still capture essential information necessary for reasonable modeling while ignoring information of lesser importance. In this report, we present an approach based on the ansatz that components of the mixture are "connected" to the neighboring zone, and the average inter-zonal connection area can simply be determined using the volume fraction. This way, modification of discretized conduction and diffusion terms is straightforward and simple. The subzonal inter-material energy exchange would still require models for the necessary information. When such models are available, e.g., Ref. [1], they can be utilized. If not, a simple energy exchange model presented in Ref. [2] can be used.

In high temperature environments, materials ionize and radiation energy transport becomes important. Complexities added in plasma-photon mixtures include required implicit numerical schemes, energy exchange between ion and electrons, and radiation-matter interactions. Transport of radiation energy is affected by the material motion. In optically thin material, material motion would hardly affect the radiation energy, while motion of optically thick material would force the radiation energy move with the material. In this report, we limit our discussion to the case radiation diffusion is a valid approach. Additional energy exchange terms in plasma-photon mixtures have been included in the presented modeling approach.

We first describe interface reconstruction techniques that have been frequently used to handle en-

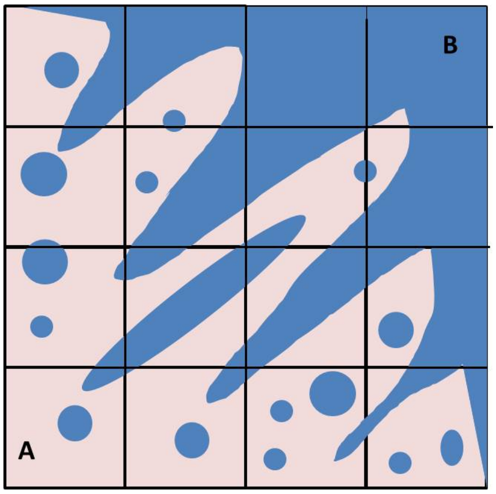

FIG. 1: Typical mixture morphology expected in mixing caused by breaking up of material B.

ergetics in multitemperature mixtures, and its issues. We then describe our approach of selective utilization of the interface reconstruction only in the zones with large scale interfaces. We also introduce simplification of combining all molecular mixtures into a composite material.

II. INTERFACE RECONSTRUCTION AND ENERGY TRANSPORT

Imagine a situation in which a material (B) is breaking off from the bulk and mixing with material A, as shown in Fig. 1. In this situation, a substantial fraction of material B is “connected” across computational zones, while another substantial fraction is dispersed. Obtaining material temperatures in this situation requires heat fluxes to be correctly calculated across the material interfaces as well as zone boundaries. This in turn would require dispersed phase size, shape, and locations. In fact, correct calculation would require mesh resolution comparable to the finest dispersed particulate size, which could be of order of the mean free path length. It is thus necessary to introduce approximations and/or numerical techniques.

One conceptually simple way is to utilize the interfaces to represent the mixture morphology. Figure 2 shows an example of the interfaces constructed between materials A and B in a computational domain. As illustrated, materials in each zone exchange energy through zone boundaries and interfaces between materials. Details of this approach can be found in Ref. [3]. This approach has advantages. It is conceptually straight forward. Subzonal information such as dispersed phase size, shape, location, and contact surface area is unnecessary. However, this approach requires a large amount of implementation effort in three dimensions.

Another difficulty is that this technique is subject to an artifact which could generate inaccurate results to the point of producing misleading computational simulations. It is highly likely that the concentration profile of material B would dictate the interface reconstruction algorithms to locate the material B toward the higher concentration side in the zone. This could lead to the “layered” structures as shown in Fig. 3, and resulting temperatures of materials A and B could have substantial amount of error. This error would be exaggerated when the material A is relatively optically thin. Radiation transport in the material A would be effective in this case, leading to a relatively uniform temperature distribution in the real situation represented in Fig. 1. However, this would not be the case in the situation shown in Fig. 3 due to the layering of material B blocking radiation transport in material A. When tracking of material A temperature is important, the technique solely based on interface reconstruction (illustrated in Fig. 2) could lead to unacceptably large errors.

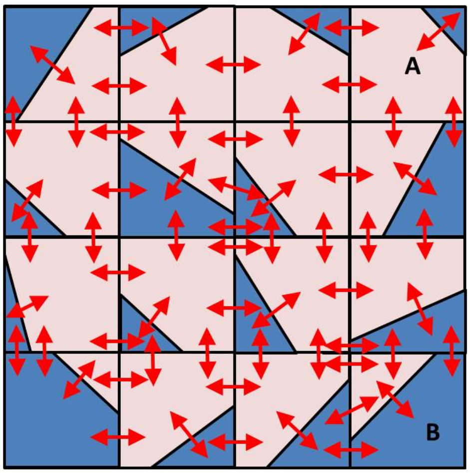

FIG. 2: Heat transfer between materials through interfaces and zone boundaries when interface reconstruction is used [3].

III. ENERGY CONSERVATION IN RANDOM PHOTON-PLASMA MIXTURES IN TEMPERATURE NONEQUILIBRIUM

III.1. Energy equations in random mixtures

As discussed above, interface reconstruction may introduce undesirable artifacts. Furthermore, materials may mix at the molecular level, increasing the level of randomness. In the technique developed previously [3], when molecular mixtures exist, material interfaces are not constructed, even when dispersed or continuous phases exist, resulting in equilibrated material temperatures. This largely alleviates the difficulty discussed above. However, it needs to be generalized in order to track material temperatures of segregated phases (continuous and dispersed), and mixed phases, separately. We combine the interface reconstruction and nonequilibrium heat flux model in the present approach. Interface reconstruction is utilized in the selected zones with resolved interfaces, while zones composed of dispersed and mixed phases

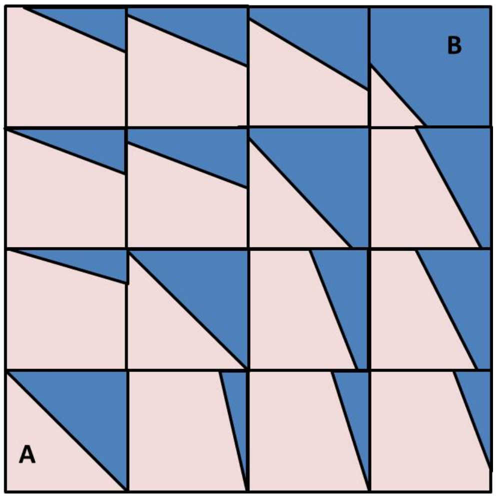

FIG. 3: Example of layered structure produced by interface reconstruction.

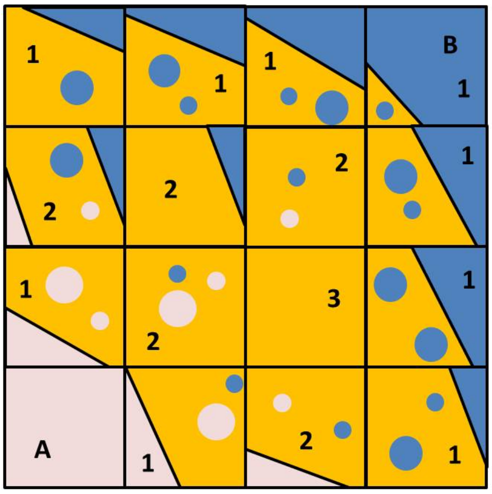

FIG. 4: Zones with various mixture morphology represented by zone typing. The background (yellow) of dispersed phases represents the mixed phase.

utilize the nonequilibrium heat flux model.

It is necessary to categorize zones according to the mixture morphology of the zone in order to apply the appropriate modeling techniques. As discussed in the extended mix model [2], mixture is presumed to be composed of segregated components and molecularly mixed components in which materials A and B are mixed at the molecular level. (We can regard the molecularly mixed region as a composite material.) In short, the mixture is composed of continuous phase of A, continuous phase of B, dispersed phase of A, dispersed phase of B, and composite mixture phase. (Dispersed phase of A is not involved in the discussions above as mixing process is presumed to occur via break up of the material B. But it is included in the discussion below.) Illustrated in Fig. 4, computation zones are categorized as:

- Type-1: Zones facing unmixed zones with pure material A or pure material B. These zones usually contain contact surfaces requiring interface reconstruction.
- Type-2: Zones containing dispersed or continuous components but not facing pure zones.
- Type-3: Zones containing only the molecularly mixed phase.

In our approach, interfaces are constructed only in Type-1 zones. When an interface is involved, heat flux is calculated using the subzonal information generated by interface reconstruction as shown in Fig. 2. In these zones, pure material energy equations are solved in subdivided zones. Pure material energy equations are well-known, thus not repeated here.

Interfaces are not constructed in Type-2 and Type-3 zones. Instead of solving pure material energy equations as in Type 1 zones, we solve the energy conservation equations for nonequilibrium mixtures given by [2]

$$\frac{\partial\left(\alpha_i^c\tilde{\rho}_i^c e_i^c\right)}{\partial t} + \nabla\cdot\left(\alpha_i^c\tilde{\rho}_i^c e_i^c \mathbf{u}_i^c\right) = \nabla\cdot\alpha_i^c k_i^c \nabla T_i^c + \dot{M}_i^c e_i^c + W_i^c + Q_i^{Vc} + Q_i^{Fc} + Q_i^{Tc} \tag{1}$$

$$\frac{\partial\left(\alpha_i^m\tilde{\rho}_i^m e_i^m\right)}{\partial t} + \nabla\cdot\left(\alpha_i^m\tilde{\rho}_i^m e_i^m \mathbf{u}_i^m\right) = \nabla\cdot\alpha_i^m k_i^m \nabla T_i^m - \dot{M}_i^c e_i^c + W_i^m + Q_i^{Vm} + Q_i^{Fm} + Q_i^{Tm} \tag{2}$$

where $\tilde{\rho}_i^c$ is the mass density of pure species i, and e_i and T_i respectively are the specific energy and temperature of material i. Superscripts c and m respectively represent pure and molecular mixture forms. 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 molecularly mixed portion is denoted by α_i^m. The mean velocities of species i in pure and molecular mixture forms are denoted by

$\mathbf{u}_i^c$ and $\mathbf{u}_i^m$, respectively. Thermal conductivities k_i^c and k_i^m are evaluated at T_i^c and T_i^m, respectively. $\dot{M}_i^c = -\dot{M}_i^m$ is the mass conversion rate from the pure component to mixed component of material i. Compression work W_i, frictional dissipation Q_i^F, dissipation of unresolved kinetic energy Q_i^Vi, and energy exchange Q_i^T are discussed in detail in Ref. [2].

III.2. Energy equations in photon-plasma mixtures

Equations (1) and (2) need to be generalized for plasma-photon mixture. In particular, electron, ion, and radiation energy need to be solved separately for each material. Note that 3-T diffusion approach, similar to the one in Ref. [4], has been employed here. Energy equations are given by

$$\frac{\partial\left(\alpha_i^c\tilde{\rho}_i^c e_i^{cI}\right)}{\partial t} + \nabla\cdot\left(\alpha_i^c\tilde{\rho}_i^c e_i^{cI}\mathbf{u}_i^c\right) = \nabla\cdot\alpha_i^c k_i^{cI}\nabla T_i^{cI} + \dot{M}_i^c e_i^{cI} + W_i^{cI} + Q_i^{VcI} + Q_i^{FcI} + Q_i^{TcI} \tag{3}$$

$$\frac{\partial\left(\alpha_i^c\tilde{\rho}_i^c e_i^{cE}\right)}{\partial t} + \nabla\cdot\left(\alpha_i^c\tilde{\rho}_i^c e_i^{cE}\mathbf{u}_i^c\right) = \nabla\cdot\alpha_i^c k_i^{cE}\nabla T_i^{cE} + \dot{M}_i^c e_i^{cE} + W_i^{cE} + Q_i^{VcE} + Q_i^{FcE} + Q_i^{TcE} \tag{4}$$

$$\frac{\partial\left(\alpha_i^c\tilde{\rho}_i^c e_i^{cR}\right)}{\partial t} + \nabla\cdot\left(\alpha_i^c\tilde{\rho}_i^c e_i^{cR}\mathbf{u}_i^c\right) = \nabla\cdot\alpha_i^c k_i^{cR}\nabla (T_i^{cR})^4 + \dot{M}_i^c e_i^{cR} + W_i^{cR} + Q_i^{TcR} \tag{5}$$

$$\frac{\partial\left(\alpha_i^m\tilde{\rho}_i^m e_i^{mI}\right)}{\partial t} + \nabla\cdot\left(\alpha_i^m\tilde{\rho}_i^m e_i^{mI}\mathbf{u}_i^m\right) = \nabla\cdot\alpha_i^m k_i^{mI}\nabla T_i^{mI} - \dot{M}_i^c e_i^{cI} + W_i^{mI} + Q_i^{VmI} + Q_i^{FmI} + Q_i^{TmI} \tag{6}$$

$$\frac{\partial\left(\alpha_i^m\tilde{\rho}_i^m e_i^{mE}\right)}{\partial t} + \nabla\cdot\left(\alpha_i^m\tilde{\rho}_i^m e_i^{mE}\mathbf{u}_i^m\right) = \nabla\cdot\alpha_i^m k_i^{mE}\nabla T_i^{mE} - \dot{M}_i^c e_i^{cE} + W_i^{mE} + Q_i^{VmE} + Q_i^{FmE} + Q_i^{TmE} \tag{7}$$

$$\frac{\partial\left(\alpha_i^m\tilde{\rho}_i^m e_i^{mR}\right)}{\partial t} + \nabla\cdot\left(\alpha_i^m\tilde{\rho}_i^m e_i^{mR}\mathbf{u}_i^m\right) = \nabla\cdot\alpha_i^m k_i^{mR}\nabla (T_i^{mR})^4 - \dot{M}_i^c e_i^{cR} + W_i^{mR} + Q_i^{TmR} \tag{8}$$

where superscripts I, E, and R respectively denote ion, electron and radiation, $e^R = a(T^R)^4$ is the radiation energy, and a is the radiation constant. Note that energies of neutral (unionized) particles are included in Eqs. (3) and (6).

The compression work W is given by

$$W_i^{cI} = -p^I\left[\frac{\partial\alpha_i^c}{\partial t} + \nabla\cdot\left(\alpha_i^c\mathbf{u}_i^c\right)\right] \tag{9}$$

$$W_i^{cE} = -p^E\left[\frac{\partial\alpha_i^c}{\partial t} + \nabla\cdot\left(\alpha_i^c\mathbf{u}_i^c\right)\right] \tag{10}$$

$$W_i^{cR} = -\frac{a(T_i^{cR})^4}{3}\left[\frac{\partial\alpha_i^c}{\partial t} + \nabla\cdot\left(\alpha_i^c\mathbf{u}_i^c\right)\right] \tag{11}$$

$$W_i^{mI} = -\frac{\alpha_i^m}{\alpha_M}\tilde{p}_i^{mI}\left[\frac{\partial\alpha_M}{\partial t} + \nabla\cdot\left(\alpha_M\mathbf{u}_i^m\right)\right] \tag{12}$$

$$W_i^{mE} = -\frac{\alpha_i^m}{\alpha_M}\tilde{p}_i^{mE}\left[\frac{\partial\alpha_M}{\partial t} + \nabla\cdot\left(\alpha_M\mathbf{u}_i^m\right)\right] \tag{13}$$

$$W_i^{mR} = -\frac{\alpha_i^m}{\alpha_M}\frac{a(T_i^{mR})^4}{3}\left[\frac{\partial\alpha_M}{\partial t} + \nabla\cdot\left(\alpha_M\mathbf{u}_i^m\right)\right] \tag{14}$$

The dissipation of unresolved kinetic energy Q^V, given in Ref. [2], is split into electron and ion energy according to the mass ratio. They are given by

$$Q_i^{VcI} = \zeta_i^I Q_i^{Vc} \tag{15}$$

$$Q_i^{VcE} = \zeta_i^E Q_i^{Vc} \tag{16}$$

where ζ_i^I is the fraction of the dissipation energy into ions in the plasma phase of material i. ζ_i^I and ζ_i^E are given by [5]

$$\zeta_i^I = \frac{m^E}{m_i^I + m^E} \tag{17}$$

$$\zeta_i^E = \frac{m_i^I}{m_i^I + m^E} \tag{18}$$

where m^E the mass of free electron, and m_I^I is the mass of ion of species i. The frictional dissipation Q_i^{Fc} given in Ref. [2] is split in the identical manner as

$$Q_i^{FcI} = \zeta_i^I Q_i^{Fc} \tag{19}$$

$$Q_i^{FcE} = \zeta_i^E Q_i^{Fc} \tag{20}$$

Energy exchange terms Q_i^{Tc} and Q_i^{Tm} described in Ref. [2] is not simply split between electrons and ions. In plasma-photon mixture, they include radiation-matter interactions such as absorption, Compton scattering, and Bremsstrahlung in addition to the energy exchange due to temperature differences between electrons and ions. They are given by

$$Q_i^{TcI} = \sum_j \alpha_i^c \alpha_j^c E_{ij}^{cI}\left(T_j^{cI} - T_i^{cI}\right) + \sum_j \alpha_i^c \alpha_j^m E_{ij}^{cI}\left(T_j^{mI} - T_i^{cI}\right) + \alpha_i^c \alpha_i^c R_{ii}^{cEI}\left(T_i^{cE} - T_i^{cI}\right) \tag{21}$$

$$\begin{aligned} Q_i^{TcE} &= \sum_j \alpha_i^c \alpha_j^c E_{ij}^{cE}\left(T_j^{cE} - T_i^{cE}\right) + \sum_j \alpha_i^c \alpha_j^m E_{ij}^{cE}\left(T_j^{mE} - T_i^{cE}\right) \\ &+ \alpha_i^c \alpha_i^c R_{ii}^{cIE}\left(T_i^{cI} - T_i^{cE}\right) + \alpha_i^c \alpha_i^c R_{ii}^{cRE}\left[(T_i^{cR})^4 - (T_i^{cE})^4\right] \end{aligned} \tag{22}$$

$$Q_i^{TcR} = \alpha_i^c \alpha_i^c R_{ii}^{cER}\left[(T_i^{cE})^4 - (T_i^{cR})^4\right] \tag{23}$$

$$\begin{aligned} Q_i^{TmI} &= \sum_j \alpha_i^m \alpha_j^c E_{ij}^{cI}\left(T_j^{cI} - T_i^{mI}\right) + \sum_j \alpha_i^m \alpha_j^m R_{ij}^{mII}\left(T_j^{mI} - T_i^{mI}\right) \\ &+ \sum_j \alpha_i^m \alpha_j^m R_{ij}^{mIE}\left(T_j^{mE} - T_i^{mI}\right) \end{aligned} \tag{24}$$

$$\begin{aligned} Q_i^{TmE} &= \sum_j \alpha_i^m \alpha_j^c E_{ij}^{cE}\left(T_j^{cE} - T_i^{mE}\right) + \sum_j \alpha_i^m \alpha_j^m R_{ij}^{mEI}\left(T_j^{mI} - T_i^{mE}\right) \\ &+ \sum_j \alpha_i^m \alpha_j^m R_{ij}^{mEE}\left(T_j^{mE} - T_i^{mE}\right) + \sum_j \alpha_i^m \alpha_j^m R_{ij}^{mER}\left[(T_j^{mR})^4 - (T_i^{mE})^4\right] \end{aligned} \tag{25}$$

$$Q_i^{TmR} = \sum_j \alpha_i^m \alpha_j^m R_{ij}^{mRE}\left[(T_j^{mE})^4 - (T_i^{mR})^4\right] \tag{26}$$

As in Ref. [2], E_{ij} is the spatial heat transport rate, and R_{ij} is the local, or collisional, energy transfer rate.

Observe that Q_i^{Tc} is composed of ion-ion, ion-electron, and electron-electron energy exchanges between segregated materials. Radiation is assumed to interact with free electrons only. This modeling approach implies that a single computational zone is composed of segregated regions with different radiation temperatures, and is modeled with insufficient mesh resolution.

For mixed composite materials, however, the forms of Q_i^{Tm} imply that each material component in the composite material has a different temperature. Furthermore, there are multiple radiation temperature in the region where materials are mixed at the molecular level, which would make radiation diffusion approximation invalid. In fact, material temperatures would be identical in the molecular mixture. However, Q_i^{Tm} presented above is still expected to produce reasonable results, since R_{ij}^{EE} and R_{ij}^{II}, are usually quite large, resulting in equilibrium of T_i^{mI} and T_i^{mE} between materials i. (T_i^{mI} and T_i^{mE} can still be quite different, since R_{ij}^{EI} may not be large enough.) Due to these large energy exchange rates, the physical situation is expected to be reasonably modeled. Radiation temperatures may still produce errors when R_{ij}^{ER} is not large. It is thus recommended to solve energy conservation of the whole composite (mixed) phase similar to the $N+1$ model described in Ref. [2], which is presented in Sec. IV.

III.3. Subzonal energy exchange

$E_{ij} = E_{ji}$ represents subzonal heat conductions such as ion-ion and electron-electron conductions. E_{ij}^m and E_{ij}^c have identical functional forms, they are just evaluated at the different temperatures of the segregated and mixed phases. They are given by

$$E_{ij}^{I} = \frac{S_{ij}k_{ij}^{I}}{\ell_i + \ell_j} + \frac{3k_B}{m_i^I + m_j^I}\frac{B_{ij}}{\mathrm{Pr}_{ij}^{I}} \tag{27}$$

$$E_{ij}^{E} = \frac{S_{ij}k_{ij}^{E}}{\ell_i + \ell_j} \tag{28}$$

where S_{ij} is the characteristic contact surface area between materials i and j, ℓ_i is the characteristic length scale of material i, k_B is the Boltzmann's constant, and m is the particle mass. B_{ij} is the momentum exchange coefficient give in Ref. [2]. For monodispersed spherical particles, S_{ij} and ℓ_i are given in Ref. [1]. The inter-material diffusivity k_{ij} between segregated pure-materials pair (i,j) is given by

$$\frac{\ell_i + \ell_j}{k_{ij}^{I}} = \frac{\ell_i}{k_i^I} + \frac{\ell_j}{k_j^I} \tag{29}$$

$$\frac{\ell_i + \ell_j}{k_{ij}^{E}} = \frac{\ell_i}{k_i^E} + \frac{\ell_j}{k_j^E} \tag{30}$$

When ℓ_i are not given, we can use the simple harmonic mean given by

$$\frac{2}{k_{ij}^{I}} = \frac{1}{k_i^I} + \frac{1}{k_j^I} \tag{31}$$

$$\frac{2}{k_{ij}^{E}} = \frac{1}{k_i^E} + \frac{1}{k_j^E} \tag{32}$$

Pr_{ij} is the Prandtl number at the segregated material interface, evaluated using electron and ion properties. If not available, unity can be used.

With a simple inspection, we can deduce that the terms involving S_{ij} in Eqs. (27) and (28) represent heat conduction. The term involving B_{ij} represents convectional heat transfer, estimated from the momentum exchange, using elementary kinetic theory [5–7]. Since the momentum exchange is dominated by ions, the electron contribution has been ignored.

Collisional energy exchange rates for the particle pair (s,t) are given by

$$R_{st} = \frac{16k_B}{(m_s + m_t)} n_s n_t \mu_{st} \Omega_{st}^{(1)}(1, T_{st}) \tag{33}$$

where n_s is the number density of the particle type s evaluated in the mixture ($n_s = \alpha_M \tilde{\rho}_s^m / m_s$), $\mu_{st} = m_s m_t/(m_s + m_t)$ is the reduced mass of the particle pair s and t, and T_{st} is the effective pair temperature given by [5, 6]

$$T_{st} = \frac{m_t T_s + m_s T_t}{m_s + m_t} \tag{34}$$

$\Omega_{st}^{(1)}(n, T)$ is the integral defined as [8]

$$\Omega_{st}^{(1)}(n, T) = \frac{1}{2\sqrt{\pi}} \left(\frac{\mu_{st}}{2k_B T}\right)^{(2n+3)/2} \int_0^\infty \exp\left(-\frac{\mu_{st} v^2}{2k_B T}\right) v^{2n+3} Q_{st}^{(1)}(v)\, dv \tag{35}$$

where T is the dummy temperature variable, and $Q_{st}^{(1)}(v)$ 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 [8]

$$Q_{st}^{(1)}(v) = 2\pi \int_0^\infty (1 - \cos\chi) b\, db \tag{36}$$

For weakly coupled plasmas R_{st} is given by

$$R_{st} = \frac{4k_B}{(m_s + m_t)} \left(\frac{\pi \mu_{st}}{2}\right)^{1/2} (k_B T_{st})^{-3/2} n_s n_t q_s^2 q_t^2 \ln\left(1 + \Lambda_{st}^2\right) \tag{37}$$

where $\Lambda_{st} = 3k_BT_{st}R_D/|q_sq_t$, q_s is the charge of the single particle of type s, and R_D is the Debye length defined as

$$R_D = \left(4\pi \sum_i \frac{n_i q_i^2}{k_B T_i^E}\right)^{-1/2} \tag{38}$$

Observe that R_D is a property of the whole plasma mixture. Note that collision between electron and neutral particle can be ignored when the degree of ionization is not small. R_{ij}^{ab}, where a and b are I or E, can be evaluated by using appropriate values. For example, R_{ij}^{IE} can be obtained from Eq. (33), using s particle as the ion of species i and t particle as the electron of species j. Radiation-electron exchange R_{ij}^{ER} is given by [4]

$$R_{ij}^{ER} = ac\sigma_{ij} \tag{39}$$

where c and $\sigma_{ij}a$ are the speed of light and extinction coefficient, respectively.

IV. COMBINED ENERGY EQUATIONS FOR MIXED PHASE

As discussed above, material temperatures in the composite material should be identical (temperature equilibrium). Therefore, Eqs. (6)–(8) can be combined into the energy equation set for the one composite material. That is, one set of energy equations is solved for the composite material instead of one set for each species. The combined energy equations are given by

$$\begin{aligned}
\frac{\partial\left(\alpha_M\tilde{\rho}_M e_M^I\right)}{\partial t} + \nabla\cdot\left(\alpha_M\tilde{\rho}_M e_M^I \mathbf{u}_M\right) &= \nabla\cdot\alpha_M k_M^I \nabla T_M^I - \sum_i \nabla\cdot\mathbf{J}_i^m h_i^{mI} - \sum_i \dot{M}_i^c e_i^{cI} \\
&+ W_M^I + Q_M^{VI} + Q_M^{FI} + Q_M^{TI} \qquad (40) \\
\frac{\partial\left(\alpha_M\tilde{\rho}_M e_M^E\right)}{\partial t} + \nabla\cdot\left(\alpha_M\tilde{\rho}_M e_M^E \mathbf{u}_M\right) &= \nabla\cdot\alpha_M k_M^E \nabla T_M^E - \sum_i \nabla\cdot\mathbf{J}_i^m h_i^{mE} - \sum_i \dot{M}_i^c e_i^{cE} \\
&+ W_M^E + Q_M^{VE} + Q_M^{FE} + Q_M^{TE} \qquad (41) \\
\frac{\partial\left(\alpha_M\tilde{\rho}_M e_M^R\right)}{\partial t} + \nabla\cdot\left(\alpha_M\tilde{\rho}_M e_M^R \mathbf{u}_M\right) &= \nabla\cdot\alpha_M k_M^R \nabla (T_M^R)^4 - \sum_i \nabla\cdot\mathbf{J}_i^m h_i^{mR} - \sum_i \dot{M}_i^c e_i^{cR} \\
&+ W_M^R + Q_M^{TR} \qquad (42)
\end{aligned}$$

where $e_M^I \equiv \sum_i \alpha_i^m \tilde{\rho}_i^m e_i^{mI}/(\alpha_M\tilde{\rho}_M)$ and $e_M^E \equiv \sum_i \alpha_i^m \tilde{\rho}_i^m e_i^{mE}/(\alpha_M\tilde{\rho}_M)$ respectively are the ion and electron specific energies of the composite material, $\alpha_M = \sum_i \alpha_i^m$ is the composite material volume fraction, $\tilde{\rho}_M = \sum_i \alpha_i^m \tilde{\rho}_i^m$ is the density of the composite material, $\mathbf{J}_i^m \equiv \alpha_i^m \tilde{\rho}_i^m/\alpha_M(\mathbf{u}_i^m - \mathbf{u}_M)$ is the diffusional mass flux of species i in the composite material, and $k_M = \sum_i \alpha_i^m k_i/\alpha_M$ is the composite material thermal conductivity. Partial ion and electron specific enthalpies are given by

$$\begin{aligned}
h_i^{mI} &= e_i^{mI} + \frac{\tilde{p}_i^{mI}}{\tilde{\rho}_i^m} \qquad (43) \\
h_i^{mE} &= e_i^{mE} + \frac{\tilde{p}_i^{mE}}{\tilde{\rho}_i^m} \qquad (44)
\end{aligned}$$

Radiation enthalpy h_i^{mR} is $(4/3)a(T_M^R)^4$ [9].

Mixture average velocity $\mathbf{u}_M$ and species velocities $\mathbf{u}_i^m$ are determined by solving species momentum equations or Stefan-Maxwell equations given in Ref. [2]. Species densities $\tilde{\rho}_i^m$ are determined from species conservation equations also given in Ref. [2]. We recommend employing the composite momentum equations, when Eqs. (40)–(42) are used.

Compression work W_M, dissipation of unresolved kinetic energy Q^V_M, frictional dissipation Q^F_M, and energy exchange Q^T_M are given by

$$
\begin{aligned}
W^I_M &= -p^I \left[\frac{\partial \alpha_M}{\partial t} + \nabla \cdot (\alpha_M \mathbf{u}_M)\right] && (45)\\
W^E_M &= -p^E \left[\frac{\partial \alpha_M}{\partial t} + \nabla \cdot (\alpha_M \mathbf{u}_M)\right] && (46)\\
W^R_M &= -\frac{a(T^R_M)^4}{3} \left[\frac{\partial \alpha_M}{\partial t} + \nabla \cdot (\alpha_M \mathbf{u}_M)\right] && (47)\\
Q^{VI}_M &= \zeta^I_M \sum_j \zeta^{Mc}_{Mj} C^V_{Mj} \alpha_M \alpha^c_j \left(\frac{D^c_j \mathbf{u}^c_j}{Dt} - \frac{D_M \mathbf{u}_M}{Dt}\right) \cdot \left(\mathbf{u}^c_j - \mathbf{u}_M\right) && (48)\\
Q^{VE}_M &= \zeta^E_M \sum_j \zeta^{Mc}_{Mj} C^V_{Mj} \alpha_M \alpha^c_j \left(\frac{D^c_j \mathbf{u}^c_j}{Dt} - \frac{D_M \mathbf{u}_M}{Dt}\right) \cdot \left(\mathbf{u}^c_j - \mathbf{u}_M\right) && (49)\\
Q^{FI}_M &= \zeta^I_M \sum_j \zeta^{Mc}_{Mj} B^c_{Mj} \alpha_M \alpha^c_j \left(\mathbf{u}^c_j - \mathbf{u}_M\right) \cdot \left(\mathbf{u}^c_j - \mathbf{u}_M\right) && (50)\\
Q^{FE}_M &= \zeta^E_M \sum_j \zeta^{Mc}_{Mj} B^c_{Mj} \alpha_M \alpha^c_j \left(\mathbf{u}^c_j - \mathbf{u}_M\right) \cdot \left(\mathbf{u}^c_j - \mathbf{u}_M\right) && (51)\\
Q^{TI}_M &= \sum_j \alpha_M \alpha^c_j E^{cI}_{ij} \left(T^{cI}_j - T^I_M\right) + \alpha_M \alpha_M R^{IE}_M \left(T^E_M - T^I_M\right) && (52)\\
Q^{TE}_M &= \sum_j \alpha_M \alpha^c_j E^{cE}_{ij} \left(T^{cE}_j - T^E_M\right) + \alpha_M \alpha_M R^{EI}_M \left(T^I_M - T^E_M\right) \\
&+ \alpha_M \alpha_M R^{ER}_M \left[(T^R_M)^4 - (T^E_M)^4\right] && (53)\\
Q^{TR}_M &= \alpha_M \alpha_M R^{RE}_M \left[(T^E_M)^4 - (T^R_M)^4\right] && (54)
\end{aligned}
$$

Collisional energy exchange rates $R^{EI}_M = R^{IE}_M$ are evaluated using Eq. (33) setting $s = M$ and $t = M$. Electron-radiation Radiation-electron exchange R^{ER}_M is obtained from Eq. (39) using the extinction coefficient for the composite material σ_M. Distribution factors ζ^I_M and ζ^E_M are determined from Eqs. (17) and (18). ζ^{Mc}_{Mj} is given by $\zeta^{Mc}_{ij} = C_{vM}/(C_{vM} + C^c_{vj})$ [2].

V. SUMMARY AND CONCLUDING REMARKS

The multifluid approach provides a natural framework, when it is necessary to model temperature dependencies on the mixture morphology. In this approach, molecular mixtures can be combined into a composite material which has its own energy equation. We have presented both the $2N$ model, where each species in the composite material has its own temperature, and the $N+1$ model, where the composite material has one temperature. In both models, ion, electron, and radiation temperatures are separately tracked, resulting in $6N$ or $3(N+1)$ energy equations. Mixture energy equations are solved in the zones with random mixtures. When material interfaces are resolved, pure material energy equations are solved with interface reconstruction. Due to the number of equations to be solved, and the complexity of the model, we recommend the $N+1$ model. When $N+1$ model is employed, corresponding $N+1$ momentum equations and Stefan-Maxwell equations can be found in Ref. [2].

The present discussion is limited to the radiation diffusion approach. It should be possible to generalize the present approach with multi-group diffusion or advanced transport models. This development will be carried out when needs arise, and reported in due course.

ACKNOWLEDGMENTS

I am grateful to William Dai and A. J. Scannapieco for their pioneering work in interface-aware radiation transport and helpful discussions, which made numerical implementation and testing possible, and to Jamie Langenbrunner for thoughtful critique of the manuscript.

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