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MECHANICS

Model of a Multicomponent Medium

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The available models of multicomponent media (MCM) were described in the most general form in [1, 2]. The following statements made in those works had a large effect on the development of MCM models: first, balance conservation equations in their general form are of little interest for the mechanics of mixtures, and, second, the main problem in the mathematical simulation of multiphase mixtures is to derive a closed system of equations both for given physical and chemical properties of each individual phase and for a given structure for the mixture as a whole. In the 20–25 years that have elapsed since the appearance of the aforementioned publications, many works have been devoted to the development of particular models based on certain specifications. So far, the problem of deriving the conservation laws for a mixture from those for individual components, as well as the problem of the closure of the system of equations for the *i*th component, remains unsolved in the general case.

CONSTRAINTS

Each component i of a mixture of N components conserves the chemical attributes of the substance irrespective of its mass and is characterized by the following physical parameters: the pressure P_i, the density ρ_i, the specific internal energy E_i, the velocity $\mathbf{U}_i$, the temperature T_i, etc. The thermodynamic parameters obey the equation of state for the ith component. After the physical parameters have been changed to the partial quantities $\alpha_i P_i$, $\alpha_i \rho_i$, $\alpha_i \rho_i \mathbf{U}_i$, $\alpha_i \rho_i E_i$, etc., which are continuous in the (t, x_k) space ($k = 1, 2, 3$), each component turns out to be a continuous medium in the entire space occupied by the mixture, so that mass, momentum, and energy conservation laws can be written for it in the form of differential equations. Thus, all components of the mixture are simultaneously present at each point of the (t, x_k) space.

To clarify the essence of the MCM model proposed, we consider ideal compressible media that are free of heat conduction, chemical reactions, and field effects and have zero deviator of the stress tensor. This consideration does not lead to any loss of generality of the model, because all the above physical processes can be incorporated into the conservation laws for the components if necessary.

INTERACTION OF COMPONENTS

Type 1. Pairwise interaction. Let the ith and jth components interact with each other independently of other components. Then the momentum (R_{ij}) and energy (Φ_{ij}) flux densities satisfy the equation

$$\mathbf{R}_{ij} = -\mathbf{R}_{ji}, \quad \Phi_{ij} = -\Phi_{ji}. \tag{1}$$

The order of the subscripts indicates the interaction direction. We will multiply Eq. (1) by α_j and sum over j under the condition that $\mathbf{R}_{ii} = 0$ and $\Phi_{ii} = 0$. The result is marked by the subscript 0:

$$\sum_{j=1}^{N} \alpha_j \mathbf{R}_{ij} = \mathbf{R}_{i0} = -\mathbf{R}_{0i}, \quad \sum_{j=1}^{N} \alpha_j \Phi_{ij} = \Phi_{i0} = -\Phi_{0i}. \tag{2}$$

Multiplying Eq. (2) by α_i, summing over i, and taking Eq. (1) into account, we obtain

$$\begin{aligned} \sum_{i=1}^{N} \alpha_i \mathbf{R}_{i0} &= \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j \mathbf{R}_{ij} = 0, \\ \sum_{i=1}^{N} \alpha_i \Phi_{i0} &= \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j \Phi_{ij} = 0. \end{aligned} \tag{3}$$

The quantities $\mathbf{R}_{i0}$ and Φ_{i0} are the sums of the independent intensities of the momentum and energy fluxes from the ith component to all N components. The pairwise interaction is taken into account in the conservation laws for the ith component in almost all MCM models (see, e.g., [1–4]).

Type 2. Cluster interaction. In terms of the partial parameters $\alpha_i P_i$, $\alpha_i \rho_i$, $\alpha_i \rho_i \mathbf{U}_i$, $\alpha_i \rho_i E_i$, etc., a virtual con-

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tinuum (VC) can be introduced with the parameters

$$P = \sum_{i=1}^{N} \alpha_i P_i, \quad \rho = \sum_{i=1}^{N} \alpha_i \rho_i, \quad \rho \mathbf{U} = \sum_{i=1}^{N} \alpha_i \rho_i \mathbf{U}_i, \quad \rho E = \sum_{i=1}^{N} \alpha_i \rho_i E_i, \tag{4}$$

which are continuous in the space occupied by the mixture. The forces and fluxes associated with the VC will be marked by the subscript *s*. The mixture and VC are nonequilibrium if one of the following conditions is not fulfilled:

$$P_i = P_p, \quad \mathbf{U}_i = \mathbf{U}_p, \quad T_i = T_p, \quad P = P_p, \quad T = T_p,$$

where P_p, $\mathbf{U}_p$, and T_p are the equilibrium state parameters. In the process of relaxation, the parameters of the components and VC change, because $\mathbf{U}$, P, ρ, and E are determined by Eq. (4). The interaction between the *i*th component and the VC will be called the cluster interaction. By analogy with Eq. (2), the forces and energy fluxes associated with the cluster interaction are related by the equations

$$\mathbf{F}_{ksi} = -\mathbf{F}_{kis}, \quad \mathbf{Q}_{si} = -\mathbf{Q}_{is}, \quad \mathbf{F}_{k0s} = \sum_{i=1}^{N} \alpha_i \mathbf{F}_{kis}, \quad \mathbf{Q}_{0s} = \sum_{i=1}^{N} \alpha_i \mathbf{Q}_{is}. \tag{5}$$

CONSERVATION LAWS

We write the conservation laws for the *i*th component:

$$\frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla(\alpha_i \rho_i \mathbf{U}_i) = 0, \tag{6}$$

$$\frac{\partial}{\partial t}(\alpha_i \rho_i \mathbf{U}_i) + \frac{\partial}{\partial x_k}(\alpha_i \rho_i U_{ki} \mathbf{U}_i) + \nabla \alpha_i P_i + \frac{\partial}{\partial x_k}(\alpha_i \mathbf{F}_{ksi}) - \alpha_i \mathbf{R}_{0i} = 0, \tag{7}$$

$$\frac{\partial}{\partial t}(\alpha_i \rho_i \varepsilon_i) + \nabla(\alpha_i \mathbf{U}_i (P_i + \rho_i \varepsilon_i)) + \frac{\partial}{\partial x_k}(\alpha_i \mathbf{F}_{ksi} \mathbf{U}_i) + \nabla \alpha_i \mathbf{Q}_{si} - \alpha_i \Phi_{0i} = 0. \tag{8}$$

In view of Eqs. (2), (3), and (5), the conservation laws for the VC are written in the form

$$\frac{\partial \rho}{\partial t} + \nabla \rho \mathbf{U} = 0, \tag{9}$$

$$\frac{\partial}{\partial t}(\rho \mathbf{U}) + \frac{\partial}{\partial x_k}(\rho U_k \mathbf{U}) + \nabla P + \frac{\partial}{\partial x_k}(\mathbf{F}_{k0s}) = 0, \tag{10}$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla(\mathbf{U}(P + \rho \varepsilon)) + \frac{\partial}{\partial x_k}(\mathbf{U} \mathbf{F}_{k0s}) + \nabla Q_{0s} = 0. \tag{11}$$

FORCE

We consider the following equation obtained by substituting Eq. (4) into Eq. (9):

$$\sum_{i=1}^{N} \left(\frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla(\alpha_i \rho_i \mathbf{U}_i) \right) = 0.$$

Each term in this sum is equal to zero, because it coincides with the left-hand side of Eq. (6). Thus, the summation of Eq. (6) yields Eq. (9).

Substituting Eqs. (2)–(5) into Eq. (10), we obtain

$$\sum_{i=1}^{N} \left(\frac{\partial}{\partial t}(\alpha_i \rho_i \mathbf{U}_i) + \frac{\partial}{\partial x_k}(\alpha_i \rho_i U_{ki} \mathbf{U}_i) + \nabla \alpha_i P_i + \frac{\partial}{\partial x_k}(\alpha_i \mathbf{F}_{kis}) - \alpha_i \mathbf{R}_{0i} \right) = 0. \tag{12}$$

We choose $\mathbf{F}_{ksi}$ so that each term in Eq. (12) coincides with Eq. (7). After simple transformations, we obtain the following expression for the force $\mathbf{F}_{ksi}$:

$$\mathbf{F}_{ksi} = 0.5 \rho_i (U_{ki} - U_k)(\mathbf{U} - \mathbf{U}_i). \tag{13}$$

NONEQUILIBRIUM KINETIC ENERGY

We consider the specific total energies of the VC and the *i*th component:

$$\varepsilon = E + 0.5 \mathbf{U}\mathbf{U} + H, \quad \varepsilon_i = E_i + 0.5 \mathbf{U}_i \mathbf{U}_i. \tag{14}$$

Expressing E and E_i from Eq. (14) and substituting the result into the fourth of Eqs. (4), we obtain

$$\rho H = \sum_{i=1}^{N} \alpha_i \rho_i H_i, \tag{15}$$

where H_i is determined by the equation

$$H_i = 0.5(\mathbf{U} - \mathbf{U}_i)^2. \tag{16}$$

We will call this quantity the nonequilibrium kinetic energy of the *i*th component.

ENERGY FLUX

The substitution of Eqs. (2)–(5), (13), and (15) into Eq. (11) yields

$$\sum_{i=1}^{N}\left(\frac{\partial}{\partial t}(\alpha_i\rho_i\varepsilon_i) + \nabla(\alpha_i(\mathbf{U}(P_i + \rho_i\varepsilon_i) - \mathbf{Q}_{si})) - \frac{\partial}{\partial x_k}(\alpha_i\mathbf{F}_{ksi}\mathbf{U}) - \alpha_i\Phi_{0i}\right) = 0. \quad (17)$$

The condition that the ith term in Eq. (17) coincides with Eq. (8) is as follows:

$$\mathbf{Q}_{si} = 0.5(P_i + \rho_i H_i)(\mathbf{U} - \mathbf{U}_i). \quad (18)$$

Requiring that the increment of the entropy of the mixture is equal to the sum of the increments of the entropies of the components, we arrive at the equation for volume concentration:

$$P_i\frac{d_i\ln\alpha_i}{dt} + \alpha_i\Phi_{si} - (\mathbf{U} - \mathbf{U}_i)\rho_i E_i\nabla\alpha_i - \alpha_i\left(E_i + \frac{P_i}{\rho_i}\right)\nabla\rho_i(\mathbf{U} - \mathbf{U}_i) = 0. \quad (19)$$

Equation (19) closes the system of equations for the ith component.

New forces $\mathbf{F}_{ksi}$ (13) and energy fluxes $\mathbf{Q}_{si}$ (18) include the parameters of the structural MCM level (mesolevel) with the subscript i and the barycentric velocity $\mathbf{U}$, which is a macrolevel parameter. This structure is typical of mesomechanical equations. These forces and fluxes vanish at velocity equilibrium.

The technique for obtaining $\mathbf{F}_{ksi}$ and $\mathbf{Q}_{si}$ is such that the conservation laws for the VC are derived by summing the conservation laws for the components.

COMPLETE EQUATIONS OF THE MODEL

The system of equations governing the behavior of the ith component includes the conservation laws given by Eqs. (6)–(8); the second of Eqs. (14); Eq. (19) for the function α_i given by Eq. (19); the equations of state $P_i = P_i(\rho_i, E_i)$ and $T_i = T_i(\rho_i, E_i)$; Eqs. (13) and (18) for the force $\mathbf{F}_{ksi}$ and energy flux $\mathbf{Q}_{si}$, respectively; the expression for the intensities of the exchange by the momentum $\mathbf{R}_{0i}$ and the energy Φ_{0i}; and Eqs. (4) for P, ρ, and $\mathbf{U}$. Thus, the complete system of equations for the mixture contains the same number of equations and functions and is closed without any additional hypotheses specifying the mixture.

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