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# Diffuse interface relaxation model for two-phase compressible flows with diffusion processes



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# ABSTRACT

The paper addresses a two-temperature model for simulating compressible two-phase flow taking into account diffusion processes related to the heat conduction and viscosity of the phases. This model is reduced from the two-phase Baer-Nunziato model in the limit of complete velocity relaxation and consists of the phase mass and energy balance equations, the mixture momentum equation, and a transport equation for the volume fraction. Terms describing effects of mechanical relaxation, temperature relaxation, and thermal conduction on volume fraction evolution are derived and demonstrated to be significant for heat conduction problems. The thermal conduction leads to instantaneous thermal relaxation so that the temperature equilibrium is always maintained in the interface region with meeting the entropy relations. A numerical method is developed to solve the model governing equations that ensures the pressure-velocity-temperature (PVT) equilibrium condition in its high-order extension. We solve the hyperbolic part of the governing equations with the Godunov method with the HLLC approximate Riemann solver. The non-linear parabolic part is solved with an efficient Chebyshev explicit iterative method without dealing with large sparse matrices. To verify the model and numerical methods proposed, we demonstrate numerical results of several numerical tests such as the multiphase shock tube problem, the multiphase impact problem, and the planar ablative Rayleigh-Taylor instability problem.

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# 1. Introduction

Numerical modeling of compressible multiphase flow have found many applications in various natural, industrial and technological areas. Typical applications include bubble dynamics [64,63], underwater explosion [53,37,33,86], cavitation flows [46,75,74], multiphase flows in the porous rock [8], inertial confinement fusion [90,65], Rayleigh–Taylor [79,44,91] and Richtmyer–Meshkov instabilities [41,10,99] and so on. In some problems where steep distributions of flow parameters occur, diffusion processes such as the heat conduction and viscous stress may have significant impact. How to properly take into account these processes in multiphase hydrodynamics with resolved interfaces is the main issue of the present paper.

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Numerical methods for simulating compressible multiphase flows can be generally classified into two categories depending on the approach to resolve material interfaces: Diffuse interface methods (DIM) [26,77,38,25,21,20,72,70,75,71,1,52,51, 17,84,85,12,27] and the sharp interface methods (SIM) [39,40,22,23,43,32,30,29,54,58,24]. The present work is done in the framework of the former - DIM. Instead of explicitly tracking sharply resolved material interfaces as in SIMs, material interfaces in DIMs are captured by allowing a numerical diffusion zone of mixture flow that is modeled as physical one. Thanks to these numerical diffusion, different components can be described with a unique set of partial differential equations and equation of state (EOS). Therefore, one can perform throughout computations on the Eulerian grid without specifying concrete interface locations. Moreover, DIMs avoid dealing with complicated grid movements and non-conservativeness issues.

The models for multiphase flows with resolved interfaces generally fall into two groups: One is based on the generalization of the conventional one-fluid Euler equations to multicomponent cases [1,84,85,35,3,4], the other is based on the reduction of non-equilibrium multi-phase flow models [6,36,75,59,56].

The first group is more concerned with numerical aspects, in particular, the property to preserve the pressure-velocity equilibrium (the PV property), and also additionally temperature equilibrium (the PVT property) when the thermal conduction is also considered. These properties are used as important numerical condition or criterion to derive such models. The definitions of these properties are given in section 3.6. For these models, material interfaces are represented by variable EOS parameters or by a characteristic function such as the Heaviside function that is interpreted as volume fraction in the context of multiphase flows. A representative of these models is the following model [85,84,11] based on the PV property, which is formulated as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0, \tag{1a}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla p = 0, \tag{1b}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + p) \boldsymbol{u}] = 0, \tag{1c}$$

$$\frac{\partial}{\partial t} \left( \frac{1}{\gamma - 1} \right) + \boldsymbol{u} \cdot \nabla \left( \frac{1}{\gamma - 1} \right) = 0, \tag{1d}$$

$$\frac{\partial}{\partial t} \left( \frac{\gamma p_{\infty}}{\gamma - 1} \right) + \boldsymbol{u} \cdot \nabla \left( \frac{\gamma p_{\infty}}{\gamma - 1} \right) = 0, \tag{1e}$$

$$\frac{\partial \rho q}{\partial t} + \nabla \cdot (\rho q \boldsymbol{u}) = 0, \tag{1f}$$

where  $\rho$ , **u**, p, E are the mixture density, velocity, pressure and specific total energy, respectively. The parameters  $\gamma$ ,  $p_{\infty}$ , q come from the EOS. Here, we consider the stiffened gas (SG) EOS for the k-th component that takes the following form:

$$\rho_k e_k = \frac{p_k + \gamma_k p_{\infty,k}}{\gamma_k - 1} + \rho_k q_k,\tag{2a}$$

$$\rho_k e_k = \rho_k C_{\nu,k} T_k + p_{\infty,k} + \rho_k q_k, \tag{2b}$$

where  $C_{y,k}$  is the specific heat at constant volume. The parameters  $\gamma_k$ ,  $p_{\infty,k}$  and  $q_k$  are constants characterizing the thermodynamic behaviors of the *k*-th phase.

When thermal conduction is considered, the temperature becomes continuous at interfaces. However, Johnsen et al. [3,34] pointed out that the system of equations (1) does not preserve temperature equilibrium. Based on similar ideas as in designing the model (1) with the PV property, they proposed a method for defining the mixture EOS that ensures the PVT property. They add the following evolution equations for  $C_{\nu}$ ,  $p_{\infty}$  to the model eq. (1)

$$\frac{\partial \rho C_{\nu}}{\partial t} + \nabla \cdot (\rho C_{\nu} \boldsymbol{u}) = 0, \tag{3a}$$

$$\frac{\partial p_{\infty}}{\partial t} + \boldsymbol{u} \cdot \nabla p_{\infty} = 0.$$
(3b)

The evolved parameters obtained from eqs. (1d) to (1f) are used to compute the pressure, while those obtained from eqs. (3a) and (3b) to compute the temperature. This model can also be formulated in volume fraction framework by replacing all the evolution eqs. (1d) to (1f), (3a), and (3b) for EOS parameters with

$$\frac{\partial \rho Y_2}{\partial t} + \nabla \cdot (\rho Y_2 \mathbf{u}) = 0, \tag{4a}$$

 $\frac{\partial \alpha_2}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_2 = 0,$ (4b)

where  $\alpha_2$  and  $Y_2$  are the volume fraction and mass fraction of the second component, respectively.

When velocity is spatially uniform, the internal energy is purely advected,

$$\frac{\mathsf{D}\rho e}{\mathsf{D}t} = 0,\tag{5}$$

where  $\rho e = \sum \alpha_k \rho_k e_k$ , the operator D·/Dt denotes the material derivative.

By using eq. (5), the following mixture rules are proposed in [3,34] to maintain the PVT property:

• To maintain pressure equilibrium, the mixture EOS parameters are defined as

$$\frac{1}{\gamma - 1} = \sum \frac{\alpha_k}{\gamma_k - 1}, \quad \frac{\gamma p_\infty}{\gamma - 1} = \sum \frac{\alpha_k \gamma_k p_{\infty,k}}{\gamma_k - 1}, \quad \rho q = \sum \alpha_k \rho_k q_k. \tag{6}$$

• While to maintain temperature equilibrium, the following mixture EOS parameters should be defined as

$$\rho C_{\nu} = \sum \alpha_k \rho_k C_{\nu,k}, \quad p_{\infty} = \sum \alpha_k p_{\infty,k}, \quad \rho q = \sum \alpha_k \rho_k q_k.$$
<sup>(7)</sup>

As can be noted, two different mixture rules are used for computing pressure and temperature, resulting in two different definitions for  $p_{\infty}$  (and interface location when the fluid distribution is represented by their own  $p_{\infty}$ ). This ambiguity in mixture EOS definition also leads to difficulties in defining some thermodynamic variables, such as the mixture entropy. Therefore, the issue of consistency with the second law of thermodynamics is a key point to cause controversy. In fact, the volume fraction based model consisting of eqs. (1a) to (1c), (4a), and (4b) formally coincides with the five-equation model [4] that lacks a mathematical entropy. In the following we refer to this model with the mixture rules eqs. (6) and (7) as the one-temperature five-equation model.

Most of the second group models for simulating compressible multiphase flows come from the seven-equation Baer-Nunziato one [6]. In the original Baer-Nunziato model, each component is described by their own velocity, temperature, and pressure. However, for certain application scenarios such as the multiphase flows where each phase occupies its own volume, the physics included in the Baer-Nunziato model is not always necessary. Therefore, a variety of reduced models are proposed, for example, the six-equation model with equilibrium velocity [36,75,59], the five-equation model with equilibrium velocity and equilibrium pressure [36,56] and the four-equation model with equilibrium velocity, pressure and temperature [46]. A complete hierarchy of these models is formulated in [48]. Since these models are compatible with the complete Baer-Nunziato one, they are more physically sound and reasonable. Besides, in [7] a one-temperature quasi-hydrodynamic multiphase model with viscosity and heat conduction has been derived with the Coleman-Noll procedure [15].

Among these models, the model with equilibrium temperature [46] is most appropriate to consider heat conduction process, however, it fails to ensure the PV or the PVT condition. Moreover, it does not provide topological information of the material interface, nor does it describe the evolution of the volume-fraction averaged material properties such as thermal conductivity and viscosity. Therefore, we are more interested in the temperature non-equilibrium models [36,56]. A seminal work has been done in this direction by Petitpas et al. [61] where a Baer-Nunziato type two-phase model with heat conduction and its reduced models have been proposed. Thanks to the nozzling term due to interface heat conduction, this model can deal with non-equilibrium heat conduction without temperature relaxation. For solving heat conduction equations in their model, they propose a discrete method under the assumption of pressure disequilibrium, temperature disequilibrium and frozen interface topology. Their approach applies to the case when the temperature relaxation and pressure relaxation times are comparable such as the boiling flow, while our work is directed at ICF plasma flows where the pressure relaxation time is negligible compared with temperature relaxation time. Bearing this purpose in mind, we investigate other possible relaxation procedures with emphasis on the one under mechanical and thermal equilibrium with non-linear diffusion. Moreover, the coupling between interface location and state parameters is taken into consideration to maintain the established pressure equilibrium. The present work is not trying to build new physical or mathematical models (except for the external energy deposition) but rather a numerical model that in a certain way treats the physical relaxation processes. Moreover, numerical issues of high-order extension for preserving PVT property and comparative analysis of existing models have also been dealt with.

We build a formally two-temperature relaxation model based on the reduction of the Baer-Nunziato one. The obtained model consists of two energy equations including thermal relaxation between phases driving temperatures into equilibrium. It includes viscosity, heat conduction and external energy source in each phase. Note that the heat conduction process is accompanied with instantaneous thermal relaxation so that temperature equilibrium is maintained. We demonstrate that the impact of these thermal relaxations (which are usually neglected in the first group models) on volume fraction is significant. The obtained model ensures the pressure and the temperature equilibria during the heat conduction. We prove that the model agrees with the second law of thermodynamics. Although the relaxation model is built under the assumption of pressure and temperature equilibria, our approach provides a methodology to consider more general disequilibrium situations. Numerically, our model is proved to satisfy the PVT property with a uniquely defined EOS.

We use the fractional step method to solve the model. The solution procedure can be divided into four steps, i.e., the hyperbolic step, the viscous step, the thermal relaxation step and the heat conduction step. The homogeneous hyperbolic

part is solved with the Godunov method coupled with the HLLC Riemann solver. The diffusion processes (viscous step and heat conduction step) are governed by a set of parabolic partial differential equations. They are solved with an efficient method of local iterations, that allows much larger time step than the traditional explicit scheme and quite straightforward for parallel implementation. The thermal relaxation procedure is realized by solving a non-linear system with two variables (equilibrium temperature and volume fraction). We prove that the thermal relaxation procedure does not undermine the PVT property.

The rest of this article is organized as follows. In Section 2, we deduce a five-equation model and a six-equation model, with more attention being devoted to the latter as it is more convenient for considering thermal processes in the multiphase system with phase energy equations. In Section 3, we design numerical methods for solving the proposed model and prove some relevant properties. In Section 4, numerical results of our model are presented and compared with those of other models.

# 2. Model formulation

#### 2.1. The Baer-Nunziato type model

The starting point of our model formulation is the complete Baer-Nunziato model [6] or its variant for compressible two-phase flows [70,61]. In this model each phase is assumed to behave as a pure fluid except when it interacts with the other fluid through relaxation terms. Including viscosity, heat conduction and external energy source to the Baer-Nunziato model, we obtain the following formulation:

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \boldsymbol{u}_k) = 0, \tag{8a}$$

$$\frac{\partial \alpha_k \rho_k \mathbf{u}_k}{\partial t} + \nabla \cdot \left( \alpha_k \rho_k \mathbf{u}_k \otimes \mathbf{u}_k + \alpha_k p_k \overline{\overline{I}} - \alpha_k \overline{\overline{\tau}}_k \right) = p_I \nabla \alpha_k - \overline{\overline{\tau}}_I \cdot \nabla \alpha_k + \mathcal{M}_k,$$
(8b)

$$\frac{\partial \alpha_k \rho_k E_k}{\partial t} + \nabla \cdot \left[ \alpha_k \left( \rho_k E_k + p_k \right) \boldsymbol{u}_k - \alpha_k \overline{\overline{\tau}}_k \cdot \boldsymbol{u}_k \right] = p_I \boldsymbol{u}_I \cdot \nabla \alpha_k$$

$$-\boldsymbol{u}_{I}\cdot\left(\overline{\boldsymbol{\tau}}_{I}\cdot\nabla\boldsymbol{\alpha}_{k}\right)-p_{I}\mathcal{F}_{k}+\boldsymbol{u}_{I}\mathcal{M}_{k}+\boldsymbol{Q}_{k}+\boldsymbol{q}_{k}+\boldsymbol{I}_{k},$$
(8c)

$$\frac{\partial \alpha_2}{\partial t} + \boldsymbol{u}_1 \cdot \nabla \alpha_2 = \mathcal{F}_2, \tag{8d}$$

where the notations used are standard:  $\alpha_k$ ,  $\rho_k$ ,  $u_k$ ,  $p_k$ ,  $\overline{\tau}_k$ ,  $E_k$  are the volume fraction, density, velocity, pressure, viscous stress, and specific total energy of *k*-th component.

For viscous stress we use the Newtonian approximation

$$\overline{\overline{\tau}}_{k} = 2\mu_{k}\overline{\overline{D}}_{k} + \left(\mu_{b,k} - \frac{2}{3}\mu_{k}\right)\nabla \cdot \boldsymbol{u}_{k},\tag{9}$$

where  $\mu_k > 0$  is the coefficient of shear viscosity and  $\mu_{b,k} > 0$  is the coefficient of bulk viscosity,  $\overline{\overline{D}}_k$  is defined as

$$\overline{\overline{D}}_k = \frac{1}{2} \left[ \nabla \boldsymbol{u}_k + (\nabla \boldsymbol{u}_k)^{\mathrm{T}} \right].$$

The total energy is  $E_k = e_k + \mathcal{K}_k$  where  $e_k$ , and  $\mathcal{K}_k = \frac{1}{2} \boldsymbol{u}_k \cdot \boldsymbol{u}_k$  are the specific internal energy and kinetic energy, respectively.

The inter-phase exchange terms include the velocity relaxation  $M_k$ , the pressure relaxation  $\mathcal{F}_k$ , and the temperature relaxation  $Q_k$ ,

$$\mathcal{M}_{k} = \vartheta \left( \boldsymbol{u}_{k^{*}} - \boldsymbol{u}_{k} \right), \quad \mathcal{F}_{k} = \eta \left( p_{k} - p_{k^{*}} \right), \quad Q_{k} = \zeta \left( T_{k^{*}} - T_{k} \right), \tag{10}$$

where  $k^*$  denotes the conjugate component of the *k*-th component, i.e., k = 1,  $k^* = 2$  or k = 2,  $k^* = 1$ . The relaxation rates are all positive  $\vartheta > 0$ ,  $\eta > 0$ ,  $\varsigma > 0$ .

The variables with the subscript "I" represent the variables at interfaces, for which there are several possible definitions [60,72]. Whatever the definitions we choose,

$$\lim_{\eta\to\infty}p_I=\lim_{\eta\to\infty}p_k=p,\quad \lim_{\vartheta\to\infty}u_I=\lim_{\vartheta\to\infty}u_k=u,\quad \lim_{\vartheta\to\infty}\overline{\overline{\tau}}_I=\lim_{\vartheta\to\infty}\overline{\overline{\tau}}_k=\overline{\overline{\tau}}_I$$

The heat conduction term is given as:

$$q_k = \nabla \cdot (\alpha_k \lambda_k \nabla T_k) \,,$$

(11)

and the external heat source term is written as:

$$I_k = \alpha_k I_k, \tag{12}$$

where  $I_k$  denotes the intensity of the external heat source released in the k-th phase, and  $I_k \ge 0$ .

For future use we can deduce the corresponding balance equations for phase internal energies and phase entropies from eq. (8). The deduction procedure is similar to that in [93,56,36,96,97] with the exception that we include viscosity, heat conduction, and external energy source here. We directly give the equation for the phase internal energy as follows:

$$\frac{\partial \alpha_k \rho_k e_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k e_k \mathbf{u}_k) = -\alpha_k p_k \nabla \cdot \mathbf{u}_k - p_I \mathcal{F}_k + p_I (\mathbf{u}_I - \mathbf{u}_k) \cdot \nabla \alpha_k + (\mathbf{u}_I - \mathbf{u}_k) \cdot \mathcal{M}_k + (\mathbf{u}_k - \mathbf{u}_I) \cdot (\overline{\overline{\tau}}_I \cdot \nabla \alpha_k) + Q_k + q_k + I_k + S_k,$$
(13)

where the viscous dissipation

$$S_k = \alpha_k \overline{\overline{\tau}}_k : \overline{\overline{D}}_k.$$
<sup>(14)</sup>

By using the Gibbs relation,

$$\Gamma_k \mathrm{d}s_k = \mathrm{d}e_k - \frac{p_k}{\rho_k^2} \mathrm{d}\rho_k \tag{15}$$

we further obtain

$$T_{k}\left[\frac{\partial \alpha_{k}\rho_{k}s_{k}}{\partial t}+\nabla \cdot (\alpha_{k}\rho_{k}\boldsymbol{u}_{k}s_{k})\right] = (p_{k}-p_{I})\mathcal{F}_{k} + (p_{I}-p_{k})(\boldsymbol{u}_{I}-\boldsymbol{u}_{k})\cdot\nabla\alpha_{k} + (\boldsymbol{u}_{I}-\boldsymbol{u}_{k})\cdot\nabla\alpha_{k} + (\boldsymbol{u}_{I}-\boldsymbol{u}_{I})\cdot\left(\overline{\overline{\tau}}_{I}\cdot\nabla\alpha_{k}\right) + Q_{k}+q_{k}+I_{k}+S_{k}.$$
(16)

Even though eq. (8) is the most complete model including relaxations in pressure, velocity and temperature, however, practical implementation of this model is rather complicated because of its complex wave structure and stiff relaxation procedures. Therefore, we will consider two possible reductions of this model that are given in the following sections.

The Baer-Nunziato model is deduced by using the Coleman-Noll procedure [16,15,6], keeping the second law of thermodynamics. Maintaining the physical consistency with the Baer-Nunziato model, the reduced models should also satisfy the second law of thermodynamics, as we demonstrate below.

**Remark 1.** The thermodynamically compatible two-phase compressible flow model proposed in [68,66,67,69] can also be reformulated in the form of Baer-Nunziato model with additional source terms describing the lift forces.

**Remark 2.** For turbulent bubbly flows, the viscous pressure has been proposed to consider the pulsation damping of the bubbles [73,60,28]. Including this viscous pressure, the relaxing pressure is

$$\widetilde{p}_k = p_k + p_{\mu,k},\tag{17}$$

with  $p_{\mu,k}$  being the viscous pressure [28]:

$$p_{\mu,k} = z_k(\alpha_k) \frac{D_I \alpha_k}{Dt} = z_k(\alpha_k) \mathcal{F}_k,$$
(18)

where  $z_k$  is a function of  $\alpha_k$ ,  $\frac{D_l}{Dt}$  denotes the material derivative related to the interface velocity  $\mathbf{u}_l$ , and  $\mathcal{F}_k = \eta (\tilde{p}_k - \tilde{p}_{k^*})$ . With the viscous pressure, the terms including  $\mathcal{F}_k$  on r.-h.s. of eq. (13) and eq. (16) should be replaced by  $\tilde{p}_l \mathcal{F}_k$  and

 $(p_k - \tilde{p}_l)\mathcal{F}_k$ , respectively. In order that the term  $(p_k - \tilde{p}_l)\mathcal{F}_k$  makes a non-negative contribution to the phase entropy in eq. (16),  $\tilde{p}_l$  should be a convex combination of  $\tilde{p}_k$  and  $z_k$  be non-positive.

It can be seen from eq. (18) that the viscous pressure  $p_{\mu,k}$  vanishes when pressure equilibrium is reached, thus, it has no impact on the solution of the reduced models (in Sections 2.2 and 2.3) derived in the limit of instantaneous mechanical relaxation. Therefore, we temporarily omit this term in the following discussions.

**Remark 3.** The heat conduction is included in the original BN model and also the model of Nigmatulin [57]. The inclusion of viscosity and capillary effects has been done in [60,76]. Petitpas et al. [61] has derived a model including an interfacial heat flux term by performing the averaging procedure [18,19]. In the present work we have included the external heat source term, which is derived with the averaging procedure as follows. Let us introduce the characteristic function:

C. Zhang, I. Menshov, L. Wang et al.

$$X_{k} = \begin{cases} 1 & \text{in the domain } V_{\Omega,k} \text{ occupied by fluid } k \\ 0 & \text{otherwise} \end{cases}$$
(19)

Performing the averaging procedure within the control volume  $V_{\Omega}$ , we have

$$\frac{1}{V_{\Omega}} \int_{V_{\Omega}} X_k I'_k \mathrm{d}V = \frac{1}{V_{\Omega}} \int_{V_{\Omega,k}} I'_k \mathrm{d}V = \alpha_k I_k = I_k, \tag{20}$$

where  $I_k$  is the average of  $I'_k$  (i.e., the heat source within  $V_{\Omega,k}$ ).

**Remark 4.** In comparison with the original BN model, the model of Petitpas et al. [61] includes a non-conservative nozzling term  $q_1 \cdot \nabla \alpha_k$  ( $q_1$  is the average interfacial heat flux) on the r.h.s. of eq. (8c). This term can be reformulated as a heat exchange term and lumped into the temperature relaxation term by modifying the temperature relaxation rate [61].

#### 2.2. The reduced five-equation model

By performing asymptotic analysis of the Baer-Nunziato model in the limit of instantaneous mechanical relaxations with the method similar to [36,88,56], one can obtain the following system of equations (for detailed derivations see Appendix):

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \boldsymbol{u}) = 0, \qquad (21a)$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot \left( \rho \boldsymbol{u} \otimes \boldsymbol{u} + p \overline{\overline{t}} \right) = \nabla \overline{\overline{\tau}},\tag{21b}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \boldsymbol{u} + p \boldsymbol{u}) = \nabla \cdot \left(\overline{\overline{\tau}} \cdot \boldsymbol{u}\right) + \sum q_k + \sum I_k,$$
(21c)

$$\frac{\partial \alpha_2}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_2 = R_{p_2} + R_{q_2} + R_{q_2} + R_{I_2} + R_{S_2},$$
(21d)

where  $\overline{I}$  is the unit tensor,  $\rho = \sum \alpha_k \rho_k$  and  $\overline{\overline{\tau}} = \sum \alpha_k \overline{\overline{\tau}}_k$  are the mixture density and the mixture viscous stress, respectively. The right hand side terms of eq. (21d) are

$$R_{p_2} = \alpha_2 \frac{A - A_2}{A_2} \nabla \cdot \boldsymbol{u}, \quad R_{q_2} = A \frac{\Gamma_2 q_2 \alpha_1 - \Gamma_1 q_1 \alpha_2}{A_1 A_2}, \quad R_{Q_2} = A \frac{\Gamma_2 Q_2 \alpha_1 - \Gamma_1 Q_1 \alpha_2}{A_1 A_2},$$
$$R_{I_2} = A \frac{\Gamma_2 I_2 \alpha_1 - \Gamma_1 I_1 \alpha_2}{A_1 A_2}, \quad R_{S_2} = A \frac{\Gamma_2 S_2 \alpha_1 - \Gamma_1 S_1 \alpha_2}{A_1 A_2},$$

where  $\Gamma_k$  is the phase Gruneisen coefficient,  $\Gamma_k = V_k \left(\frac{\partial p_k}{\partial e_k}\right)_{V_k}$ ,  $V_k = 1/\rho_k$ ,  $a_k^2 = \overline{\gamma}_k p_k V_k$  is the phase speed of sound,  $\overline{\gamma}_k = -\frac{V_k}{p_k} \left(\frac{\partial p_k}{\partial V_k}\right)_{s_k}$  is the phase adiabatic exponent,  $A_k = \rho_k a_k^2$ , and  $1/A = \sum (\alpha_k/A_k)$ .

In the case of the SG EOS (2a), these parameters are

$$\Gamma_k = \gamma_k - 1, \tag{23}$$

$$\overline{\gamma_k} = \gamma_k \frac{p_k + p_{\infty,k}}{p_k} > \gamma_k > \Gamma_k, \tag{24}$$

$$A_{k} = \gamma_{k}(p_{k} + p_{\infty,k}) = \frac{\gamma_{k}(\gamma_{k} - 1)C_{\nu,k}T_{k}}{V_{k}}.$$
(25)

The first term on the right hand side (r.-h.s.) of eq. (21d)  $R_{p_k}$  comes from pressure relaxation. In fact,  $W_{p_k} = -pR_{p_k}$  represents the rate of work performed on material interfaces to maintain pressure equilibrium under compression or expansion [42]. The significance of this term for spherical bubble dynamics and multiphase flows has been demonstrated in [78] and [56], respectively.

In the limit of the sharp material interface, i.e.  $\alpha_k = 1$ ,  $\alpha_l = 0$  ( $l \neq k$ ), the first r.-h.s. term of eq. (21d)  $R_{p_k}$  vanishes. The terms  $R_{q_k}$ ,  $R_{I_k}$ , and  $R_{S_k}$  also vanish in accordance of the definitions eq. (11), eq. (12) and eq. (14). However, the term  $R_{Q_k}$  due to temperature relaxation still remains. This means that for compressible multicomponent problem with heat conduction, the thermal relaxation can not be neglected even for interface-tracking methods where the diffused zone is absent. Therefore, vanishing the r.-h.s. of eq. (21d) and using just the pure advection equation for volume fraction may lead to errors that come from physical defects instead of numerical ones.

If we define the mixture entropy as

$$s = Y_1 s_1 + Y_2 s_2, (26)$$

from eq. (16) one can deduce

$$\frac{\partial \rho s}{\partial t} + \nabla \cdot (\rho \mathbf{u} s) = \frac{\alpha_1 \overline{\overline{\tau}}_1 : \overline{D}_1}{T_1} + \frac{\alpha_2 \overline{\overline{\tau}}_2 : \overline{D}_2}{T_2} + \frac{Q_1 + q_1 + I_1}{T_1} + \frac{Q_2 + q_2 + I_2}{T_2}.$$
(27)

**Proposition 1.** In the absence of heat flows through the external boundaries of the control volume, eq. (27) is non-negative.

**Proof 1.** The first two terms on the r.-h.s. of eq. (27) can be proven to be non-negative,  $\alpha_k \overline{\overline{\tau}}_k : \overline{\overline{D}}_k \ge 0$ , by using the definition eq. (9) and simple tensor manipulations.

Also, due to eq. (10)

$$\frac{Q_1}{T_1} + \frac{Q_2}{T_2} = \varsigma \frac{(T_2 - T_1)^2}{T_1 T_2} \ge 0.$$
(28)

The heat conduction term can be recast as

$$\frac{q_k}{T_k} = -\frac{\nabla \cdot \mathbf{q}_k}{T_k} = -\nabla \cdot (\frac{\mathbf{q}_k}{T_k}) + \mathbf{q}_k \cdot \nabla (\frac{1}{T_k})$$
(29)

The first term is of the divergence type and represents external heat inflow to the phase material particle. The second term is positive due to the Fourier's law of heat conduction  $\boldsymbol{q}_k = -\alpha_k \lambda_k \nabla T_k$ ,  $\alpha_k \ge 0$ ,  $\lambda_k \ge 0$  and  $\mathcal{I}_k \ge 0$ . Therefore, except the heat inflow terms, the r.-h.s of the mixture entropy equation (2.11) is non-negative. This means that the mixture entropy respects the second law of thermodynamics.

Note that a similar five equation model is presented in [76] where only  $R_{p2}$  retains on r.h.s. of the volume fraction equation.

The model eq. (21) assumes two temperatures and only one pressure. It is a counterpart of Kapila's five-equation model [36,56] in the presence of dissipation processes, which has certain numerical constraints such as the non-monotonic behavior of sound speed across interface and lack of robustness due to volume fraction positivity issues. To circumvent these issues, we turn to the six-equation formulation, whose advantages include: (a) robust numerical solution, (b) more relaxation freedoms that allow considering the difference between relaxation time scales, (c) equipment with phase energy equations that brings convenience to deal with phase energy exchanges.

Moreover, in the following model formulation we maintain thermal equilibrium in the course of heat conduction, which is shown to be more computationally efficient than heat conduction in thermal disequilibrium. This leads to an original model valuable from a physical point of view as able to treat two situations: (a) flows in thermal equilibrium/disequilibrium without heat conduction, (b) flows in thermal equilibrium with heat conduction.

# 2.3. The reduced six-equation model

We first separate the physical process into three stages: the mechanical stage, the thermal relaxation stage and the heat conduction stage, and then build thermodynamical consistency for each stage.

In the mechanical stage the pressure equilibrium is reached with the instantaneous pressure relaxation. The thermal relaxation drives the phase temperatures to equilibrium. The thermal and mechanical relaxation time scales vary for different fluids and application problems. We are attempting to take the difference between relaxation time scales into consideration without relaxation parameters. These parameters are yet to be evaluated or improved for complicated processes, for example, the ICF plasma flows that we are concerned with.

The heat conduction can proceed under different physical relaxation assumptions of mechanical/thermal equilibrium/disequilibrium. The work of Petitpas et al. [61] provides a model/numerical method where the heat conduction takes place during the pressure and temperature disequilibrium. For many applications (for example, detonation [36,14,62], phase transition in metastable liquids [74,92] and bubble dynamics [9,31,55], etc.), it is estimated that the mechanical relaxation takes place much faster than the thermal one, approximately meaning that temperature relaxation goes under pressure equilibrium. Moreover, thermal relaxation is caused by the heat convection and conduction, which are the results of collective and random molecule motions. Due to the similarity in physical mechanism, we assume that these thermal processes happen at similar time scales and accompany each other. On the basis of such considerations, we consider the heat conduction under pressure equilibrium.

*Mechanical stage* For the mechanical stage, we temporarily omit thermal relaxation and conduction. In the limit of instantaneous velocity relaxation, one can obtain the following six-equation model with one velocity from the Baer-Nunziato model eq. (8)

Journal of Computational Physics 466 (2022) 111356

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \boldsymbol{u}) = 0, \tag{30a}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla (\alpha_1 p_1 + \alpha_2 p_2) = \nabla \cdot \overline{\overline{\tau}},$$
(30b)

$$\frac{\partial \alpha_k \rho_k e_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k e_k \boldsymbol{u}) + \alpha_k p_k \nabla \cdot \boldsymbol{u} = -p_I \mathcal{F}_k + \alpha_k \overline{\overline{\tau}}_k : \overline{\overline{D}},$$
(30c)

$$\frac{\partial \alpha_2}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_2 = \mathcal{F}_2. \tag{30d}$$

The corresponding balance equation for mixture entropy is

$$\frac{\partial \rho s}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} s) = \frac{\alpha_1 \overline{\tau}_1 : \overline{D}_1}{T_1} + \frac{\alpha_2 \overline{\tau}_2 : \overline{D}_2}{T_2} + \frac{(p_1 - p_I)\mathcal{F}_1}{T_1} + \frac{(p_2 - p_I)\mathcal{F}_2}{T_2}$$
(31)

As long as the interface pressure  $p_1$  is assumed to be a convex combination of  $p_1$  and  $p_2$ , i.e.,

$$p_{I} = Z_{1}p_{1} + Z_{2}p_{2} \quad (Z_{1}, Z_{2} \in [0, 1], Z_{1} + Z_{2} = 1),$$
(32)

the term  $(p_k - p_l)\mathcal{F}_k$  remains non-negative and the second law of thermodynamics is respected.

When solving internal energy equations (30c), the total energy equation (21c) will have to be supplemented to keep the energy conservation as in [75].

This stage consists of the hydrodynamic, the viscous and the pressure relaxation processes. The last relaxation process drives the phase pressures into an equilibrium pressure  $p = \lim_{\eta \to \infty} p_1 = \lim_{\eta \to \infty} p_2$ .

*Thermal relaxation stage* The procedure is similar to that for deducing the model for phase transition in [92]. Having reached the pressure equilibrium after the mechanical stage, we continue to build our model for the thermal relaxation on the basis of the following physical assumptions:

• The mechanical relaxation happens much faster than the thermal relaxation, which means that the temperature relaxation goes in the state of pressure equilibrium.

The thermal relaxation process is assumed to be governed by the following equations:

$$\frac{\partial \alpha_k \rho_k}{\partial t} = 0, \tag{33a}$$

$$\frac{\partial \rho \alpha}{\partial t} = 0,$$
(33b)
$$\frac{\partial \alpha_1 \rho_1 e_1}{\partial t} = Q'_1.$$
(33c)

$$\frac{\alpha_1 \rho_1 c_1}{\partial t} = Q_1', \tag{33c}$$

$$\frac{\partial \alpha_2 \rho_2 e_2}{\partial t} = Q'_2,$$
(33d)

$$\frac{\partial \alpha_2}{\partial t} = r_0 \frac{\alpha_2}{p},\tag{33e}$$

where  $Q'_k$  is the thermal relaxation term defined in eq. (10), which results in the variation of the phase temperature and the volume fraction. The term  $Q'_2/p$  represents the volume fraction change rate if no phase temperature variation is considered.

The parameter  $r_0$  is a dimensionless coefficient, balancing the phase temperature change and volume fraction change. It is determined in such a way that the pressure equilibrium condition is maintained, i.e.,

$$\frac{\partial p_1}{\partial t} = \frac{\partial p_2}{\partial t}.$$
(34)

Thus one can obtain

$$r_{0} = \frac{\Gamma_{1}/\alpha_{1} + \Gamma_{2}/\alpha_{2}}{(A_{1}/\alpha_{1} + A_{2}/\alpha_{2})/p - (\Gamma_{1}/\alpha_{1} + \Gamma_{2}/\alpha_{2})},$$
(35)

or

$$r_0 = \frac{\Gamma_1/\alpha_1 + \Gamma_2/\alpha_2}{\left(\overline{\gamma}_1 - \Gamma_1\right)/\alpha_1 + \left(\overline{\gamma}_2 - \Gamma_2\right)/\alpha_2},\tag{36}$$

According to eqs. (25), (33a), and (35),  $r_0$  is a function of  $T_1$ ,  $T_2$  and  $\alpha_2$ , and from eq. (24), it satisfies

$$r_0 = r_0 (T_1, T_2, \alpha_2) > 0.$$
(37)

By using eqs. (10), (15), (26), and (37) one can deduce

$$\frac{\partial \rho s}{\partial t} + \nabla \cdot (\rho s \boldsymbol{u}) = (1 + r_0) \left( \frac{1}{T_2} - \frac{1}{T_1} \right) \boldsymbol{Q}_2^{\prime} \ge 0$$
(38)

This means that the model for the thermal relaxation is consistent with the second law of thermodynamics.

*Heat conduction stage* We build our model for thermal conduction under the physical assumption of both pressure and temperature equilibrium. This assumption means that the heat conduction time scale is larger enough than the heat transfer scale so that temperature equilibrium always holds. In fact, this is a default assumption for models based on single temperature formulation, for example, the four-equation conservative model in [46].

The heat conduction process (including the external heat source) is modeled by the following system of equations:

$$\frac{\partial \alpha_k \rho_k}{\partial t} = 0, \tag{39a}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} = \boldsymbol{0},\tag{39b}$$

$$\frac{\partial \alpha_1 \rho_1 e_1}{\partial t} = \delta q_1 + q_1 + I_1, \tag{39c}$$

$$\frac{\partial \alpha_2 \rho_2 e_2}{\partial t} = \delta q_2 + q_2 + I_2, \tag{39d}$$

$$\frac{\partial \alpha_2}{\partial t} = \frac{r_{10}}{p} \delta q_2 + \frac{r_1}{p} \left( q_1 + I_1 \right) + \frac{r_2}{p} \left( q_2 + I_2 \right).$$
(39e)

Here, the term  $\delta q_k$  represents an interphase energy interaction term, and  $\delta q_1 + \delta q_2 = 0$  for energy conservation. It consists of three components including the heat convection, the nozzling term, and the work done due to the interface motion, i.e.,

$$\delta q_k = \widetilde{Q}'_k + \boldsymbol{q}_I \cdot \nabla \alpha_k - p \frac{\partial \alpha_k}{\partial t}.$$
(40)

The first two terms can be written in the form of temperature relaxation (similar to eq. (10)) with their own non-negative relaxation rate [61] as follows:

$$Q_k'' = \widetilde{Q}_k' + \boldsymbol{q}_I \cdot \nabla \alpha_k. \tag{41}$$

The interphase interaction is defined as a linear combination of  $q_k$  and  $I_k$ ,

$$\delta q_2 = \hat{r}_1(q_1 + I_1) + \hat{r}_2(q_2 + I_2). \tag{42}$$

We then define the parameters  $r_{10}$ ,  $r_1$ ,  $r_2$ ,  $\hat{r}_1$ ,  $\hat{r}_2$  in this model in the following manner.

• Defining the parameters  $r_{10}$ ,  $r_1$ ,  $r_2$ 

. .

The pressure equilibrium condition eq. (34) should be maintained, thus, one can obtain

$$r_{10} = r_0,$$
 (43a)

$$r_1 = \frac{-\Gamma_1/\alpha_1}{\left(\overline{\gamma}_1 - \Gamma_1\right)/\alpha_1 + \left(\overline{\gamma}_2 - \Gamma_2\right)/\alpha_2},\tag{43b}$$

$$r_2 = \frac{\Gamma_2/\alpha_2}{\left(\overline{\gamma}_1 - \Gamma_1\right)/\alpha_1 + \left(\overline{\gamma}_2 - \Gamma_2\right)/\alpha_2}.$$
(43c)

• Defining the parameters 
$$\hat{r}_1, \hat{r}_2$$

The temperature equilibrium condition should be satisfied, i.e.,

$$\frac{\partial T_1}{\partial t} = \frac{\partial T_2}{\partial t},\tag{44}$$

which yields the coefficients in eq. (42) as

$$\widehat{r}_{1} = -\frac{r_{1}\mathcal{Y} - m_{2}C_{\nu,2}}{r_{0}\mathcal{Y} - m_{1}C_{\nu,1} - m_{2}C_{\nu,2}},\tag{45a}$$

$$\widehat{r}_2 = -\frac{r_2 \mathcal{Y} + m_1 \mathcal{C}_{\nu,1}}{r_0 \mathcal{Y} - m_1 \mathcal{C}_{\nu,1} - m_2 \mathcal{C}_{\nu,2}},\tag{45b}$$

$$\mathcal{Y} = m_1 C_{\nu,1} G_2 + m_2 C_{\nu,2} G_1, \tag{45c}$$

where  $m_k = \alpha_k \rho_k$ ,  $G_k = 1 + \Gamma_k / c_{v,k}$ , with  $c_{v,k}$  being the dimensionless specific heat,  $c_{v,k} = pV_k / (C_{v,k}T_k)$ .

By using eq. (39) and the Gibbs relation eq. (15), one can deduce

$$\frac{\partial \rho s}{\partial t} + \nabla \cdot (\rho s \boldsymbol{u}) = \frac{q_1}{T_1} + \frac{q_2}{T_2} + \frac{I_1}{T_1} + \frac{I_2}{T_2} + \left(\frac{1}{T_2} - \frac{1}{T_1}\right) Q_2''.$$
(46)

The last r.h.s. term can be shown to be non-negative by inserting the temperature relaxation expression. As for the first two terms, according to proof 1, we have

$$\int_{V} \frac{q_k}{T_k} \, \mathrm{d}\tau \ge 0,\tag{47}$$

if the net heat flux across the surface of the volume V vanishes.

We further deduce

$$\int_{V} \left[ \frac{\partial \rho s}{\partial t} + \nabla \cdot (\rho s \boldsymbol{u}) \right] d\tau \ge 0, \tag{48}$$

and as V is an arbitrary closed domain, one can write the entropy inequality

$$\frac{\partial \rho s}{\partial t} + \nabla \cdot (\rho s \boldsymbol{u}) \ge 0. \tag{49}$$

**Remark 5.** Thanks to eq. (44),  $\delta q_k$  can be expressed as a function of  $q_k$  and  $\mathcal{I}_k$ . One can also consider the more general situation where heat conduction goes in temperature disequilibrium by abandoning the complete temperature relaxation assumption (i.e., eq. (44)) and specify concrete closure law for Q' or Q''.

Moreover, under the assumption of complete relaxations within every time step, different relaxation sequences are also possible (see Table 1 and section 3.4.2).

#### 2.4. The final model

We summarize the finial model for compressible two-phase flows with viscosity and heat conduction as follows:

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \boldsymbol{u}) = 0, \tag{50a}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla (\alpha_1 p_1 + \alpha_2 p_2) = \nabla \cdot \overline{\tau},$$
(50b)

$$\frac{\partial \alpha_k \rho_k e_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k e_k \boldsymbol{u}) + \alpha_k p_k \nabla \cdot \boldsymbol{u} = -p_I \mathcal{F}_k + \alpha_k \overline{\overline{\tau}}_k : \overline{\overline{D}} + Q'_{\boldsymbol{\mu}} + \delta q_k + q_k + I_k,$$
(50c)

$$\frac{\partial \alpha_2}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_2 = \mathcal{F}_2 + \frac{r_0}{p} \left( \mathcal{Q}_2' + \delta q_2 \right)$$

$$+\frac{r_1}{p}(q_1+I_1)+\frac{r_2}{p}(q_2+I_2).$$
(50d)

The mechanical stage can violate the temperature equilibrium state of the phases that is reached and maintained through following temperature relaxations. One can see that the temperature relaxation in the considered model eq. (8) consists of two parts: the thermal relaxation before heat conduction  $Q'_k$  and that during heat conduction  $Q''_k$  (see eq. (41)), with the former being much faster than the latter. The former ensures the initial temperature equilibrium before the heat conduction progresses, the latter maintains this temperature equilibrium while the heat conduction in and between the phases. Thus, temperature equilibrium is still maintained after the heat conduction.

For each stage, the entropy inequality remains valid. Thus, after implementing the fractional step method corresponding to the three relaxation stages, the solution obtained should not be contrary to the second law of thermodynamics.

Since the final model is non-conservative for the mixture total energy, we supplement it with the mixture total energy equation of the five-equation model eq. (21c) in order to correct the non-conservativeness. Similar idea is adopted in [75] in the absence of the diffusion processes.

#### 3. Numerical methods

In this section we describe the numerical methods for solving the above proposed model. The numerical method is based on the operator splitting technique that consists of three stages: the mechanical (solving the hyperbolic, viscous, and the pressure relaxation parts of the equations), the temperature relaxation, and the heat conduction stage. We address these steps separately. These steps can be arranged in different orders to mimic different physical assumptions (as listed in Table 1 below).

#### 3.1. Hyperbolic part

The homogeneous hyperbolic part of the governing equations eq. (50) to be solved first is as follows:

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \boldsymbol{u}) = 0, \tag{51a}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla (\alpha_1 p_1 + \alpha_2 p_2) = 0, \tag{51b}$$

$$\frac{\partial \alpha_k \rho_k e_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k e_k \boldsymbol{u}_k) + \alpha_k p_k \nabla \cdot \boldsymbol{u} = 0,$$
(51c)

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left[ \left( \rho E + \alpha_1 p_1 + \alpha_2 p_2 \right) \boldsymbol{u} \right] = 0, \tag{51d}$$

$$\frac{\partial \alpha_2}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_2 = 0. \tag{51e}$$

As mentioned above, we adopt the idea similar to that of [75], i.e., using a redundant equation for the mixture total energy eq. (51d) to correct the solution of the non-conservative equations for phase internal energies eq. (51c). One can rewrite eq. (51) (without the redundant equation) into the following system with respect to the primitive variable  $\mathbf{Z} = [\rho_1 \ \rho_2 \ u \ v \ p_1 \ p_2 \ \alpha_2]^T$ 

$$\frac{\partial \mathbf{Z}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{Z}}{\partial x} = 0.$$
(52)

It can be shown that the matrix **A** has 7 real eigenvalues (i.e.  $u \pm c$  and u of multiplicity 5) and the corresponding set of six linearly independent right eigenvectors. Thus, the system is hyperbolic.

The mixture speed of sound for this model is

$$c^2 = Y_1 c_1^2 + Y_2 c_2^2. ag{53}$$

This ensures monotonic variation of the characteristic velocity across the interface zone and therefore more robust compared with the five-equation model eq. (21) where the mixture speed of sound is given by non-monotonic Wood's formulae. We recast eq. (51) in the vector compact form (in 1D) as:

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}(\boldsymbol{U})}{\partial x} + \boldsymbol{R}(\boldsymbol{U}) \frac{\partial \boldsymbol{u}}{\partial x} = 0,$$
(54)

where

 $U = [\alpha_1 \rho_1 \ \alpha_2 \rho_2 \ \rho u \ \rho v \ \alpha_1 \rho_1 e_1 \ \alpha_2 \rho_2 e_2 \ \rho E \ \alpha_2]^{\mathrm{T}},$   $F (U) = uU + (\alpha_1 p_1 + \alpha_2 p_2)D,$   $D (U) = [0 \ 0 \ 1 \ 0 \ 0 \ u \ 0]^{\mathrm{T}},$  $R (U) = [0 \ 0 \ 0 \ \alpha_1 p_1 \ \alpha_2 p_2 \ 0 \ -\alpha_2]^{\mathrm{T}}.$ 

We use the Godunov method coupled with the approximate Riemann solver HLLC to solve eq. (54):

$$\boldsymbol{U}_{i}^{n+1} = \boldsymbol{U}_{i}^{n} - \frac{\Delta t}{\Delta x} \left[ \boldsymbol{F} \left( \boldsymbol{U}_{i+1/2}^{*} \right) - \boldsymbol{F} \left( \boldsymbol{U}_{i-1/2}^{*} \right) \right] - \frac{\Delta t}{\Delta x} \boldsymbol{R} \left( \boldsymbol{U}_{i}^{n} \right) \left( \boldsymbol{u}_{i+1/2}^{*} - \boldsymbol{u}_{i-1/2}^{*} \right),$$
(55)

where  $U_{i+1/2}^* = U_{i+1/2}^* (U_i, U_{i+1})$  is the Riemann solution at the cell face i + 1/2. Here we use the three-wave approximate Riemann solver HLLC [80–82,89]. The dimensional spitting method is used for extension to multiple dimensions.

# 3.2. Viscous part

Viscous terms have no impact on the mass balance equations and affect only the momentum and energy equations. The corresponding splitted equations are read as

$$\frac{\partial \alpha_k \rho_k}{\partial t} = 0, \quad \frac{\partial \alpha_k}{\partial t} = 0, \quad \frac{\partial \rho \mathbf{u}}{\partial t} = \nabla \cdot \overline{\tau},$$

$$\frac{\partial \alpha_k \rho_k e_k}{\partial t} = \alpha_k \overline{\tau_k} : \overline{D}, \quad \frac{\partial \rho E}{\partial t} = \nabla \cdot \left(\overline{\tau} \cdot \mathbf{u}\right).$$
(56)

To solve the parabolic PDE for velocity, we use an efficient method of local iterations based on Chebyshev parameters [100,83]. A brief introduction on this method is given below.

Consider the following 1D parabolic PDE

$$\frac{\partial v}{\partial t} = Lv + f(x, t), \quad x \in G \subset \mathbb{R}$$
(57)

where *L* is a linear elliptic self-adjoint positive-definite operator.

Given a grid  $\Omega_h = \bigcup [x_{j-1/2}, x_{j+1/2}]$  with a space step *h*, consider also a discrete operator  $L_h v_j$  that approximates the operator *L* with  $O(h^2)$  on smooth solutions. For example, it can be the 1D reduction of the 7-point (in 3D) symmetric discretization of *L* obtained with the finite volume method used in the present paper (see below). The operator  $L_h$  is self-adjoint and has real positive eigenvalues within an interval  $[\lambda_{min}, \lambda_{max}]$ .

The method of local iterations [100] is realized as 2P - 1 explicit iterations, where  $P = \lceil \pi/4\sqrt{\tau\lambda_{max} + 1} \rceil$ , with  $\tau$  being the time step and  $\lceil x \rceil$  denoting the maximal integer to be greater than or equal to x. These explicit iterations are written as follows (for details see [100]):

$$\nu^{(m)} = \frac{1}{1 + \tau b_m} \left( \nu^n + \tau b_m \nu^{(m-1)} - \tau L_h \nu^{(m-1)} + \tau f^{(n)} \right), \quad m = 1, 2, \cdots, 2P - 1,$$
(58)

where  $v^{(m)}$  is the solution after *m*-th iteration,  $b_m$  is a set of iteration parameters,

$$(b_1, b_2, \cdots, b_{2P-1}) = (a_P, a_{P-1}, \cdots, a_2, a_P, a_{P-1}, \cdots, a_1),$$

Here,

$$a_m = \frac{\lambda_{max}}{1+\beta_1} (\beta_1 - \beta_m), \quad m = 1, \cdots, P,$$
(59)

and the sequence  $(\beta_1, \dots, \beta_P)$  represents the roots of the Chebyshev polynomial  $T_P(x)$ :  $\cos \frac{(2j-1)\pi}{2P}$ ,  $j = 1, \dots, P$ , arranged in the increasing order.

Since  $b_{2P-1} = 0$ , the last iteration becomes

$$v^{(2P-1)} = v^n + \tau L_h v^{(2P-2)} + \tau f^n, \tag{60}$$

which is the pure explicit step and  $v^{(2P-2)}$  can be viewed as a predicted solution.

This scheme ensures the monotonicity of the solution [100]. Each explicit iteration of eq. (58) is a conventional explicit step, making its parallel realization quite straightforward.

According to eq. (56), the mixture density  $\rho$  does not vary with time at this stage. Therefore, the momentum equation takes in 1D the following form:

$$\rho \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( \frac{4}{3} \mu \frac{\partial u}{\partial x} \right). \tag{61}$$

The above method of local iterations is applied to eq. (61). The operator  $L_h$  that approximates the r.-h.s. is given by central differences as

$$L_{h} = \frac{1}{\Delta x} \left( F_{i+1/2}^{vis} - F_{i-1/2}^{vis} \right), \tag{62}$$

where

$$F_{i+1/2}^{vis} = \frac{4}{3} \mu_{i+1/2} \frac{\partial u}{\partial x} \Big|_{i+1/2}$$

represents the viscous flux across the cell face i + 1/2.

The last iteration step is given in the conservative form,

$$\frac{(\rho u)_i^{n+1} - (\rho u)_i^n}{\Delta t} = L_h(\widehat{u}_i)$$

with  $\hat{u}$  being the predicted velocity after the first (2P - 2) iterations.

Once the velocity is calculated, the total energy is then updated as follows:

$$\frac{(\rho E)_{i}^{n+1} - (\rho E)_{i}^{n}}{\Delta t} = \frac{1}{\Delta x} \left( \widehat{u}_{i+1/2} F_{i+1/2}^{vis} - \widehat{u}_{i-1/2} F_{i-1/2}^{vis} \right), \tag{63}$$

where  $F_{i+1/2}^{vis}$  is determined by the velocity  $\hat{u}$  calculated in the first 2P - 2 local iteration.

Note that  $\alpha_k \overline{\overline{\tau}}_k : \overline{\overline{D}} = \nabla \cdot \left( \alpha_k \overline{\overline{\tau}}_k \cdot \mathbf{u} \right) - \left[ \nabla \cdot \left( \alpha_k \overline{\overline{\tau}}_k \right) \right] \cdot \mathbf{u}$ , then one can update the internal energies as follows:

$$\frac{(\alpha_k \rho_k e_k)_i^{n+1} - (\alpha_k \rho_k e_k)_i^n}{\Delta t} = \frac{1}{\Delta x} \left( \alpha_{k,i+1/2} \widehat{u}_{i+1/2} F_{i+1/2}^{vis} - \alpha_{k,i-1/2} \widehat{u}_{i-1/2} F_{i-1/2}^{vis} \right) - \frac{1}{\Delta x} u_i \left( \alpha_{k,i+1/2} F_{i+1/2}^{vis} - \alpha_{k,i-1/2} F_{i-1/2}^{vis} \right).$$
(64)

Extensions of the above algorithm to multiple dimensions can be done straightforwardly in the directional splitting manner.

#### 3.3. Pressure relaxation part

Next step is to drive phase pressures into an equilibrium state by performing instantaneous pressure relaxation procedures when  $\tau = 1/\eta \rightarrow 0$ . The process can be described with the following equations:

$$\frac{\partial \alpha_k \rho_k}{\partial t} = 0, \quad \frac{\partial \rho \mathbf{u}}{\partial t} = 0, \quad \frac{\partial \alpha_k \rho_k e_k}{\partial t} = -p_1 \mathcal{F}_k, \quad \frac{\partial \alpha_k}{\partial t} = \mathcal{F}_k, \tag{65}$$

where  $\mathcal{F}_k$  is defined in eq. (10).

Here we use the relaxation algorithm proposed in [75]. This algorithm consists of the following basic steps:

- (1) Combining eq. (65) and eq. (2a), one can obtain the relaxed volume fraction as a function of the equilibrium pressure *p*<sup>(1)</sup>, i.e., *α*<sub>k</sub><sup>(1)</sup> = *α*<sub>k</sub>(*p*<sup>(1)</sup>). By using the saturation constraint ∑*α*<sub>k</sub>(*p*<sup>(1)</sup>) = 1, we can find *p*<sup>(1)</sup> and *α*<sub>k</sub><sup>(1)</sup>.
   (2) Having *α*<sub>k</sub><sup>(1)</sup>, we then re-evaluate the pressure by using the mixture total energy *ρE* (solved from the mechanical
- (2) Having  $\alpha_k^{(1)}$ , we then re-evaluate the pressure by using the mixture total energy  $\rho E$  (solved from the mechanical part of eq. (21c)) to ensure the conservativeness of energy and obtain the final pressure as  $p^{(2)} = p(\alpha_k^{(1)}, \rho e)$ , where  $\rho e = \rho E \rho \mathbf{u} \cdot \mathbf{u}/2$ .
- (3) The phase internal energies are recalculated according to  $e_k = e_k(p^{(2)}, \alpha_k^{(1)})$ .

It is reported that this solution algorithm turns to be only about 5% more expensive than that of the five-equation model [78].

# 3.4. Temperature relaxation and heat conduction parts

The system of equations for the temperature relaxation read:

$$\frac{\partial \alpha_k \rho_k}{\partial t} = 0, \tag{66a}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} = 0, \tag{66b}$$

$$\frac{\partial \alpha_k \rho_k e_k}{\partial t} = Q'_k,\tag{66c}$$

$$\frac{\partial \alpha_2}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_2 = \frac{r_0}{p} \boldsymbol{Q}_2. \tag{66d}$$

And the heat conduction process is described by

$$\frac{\partial \alpha_k \rho_k}{\partial t} = 0, \tag{67a}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} = \boldsymbol{0},\tag{67b}$$

$$\frac{\partial \alpha_k \rho_k e_k}{\partial t} = \delta q_k + q_k + \mathcal{I}_k,\tag{67c}$$

$$\frac{\partial \alpha_2}{\partial t} = \frac{r_0}{p} \delta q_2 + \frac{r_1}{p} \left( q_1 + I_1 \right) + \frac{r_2}{p} \left( q_2 + I_2 \right).$$
(67d)

We see that formally eq. (66) is a particular case of eq. (67) when  $q_k + I_k = 0$ ,  $\delta q_k = Q'_k$ . Therefore, we first deal with numerical solutions of eq. (67) and then extend to eq. (66).

Considering  $e_k = e_k(T_k, \rho_k)$  and eliminating  $\delta q_2$  from eq. (67), one can deduce the following relation between phase temperatures and volume fraction  $\alpha_2$ :

$$C_2 \frac{\partial T_2}{\partial t} + \mathcal{B}_2 \frac{\partial \alpha_2}{\partial t} = \mathcal{R}_1 \left( q_1 + \mathcal{I}_1 \right) + \mathcal{R}_2 \left( q_2 + \mathcal{I}_2 \right).$$
(68)

$$\mathcal{B}_2 C_1 \frac{\partial T_1}{\partial t} + (\mathcal{B}_1 + \mathcal{B}_2) C_2 \frac{\partial T_2}{\partial t} = (\mathcal{B}_2 + \mathcal{B}_1 \mathcal{R}_1) (q_1 + \mathcal{I}_1) + (\mathcal{B}_2 + \mathcal{B}_1 \mathcal{R}_2) (q_2 + \mathcal{I}_2),$$
(69)

where

$$\begin{split} & C_k = m_k C_{v,k}, \\ & \mathcal{B}_1 \left( T_k, \alpha_2 \right) = p \left( T_k, \alpha_2 \right) \left( G_2 - G_1 \right), \\ & \mathcal{B}_2 \left( T_k, \alpha_2 \right) = p \left( T_k, \alpha_2 \right) \frac{1 - r_0 \left( T_k, \alpha_2 \right) G_2}{r_0 \left( T_k, \alpha_2 \right)} \\ & \mathcal{R}_1 \left( \alpha_2 \right) = \frac{-\Gamma_1 / \alpha_1}{\Gamma_1 / \alpha_1 + \Gamma_2 / \alpha_2}, \\ & \mathcal{R}_2 \left( \alpha_2 \right) = 1 + \frac{\Gamma_2 / \alpha_2}{\Gamma_1 / \alpha_1 + \Gamma_2 / \alpha_2}. \end{split}$$

In the case of the SG EOS, we have:

$$\mathcal{B}_{1} = p_{\infty,1} - p_{\infty,2},$$

$$\mathcal{B}_{2} = \frac{p}{r_{0}} + p_{\infty,2}.$$
(70)
(71)

It can be seen that  $C_1$ ,  $C_2$ ,  $\mathcal{B}_1$  are all constants in this case, while  $\mathcal{B}_2$  is a function of  $\alpha_2$ ,  $T_1$ ,  $T_2$  due to eq. (37)) and  $p = p(T_k, \rho_k) = p(T_k, \frac{m_k}{\alpha_k})$ . Here,  $m_k$  is constant as a result of eq. (66a).

Using eqs. (25), (35), and (71),  $\mathcal{B}_2(T_1, T_2, \alpha_2)$  can be explicitly written as

$$\mathcal{B}_{2}(T_{1}, T_{2}, \alpha_{2}) = \frac{\Gamma_{1}C_{1}T_{1}/\alpha_{1}^{2} + \Gamma_{1}p_{\infty,1}/\alpha_{1} + \Gamma_{2}C_{2}T_{2}/\alpha_{2}^{2} + \Gamma_{2}p_{\infty,2}/\alpha_{2}}{\Gamma_{1}/\alpha_{1} + \Gamma_{2}/\alpha_{2}} + p_{\infty,2}.$$
(72)

#### 3.4.1. Temperature relaxation

The temperature relaxation process is assumed to be much faster than phase heat conduction so that we take  $q_1 = q_2 = 0$  and  $I_1 = I_2 = 0$ . In this case, eqs. (68) and (69) are reduced to the following:

$$C_2 \frac{\partial T_2}{\partial t} + \mathcal{B}_2 \frac{\partial \alpha_2}{\partial t} = 0, \tag{73a}$$

$$\mathcal{B}_2 C_1 \frac{\partial T_1}{\partial t} + (\mathcal{B}_1 + \mathcal{B}_2) C_2 \frac{\partial T_2}{\partial t} = 0.$$
(73b)

In the model considered, we neglect a finite temperature relaxation time and assume the temperature equilibrium to occur within the time step. Using the superscript "0" and "/" to denote parameters before and after the temperature relaxation stage, an implicit discretization of eqs. (73a) and (73b) can be written as

$$C_2\left(T' - T_2^0\right) + \mathcal{B}_2(T_1^{a\nu}, T_2^{a\nu}, \alpha_2^{a\nu})\left(\alpha_2' - \alpha_2^0\right) = 0,$$
(74a)

$$\mathcal{B}_{2}(T_{1}^{av}, T_{2}^{av}, \alpha_{2}^{av})C_{1}\left(T' - T_{1}^{0}\right) + \left(\mathcal{B}_{1} + \mathcal{B}_{2}(T_{1}^{av}, T_{2}^{av}, \alpha_{2}^{av})\right)C_{2}\left(T' - T_{2}^{0}\right) = 0.$$
(74b)

Here the parameters  $C_1$ ,  $C_2$ , and  $\mathcal{B}_1$  are all constants, while  $\mathcal{B}_2$  is a function of the phase temperatures and the volume fraction,  $\mathcal{B}_2 = \mathcal{B}_2(T_1, T_2, \alpha_2)$  that is approximated by the average values  $T_k^{av} = (T_k^0 + T')/2$  and  $\alpha_2^{av} = (\alpha_2^0 + \alpha_2')/2$ , i.e.,  $\mathcal{B}_2 = \mathcal{B}_2(T_1^{av}, T_2^{av}, \alpha_2^{av})$ . This system is solved with the Newton method or the simple iterative method. In the present work we use the latter.

**Remark 6.** If we look at eq. (7) from the perspective of the temperature relaxation, the relaxed temperature defined by the one-temperature five-equation model can be viewed as an averaged temperature:

$$\rho e = \sum \left( \alpha_k \rho_k C_{\nu,k} T_k^0 + \alpha_k p_{\infty,k} + \alpha_k \rho_k q_k \right) = \rho C_\nu T' + p_\infty + \rho q, \tag{75}$$

with

$$T' = \frac{C_1 T_1^0 + C_2 T_2^0}{C_1 + C_2}.$$
(76)

In fact, in the case when  $p_{\infty,1} = p_{\infty,2}$  the solution of eq. (73b) coincides with eq. (76). Otherwise, we obtain a solution different from eq. (76). Moreover, no corresponding volume fraction variation is considered in the one-temperature five-equation model.

# 3.4.2. Heat conduction

*Heat conduction under temperature equilibrium* The heat conduction process goes under the temperature equilibrium condition  $T_1 = T_2 = T$ , so that eqs. (68) and (69) describe the change in time of temperature and volume fraction:

$$\frac{\partial T}{\partial t} = \mathcal{V}_1 \left( q_1 + I_1 \right) + \mathcal{V}_2 \left( q_2 + I_2 \right), \tag{77a}$$

$$\frac{\partial \alpha_2}{\partial t} = \mathcal{U}_1 \left( q_1 + I_1 \right) + \mathcal{U}_2 \left( q_2 + I_2 \right), \tag{77b}$$

where

$$\mathcal{V}_1 = \frac{\mathcal{B}_2 + \mathcal{B}_1 \mathcal{R}_1}{(\mathcal{B}_1 + \mathcal{B}_2) C_2 + C_1 \mathcal{B}_2}, \quad \mathcal{V}_2 = \frac{\mathcal{B}_2 + \mathcal{B}_1 \mathcal{R}_2}{(\mathcal{B}_1 + \mathcal{B}_2) C_2 + C_1 \mathcal{B}_2}$$

and

$$\mathcal{U}_1 = \frac{\mathcal{R}_1 - C_2 \mathcal{V}_1}{\mathcal{B}_2}, \quad \mathcal{U}_2 = \frac{\mathcal{R}_2 - C_2 \mathcal{V}_2}{\mathcal{B}_2}.$$

Note that  $\mathcal{B}_k$ ,  $\mathcal{V}_k$ ,  $\mathcal{U}_k$ ,  $\mathcal{R}_k$  are dependent on  $\alpha_2$  and T.

Initial data for this system of ODE are T' and  $\alpha'$  obtained as the result of solving the temperature relaxation step (see section 3.4.1).

Note that the coefficients  $\mathcal{V}_1$ ,  $\mathcal{V}_2$ ,  $\mathcal{U}_1$ ,  $\mathcal{U}_2$  are functions of T and  $\alpha_2$ . The heat conduction coefficients commonly depend on temperature, i.e.,  $\lambda_k = \lambda_k(T_k)$ . For example, for the thermal conductivity in completely ionized gas  $\lambda_k = O(T_k^{\frac{5}{2}})$  [87]. Therefore, eqs. (77a) and (77b) represent a system of non-linear PDEs, with the spatial differential operator being applied only to T.

To solve this system of parabolic equations we implement the method of local iterations described above (eq. (58)). The term due to heat conduction  $q_k$  is approximated with the central difference scheme. For example, assuming the 1D case on a uniform grid,  $q_k$  is discretized as

$$(q_k)_i = \frac{\Lambda_{k,i+1/2}T_{i+1} - \left(\Lambda_{k,i+1/2} + \Lambda_{k,i-1/2}\right)T_i + \Lambda_{k,i-1/2}T_{i-1}}{\Delta x^2}$$
(78)

where  $\Lambda_k = \alpha_k \lambda_k$ .

The method of local iterations is applied to solve eq. (77a) for temperature with iterative recalculation of volume fraction in eq. (77b). The computational algorithm is formulated in Algorithm 1.

# Algorithm 1 The iterative algorithm for solving eqs. (77a) and (77b).

```
Define the discretized solution

T := \{T_1, T_2, ..., T_N\}, \quad A := \{\alpha_{2,1}, \alpha_{2,2}, ..., \alpha_{2,N}\}, \quad T^{(1)} := T', \quad A^{(1)} := A'
Define it := 1, \quad Conv := -1, \quad tol

while Conv < 0 do

Calculate the parameters \mathcal{V}_k, \mathcal{U}_k, \Lambda_k by using T^{(it)}, A^{(it)}

Solve eq. (77a) with respect to T by using the method of local iterations (or a conventional implicit scheme) to obtain T'

Solve eq. (77b) with respect to \alpha_2 with T' and A^{(it)} to obtain A'

Set T^{(it+1)} = T', \quad A^{(it+1)} = A'

Calculate err = \|T^{(it+1)} - T^{(it)}\|

if err < tol then

Conv = 1

end if

Update it := it + 1

end while

return T^{(it+1)}, \quad A^{(it+1)}
```

*Heat conduction under temperature disequilibrium* Although in the present work we focus on the case where phase temperatures reach equilibrium at the end of each time step, one can also consider disequilibrium heat conduction. The role of the temperature relaxation term Q'' (inside  $\delta q_k$ ) accompanying the heat conduction is to drive the phase temperatures into equilibrium. Temporarily abandoning this term under the temperature disequilibrium, eqs. (39c) to (39e) become:

$$\frac{\partial \alpha_k \rho_k e_k}{\partial t} = q_k + I_k - p \frac{\partial \alpha_k}{\partial t},$$

$$(1+r_{10}) \frac{\partial \alpha_2}{\partial t} = \frac{r_1}{p} \left( q_1 + I_1 \right) + \frac{r_2}{p} \left( q_2 + I_2 \right).$$
(79a)
(79b)

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Table I
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Different relaxation procedures.

Procedure (A)	Procedure (B)	Procedure (C)	
HC under disequilibrium of pressure and temperature	HC under equilibrium of pressure and temperature	HC under temperature disequilibrium and pressure equilibrium	
HD	HD	HD	
$p_1 \neq p_2, T_1 \neq T_2$	$p_1 \neq p_2, T_1 \neq T_2$	$p_1 \neq p_2, T_1 \neq T_2$	
<b>HC</b> $p_1 \neq p_2, T_1 \neq T_2$ Solve 2 HEs	<b>PR</b> $p_1^0 \neq p_2^0, \ p_1' = p_2', \ T_1 \neq T_2$	<b>PR</b> $p_1^0 \neq p_2^0, \ p_1' = p_2', \ T_1 \neq T_2$	
<b>PR</b> $p_1^0 \neq p_2^0, p_1' = p_2', T_1 \neq T_2$	<b>TR</b> $p_1 = p_2, T_1^0 \neq T_2^0, T_1' = T_2'$	<b>HC</b> $p_1 = p_2, T_1 \neq T_2$ Solve 2 HEs	
<b>TR</b> $p_1 = p_2 \ T_1^0 \neq T_2^0, \ T_1' = T_2'$	<b>HC+TR</b> $p_1 = p_2, T_1^0 = T_2^0, \ \frac{\partial T_1}{\partial t} = \frac{\partial T_2}{\partial t}$ Solve 1 HF	<b>TR</b> $p_1 = p_2, T_1^0 \neq T_2^0, T_1' = T_2'$	
$t_{ex1}$ = 79.95 s $t_{ex2}$ = 2757.78 s $t_{ex3}$ = 3399.52 s	$t_{ex1} = 69.04 \text{ s}$ $t_{ex2} = 1570.20 \text{ s}$ $t_{ex3} = 40.69 \text{ s}$	$t_{ex1} = 77.71 \text{ s}$ $t_{ex2} = 2733.53 \text{ s}$ $t_{ex3} = 3577.38 \text{ s}$	

HD = hydrodynamic, HC = heat conduction, PR = pressure relaxation, TR = temperature relaxation, HE = heat equation.

Superscripts "0" and "r" represent values at the beginning and the end of the current stage, respectively.

The last row displays the computation times of sample test problems with the explicit scheme below. The first, second, third row correspond to the shock tube test with  $\lambda_1 = \lambda_2 = 10^6$  W/(m · K) on 200-cell and 1000-cell grid, the two-phase problem with  $\lambda_1 = \lambda_2 = 10^7$  W/(m · K), respectively.

The computations are performed on processor Intel(R) Xeon(R) W-2012 CPU @ 2.90 GHz and MATLAB 2017.

For SG EOS, eq. (79a) becomes

$$\alpha_k \rho_k C_{\nu,k} \frac{\partial T_k}{\partial t} = q_k + \mathcal{I}_k - (p + p_{\infty,k}) \frac{\partial \alpha_k}{\partial t}.$$
(80)

After disequilibrium heat conduction, the complete temperature relaxation (including the nozzling term) is performed at the end of each time step.

For the case of finite temperature relaxation rate, one has to add the nozzling terms  $\mathbf{q}_I \cdot \nabla \alpha_k$  and  $\frac{r_{10}}{p} \mathbf{q}_I \cdot \nabla \alpha_k$  to the r.-h.s. of eq. (79a) and eq. (79b), respectively.

Equations (79b) and (80) are solved with the iterative method similar to Algorithm 1. Note that here we have two disequilibrium temperatures and one volume fraction as unknowns. For the numerical approximation of the nozzling terms, see [61].

#### 3.5. Relaxation procedures

On the basis of different physical assumptions, several relaxation procedures are possible, as summarized in Table 1. Procedure (A) is the solution procedure similar to that of Petitpas et al. for their model [61]. In their procedure, the heat conduction proceeds under pressure and temperature disequilibrium and frozen interface topology. Heat conduction contributes to this disequilibrium, which is then erased with the pressure relaxation and temperature relaxation successively.

Our work focuses on the heat conduction under pressure equilibrium. Possible candidates are procedures (B) and (C). The heat conduction and temperature relaxation may undermine the obtained pressure equilibrium. To balance the arising pressure disequilibrium, the interface is in motion. The last three r.h.s. terms in eq. (50d) account for the mechanism of maintaining the pressure equilibrium obtained through the first term  $\mathcal{F}_k$ . The coupling between volume fraction and temperature is taken into consideration, adding some computational complexity.

In the application context of the high-energy-density plasma flows the heat equation is strongly non-linear and timeconsuming to solve. Therefore, computational efficiency is an important aspect in choosing relaxation procedures. The procedure (B) has better efficiency than procedures (A) and (C), especially for problems where temperature relaxation time approaches zero. One reason is that the procedure (B) solves only one heat equation for the equilibrium temperature, while others need to solve the heat equation for each phase in temperature disequilibrium. In addition, the explicit stable time step required by the phase heat equation is smaller than that of an equilibrium mixture heat equation in general. In procedure (B), the stable explicit time step required by the heat equation (77a) is

$$\Delta t < \frac{\Delta x^2}{(\alpha_1 \lambda_1)_{i+1/2} (\mathcal{V}_1)_i + (\alpha_1 \lambda_1)_{i-1/2} (\mathcal{V}_1)_i + (\alpha_2 \lambda_2)_{i+1/2} (\mathcal{V}_2)_i + (\alpha_2 \lambda_2)_{i-1/2} (\mathcal{V}_2)_i}.$$
(81)



Fig. 1. Initial stable explicit time step for the relaxation procedures (A) and (B).

In the case when  $\mathcal{B}_1 = 0$  (or  $p_{\infty,1} = p_{\infty,2}$ ) and constant conductivity, this is reduced to the following familiar formulation:

$$\Delta t < \frac{\rho C_v \Delta x^2}{2\lambda},\tag{82}$$

see eq. (3a) for the definition of  $C_{\nu}$ .

Fig. 1 demonstrates the stable time steps required by the explicit scheme for the two-phase problem in Section 4.5. Here the time step for the phase heat equation is determined with the method proposed in Petitpas et al. [61]. We see that the time step for phase 2 is very small, which leads to a significant increase in the computation time. We have compared the computation time consumed by different relaxation procedures for several sample problems in Table 1, where one can see that the proposed relaxation procedure (B) has obvious advantage in explicit implementation.

#### 3.6. Evolution of constant pressure and temperature profiles

For the interface-capturing schemes, an important property is the preservation of constant velocity and pressure profiles, which is referred to as the PV property in literature and given by the following definition.

Definition 1. Say that an interface-capturing numerical scheme has the PV property if it ensures

$$u_i^{n+1} = u = \text{const}, \ p_i^{n+1} = p = \text{const}$$

providing that

$$u_i^n = u = \text{const}, \ p_i^n = p = \text{const}.$$

The numerical methods/models with this property have been studied, for example, in [1,2,84,85,50,98,4]. However, as pointed out in [35,3], the methods with the PV property may result in erroneous temperature spikes in the vicinity of the material interfaces. This phenomenon is not problematic when dissipative processes are not considered. However, when heat conduction is involved, the numerical errors in temperature may affect the pressure through the energy equation. Therefore, for compressible multi-fluid problems, instead of the above PV property we require the following PVT property

Definition 2. An interface-capturing numerical scheme has the PVT property if it ensures

$$u_i^{n+1} = u = \text{const}, \ p_i^{n+1} = p = \text{const}, \ T_i^{n+1} = T = \text{const},$$

providing that

$$u_i^n = u = \text{const}, \ p_i^n = p = \text{const}, \ T_i^n = T = \text{const}$$

Johnsen et al. [35,3] have proposed a methodology to get rid of the temperature spikes by introducing rules to define different mixture EOS for computing pressure and temperature. Their idea is similar to that of [1] for designing numerical methods to ensure the PV property. They developed their method based on the one-fluid formulation with single velocity, pressure and temperature. In this model the interfaces are represented by discontinuity in material properties.

However, this method may result in multiple definitions of material properties, and thus ambiguity in interface locations. In fact, although they assume that the fluids are in temperature equilibrium, the resultant model formally allows two temperatures. Their definitions of the mixture EOS for computing temperature are equivalent to averaging the phasic temperatures according to eq. (76).

If we look at the problem from the perspective of the two-temperature model, the temperature averaging procedure (by defining the mixture EOS) should be interpreted as a physical process – temperature relaxation. The impact of temperature relaxation process on volume fraction evolution is significant, as we demonstrate below. In the model of [35,3] this impact is neglected and volume fraction is purely advected. As can be seen in our model formulation (see Section 2), the impact of temperature relaxations ( $Q'_k$  in eq. (33) and  $\delta q_2$  in eq. (39)) on volume fraction evolution has been included and numerically treated properly in section 3.4.

In the case of ideal gas EOS, we have

$$p_{\infty,k} = 0, \ q_k = 0, \ \mathcal{B}_1 = 0.$$

Then the solution of our temperature-relaxations equations (73b) reproduces eq. (76). In fact, as long as  $p_{\infty,1} = p_{\infty,2}$ , eq. (76) holds. If the phasic temperatures before thermal relaxation are in equilibrium, then the averaging procedure does not change the temperature, nor the volume fraction.

Next we demonstrate that the proposed model preserves the PVT property, and is free of the temperature spike problem. Let us consider the following Riemann problem with the initial discontinuity:

$$u^{L} = u^{R} = u > 0$$
  

$$\rho_{k}^{L} = \rho_{k}^{R} = \rho_{k}, \quad k = 1, 2$$
  

$$e_{k}^{L} = e_{k}^{R} = e_{k}, \quad k = 1, 2$$
  

$$\alpha_{2}^{L} \neq \alpha_{2}^{R},$$
  

$$T_{1} = T_{2} = T,$$
  

$$\gamma_{1} \neq \gamma_{2}.$$
  
(83)

This problem is similar to that in [4,98], the difference consists in that we additionally require an initial temperature equilibrium and consider the thermal relaxation process.

Proposition 2. The solution to our model equations with initial discontinuity (83) ensures that

$$u^{*} = u$$

$$\rho_{k}^{*} = \rho_{k}, \quad k = 1, 2$$

$$e_{k}^{*} = e_{k}, \quad k = 1, 2$$

$$T_{1}^{*} = T_{2}^{*} = T,$$
(84)

where the superscript "\*" denotes the solution in the cell downstream the discontinuity after one time step.

**Proof 2.** We apply a Riemann solver that resolves isolated contact discontinuity exactly (for example HLLC [89,82]). After one time step, we have

$$\boldsymbol{U}_{i}^{*} = \boldsymbol{\xi} \boldsymbol{U}_{i-1} + (1-\boldsymbol{\xi}) \boldsymbol{U}_{i}, \tag{85}$$

where **U** is the solution vector defined in eq. (54) and  $\xi = u \Delta t / \Delta x$ . After some algebraic manipulations, one can obtain that

$$u^* = u, \quad p_1^* = p_2^* = p, \quad e_k^* = e_k, \quad \rho_k^* = \rho_k.$$
 (86)

By using the EOS of each phase, one can deduce

$$T_{k}^{*} = T_{k}(p_{k}^{*}, \rho_{k}^{*}) = T.$$
(87)

Next we prove that the temperature relaxation eqs. (73a) and (73b) with  $T_k^0 = T_k^*$  allows only one physically admissible solution T' = T.

For the case  $p_{\infty,1} = p_{\infty,2}$ , this consequence immediately comes from eq. (76).

For the case  $p_{\infty,1} \neq p_{\infty,2}$ , the proof is not so straightforward. For this case, let us assume that there exists another solution that  $T'' \neq T$  and satisfies eqs. (73a) and (73b). By using eq. (74b) and having in mind  $T'' - T \neq 0$ , one obtains

$$\mathcal{B}_2\left(T^{a\nu},\alpha_2^{a\nu}\right) = -\frac{C_2\mathcal{B}_1}{C} = B_2 = \text{const},\tag{88}$$

where

$$C = C_1 + C_2,$$
  

$$T^{av} = T_1^{av} = T_2^{av} = (T'' + T)/2$$
  

$$\alpha_2^{av} = (\alpha_2'' + \alpha_2)/2.$$

By using eqs. (72) and (88), one can obtain

$$\Gamma^{av} = \frac{b_1 \Gamma_1 / \alpha_1^{av} + b_2 \Gamma_2 / \alpha_2^{av}}{\Gamma_1 C_1 / (\alpha_1^{av})^2 + \Gamma_2 C_2 / (\alpha_2^{av})^2},\tag{89}$$

where  $b_1 = B_2 - p_{\infty,2} - p_{\infty,1}$ ,  $b_2 = B_2 - 2p_{\infty,2}$ ,  $\alpha_1^{av} = 1 - \alpha_2^{av}$ . By using eqs. (74a) and (88), one obtains

$$T'' = T - 2\frac{B_2}{C_2} \left( \alpha_2^{av} - \alpha_2^0 \right), \tag{90}$$

or

$$T^{av} = T - \frac{B_2}{C_2} \left( \alpha_2^{av} - \alpha_2^{\ 0} \right), \tag{91}$$

Combination of eqs. (89) and (91) leads to  $\gamma_1 = \gamma_2$ , which contradicts the initial condition (eq. (83)). Thus, the temperature relaxation procedure does not violate the temperature equilibrium. Moreover, since velocity and temperature are spatially uniform, the diffusion processes (heat conduction and viscosity) do not have any impact on the solution.

**Remark 7.** The conservative four-equation model [46] preserves the PV/PVT property in the case of uniform pressure and temperature distribution. When discontinuity exists in temperature, the four-equation model fails to preserve the PV property, while the six-equation model preserves this property without temperature relaxation.

#### 3.7. Extension to high order and interface sharpening

The scheme can be extended to higher orders with the MUSCL or WENO scheme. Moreover, to minimize numerical diffusion of material interfaces, we apply special interface-sharpening schemes [95,86,12,13,94]. One principle for implementing these schemes is that the reconstruction schemes for volume fractions and phase densities should be consistent, otherwise, the PVT property is violated. We give some explanations on the principles or issues for implementing high-order reconstruction schemes maintaining the PVT property for both the conservative four-equation model [46] and the quasi-conservative models (the six-equation model and the one-temperature five-equation model [3]).

# 3.7.1. Reconstruction principle for the quasi-conservative model

Observing the above proof of the PVT property (proof 2), one can see that an important condition for proving the temperature equilibrium is  $\rho_k^* = \rho_k$ . The high-order extensions should also ensure this condition. This is deduced from

$$(\alpha_k \rho_k)_i^* = \xi \,(\alpha_k \rho_k)_{i-1} + (1 - \xi) \,(\alpha_k \rho_k)_i \tag{92a}$$

$$(\alpha_k)_i^* = \xi \,(\alpha_k)_{i-1} + (1-\xi) \,(\alpha_k)_i \,. \tag{92b}$$

The corresponding high-order formulation is given as follows:

$$(\alpha_k \rho_k)_i^* = (\alpha_k \rho_k)_i - \xi \left[ (\alpha_k \rho_k)_{i,RF} - (\alpha_k \rho_k)_{i-1,RF} \right], \tag{93a}$$

$$(\alpha_k)_i^* = (\alpha_k)_i - \xi \left[ (\alpha_k)_{i,RF} - (\alpha_k)_{i-1,RF} \right], \tag{93b}$$

where we use the subscript "RF" to represent the reconstructed values on the right face of the current cell.

Assume that we use a reconstruction scheme that is a homogeneous function of degree 1 with respect to the reconstruction stencil, i.e., Rec ( $\beta P$ ) =  $\beta$ Rec (P),  $\beta$  = const > 0. Note that the TVD schemes are such functions. Then the reconstructed values are as follows:

$$(\alpha_k)_{i,RF} = \operatorname{Rec}\left(\mathcal{P}\right),\tag{94a}$$

$$(\alpha_k \rho_k)_{i,RF} = \overline{\text{Rec}} \left( \rho_k \mathcal{P} \right) = \rho_k \overline{\text{Rec}} \left( \mathcal{P} \right), \tag{94b}$$

where  $\mathcal{P}$  is the reconstruction stencil, for example, for the MINMOD scheme,  $\mathcal{P} = \{(\alpha_k)_{i-1}, (\alpha_k)_i, (\alpha_k)_{i+1}\}$ . Rec and  $\overline{\text{Rec}}$  are the reconstruction scheme for  $\alpha_k$  and  $\alpha_k \rho_k$ , respectively.

Combination of eqs. (93a), (93b), (94a), and (94b) leads to the conclusion that  $\rho_k^* = \rho_k$  holds only when  $\text{Rec}(\mathcal{P}) = \overline{\text{Rec}}(\mathcal{P})$ . This means that the same scheme should be used for reconstruction of  $(\alpha_k)_{i,RF}$  and  $(\alpha_k\rho_k)_{i,RF}$ ; Otherwise, the temperature equilibrium is violated. The numerical results presented in Section 4 also confirm this fact.

# 3.7.2. Reconstruction principle for the fully conservative model

As remarked above, for this model the standard first order FVM-HLLC ensures the PVT property in the case of uniform pressure and temperature. However, when extended to high-orders with the MUSCL scheme, one must cautiously select the reconstruction variables, otherwise, spurious oscillations arise. Two possible reconstruction candidates are  $[\rho \rho Y u p]$  or  $[\rho Y u p]$ . The latter is preferred in [45] for preserving the positivity of the mass fraction Y. This is reasonable because for the first candidate the monotonicity-preserving property of  $(\rho)_{RF}$  and  $(\rho Y)_{RF}$  does not mean no new extrema appear in  $Y_{RF} = (\rho Y)_{RF}/(\rho)_{RF}$ . In implementing TVD reconstruction with the first candidate, we encounter some robustness issues, i.e., computation breakdown in the case of complicated EOS and strong discontinuity. However, if both schemes converge, they do tend to converge to the same solution.

Although the second candidate is beneficial to positivity and robustness, it may ruin the PVT property. To avoid complicated mathematical manipulations, we show the problem with the IG EOS. Given spatially uniform initial temperature  $T_i$  and  $p_i$ , with the IG EOS and the relation  $Y_1V_1 + Y_2V_2 = 1$ , we deduce that the following quantity should also be spatially uniform

$$\frac{p_i}{T_i} = \rho_i Y_{1,i} \tilde{R}_1 + (\rho_i - \rho_i Y_{1,i}) \tilde{R}_2 = (\rho \tilde{R})_i = \text{const}, \quad \tilde{R}_k = (\gamma_k - 1) C_{\nu,k}.$$
(95)

The PVT property requires that  $(\rho \tilde{R})_i$  should remain unchanged in space and time. When the velocity is uniform, with the first reconstruction candidate, we have

$$(\rho)_{i}^{*} = (\rho)_{i} - \xi \left[ (\rho)_{i,RF} - (\rho)_{i-1,RF} \right],$$
(96a)

$$(\rho Y_1)_i^* = (\rho Y_1)_i - \xi \left[ (\rho Y_1)_{i,RF} - (\rho Y_1)_{i-1,RF} \right].$$
(96b)

With the second set of reconstruction variables where  $Y_1$  is reconstructed, we deduce

$$(\rho Y_1)_i^* = (\rho Y_1)_i - \xi \left[ \rho_{i,RF} (Y_1)_{i,RF} - \rho_{i-1,RF} (Y_1)_{i-1,RF} \right].$$
(97)

According to eq. (95), the limited slope for the linearly related variables  $\rho$  and  $\rho Y_k$  are equal, and different from that for  $Y_1$  in general. Once the reconstruction slope is determined,  $(\rho Y_1)_{i,RF}$  is a linear combination of its stencil, whereas  $\rho_{i,RF}(Y_1)_{i,RF}$  is not. One can check that eq. (96b) leads to  $(\rho \tilde{R})_i^* = (\rho \tilde{R})_i$ , while eq. (97) fails. Therefore, one can ascertain that first reconstruction candidate is compatible with the PVT property, which cannot be done for the second.

On the basis of the above analysis in this section, we define the following Temperature Non-Oscillatory (TNO) reconstruction schemes.

**Definition 3.** High order schemes that ensure the same TVD reconstruction or the same interpolation weights for  $\alpha_k \rho_k$  and  $\alpha_k$  for the five-equation and six-equation models (or  $\rho$  and  $\rho Y_k$  for the four-equation model) are termed as temperature non-oscillatory (TNO). Otherwise, the schemes are termed as non-TNO.

#### 4. Numerical results

In this section we perform several numerical tests with the purpose to verify our model and numerical methods and also compare with some other methods presented in literature. In the laser ablation problem (section 4.6), the variables are measured in the centimeter-gram-microsecond system of units, and in SI units for other tests.

# 4.1. Preservation of the PVT property

The purpose of this test is to check the capability of different models and numerical schemes to keep the PVT property. We consider the translation of material interface with initially uniform velocity  $u = 1.00 \times 10^3$  m/s and pressure  $p = 1.00 \times 10^5$  Pa. Initial phase pressures and temperatures are all in equilibrium. The computational domain is [0 m, 1 m] and the material interface is initially located at x = 0.20 m. The EOS parameters for the left component are  $\gamma = 4.40$ ,  $C_v = 58.82$  J/(kg·K), and parameters for the right component are  $\gamma = 1.40$ ,  $C_v = 125.00$  J/(kg·K),  $p_{\infty} = 0.00$  Pa. The right (left) pure component is approximated as a mixture with negligible amount (mass fraction  $10^{-8}$ ) of the left (right) component.

We consider the following three cases:

- (a) IG EOS without temperature discontinuity. The left component has the parameter  $p_{\infty,1} = 0.00$  Pa and the temperature is spatially uniform T = 3000.00 K. Such setting leads to a density of 0.17 kg/m<sup>3</sup> on the left and 0.67 kg/m<sup>3</sup> on the right.
- (b) SG EOS without temperature discontinuity. The left component has the parameter  $p_{\infty,1} = 6.00 \times 10^8$  Pa and the temperature is spatially uniform T = 3000.00 K. Such setting leads to a density of 1000.15 kg/m<sup>3</sup> on the left and 0.67 kg/m<sup>3</sup> on the right.



Fig. 2. Pure translation of a two-fluid system: numerical solutions for initial condition without temperature discontinuity. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

(c) IG EOS with temperature discontinuity. The left component has the parameter  $p_{\infty,1} = 0.00$  Pa. The temperature is discontinuous at the interface with 3000.00 K for the left component and 1000.00 K for the right component. Such setting leads to a density of 0.17 kg/m<sup>3</sup> on the left and 2.00 kg/m<sup>3</sup> on the right.

Non-physical oscillations can be caused by both models and numerical methods. We demonstrate this below.

*Comparison of models* Here and in the following subsections, we evaluate four different models:

- (a) The conservative four-equation model with one temperature (4-eqn model 1T.) [46],
- (b) The five-equation model with one temperature and one pressure (5-eqn model 1T.) [3],
- (c) The six-equation model with two temperatures (6-eqn model 2T.) [75],
- (d) The proposed six-equation model with two temperatures and thermal relaxation (6-eqn model 2T. relaxed).

To shield the impact of numerical methods, we use the TNO reconstruction schemes in solving all the above models. Computations with the above models are performed on a 100-cell grid to the moment  $t = 5.00 \times 10^{-4}$  s. The numerical results for Case (a) and (b) are illustrated in Fig. 2. From Figs. 2a and 2b, it can be seen that all models with TNO schemes maintain the PVT property without triggering oscillations for Case (a). However, in Case (b), when solving the conservative four-equation model with the TNO scheme, the computation fails after a few steps due to complex wave speed. In this case, the quasi-conservative models show more robustness and are free of oscillations at the interface (see Figs. 2c and 2d). As demonstrated in Fig. 3, in Case (c) with temperature discontinuity, both the conservative four-equation model and the six-equation model with temperature relaxation lead to oscillations, the other models maintain the pressure-velocity equilibrium.

*Comparison of numerical schemes* As mentioned above, in Case (b) when solving the conservative four-equation model with the TNO reconstruction scheme, the computation fails due to lack of robustness. Here we have used the reconstruction



Fig. 3. Pure translation of a two-fluid system: numerical solutions for initial condition with temperature discontinuity.



Fig. 4. Pure translation of a two-fluid system: numerical solutions to the conservative four-equation model with non-TNO reconstruction.



Fig. 5. Pure translation of a two-fluid system: numerical solutions to the six-equation model with non-TNO reconstruction.

variable [ $\rho u p Y_1$ ], which is non-TNO. From Fig. 4 we see that the non-physical pressure/temperature spikes arise in the numerical results obtained with the conservative four-equation model. This error can infect the solution in the computational domain through the heat conduction.

We continue to show that non-TNO scheme leads to non-physical oscillations of the six-equation model. If we use the interface-sharpening scheme Overbee [12] for reconstructing the volume fraction, and MINMOD for the phase densities, we obtain the results shown in Fig. 5. One can see that the oscillations appear as a result of this non-TNO scheme.

#### Table 2

The performance of different model/scheme combinations for the pure translation pro-
--

Initial condition	Model	Scheme	Oscillation
Without temperature discontinuity	Four-equation [46]	TNO	NO
	Five-equation [3]	TNO	NO
	Six-equation without TR	TNO	NO
	Six-equation with TR	TNO	NO
With temperature discontinuity	Four-equation [46]	TNO	YES
	Five-equation [3]	TNO	NO
	Six-equation without TR	TNO	NO
	Six-equation with TR	TNO	YES
With/without temperature discontinuity	All models	Non-TNO	YES

TR = temperature relaxation.

For clarity, we summarize the performance of different model/scheme combinations in Table 2.

**Remark 8.** In the following tests the six-equation model is solved with Procedure (B) of Table 1 under instantaneous pressure relaxation and temperature relaxation. In this case, in fact, the solution to the conservative four-equation model [46] is obtained but with a different numerical scheme.

Both the six-equation model and the four-equation model are reduced systems of the BN model which is a relaxation system. Different reduced models have different wave structures and numerical performance for a finite computational time step. It is well known that the thermal equilibrium assumption results in non-physical oscillations at interface in the hydrodynamic step. Unlike the four-equation model, the six-equation model does not assume thermal equilibrium at the hydrodynamic stage. Moreover, the six-equation model retains more degrees of freedom for relaxation than the four-equation model, allowing to consider difference in relaxation time scales.

#### 4.2. Convergence test

We check the convergence performance of our algorithm with a manufactured exact solution as follows:

$$(\alpha_k \rho_k)(x,t) = 0.5 \text{ kg/m}^3, \ p(x,t) = 100 \text{ Pa}, \ \alpha_1(x,t) = 0.6,$$

and the velocity is the solution of the viscous Burgers equation (see [49])

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = v \frac{\partial^2 u}{\partial^2 x},$$
  

$$u(x,t) = \frac{1 + (2a - 1)\exp((1 - a)\xi/v)}{1 + \exp((1 - a)\xi/v)}, \quad \xi = x - at - x_0.$$
(98)

The constant are a = 0.5 m/s,  $x_0 = 0.1$  m,  $\nu = 0.01$  m<sup>2</sup>/s. The properties of two fluids are  $\gamma_1 = 4.4$ ,  $C_{\nu,1} = 40$  J/(kg·K) and  $\gamma_2 = 1.4$ ,  $C_{\nu,2} = 340$  J/(kg·K), which ensures initial temperature equilibrium. Inserting these manufactured solutions to the model equations, one can obtain additional r.h.s. source terms that make exact solution valid. We take the solutions at t = 0.1 s as the initial condition and numerically evolve solution of the model with additional source terms to t = 0.2 s. The dependence of numerical error with the spatial step  $\Delta x$  is demonstrated in Fig. 6. The orders of accuracy in  $L_1$ ,  $L_2$  and  $L_\infty$  space are 1.52, 1.70, and 1.90, respectively.

#### 4.3. Multicomponent heat conduction problem

We consider the multicomponent heat conduction problem from [61]. The material interface is located at the center of the computational domain [0 m, 1 m]. The fluid on the left is characterized by parameters

$$\gamma_1 = 3.42, \ P_{\infty,1} = 8.99 \times 10^8$$
 Pa,  $C_{\nu,1} = 1231$  J/(kg · K),  $\lambda_1 = 1 \times 10^6$  W/(m · K),  $T_1 = 360$  K

and that on the right

$$\gamma_2 = 1.40, P_{\infty,2} = 1.00 \times 10^8 \text{ Pa}, C_{v,2} = 1000.00 \text{ J}/(\text{kg} \cdot \text{K}), \lambda_2 = 1 \times 10^5 \text{ W}/(\text{m} \cdot \text{K}), T_2 = 300 \text{ K}.$$

The initial pressure is uniform  $p_1 = p_2 = 1 \times 10^5$  Pa. The insulated wall boundary conditions are imposed on both sides. As time evolves, the fluids reach a steady state where the interface location x = 0.48 m, the density on the left 872.24 kg/m<sup>3</sup> and on the right 802.06 kg/m<sup>3</sup>, and the equilibrium temperature 350.30 K [61]. The heat exchange between phases is realized through the nozzling term in [61]. In our approach this effect is considered through the temperature relaxation procedure. Our numerical results in Fig. 7 show the evolution of density, temperature, pressure and velocity towards the steady state. Good agreement with the analytical solutions is observed.



Fig. 6. The error dependence on the grid size.



Fig. 7. Evolution of the numerical solutions of the six-equation model toward the analytical steady solution.

# 4.4. Shock tube problem with heat conduction

In this section we consider a two-fluid shock tube problem with the purpose of evaluating different models. Two fluids are initially at rest and separated by the material interface located at x = 0.7 m separating them. The fluid on the left has the EOS parameters as  $\gamma = 4.40$ ,  $p_{\infty} = 6.00 \times 10^8$  Pa,  $C_{\nu} = 1606.00$  J/(kg·K), and that on the right  $\gamma = 1.40$ ,  $p_{\infty} = 0.00$  Pa,  $C_{\nu} = 714.00$  J/(kg·K). The initial pressure and temperature on both sides are given as follows:

0.00 < x < 0.70 m:  $p = 1.00 \times 10^9 \text{ Pa}$ , T = 293.02 K,



Fig. 8. Numerical results for the two-fluid shock tube problem without heat conduction.

0.70 < x < 1.00 m:  $p = 1.00 \times 10^5 \text{ Pa}$ , T = 7.02 K.

The initial densities are determined from the corresponding EOS.

*Test without heat conduction* Computations are performed on a 1000-cell uniform grid. The obtained numerical results obtained at the time moment  $t = 2.00 \times 10^{-4}$  s are compared to the exact Riemann solution in Fig. 8. The exact solution consists of a leftward rarefaction wave, a rightward contact wave (interface) and a rightward shock wave.

From the density profiles Fig. 8b and temperature profiles Fig. 8d, one can see that the shock wave velocity in the fiveequation model with one temperature appears to be overestimated. This stems from the different estimation of mixture acoustic velocity inside the diffused zone.

Note that as a solution to the Euler equations, the exact Riemann solution does not include any thermal relaxation. Therefore, the solution to the two-temperature six-equation model with no thermal relaxation is expected to better match the exact solution than that with thermal relaxation. In Fig. 8e we plot the two temperatures of fluids calculated in the temperature-disequilibrium six-equation model without temperature relaxation. As seen, the temperature of the first fluid quite well matches the exact solution on the left of the interface, while the temperature of the second fluid similarly does on the right. Thermal relaxation drives the two temperatures into an equilibrium temperature – the profile denoted as "6-eqn model 2T. relaxed" in Figs. 8c and 8d.

Test with equal phase thermal conductivity The above two-fluid shock tube problem is now considered with taking into account the phase heat conduction effect. The diffusion PDEs are solved with the explicit method of local iterations if not mentioned. The thermal conductivity is set to be a large number for comparison purpose. We first assign the same heat conduction coefficient for the two fluids  $\lambda_1 = \lambda_2 = 1.00 \times 10^6$  W/(m·K). The numerical results obtained with different models are compared in Fig. 9. The results marked as converged ("Conv") are computed on a fine grid consisting of 20000 computational cells. The difference between the converged solutions of different models is indiscernible and they are taken as the reference solution for comparison. To demonstrate the difference between the models, we show also the numerical solutions for a coarse grid of 200 cells. The results for the proposed model (6-eqn model 2T.R.) agree much better with the reference solution than the five-equation model (see Figs. 9c and 9d). The results of the four-equation model are also satisfactory since the heat conduction seems to be not strong enough to spread its erroneous temperature spikes.

We then compare the results of different relaxation procedures A, B, C and the fully conservative four-equation model in Fig. 10. The relaxation procedure (C) produces numerical results that are slightly different from others. The computation time consumed on a grid of 200 cells are 79.95 s, 69.04 s, 77.71 s, and 57.20 s, respectively. On a grid of 1000 cells they are 2757.78 s, 1570.20 s, 2733.53 s, and 1307.24 s, respectively.

As the thermal conductivity is increased to  $\lambda_1 = \lambda_2 = 1.00 \times 10^7 \text{ W/(m \cdot K)}$ , we find that these models do not converge to the same solution. This is demonstrated in Fig. 11, and is more clearly seen in the temperature profiles. The results of the four-equation model on a 20000-cell grid diverge from those of the five-equation and six-equation models to the right of the material interface. This can be explained by the numerical errors in the diffused zone, which then contaminate the results in the second fluid due to large thermal conductivity.

In Fig. 12 we verify the explicit method of local iterations that is used to solve efficiently the parabolic part of the model (heat conduction). Here we compare this method with the implicit scheme solved by conventional Newtonian iterations. In the implicit scheme, the preconditioned conjugate gradient method is used for solving the system of algebraic equations. We see that the results obtained with both schemes on a 100-cell grid agree very well with the reference solution.

Test with non-uniform thermal conductivity and viscosity This test considers the shock tube problem for two fluids which have different thermal conductivities and viscosities. For the left fluid, the thermal conductivity and dynamic viscosity are assumed to be  $\lambda_L = 1.00 \times 10^7 \text{ W/(m \cdot K)}$  and  $\mu_L = 5.00 \times 10^2 \text{ Pa} \cdot \text{s}$  and those for the right are  $\lambda_R = 1.00 \times 10^6 \text{ W/(m \cdot K)}$  and  $\mu_R = 1.00 \text{ Pa} \cdot \text{s}$ . The viscosity and thermal conductivity are averaged with volume fractions, i.e.  $\lambda = \sum_k \alpha_k \lambda_k$ ,  $\mu = \sum_k \alpha_k \mu_k$ . Here, we compare the performance of the five-equation model and the six-equation model. From Fig. 13 one can see that the convergence performance of the proposed six-equation model is still superior to that of the five-equation model.

#### 4.5. Two-phase problem

In this section, numerical experiments are performed for two-phase flows where the phases are mixed and may occupy the same location in space.

*Shock propagation in a water-gas mixture* The material properties of the phases are the same as in the previous test. The volume fraction of each component is initially 0.50 in the whole computational domain. Other initial data is given as follows:

$$x < 0.5 \text{ m}$$
:  $P = 1.00 \times 10^9 \text{ Pa}$ ,  $T = 1000.00 \text{ K}$ ;  
 $x > 0.5 \text{ m}$ :  $P = 1.00 \times 10^5 \text{ Pa}$ ,  $T = 300.00 \text{ K}$ .

Here, the heat capacities of the fluids described by the SG EOS and IG EOS are 588.33 J/(kg·K) and 833.33 J/(kg·K), respectively. Initial densities are determined by the corresponding EOS of each phase. For comparison purpose, the conductivities of gas and water are set by effective values of  $1.00 \times 10^7$  W/m/K and  $1.00 \times 10^5$  W/m/K, respectively. Computations are performed to the moment  $t = 2.00 \times 10^{-4}$  s on a 1000-cell uniform grid. The numerical results are shown in Fig. 14. One



**Fig. 9.** Numerical results for the two-fluid shock tube problem with equal phase heat conductivity  $\lambda = 1.00 \times 10^6$ .

can see that including temperature relaxation changes considerably the solution. The heat conduction process smears the temperature profile near the contact discontinuity, also resulting in corresponding changes in other variables.

Comparison between different relaxation procedures We compare the numerical results when  $\lambda_1 = \lambda_2 = 10^7 \text{ W/m/K}$  obtained with different relaxation procedures on a grid of 200 cells in Fig. 15. Again, it can be seen that the results of the procedure (C) deviate from the others. The relaxation procedure (B) accomplishes the computation within 40.69 s with the explicit scheme, while the others take more than 3000 s. This is because in procedures (A)(C) we have to solve the heat equation for each phase whose stable time step is much smaller than the mixture heat equation.



Fig. 10. Numerical results with different relaxation procedures. All the relaxations are achieved within each computational time step.

Shock wave in solid alloys We further consider an alloy impact problem from [56]. The alloy is composed of two components epoxy and spinel. The volume fractions of these two components are 0.595 and 0.415, respectively. We solve this problem as a two-phase one with the six-equation model. The materials are characterized by the following EOS parameters:

- Epoxy  $\gamma = 2.94$ ,  $P_{\infty,1} = 3.20 \times 10^9$  Pa,  $\rho = 1185.00$  kg/m<sup>3</sup>, Spinel  $\gamma = 1.62$ ,  $P_{\infty,2} = 1.41 \times 10^{11}$  Pa,  $\rho = 3622.00$  kg/m<sup>3</sup>.

The schematic of this problem is displayed in Fig. 16. Calculations are carried out in the model without thermal relaxation, as the time scale of this problem is much smaller than the characteristic relaxation time. However, the mechanical relaxation is implemented.

For many metals, the shock velocity S linearly depends on the impact velocity  $u_L$ . Calculations of the shock wave propagation are done for different velocities  $u_I$ . The results obtained are plotted in Fig. 17 and compared with the experimental data that is available from [56]. As can be seen, a linear profile of S well agrees with the experimental data.

#### 4.6. Laser ablation problem

This section addresses an application problem related to the field of inertial confinement fusion (ICF) - the laser ablation problem. In the direct-drive ICF capsule, the laser is used as an energy source to accelerate the plastic (CH, i.e., phenylethylene  $C_8H_8$ ) target creating high temperature and high pressure environment for inward implosion.

One-dimensional planar target First, the laser ablation problem is considered in the 1D approximation. It is assumed that the target is plane, and the laser emission is uniform and normal to the target surface. The target is placed in vacuum that is approximated as a fluid with extremely low density. As shown in Fig. 18, the laser radiation comes from the right and its energy is absorbed by the CH material that then turns to high temperature ablated plasma. The energy absorption occurs up to the critical density point (where the incident power energy equals the reflected one) and over a distance  $d_S$  (absorption area) to the right of the critical density point. We consider the following composite target consisting of two different CH materials separated by the material interface at a distance  $x_I$ 

- $\rho = 1.00, \ \gamma = 1.666, \ C_{\nu} = 86.27,$ • CH #1
- $\rho = 0.80, \gamma = 1.220, C_v = 76.27,$ • CH #2

hereinafter dimensions used are centimeter, gram and microsecond.

The vacuum is approximated as the material CH #2 with a density of  $8.00 \times 10^{-6}$ . The critical density is  $\rho_{crt} = 0.39$  that can be calculated according to the inverse bremsstrahlung absorption theory.

The electron, ion and photon in the plasma are assumed to be in thermal equilibrium. The thermal conductivity of the plasma is approximated with the one-temperature Spitzer-Harm model [87,47] and is a nonlinear function of density and temperature:

$$\lambda_{SH} = 9.44 \left(\frac{2}{\pi}\right)^{3/2} \frac{(k_B T_e)^{5/2} k_B N_e}{\sqrt{m_e} e^4} \frac{1}{N_i Z_e \left(Z_e + 4\right) \ln \Lambda_{ei}},\tag{99}$$



**Fig. 11.** Numerical results for the two-fluid shock tube problem with equal phase heat conductivity  $\lambda = 1.00 \times 10^7$ .

where  $k_B$  is the Boltzmann constant,  $T_e$  is the electronic temperature,  $N_e$  is the electron density, e is the electronic charge,  $m_e$  is the electronic mass,  $N_i$  is the ion density,  $Z_e$  is the degree of ionization. For a certain plasma,

$$N_i = \frac{N_0}{A_c}\rho, \quad N_e = Z_e N_i, \tag{100}$$

where  $A_c$  is the average atomic number,  $N_0$  is the Avogadro's number.



Fig. 12. Numerical results for the two-fluid shock tube problem obtained with the explicit and implicit scheme on a 100-cell grid.



Fig. 13. Numerical results for the two-fluid shock tube problem with for the case of different phase coefficients of viscosity and heat conductivity.

 $\ln \Lambda_{ei}$  is the Coulomb logarithm of laser absorption and determined with

$$\ln \Lambda_{ei} = \begin{cases} \max\left(1, \ln \frac{l_D}{l_{LD}}\right), & \frac{Z_e^2}{3k_B T_e} \ge l_{dB}, \\ \max\left(1, \ln \frac{l_D}{l_{dB}}\right), & \frac{Z_e^2}{3k_B T_e} < l_{dB}, \end{cases}$$
(101)

where  $l_D$  is Debye length,  $l_{LD}$  is Landau length,  $l_{dB}$  is De Broglie wavelength.

Here, for simplicity, we assume equal phase conductivity defined with the same Spitzer-Harm relation.

Within the absorption distance  $d_S = 2.00 \times 10^{-3}$ , the deposited laser power intensity is assumed to be constant,  $I = 1.00 \times 10^3$ . In the vicinity of the right interface, the density is smoothed in the region from  $x_R$  to  $x_{RR}$  by an exponential function of the spatial coordinate. The geometry of the computational domain is specified as  $L = 1.00 \times 10^{-1}$  and  $x_L = 0.45L$ ,  $x_R = 0.50L$ ,  $x_{RR} = 0.51L$ . The initial temperature  $T = 3.00 \times 10^{-4}$  in the whole computational domain. Pressure is calculated with the EOS of each material.

Calculations are performed with three models (the four-equation model, the one-temperature five-equation model and the proposed six-equation model) and two grids consisting of 1200 and 9600 equally distributed cells. To improve the material interface resolution, we implement the MUSCL scheme with the Overbee limiter [13]. This scheme is applied to phase masses  $\alpha_k \rho_k$  and the volume fraction  $\alpha_1$  for the five- and six-equation model, and to mixture density  $\rho$  and mass fraction  $Y_1$  for the four-equation model.

The numerical results of these three models at  $t = 6.00 \times 10^{-3}$  are compared in Fig. 19. All three models tend to converge to the same solution. The results show only minor differences. For example, convergence in density for the four-equation model and convergence in temperature for the six-equation model are found to be worse in comparison with the other two (Figs. 19a, 19b, 19e, and 19f). There is also small difference in the interface velocity, as seen in Figs. 19c and 19d.



Fig. 14. The numerical results for the water-gas multiphase shock tube problem. The lines 'no T.R.', 'with T.R.', 'with T.R.', represent the numerical results without temperature relaxation, with temperature relaxation, with temperature relaxation and heat conduction, respectively.



**Fig. 15.** The numerical results with different relaxation procedures for the water-gas multiphase problem. The time consumption of procedures (A), (B), and (C) are 3399.52 s, 40.69 s, and 3577.38 s, respectively.

To demonstrate the interface-sharpening effect, we compare the results obtained with the MINMOD limiter to those obtained with the Overbee scheme in Fig. 20. One can see that with the Overbee limiter, the diffused interface is within 2-3 computational cells, which is much less in comparison to the MINMOD scheme.

For the present problem, all materials are described with the ideal gas EOS. In this case, the effective temperature averaging procedure (eq. (76)) of the one-temperature five-equation model and the temperature relaxation procedure (eq.



Fig. 16. Schematic of the alloy impact problem.



Fig. 17. Shock velocity diagram for the epoxy/spinel alloy impact problem. The experimental data is from [56].



(b) Critical density  $\rho_{crt}$  and absorption distance  $d_S$ 

Fig. 18. The laser ablation of a multicomponent planar target.

(73b)) of the six-equation model yield the same result for temperature. The former neglects the effect of temperature relaxation on volume fraction within the diffused interface. This diffused interface is narrowed into 2-3 computational cells thanks to the interface-sharpening technique. Therefore, the advantage of the proposed model for this problem is not so evident as that for the water-air shock tube problem in section 4.4.

*Laser ablative Rayleigh–Taylor instability in a 2D thin target* Next we consider the laser ablation problem in the 2D formulation. The interface is initially perturbed and has the following form:

$$x_{interface} = x_R - A_m \cos(2\pi y/L_y)$$
,

where  $A_m$  is the perturbation amplitude taken as  $A_m = 0.02L_y$ .



Fig. 19. Numerical results for the laser ablation of a multicomponent planar target.

The laser ablation of a thin target is considered, which is accompanied with the development of Rayleigh–Taylor instability. The problem is a two-phase version of that in [47]. The problem set-up is displayed in Fig. 21. The left and right ends of the target are located at  $x_{LL} = 0.50L$  and  $x_R = 0.70L$ , respectively. The two CH materials are separated by a planar interface at  $x_L = 0.65L$ . The evolution of the ablated target modeled with the proposed six-equation model is demonstrated in Fig. 22. Here, the numerical Schlieren is qualitatively compared with the experimental results for single material from GEKKO XII [5].

The numerical results obtained with different models are compared in Fig. 23. We can see that although the density distributions obtained with the three models are similar in appearance, the shapes of the material interfaces are different



Fig. 20. Comparison of the numerical results obtained the Overbee and MINMOD limiter schemes.



Fig. 21. Schematic of the laser ablation of a thin two-phase target.



Fig. 22. Evolution of the numerical Schlieren obtained with the proposed six-equation model. The figures on the right are experimental images from [5].

from each other. The material interface obtained with the five-equation model is more diffusive and quite different from the others. The difference in critical density distribution can be seen from the laser absorption area. Again the one-temperature five-equation model result is found to be much different from the other two, mostly due to the exceeded numerical diffusion of the material interface and violation of the second law of thermodynamics in the diffused zone.

As demonstrated in Fig. 24, with physical diffusions being included, the numerical results tend to converge with the grid refinement and approach the fully resolved DNS (direct numerical simulation).



Fig. 23. Comparison of the numerical results obtained with the four- (the first row), five- (the second row) and the six-equation model (the third row). Displayed results from left to right: density, volume fraction, temperature, laser absorption area, numerical Schlieren.



**Fig. 24.** Numerical results on grids with different resolution (from top to bottom  $720 \times 120$ ,  $960 \times 160$ ,  $1440 \times 240$ ,  $1920 \times 320$  cells). The columns from left to right display the results for density, pressure and temperature, respectively.

# Conclusion

In this paper we have established a temperature disequilibrium model for modeling compressible two-phase flows with taking into account the dissipative thermal conduction and viscosity. We have proposed numerical methods based on the fractional step approach for solving the proposed model. In this approach, the hyperbolic part of the governing equations is solved with the Godunov-HLLC scheme, and the parabolic part with the method of local iterations based on Chebyshev parameters.

The proposed model has demonstrated the following advantages.

- It is thermodynamically consistent.
- It ensures temperature equilibrium during the heat conduction process by implementing a special phase thermal relaxation.
- It includes the effect of mechanical relaxation, thermal relaxation and heat conduction on the volume fraction.
- Numerically, it maintains the pressure, velocity and temperature equilibrium, thus avoids spurious oscillations in the vicinity of material interfaces.
- It shows superior convergence performance when compared to other models with non-physical diffused mixture.
- Tanks to its special relaxation procedure, it has better computational efficiency in solving the heat conduction equation, especially non-linear ones.
- Thanks to its physical consistency with the most complete Baer-Nunziato model, our model can be used for simulating two-phase flows with both resolved and non-resolved interfaces.

We have compared the proposed six-equation model with the one temperature, one pressure five-equation model both analytically and numerically. Our analysis shows that this five-equation model is not consistent with the second law of thermodynamics. Numerical experiments on the laser ablation of a CH target demonstrate that the temperature-equilibrium five-equation model yields numerical results much different from those of the four-equation and six-equation models. In our future work we plan to include mass diffusion into our model.

# **CRediT authorship contribution statement**

**Chao Zhang:** Conceptualization, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft. **Igor Menshov:** Methodology, Writing – original draft, Writing – review & editing. **Lifeng Wang:** Formal analysis, Funding acquisition, Validation, Writing – review & editing. **Zhijun Shen:** Formal analysis, Writing – review & editing.

# **Declaration of competing interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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# Appendix A. Derivation of the five-equation model (21) with asymptotic analysis

By performing manipulations of the conservative form (21) with the method similar to [56,93], one can obtain the equations for the primitive variables  $z = [s_k, u_k, p_k, \alpha_k]$  as follows:

$$\alpha_k \rho_k T_k \frac{D_k s_k}{Dt} = (\boldsymbol{u}_I - \boldsymbol{u}_k) \cdot \mathcal{M}_k + (p_k - p_l) \mathcal{F}_k + (p_l - p_k) (\boldsymbol{u}_I - \boldsymbol{u}_k) \cdot \nabla \alpha_k + (\boldsymbol{u}_k - \boldsymbol{u}_I) \cdot \left(\overline{\overline{\tau}}_I \cdot \nabla \alpha_k\right) + \mathcal{G}_k$$
(102a)

$$\alpha_k \rho_k \frac{\mathsf{D}_k \boldsymbol{u}_k}{\mathsf{D}t} = \nabla \cdot \left( \alpha_k \overline{\overline{\tau}}_k - \alpha_k p_k \overline{\overline{t}} \right) - \left( \overline{\overline{\tau}}_I - p_I \overline{\overline{t}} \right) \cdot \nabla \alpha_k + \mathcal{M}_k \tag{102b}$$

$$\frac{\mathsf{D}_{k}p_{k}}{\mathsf{D}t} = -\frac{\rho_{k}a_{lk}^{2}}{\alpha_{k}}\mathcal{F}_{k} + \Gamma_{k}\frac{\mathbf{u}_{k} - \mathbf{u}_{l}}{\alpha_{k}}\left[\left(\overline{\overline{\tau}}_{l} - \frac{\rho_{k}a_{lk}^{2}}{\Gamma_{k}}\overline{\overline{l}}\right) \cdot \nabla\alpha_{k} - \mathcal{M}_{k}\right] + \frac{\Gamma_{k}\mathcal{G}_{k}}{\alpha_{k}} - \rho_{k}a_{k}^{2}\nabla \cdot \mathbf{u}_{k}$$
(102c)

$$\frac{\mathsf{D}_{I}\alpha_{k}}{\mathsf{D}t} = \mathcal{F}_{k} \tag{102d}$$

where

$$\frac{\rho_k a_{lk}^2}{\alpha_k} = \frac{\rho_k a_k^2}{\alpha_k} + \Gamma_k \frac{p_l - p_k}{\alpha_k}, \quad \mathcal{G}_k = \mathcal{S}_k + Q_k + q_k + \mathcal{I}_k,$$

the material derivative of a variable  $\Phi$  related to the velocity  $\mathbf{u}_m$  (m = k, I) is

C. Zhang, I. Menshov, L. Wang et al.

$$\frac{\mathsf{D}_m\Phi}{\mathsf{D}t}=\frac{\partial\Phi}{\partial t}+\boldsymbol{u}_m\cdot\nabla\Phi.$$

We aim to reduce eq. (102) in the limit of zero mechanical relaxation time, i.e.,

$$\epsilon \sim \frac{1}{\vartheta} \sim \frac{1}{\eta} \to 0.$$

We assume an asymptotic solution in the following form

$$\boldsymbol{z} = \boldsymbol{z}^{(0)} + \boldsymbol{\epsilon} \boldsymbol{z}^{(1)} + \boldsymbol{O}(\boldsymbol{\epsilon}^2)$$

In the order  $O(1/\epsilon)$ , only terms involving relaxations  $\mathcal{M}_k$  and  $\mathcal{F}_k$  of eq. (102) retain, which yields

$$\begin{aligned} \mathbf{u}_{1}^{(0)} &= \mathbf{u}_{1}^{(0)} = \mathbf{u}_{2}^{(0)} = \mathbf{u}^{(0)}, \\ p_{1}^{(0)} &= p_{1}^{(0)} = p_{2}^{(0)} = p^{(0)}. \end{aligned}$$
(103a)  
(103b)

In the order O(1), with eqs. (103a) and (103b), eq. (102) becomes

$$\alpha_k \rho_k T_k \frac{\mathrm{D}s_k}{\mathrm{D}t} = \mathcal{G}_k,\tag{104a}$$

$$\alpha_k \rho_k \frac{\mathsf{D}\boldsymbol{u}}{\mathsf{D}\boldsymbol{t}} = \nabla \cdot \left( \alpha_k \overline{\overline{\tau}}_k - \alpha_k p \overline{\overline{I}} \right) - \left( \overline{\overline{\tau}}_I - p \overline{\overline{I}} \right) \cdot \nabla \alpha_k + \mathcal{M}_k^{(0)}, \tag{104b}$$

$$\frac{\mathrm{D}p}{\mathrm{D}t} = -\frac{\rho_k a_{Ik}^2}{\alpha_k} \mathcal{F}_k^{(0)} + \frac{\Gamma_k \mathcal{G}_k}{\alpha_k} - \rho_k a_k^2 \nabla \cdot \boldsymbol{u}, \qquad (104c)$$

$$\frac{\mathrm{D}\alpha_k}{\mathrm{D}t} = \mathcal{F}_k^{(0)},\tag{104d}$$

where the superscripts "(0)" over the primitive variables are omitted for simplicity.

With eq. (104c) and the relation  $\sum \mathcal{F}_k^{(0)} = 0$ , one can solve

$$\mathcal{F}_{2}^{(0)} = \alpha_{2} \frac{A - A_{2}}{A_{2}} \nabla \cdot \boldsymbol{u} + A \frac{\Gamma_{2} \mathcal{G}_{2} \alpha_{1} - \Gamma_{1} \mathcal{G}_{1} \alpha_{2}}{A_{1} A_{2}}, \quad \mathcal{F}_{1}^{(0)} = -\mathcal{F}_{2}^{(0)}.$$
(105)

Eliminating  $\mathcal{M}_{k}^{(0)}$  and  $\mathcal{F}_{k}^{(0)}$ , eqs. (104b) and (104c) become

$$\frac{\mathbf{D}\boldsymbol{u}}{\mathbf{D}\boldsymbol{t}} = \frac{1}{\rho} \nabla \cdot \left(\overline{\overline{\tau}} - p\overline{\overline{l}}\right),\tag{106a}$$

$$\frac{\mathsf{D}p}{\mathsf{D}t} + A\nabla \cdot \boldsymbol{u} = A \sum \frac{\Gamma_k \mathcal{G}_k}{A_k}.$$
(106b)

Reformulations of eqs. (104a), (104d), (106a), and (106b) give the conservative form of the reduced five-equation model eq. (21).

# Appendix B. Supplementary material

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.jcp.2022.111356.

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