

NEW MODELS OF CONTINUUM MECHANICS

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Possible ways of transition from traditional models of continuum mechanics to new-generation models, using a model of a multicomponent model as an example, are considered.

Keywords: *conservation laws, continuous medium, differential equations, mixture, component, concentration, interaction of components, particles.*

Introduction. The models of continuum mechanics widely used for solving various problems of physics, chemistry, and technology usually rely on simplifying hypothesis and empirical parameters. This made it possible to subdivide the science — continuum mechanics (CM) — into the following parts: gas dynamics, hydrodynamics, elasticity theory, plasticity theory, plasma theory, in each of which additional simplifying hypotheses are formulated and original methods are used to find solutions. Even though such an approach has turned out to be very effective for constructing analytical solutions, the use of CM models based on simplifying hypotheses for mathematical simulation of complex dynamic processes does not allow one to employ in full measure the potentialities provided by the computation engineering of the 21st century. The accuracy of CM models has approached its limit. This has led to the necessity of creating a new generation of CM models. All of the CM models are based on three laws of mass, momentum, and energy conservation. They are written in the form of partial differential equations for a continuous medium which in the course of several centuries was considered as a material substance continuously filling the considered volume of space. The laws of conservation of continuous media were formulated in the period from 1640 to 1900. We will recall briefly the basic dates at which they were invented. In 1660 R. Hooke formulated an empirical law of elastic deformations — a linear dependence of stresses on strains. In 1748 M. V. Lomonosov found the law of mass conservation. In 1755 L. Euler gave a differential formulation of the momentum conservation law of an ideal continuous medium. Within the years 1822–1847 L. Navier and D. Stokes created a model of an incompressible viscous fluid, that is, the law of mass and momentum conservation. For the period of 1842–1847 J. Mayer, J. Joule, and G. Helmholtz formulated the energy conservation law. In 1870 B. Saint-Venant published equations for the plastic flow of a body. The governing equations that describe dependences between a stress tensor and strain tensor were derived in the same years as the conservation laws. In the region of low pressures the results satisfying the industry were provided by the model of an incompressible fluid and the elastic-plastic model of a solid body; in the region of gas states the simplest equation of the ideal gas state was used.

Up to the mid-1950's, the development of CM tended toward construction of analytical solutions, usually for simplified statements of problems and simplified properties of substances. The value of analytical solutions is indisputable. However, at the beginning of the 21st century their role underwent a change. Since, by the year 2010, computer speed has attained 10^{15} operations per second and the theory of the numerical methods of the CM has been well developed, analytical solutions came to be widely used as standard solutions to control the accuracy of the methods of mathematical simulation. Despite the fact that the physical experiment was increasingly frequently replaced by the mathematical one, any progress along this line is impossible unless new generation models accounting for the inhomogeneity and real properties of substances are devised.

The atomic-molecular theories of the structure of material were developed notably later than the basic equations of mechanics, although assumptions on the existence of microparticles were already made by philosophers before the Common Era. However, a concrete step was made in 1803, when J. Dalton introduced the notion of atomic weight

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and compiled a table of atomic weights of the elements. The next important discovery was made in 1869 by D. Mendeleev who compiled a periodic table of the elements. Finally, in 1903 G. Thomson devised an electronic model of the atom. Thus, the substance came to be considered at two levels: at the macrolevel — this is a continuous medium, and at the microlevel — this is an aggregate of microparticles. However, over many years no combined use of the models of macro- and microlevels has been made. Throughout the entire 20th century micromodels were mainly employed for constructing and improving the accuracy of the equations of state of a substance that close the system of conservation equations of a continuous medium.

According to current concepts, the notion of a continuous medium is nothing more than mathematical abstraction. Any body — a liquid, gas, solid, or a plasma — consists of microparticles (molecules, atoms, electrons, ions, etc.), each of which has its own mass, velocity, and internal energy. If this is a multiatomic molecule, then its internal energy is composed of the energy of its formation, the energy of each of the atoms it comprises, the proportional energy of binding an electron with the "atom's" nucleus, and the energy of the nucleus determined by the binding energy of nucleons that form the atomic nucleus. It goes without saying that a set of microparticles is a discrete medium. Simulation of a discrete medium at the microlevel is beyond the powers even of contemporary computers because of the enormous density of microparticles (about $3 \cdot 10^{19}$ molecules in 1 cm^3 of air) and because it is impossible, by virtue of the uncertainty principle, to provide accurate initial data for each particle at a certain fixed instant of time. It is precisely for the above-indicated reasons that in the second half of the 20th century attempts were made to create models that combine continuous medium elements with the elements of micromodels.

Coupling between Microparticles and a Continuous Medium. A continuous medium is characterized by mass M , momentum \mathbf{K} , and energy Q_0 . These quantities are continuous in a four-dimensional space x, y, z, t . The partial derivatives of the parameters M , \mathbf{K} , and Q_0 with respect to volume at a constant time t determine the density ρ , velocity \mathbf{U} , and the specific energy ε of the medium:

$$\rho = \left(\frac{\partial M}{\partial \theta} \right)_t, \quad \rho \mathbf{U} = \left(\frac{\partial \mathbf{K}}{\partial \theta} \right)_t, \quad \rho \varepsilon = \left(\frac{\partial Q_0}{\partial \theta} \right)_t.$$

The continuity of these quantities allows one, in turn, to determine their partial derivatives with respect to spatial variables and time and to write conservation laws in the form of partial differential equations. To maximally facilitate the understanding of the basic ideas, we will confine ourselves only to the adiabatic core [1] of conservation laws in the form

$$\frac{\partial \rho}{\partial t} + \nabla \rho \mathbf{U} = 0, \quad (1)$$

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \frac{\partial}{\partial x_k} (\rho \mathbf{U} U_k) + \nabla P = 0, \quad (2)$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \mathbf{U} (\rho \varepsilon + P) = 0, \quad (3)$$

where P is the pressure, $k = 1, 2, 3$. In the phenomenological theory of a continuous medium, ρ , \mathbf{U} , and ε are first considered as average quantities in a certain finite volume θ such that it contains many microparticles. Next, it is postulated [2] that on shrinking of the finite volume to a point, the average quantities ρ , \mathbf{U} , and ε have finite limits which are precisely the characteristics of the continuous medium at the point. Here, usually, the physical content of the notion "many particles" is not refined, thus making it difficult to establish the quantitative correspondence between the parameters of a continuous medium (macrolevel) and those of a discrete medium (microlevel).

Now, we will consider a discrete medium of microparticles. Let, in a certain arbitrary finite volume θ , there be n microparticles. Each particle has a number v , mass m_v , velocity \mathbf{U}_v , and internal energy q_v . At a certain fixed

instant of time t^* the mass M , momentum \mathbf{K} , and energy Q_0 of all the n particles are determined by means of summation:

$$M = \sum_{v=1}^n m_v, \quad \mathbf{K} = \sum_{v=1}^n m_v \mathbf{U}_v, \quad Q_0 = \sum_{v=1}^n m_v (q_v + 0.5 \mathbf{U}_v^2).$$

Thus, at any time instant t the laws of conservation of M , \mathbf{K} , and Q_0 in transition from the micro- to macrolevel and back have the form

$$\int_0^\theta \rho d\theta = \sum_{v=1}^n m_v, \quad \int_0^\theta \rho \mathbf{U} d\theta = \sum_{v=1}^n m_v \mathbf{U}_v, \quad \int_0^\theta \rho \varepsilon d\theta = \sum_{v=1}^n m_v (q_v + 0.5 \mathbf{U}_v^2). \quad (4)$$

In such an approach, the principle of uncertainty is not disturbed, since there is no need to indicate the position of each particle. Either micro- or macromodels are preferable for solving various problems. To describe the behavior of dense gases and liquids in dynamic processes, a model of a continuous medium with a corresponding equation of state is used to advantage.

During the second half of the 20th century, many models appeared that combined a continuous description of a substance with a discrete one, when the trajectory of a particle with the number v is determined by the Newton equation:

$$m_v \frac{d\mathbf{U}_v}{dt} = \mathbf{F}_v.$$

The particle can be "large" and contain so many microparticles that its properties are determined as those of a continuous medium on a mesolevel. The forces acting on a mesoparticle can be determined differently.

In hydrodynamics, for example, wide use was made of the model of particles that originated from the model of "particles in cells" devised in 1955 by F. Harlow with co-workers [3, 4] for numerical solution of Eqs. (1)–(3). In the method of particles, the quantities ∇P and $\nabla \mathbf{U}$ are determined on the macrolevel of a continuous medium whose parameters are determined from equations of type (4) and from the equation of state. These quantities ∇P and $\nabla \mathbf{U}$ act then on mesoparticles that preserve "their" mass with time and move along their "own" paths. The methods of particles turned out to be most efficient in solving the problems of plasma physics [5, 6]. Some of these methods have their drawbacks, among which the most significant is the absence of invariance with respect to the G. Galilei transformation.

To increase the effectiveness of mathematical simulation of the properties of substances, a method of molecular dynamics has been devised [7, 8]. In this method the laws of interaction of microparticles with one another are extended to mesoparticles, that is, to large molecules. The method of molecular dynamics has turned out to be very efficient in constructing the equations of state of a substance; it successfully complemented the methods of statistical physics, physical and quantum mechanics, and thermodynamics. In the kinetic theory of gases, when the free path of microparticles from interaction to interaction is much larger than the dimensions of a particle, discrete models based on the probabilistic description of the behavior of an ensemble of particles with the aid of the Boltzmann equation turned out to be effective.

The necessity of increasing the accuracy of mathematical simulation of the behavior of solid bodies subjected to plastic deformation has led to the appearance of models in which a model of a continuous medium is applied on several mesolevels. Such an approach to simulation of the behavior of a solid body is called mesomechanics. In [9], models of plastic deformation are considered in which the carriers of plastic deformation are structural elements responsible for both shifts and mutual rotations. Their dimensions, intensity, and interaction are determined by micro-, meso-, and macrovortices. This model of the mechanics is replaced (approximated) by a certain mathematical model that can be used for carrying out calculations on computers. In [10], the results of calculations of the behavior of solid bodies in the region of plastic deformations are presented that were obtained with the aid of the two-level model of mesomechanics.

In [3–8], many variants of the method of particles and of the method of molecular dynamics are described. These and other methods have again attracted attention in the recent decade on the revolutionary introduction of nanotechnology. A detailed survey of multilevel models lying between the models that describe substances on micro- and macrolevels is given in [11].

The History of the Models of Multicomponent Media. Very few pure substances exist in nature. There are mainly mixtures of substances. Substances can be mixed on both the molecular level (homogeneous mixtures) and on the level of large macroparticles (heterogeneous mixtures). Within these frames there are virtually all mixtures — multicomponent media (MCM). A continuous medium in an arbitrary volume is called [12] multicomponent if several substances ($N > 1$) are mixed in this volume. Each component may be in any state of aggregation: S (solid), L (liquid), G (gas), and P (plasma). Any combinations of the states of aggregation of components are possible in a multicomponent medium. Since different components of a multicomponent medium differ in heat capacities, speeds of sound, compressibilities, and in other physical characteristics, a multicomponent medium subjected to external effects usually develops a nonequilibrium state that is characterized by different pressures, temperatures, and velocities. Efforts to raise the accuracy of prediction of processes occurring in a multicomponent medium by taking into account these nonequilibrium states and describing relaxation processes sharply complicate the models. In the course of phase transitions, some components change substantially the character of their interaction with one another, forcing one to consider a multitude of properties displayed in pair interactions.

The history of devising multicomponent medium models goes back to the mid-1850's and began with the works of H. Darcy, N. E. Zhukovskii, and I. Prigogine. Vigorous development of the multicomponent medium models occurred in the mid-1950's in connection with the advent of computers. In the Soviet Union, a great contribution to the theory of a multicomponent medium was made by L. D. Landau (1945), G. S. Chernyi (1951), Kh. A. Rakhmatulin, S. S. Kutateladze (1956), V. V. Struminskii, R. I. Nigmatulin (1961), A. N. Kraiko (1965), V. P. Myasnikov (1966), V. E. Nakoryakov (1971), N. N. Yatsenko, V. M. Fomin, and R. I. Soloukhin (1976). Abroad, these were T. Cowling, R. Toupin, S. Truesdell, S. Chapman (1956), A. Green, P. Cayley, G. Cliegel, P. Naghdi (1961), G. Batchelor, G. Müller (1966), and L. Wijngaarden (1971). This, by no means complete, list shows that the most prominent scientists were long involved in developing MCM models.

The necessity of modeling the behavior of MCM arises in many areas of human activity [13]. This gives rise to the appearance of various MCM models intended for simulation of the MCM behavior on being subjected to external effects — from very simple to very complicated ones. Most often, the simplicity of a model is attained due to simplifying hypotheses. Thus, for example, in solving many problems, air (a mixture of nitrogen, oxygen, and of other gases) is considered as a single substance with its own equation of state. In this case, an MCM model is the simplest one — this is the classical equation of gas dynamics. Next in complexity are models in which in an MCM we isolate one or more components moving with the same velocity and having the same temperature and pressure. Here, for describing the mixing of components, the equation of diffusion or equation of filtration is used (the models of H. Darcy, Buckley–Leverett, et al. [12]), although the use of diffusion equations for describing the motion of components relative to one another contradicts the assumption on the equality of their velocities.

Most complete and promising are models based on the hypothesis of interpenetrating interacting continua [12–18]. The class of these models involves both simple and more complex ones. The complexity of a model depends on the simplifications made. Since models are complex, in the process of changing over from a general model to a particular one, physical controversies may arise similar to the fundamental controversy inherent in diffusion models.

At the present time, the theory of MCM models is being intensely developed. Studying and applying particular models leads to the process of accumulation of information and experience. There remain diffusion models and models based on the theory of multivelocitly interacting continua. A weak spot in all of the models remains the description of the interaction of components. An advance in the theory of MCM is the solution of the problem on the agreement of the laws of conservation of components with the laws of conservation of a mixture [17]. The need for such a matching has led to the appearance of a new type of interaction of components — the cluster interaction, which is independent either of the states of aggregation of the components, or of their physical properties. Below, we will consider one of the contemporary MCM models.

Models of Multivelocitly Continua. In multivelocitly continua models, the behavior of each component is determined by conservation laws written for the macrolevel quantities. This means that for each component the transition

from consideration on a microlevel to the macrolevel quantities has already occurred, as a result of which each component numbered i has the following physical characteristics: pressure P_i , temperature T_i , density ρ_i , specific internal energy E_i , velocity \mathbf{U}_i , entropy S_i , etc. The thermodynamic characteristics of the i th component are interrelated by the equation of state.

We will consider the volume θ in which there is a mixture of mass M consisting of N components. We will divide M and θ among all the components:

$$M = \sum_{i=1}^N M_i, \quad \theta = \sum_{i=1}^N \theta_i. \quad (5)$$

The ratios

$$\eta_i = \frac{M_i}{M}, \quad \alpha_i = \frac{\theta_i}{\theta} \quad (6)$$

are called [12–18] the mass and volume concentration of the i th component. By definition, the density is the mass of a substance in a unit volume. Consequently,

$$\rho_i = \frac{M_i}{\theta_i}, \quad \rho = \frac{M}{\theta}, \quad (7)$$

where ρ is the density of the mixture. Let us imagine that the mass M_i is "smeared" over the entire volume θ . The quantity

$$\alpha_i \rho_i = \frac{M_i}{\theta} \quad (8)$$

is a virtual quantity and is called the partial density of the component i . From Eqs. (5)–(8) it is seen that $\alpha_i \rho_i$ and ρ are interrelated as

$$\alpha_i \rho_i = \eta_i \rho. \quad (9)$$

For the specific volume $V = 1/\rho$ relation (9) takes the form

$$\alpha_i V = \eta_i V_i.$$

From Eqs. (5), (7), and (8) it follows that the mixture density is equal to the sum of the partial densities of the components:

$$\rho = \sum_{i=1}^N \alpha_i \rho_i. \quad (10)$$

Each mixture component has the momentum $\mathbf{U}_i M_i$. From the momentum conservation law at a fixed time t it follows that

$$\mathbf{U} M = \sum_{i=1}^N \mathbf{U}_i M_i.$$

Having replaced M_i by $\eta_i M$ with the aid of (6) and dividing it by M , we obtain that the mixture velocity \mathbf{U} is equal to the sum of partial velocities $\eta_i \mathbf{U}_i$ of the components:

$$\mathbf{U} = \sum_{i=1}^N \eta_i \mathbf{U}_i. \quad (11)$$

From Eqs. (9) and (11) it follows that the specific momentum of the mixture $\rho\mathbf{U}$ is equal to the sum of the specific momenta of the components:

$$\rho\mathbf{U} = \sum_{i=1}^N \alpha_i \rho_i \mathbf{U}_i. \quad (12)$$

The total specific energy of the mixture ε consists of the specific internal energy E and specific kinetic energy $0.5\mathbf{U}^2$. A similar coupling exists also for the i th component:

$$\varepsilon = E + 0.5\mathbf{U}^2, \quad \varepsilon_i = E_i + 0.5\mathbf{U}_i^2. \quad (13)$$

From the energy conservation law at a fixed time it follows that

$$\varepsilon M = \sum_{i=1}^N \varepsilon_i M_i.$$

After division by M and use of (6) we obtain that the total specific energy of the mixture is equal to the sum of partial total specific energies of the components:

$$\varepsilon = \sum_{i=1}^N \eta_i \varepsilon_i. \quad (14)$$

From Eqs. (13) and (14) it follows that

$$E = \sum_{i=1}^N \eta_i (E_i + 0.5\mathbf{U}_i^2 - 0.5\mathbf{U}^2). \quad (15)$$

In the process of relaxation of velocities, $\mathbf{U}_i \neq \mathbf{U}$, hence the internal specific energy of the mixture is not equal to the sum of partial internal energies of the components. It can be easily verified that expression (15) for E is not invariant with respect to the Galilei transformation. We will transform Eq. (15) so that it is independent of the choice of the coordinate system moving with a constant velocity. We will multiply (11) by \mathbf{U} and write the resulting equation in the form

$$\sum_{i=1}^N \eta_i \mathbf{U}^2 = \sum_{i=1}^N \eta_i (2\mathbf{U}_i \mathbf{U} - \mathbf{U}^2). \quad (16)$$

Putting (16) into (15), we obtain an expression for E that satisfies the Galilei transformation:

$$E = \sum_{i=1}^N \eta_i (E_i + H_i), \quad (17)$$

where

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

We will call quantity $H = \sum_{i=1}^N \eta_i H_i$ the nonequilibrium kinetic energy of the mixture. In the process of relaxa-

tion of velocities, when $\mathbf{U} - \mathbf{U}_i \rightarrow 0$, this energy goes over into the internal energy, which increases in this way.

The physical quantities P_i , ρ_i , E_i , T_i , \mathbf{U}_i and others are quantities of the macrolevel of the i th component, whereas the partial quantities $\alpha_i \rho_i$, $\alpha_i P_i$, $\eta_i \mathbf{U}_i$, $\eta_i E_i$, $\eta_i \varepsilon_i$ and others describe its behavior as that of a continuous medium. However, each component is a structural element of the mixture. Thus, the indicated quantities relative to the mixture are quantities of the intermediate level — the mesolevel. The quantities of the macrolevel that characterize the behavior of the mixture result from the quantities of the mesolevel as follows from Eqs. (10), (11), (14), and (17).

Interaction of Components. A multicomponent mixture can be in a nonequilibrium state. The conditions of the mixture equilibrium have the form

$$P_i = P_j, \quad T_i = T_j, \quad \mathbf{U}_i = \mathbf{U}_j.$$

If at least one of these conditions is not fulfilled, the mixture is nonequilibrium. Relaxation processes of the establishment of equilibrium in which the components exchange momentum and energy occur in the mixture.

For a long time, when models of multicomponent media were constructed, only pair interactions were considered, in the process of which the i th and j th components interact independently of the remaining components [12, 14–16, 18]. In the case where $\mathbf{U}_i \neq \mathbf{U}_j$, the momentum exchange is determined most often by the vector

$$\bar{\mathbf{R}}_{ij} = a_{ij} (\mathbf{U}_j - \mathbf{U}_i) / \tau_{ij}^U. \quad (18)$$

The functions a_{ij} and τ_{ij}^U depend on the degree of mixture heterogeneity, on the properties of the i th and j th components, on the dimensions and shape of the particles of the components, on the speed of sound, compressibility, the equations of state of the components, on the states of aggregation of components, and their adhesion properties so that they satisfy the Onsager reciprocity condition:

$$a_{ij} = a_{ji}, \quad \tau_{ij}^U = \tau_{ji}^U,$$

as a result of which the vector \mathbf{R} satisfies the condition

$$\mathbf{R}_{ij} = -\mathbf{R}_{ji}. \quad (19)$$

The specific form of these relations is established with allowance for the conditions of each specific problem. Often, in order to justify them, an elementary two-component cell is constructed. The order of the subscripts ij points to the fact that the i th component acts on the j th one. The action experienced by the i th component from all the N components, i.e., from the mixture, is determined by summation over j :

$$\mathbf{R}_i = \sum_{j=1}^N \alpha_j \mathbf{R}_{ji}.$$

By virtue of conditions (19), the vector \mathbf{R} acting on the mixture from the side of all the components turns out to be equal to zero:

$$\mathbf{R} = \sum_{j=1}^N \sum_{i=1}^N \alpha_i \alpha_j \mathbf{R}_{ij} = 0. \quad (20)$$

Analogous reasoning relates also to the scalar function Φ_{ij} that describes the energy exchange between the i th and j th components. According to [17], we will write this function in the form

$$\Phi_{ji} = \frac{b_{ji}}{\tau_{ji}^P} (P_j - P_i) + \frac{c_{ji}}{\tau_{ji}^T} (\alpha_i \rho_i C_{vi} + \alpha_j \rho_j C_{vj}) (T_j - T_i), \quad (21)$$

where $b_{ij} = b_{ji}$, $c_{ij} = c_{ji}$, $\tau_{ij}^P = \tau_{ji}^P$, $\tau_{ij}^T = \tau_{ji}^T$, and $\Phi_{ij} = -\Phi_{ji}$, C_V is the specific heat at constant volume. The functions b_{ij} and c_{ij} are dimensionless. Just as a_{ij} , they depend on the degree of heterogeneity and on the properties of the i th and j th components. The energy flux to the i th component from the side of the remaining mixture components are obtained by summation:

$$\Phi_i = \sum_{j=1}^N \alpha_j \Phi_{ji}.$$

The energy flux acting on the mixture from the side of all the components is equal to zero:

$$\Phi = \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j \Phi_{ij} = 0. \quad (22)$$

Equations (20) and (22) represent a principal specific feature of the model of pair interactions.

Laws of Conservation of the i th Component. We will write the laws of mass, momentum, and energy conservation of an ideal continuous medium without thermal conductivity in the form

$$\frac{\partial}{\partial t} (\alpha_i \rho_i) + \nabla (\alpha_i \rho_i \mathbf{U}_i) = 0, \quad (23)$$

$$\frac{\partial}{\partial t} (\alpha_i \rho_i \mathbf{U}_i) + \nabla \alpha_i P_i + \sum_{k=1}^3 \frac{\partial}{\partial x_k} (\alpha_i \rho_i \mathbf{U}_i U_{ik} + \alpha_i \mathbf{F}_{ik}) - \alpha_i \mathbf{R}_i = 0, \quad (24)$$

$$\frac{\partial}{\partial t} (\alpha_i \rho_i \varepsilon_i) + \nabla (\alpha_i \mathbf{U}_i (P_i + \rho_i \varepsilon_i)) + \sum_{k=1}^3 \frac{\partial}{\partial x_k} (\alpha_i \mathbf{F}_{ik} \mathbf{U}_i) + \nabla \alpha_i \mathbf{Q}_i - \alpha_i \Phi_i = 0. \quad (25)$$

The system of equations (23)–(25) should be supplemented with the equation of state in the form

$$P_i = P_i(\rho_i, E_i), \quad T_i = T_i(\rho_i, E_i) \quad (26)$$

and with ε_i expressed in terms of E_i and $0.5\mathbf{U}_i^2$:

$$\varepsilon_i = E_i + 0.5\mathbf{U}_i^2. \quad (27)$$

As compared to [12], [14–16], the new quantities in these equations are the vector \mathbf{F}_{ik} formed by the elements of the k th line of the tensor F_i and the vector \mathbf{Q}_i .

Equations (23)–(27) are closed by the equation for the volume concentration α_i .

Mixture Conservation Laws. The quantities of the macrolevel P , ρ , E , \mathbf{U} , ε , and T are the characteristics of a certain continuous medium (mixture). We will write the mass, momentum, and energy conservation laws for a mixture of real substances without heat conduction. They have the form

$$\frac{\partial \rho}{\partial t} + \nabla \rho \mathbf{U} = 0, \quad (28)$$

$$\frac{\partial}{\partial t} (\rho \mathbf{U}) + \mathbf{U} \nabla (\rho \mathbf{U}) + \rho (\mathbf{U} \nabla) \mathbf{U} + \nabla P + \sum_{k=1}^3 \frac{\partial}{\partial x_k} \mathbf{F}_k = 0, \quad (29)$$

$$\frac{\partial}{\partial t} (\rho \epsilon) + \nabla \mathbf{U} (P + \rho \epsilon) + \sum_{k=1}^3 \frac{\partial}{\partial x_k} (\mathbf{U} \mathbf{F}_k) + \nabla \mathbf{Q} = 0. \quad (30)$$

Within the framework of the hypotheses adopted above, the equation of state of a mixture does not exist. The interaction tensor F and the energy flux \mathbf{Q} must be such that the mixture conservation laws could be coordinated with the conservation laws of the components, i.e., that they could be obtained by summing up the laws of the conservation of components.

Necessary Conditions for the Consistency of Conservation Laws. In the absence of chemical reactions the laws of mass conservation of the i th component and of the mixture have the form of Eqs. (23) and (28). Since Eqs. (10) and (12) are valid, summation of Eq. (23) yields (28). Thus, the mass conservation laws of a mixture result from summation of the mass conservation laws of components without any necessary or sufficient conditions.

We will sum the momentum conservation law of the motion of the i th component over i :

$$\sum_{i=1}^N \left(\frac{\partial \alpha_i \rho_i \mathbf{U}_i}{\partial t} + \sum_{k=1}^3 \frac{\partial}{\partial x_k} (\alpha_i \rho_i \mathbf{U}_i U_{ik} + \alpha_i \mathbf{F}_{ik}) + \nabla \alpha_i P_i \right) = 0. \quad (31)$$

With the aid of Eqs. (12) and the equation

$$P = \sum_{i=1}^N \alpha_i P_i$$

we transform Eq. (31) to give

$$\frac{\partial}{\partial t} (\rho \mathbf{U}) + \mathbf{U} \nabla (\rho \mathbf{U}) + \rho (\mathbf{U} \nabla) \mathbf{U} + \nabla P + \sum_{k=1}^3 \frac{\partial}{\partial x_k} \mathbf{F}_k + \omega_1 = 0, \quad (32)$$

where

$$\omega_1 = \sum_{k=1}^3 \frac{\partial}{\partial x_k} \left(\sum_{i=1}^N (\alpha_i \rho_i \mathbf{U}_i U_{ik} + \alpha_i \mathbf{F}_{ik}) - \mathbf{F}_k - \rho \mathbf{U} U_k \right) = 0. \quad (33)$$

From comparison Eqs. (32) and (29) it follows that the necessary condition for obtaining the momentum conservation law of a mixture by summing over all the components of Eqs. (24) has the form $\omega_1 = 0$. The force $\alpha_i \mathbf{F}_{ik}$ acts on the i th component from the side of the mixture as a totality of components. The force \mathbf{F}_k is the resultant of the forces with which each component acts on the mixture. According to Newton's third law

$$\mathbf{F}_k = - \sum_{i=1}^N \alpha_i \mathbf{F}_{ik}. \quad (34)$$

Substituting (34) into (33) and equating ω_1 to zero, we obtain the equation

$$\sum_{k=1}^3 \frac{\partial}{\partial x_k} \left(\sum_{i=1}^N (2\alpha_i \mathbf{F}_{ik} + \alpha_i \rho_i \mathbf{U}_i U_{ik}) - \rho \mathbf{U} U_k \right) = 0. \quad (35)$$

With the aid of Eq. (12) we represent $\rho \mathbf{U} U_k$ as a sum over the components

$$\rho \mathbf{U} U_k = \sum_{i=1}^N \alpha_i \rho_i ((\mathbf{U}_i - \mathbf{U}) U_k + \mathbf{U} U_{ik}). \quad (36)$$

Equations (35) and (36) yield the equation

$$\sum_{k=1}^3 \frac{\partial}{\partial x_k} \left(\sum_{i=1}^N (2\alpha_i \mathbf{F}_{ik} + \alpha_i \rho_i (\mathbf{U}_i - \mathbf{U}) (U_{ik} - U_k)) \right) = 0.$$

Equating each term to zero in the sum over i , we obtain the following expression for the vector \mathbf{F}_{ik} :

$$\mathbf{F}_{ik} = -0.5 \rho_i (\mathbf{U} - \mathbf{U}_i) (U_k - U_{ik}). \quad (37)$$

The i th component experiences the force $\alpha_i \mathbf{F}_{ik}$ acting from the side of the mixture over the area orthogonal to the Ok axis.

Next, we will consider the energy conservation law. We will sum up (25) over all the components, then add and subtract the value

$$\nabla (P\mathbf{U} + \rho \varepsilon \mathbf{U} + \mathbf{Q}) + \sum_{k=1}^3 \frac{\partial}{\partial x_k} \mathbf{F}_k \mathbf{U}$$

and bring the resulting equation to the form

$$\frac{\partial}{\partial t} (\rho \varepsilon) + \nabla \mathbf{U} (P + \rho \varepsilon) + \nabla \mathbf{Q} + \sum_{k=1}^3 \frac{\partial}{\partial x_k} \mathbf{F}_k \mathbf{U} + \omega_2 = 0, \quad (38)$$

where

$$\omega_2 = \sum_{i=1}^N \sum_{k=1}^3 \frac{\partial}{\partial x_k} (\alpha_i ((P_i + \rho_i \varepsilon_i) (U_{ik} - U_k) + Q_{ik} + \mathbf{F}_{ik} (\mathbf{U}_i + \mathbf{U}))) - \nabla \mathbf{Q}. \quad (39)$$

From a comparison of Eq. (38) with the energy conservation law of the mixture (30), it is seen that the prerequisite for obtaining the energy conservation law of a mixture by means of summing up the energy conservation laws of components has the form $\omega_2 = 0$.

Expression (39) involves the vector \mathbf{Q} and vectors \mathbf{Q}_i . The vector \mathbf{Q} represents an energy flux directed to the mixture from all the components, and the vector $\alpha_i \mathbf{Q}_i$ represents an energy flux directed to the i th component. According to the energy conservation law, the following should hold:

$$\mathbf{Q} = - \sum_{i=1}^N \alpha_i \mathbf{Q}_i. \quad (40)$$

Equations (13), (37), (39), and (40) and the condition $\omega_2 = 0$ yield the equation

$$\sum_{i=1}^N (\nabla (2\alpha_i \mathbf{Q}_i - \alpha_i (\mathbf{U} - \mathbf{U}_i) (P_i + \rho_i E_i))) = 0.$$

Equating each term to zero, we obtain an expression for the energy flux:

$$\mathbf{Q}_i = 0.5 (\mathbf{U} - \mathbf{U}_i) (P_i + \rho_i E_i). \quad (41)$$

The model considered contains a new type of interaction of components — cluster interaction or interaction of each component with the mixture as a whole. This form of interaction is described by universal forces \mathbf{F}_{ik} (37) and energy fluxes \mathbf{Q}_i (41), which are independent either of the physical properties of the components or of their equations of state. The model is based on two requirements: strict fulfillment of conservation laws and the observance of the invariance with respect to the Galilei transformation.

Closure of the System of Equations. The system of equations of the i th component contains $11N$ independent quantities:

$$P_i, \rho_i, E_i, \varepsilon_i, T_i, \mathbf{U}_i, \alpha_i, \mathbf{R}_i, \Phi_i, \mathbf{F}_{ik}, \mathbf{Q}_i$$

and $10N$ independent equations:

- a) $3N$ conservation laws (28)–(30);
- b) N equations that connect the specific values of the total, internal, and kinetic energies (27);
- c) $2N$ equations of state (26);
- d) $4N$ equations for the interaction functions (18), (21), (37), and (41).

For the system of equations to be closed, the above-indicated equations should be supplemented with N equations to determine α_i . These equations must not depend on the already available equations.

As the first step, we will differentiate the equation

$$\sum_{i=1}^N \alpha_i = 1$$

along the trajectory of the mixture:

$$\sum_{i=1}^N \left(\frac{\partial \alpha_i}{\partial t} + \mathbf{U} \nabla \alpha_i \right) = 0. \quad (42)$$

The resulting equation (42) is invariant with respect to the Galilei transformation. Each term in it is not equal to zero, since α_i changes with time along the mixture trajectory. To Eq. (42) we will add the function Ω_i , which satisfies the following conditions:

- 1) the function Ω_i should be invariant with respect to the Galilei transformation;
- 2) the sum Ω_i should be equal to zero:

$$\sum_{i=1}^N \Omega_i = 0. \quad (43)$$

After summation of Eqs. (42) and (43), we obtain the equation

$$\sum_{i=1}^N \left(\frac{\partial \alpha_i}{\partial t} + \mathbf{U} \nabla \alpha_i + \Omega_i \right) = 0. \quad (44)$$

The next condition that should be satisfied by the function Ω_i is that it must convert each term of the sum in (44) into zero. Thus, to determine α_i we obtain the equation

$$\frac{\partial \alpha_i}{\partial t} + \mathbf{UV}\alpha_i + \Omega_i = 0. \quad (45)$$

The volume concentration α_i depends on the interaction of components. The two functions \mathbf{R}_i and Φ_i that describe pair interactions of components satisfy the above-enumerated requirements. Since Eq. (45) is scalar, it is natural to take the function Ω_i in the form close to that of the function Φ_i . These functions have different dimensions, since they are terms of different equations. To determine the differences between them, we will consider the simplest system consisting of two plane layers of different substances located between two rigid walls orthogonal to the Ox axis. Each layer is characterized by a set of physical parameters P_l, ρ_l, E_l, c_l , and P_r, ρ_r, E_r, c_r and has thickness Δx_l and Δx_r . The velocities are equal to zero, whereas the pressures are different at $t = 0$. Therefore, when $t > 0$, the contact boundary will start to move with velocity

$$U_{c.b} \approx - \frac{2(P_r - P_l)}{h_r - h_l} t, \quad (46)$$

where $h_r = \rho_r \Delta x_r$, $h_l = \rho_l \Delta x_l$. According to the problem, conditions Δx_l and Δx_r change so that $\Delta x_l + \Delta x_r = \text{const}$. Let us introduce the average volume concentration of the right and left substance:

$$\alpha_l = \frac{\Delta x_l}{\Delta x_l + \Delta x_r}, \quad \alpha_r = \frac{\Delta x_r}{\Delta x_l + \Delta x_r}. \quad (47)$$

From Eqs. (46) and (47) there follows the equation

$$\frac{\partial \alpha_l}{\partial t} \approx - \frac{2(P_r - P_l) t}{(\Delta x_l + \Delta x_r)(h_l + h_r)}. \quad (48)$$

In the acoustic approximation we will express Δx and h in terms of the speed of sound and relaxation time τ :

$$\Delta x_l + \Delta x_r \approx (c_l + c_r) \tau, \quad h_l + h_r \approx (\rho_l c_l + \rho_r c_r) \tau,$$

and we will consider that the time t is proportional to the time of relaxation $t \approx b\tau$. With these hypotheses Eq. (48) will take the form

$$\frac{\partial \alpha_l}{\partial t} \approx - \frac{(P_r - P_l) b}{(c_r + c_l)(\rho_r c_r + \rho_l c_l) \tau}.$$

With allowance for the foregoing we will multiply the function Φ_{ij} (23) by the function

$$f_{ij} = \frac{1}{(c_i + c_j)(\rho_i c_i + \rho_j c_j)},$$

as a result of which the quantity Ω_i will take the form

$$\Omega_i = \alpha_i \sum_{j=1}^N \alpha_j f_{ij} \Phi_{ij}.$$

Molecular-Kinetic Justification of the Force of Cluster Interaction. The expressions for \mathbf{F}_{ik} and \mathbf{Q}_i were obtained on the macrolevel as the necessary conditions of coordination of the conservation laws of the components and

mixture. We will obtain an expression for the forces \mathbf{F}_{ik} by a quite different method applied for determining the equation of state of an ideal gas.

The relationship between the pressure and internal specific energy is determined in this method as the result of the interaction of molecules with the vessel walls. For transition from the microlevel of molecules to the macrolevel of a component, we will make some assumptions as suggested in physics textbooks [19–21]:

- 1) the molecules have a mass and do not have a volume;
- 2) the molecules move at random and each molecule has its own velocity;
- 3) the molecules do not interact with one another and interact only with the walls of the vessel in which they reside.

Let each component be an ideal gas. Its molecules have mass m_{vi} and velocity \mathbf{U}_{vi} . The mass and the values of the density ρ_i and velocity \mathbf{U}_i of the gas are defined by the equations

$$M_i = \sum_{v=1}^{n_i} m_{vi}, \quad \rho_i = \frac{M_i}{\theta_i}, \quad \mathbf{U}_i = \sum_{v=1}^{n_i} \eta_{vi} \mathbf{U}_{vi}, \quad (49)$$

where η_{vi} is the mass concentration of the v th molecule in the gas i . The velocity \mathbf{U}_i determines the kinetic energy of the i th component, which is smaller than the full kinetic energy of all n_i molecules. Their difference divided by M_i determines the specific internal energy:

$$E_i = \sum_{v=1}^{n_i} 0.5 \eta_{vi} (\mathbf{U}_{vi} - \mathbf{U}_i)^2. \quad (50)$$

Assuming that the collisions of molecules with the vessel walls are elastic, we will obtain an expression for the force acting on the gas from the side of a unit area of the faces S_x, S_y, S_z orthogonal to Ox, Oy, Oz :

$$\begin{aligned} \varphi_{ix} &= -\rho_i \sum_{v=1}^{n_i} \eta_{vi} (U_{vix} - U_{ix})^2 \mathbf{i}, \\ \varphi_{iy} &= -\rho_i \sum_{v=1}^{n_i} \eta_{vi} (U_{viy} - U_{iy})^2 \mathbf{j}, \\ \varphi_{iz} &= -\rho_i \sum_{v=1}^{n_i} \eta_{vi} (U_{viz} - U_{iz})^2 \mathbf{k}. \end{aligned}$$

The vectors $\varphi_{ix}, \varphi_{iy}, \varphi_{iz}$ are formed by the diagonal elements of the tensor φ . According to the rules of mechanics, the pressure is equal to the sum of diagonal terms with the opposite sign divided by 3:

$$P_i = \frac{1}{3} \rho_i \sum_{v=1}^{n_i} \eta_{vi} (\mathbf{U}_{vi} - \mathbf{U}_i)^2. \quad (51)$$

Having eliminated the sum in (50) and (51), we obtain the classical equation of state of a monatomic ideal gas of the i th component:

$$P_i = \frac{2}{3} \rho_i E_i.$$

This equation is correct if the gas is in a vessel of volume θ_i and there are no any other gases in this vessel. If now we take the volume θ , then the pressure and density become partial quantities and the equation of state takes the form

$$\alpha_i P_i = \frac{2}{3} \alpha_i \rho_i E_i.$$

In a mixture, transition from the microlevel to the macrolevel consists of two stages. First, in accordance with the above-described procedure, a transition from the microlevel to the macrolevel of the component occurs. The latter macrolevel is the intermediate level of the mixture — a mesolevel. Thereafter, transition from the mesolevel to the macrolevel of the mixture occurs. Let, in the volume θ of the mixture, there be N ideal gases. For each gas the mass M_i , velocity \mathbf{U}_i , and the energy E_i have the form of Eqs. (49) and (50). From the conservation law

$$M = \sum_{i=1}^N M_i, \quad \mathbf{K} = \sum_{i=1}^N \mathbf{K}_i$$

and definitions

$$\mathbf{K} = \mathbf{U}M, \quad \mathbf{K}_i = \mathbf{U}_i M_i, \quad \eta_i = M_i/M$$

the expression for the mixture velocity (11) follows. This is the velocity at which the volume θ and its faces move. Since $\mathbf{U}_i \neq \mathbf{U}$, this means that the components move inside the volume θ and interact with the walls that bound this volume. To describe the interaction of the i th component with the walls of the volume θ we will make three assumptions:

- 1) the i th component is a large particle;
- 2) the interaction of the i th component with the faces S_x , S_y , and S_z is inelastic;
- 3) the change in the momentum of the i th component in the case of normal and tangent interaction with the wall is different.

From the side of the face S_x the i th component experiences the action of the force \mathbf{F}_{ix} . It has normal F_{ixx} and tangential F_{ixy} , F_{ixz} components. In interaction with the face S_x , the normal U_{ix} and tangential U_{iy} , U_{iz} components of the velocity \mathbf{U}_i satisfy the inequalities

$$\begin{aligned} (U_{ix}^f - U_x)(U_{ix} - U_x) < 0, \\ (U_{iy}^f - U_y)(U_{iy} - U_y) > 0, \quad (U_{iz}^f - U_z)(U_{iz} - U_z) > 0, \end{aligned}$$

where U_{ix} , U_{iy} , and U_{iz} are the velocity components of the i th component before its impact on the wall; U_x , U_y , and U_z are the velocity components of the wall; U_{ix}^f , U_{iy}^f , and U_{iz}^f are the velocity components of the i th component after the interaction with the wall. We restrict ourselves to the simplest law of interaction:

on reflection

$$U_{ix}^f - U_x = -\gamma(U_{ix} - U_x), \tag{52}$$

on contact

$$U_{iy}^f - U_y = \beta(U_{iy} - U_y), \quad U_{iz}^f - U_z = \beta(U_{iz} - U_z). \tag{53}$$

The values of γ and β change in a unit interval $0 \leq \gamma \leq 1$, $0 \leq \beta \leq 1$. The boundary values $\gamma = 0$, $\beta = 0$ characterize the regime of absolute adhesion to the wall, and the values $\gamma = 1$ and $\beta = 1$ characterize the regime of an absolutely elastic interaction.

The force F_{ixx} that acts on the i th component from the side of the unit area S_x in the direction from Ox will be found from the condition that its pulse in time

$$\Delta t_{ixx} = \frac{(U_{ix}^f - U_{ix}) \theta^{1/3}}{(U_{ix} - U_x) (U_{ix}^f - U_x)}$$

is equal to the change in momentum of the i th component in interaction with the wall:

$$F_{ixx} = \frac{M_i (U_{ix}^f - U_{ix})}{\Delta t_{ixx}}.$$

Having substituted U_{ix}^f from (52) into the expression of the force F_{ixx} , as well as the value of M_i from (8) and dividing it by $\theta^{2/3}$ (the area of the face S_x), we obtain the expression for the force F_{ixx} in the form

$$F_{ixx} = -\gamma \alpha_i \rho_i (U_{ix} - U_x)^2.$$

Along the Oy axis, a change in the tangential component of the momentum is equal to the pulse of the acting force F_{ixy} :

$$M_i (U_{iy}^f - U_{iy}) = F_{ixy} \Delta t_{ixy}. \quad (54)$$

It is not difficult to write the expression for Δt_{ixy} . Let us assume that Δt_{ixy} is related to Δt_{ixx} by the equation

$$\Delta t_{ixy} = R(\beta) \Delta t_{ixx}. \quad (55)$$

Equations (52)–(55) yield the equation for the force acting on the i th component of the mixture along the tangent from the side of the unit area of the face S_x in time Δt_{ixy} :

$$F_{ixy} = -\alpha_i \rho_i \frac{\gamma(1-\beta)}{R(1+\gamma)} (U_{iy} - U_y) (U_{ix} - U_x).$$

The expression for F_{ixz} is obtained analogously. The vector \mathbf{F}_{ix} with the components F_{ixx} , F_{ixy} , and F_{ixz} has the form

$$\mathbf{F}_{ix} = -\gamma \alpha_i \rho_i (U_{ix} - U_x) \left((U_{ix} - U_x) \mathbf{i} + \frac{(1-\beta)}{R(1+\gamma)} \left((U_{iy} - U_y) \mathbf{j} + (U_{iz} - U_z) \mathbf{k} \right) \right).$$

The vectors \mathbf{F}_{iy} and \mathbf{F}_{iz} are obtained analogously. We fail to refine the parameters of the model α , β , and R with the aid of the theory. However, in the case of a concrete choice of the values of these parameters:

$$\gamma = \frac{1}{2}, \quad R = \frac{2}{3} (1 - \beta)$$

the expression \mathbf{F}_{ik} ($k = x, y, z$) strictly coincides with expression (37) obtained above on the macrolevel.

The utterly different methods of obtaining the dependence of the force of cluster interaction on the velocities of the mixture U and of the i th component U_i lead to the same result.

Conditions on a Strong Discontinuity. In many earlier published works [22–28] the shock adiabats of mixtures were determined experimentally by measuring the shock wave velocity D in a mixture and recovering the mass velocity \mathbf{U} by the method of reflection over the velocities in screens and strikers. Usually, the shock adiabat of a mixture was determined on the assumption that the mixture is a homogeneous substance. Such an approach can be justified for components with close properties and in a narrow range of volume concentrations. In the case where the densities of the components differ greatly or the volume concentration of one of them is close to zero or unity, the validity of such an approach is doubtful. One convincing attempt to disturb the classical approach to the determination of the shock adiabat of a mixture was set forth in [28]. It is shown that in some mixtures with volume concentration of the heavy component $\alpha = 0.2$ the pressure at the shock wave undergoes a change as a result of relaxation processes long before it is overtaken by an unloading wave from the rear surface of a striker.

Numerous experimental and theoretical investigations pertaining to the study of the propagation of shock waves in multicomponent media [22–30] allow a conclusion that a shock wave in a multicomponent medium does not split into several strong discontinuities. Based on these observations, we will introduce into consideration the velocity of the propagation of a strong discontinuity in a mixture in the Lagrangian coordinates $W = \frac{dm}{dt}$. A strong discontinuity is the surface on which all the characteristics of the components and mixture change jumpwise. Irrespective of the state of the components ahead of the discontinuity, their state behind the discontinuity is always nonequilibrium: $U_i \neq U_j$, $P_i \neq P_j$, and $T_i \neq T_j$. On the surface of a strong discontinuity (behind it) relaxation processes of establishment of equilibrium begin: $U_i - U_j \rightarrow 0$, $P_i - P_j \rightarrow 0$, and $T_i - T_j \rightarrow 0$. These processes proceed in a finite-dimensional region Δx that is treated as the width of the shock wave front. Thus, the conditions on a shock wave in a mixture are the conservation laws written for the state of a substance before a strong discontinuity and at the end of the relaxation region. They cannot be obtained by summation of equations at strong discontinuities of the mixture components. The above-described structure of quantities in a shock wave agrees qualitatively with the experimental data obtained in [28].

We will consider the laws of conservation of the i th component on a strong discontinuity. We will "gather" each component into a volume θ_i that does not contain any other components. On the surface of a strong discontinuity the tangential velocity component is continuous. Therefore we will consider a transition through the discontinuity in one-dimensional statement. We will direct the Ox axis along the normal to the discontinuity surface. In a one-dimensional plane case the equations of the i th component (23)–(25) and (45) after transition from the Eulerian coordinate x to the Lagrangian one m_i will be written in the form

$$\frac{d_i}{dt} \left(\frac{1}{\rho_i} \right) - \frac{\partial U_i}{\partial m_i} = 0, \quad (56)$$

$$\frac{d_i U_i}{dt} + \frac{\partial}{\partial m_i} (P_i + F_i) - \frac{R_i}{\rho_i} = 0, \quad (57)$$

$$\frac{d_i \varepsilon_i}{dt} + \frac{\partial}{\partial m_i} (u_i (P_i + F_i) + Q_i) - \frac{\Phi_i + A_i}{\rho_i} = 0, \quad (58)$$

$$\frac{d_i \alpha_i}{dt} + \alpha_i \rho_i (U - U_i) \frac{\partial \alpha_i}{\partial m_i} + \Omega_i = 0. \quad (59)$$

We will begin the consideration of the conditions of a strong discontinuity from Eq. (59). We will multiply it by $dm_i dt$ and integrate over the rectangle $0 \leq m_i \leq \Delta m_i$, $0 \leq t \leq \Delta t_i$, where Δm_i and Δt_i are interrelated as

$$\Delta m_i = W_i \Delta t_i.$$

We will consider three integrals separately. The first integral

$$J_1 = \int_0^{\Delta m_i} \int_0^{\Delta t_i} \frac{d_i \alpha_i}{dt} dt dm_i$$

after integration over t and application of the mean value theorem has the form

$$J_1 = (\alpha_{i+} - \alpha_{i-}) \Delta m_i.$$

Here and everywhere, quantities with the subscript "+" characterize the state behind a strong discontinuity, and quantities with the subscript "-" — those ahead of the strong discontinuity. In the second integral

$$J_2 = \int_0^{\Delta t_i} \int_0^{\Delta m_i} \alpha_i \rho_i (U - U_i) \frac{d_i \alpha_i}{dm_i} dm_i dt$$

we will apply the generalized mean value theorem, after which it will take the form

$$J_2 = \left[\frac{1}{2} \Delta t_i^2 \left((\alpha_{i+} \rho_{i+} (U_+ - U_{i+}) - \alpha_{i-} \rho_{i-} (U_- - U_{i-})) W_i + \alpha_{i-} \rho_{i-} (U_- - U_{i-}) \Delta m_i \Delta t_i \right) \right] (\alpha_{i-} - \alpha_{i+}).$$

With the aid of the mean value theorem, the third integral will be presented in the form

$$J_3 = \int_0^{\Delta t_i} \int_0^{\Delta m_i} \Omega_i^* dt dm_i = \Omega_i^* \Delta t_i \Delta m_i.$$

where the asterisk means that the value of Ω_i^* lies inside of the rectangle considered. Dividing the sum of the three integrals by Δt_i and passing to the limit when $\Delta t_i \rightarrow 0$, we at $W_i \neq 0$ obtain on a strong discontinuity that

$$\alpha_{i+} - \alpha_{i-} = 0. \quad (60)$$

Following the above-given procedure of transition from differential equations (56)–(58) to equations on discontinuity, we obtain three laws of conservation of the i th component on the surface of a strong discontinuity in the form

$$\frac{1}{\rho_{i+}} W_i + U_{i+} = \frac{1}{\rho_{i-}} W_i + U_{i-}, \quad (61)$$

$$U_{i+} W_i - P_{i+} - F_{i+} = U_{i-} W_i - P_{i-} - F_{i-}, \quad (62)$$

$$\varepsilon_{i+} W_i - U_{i+} (P_{i+} + F_{i+}) - Q_{i+} = \varepsilon_{i-} W_i - U_{i-} (P_{i-} + F_{i-}) - Q_{i-}. \quad (63)$$

The quantities with the subscript "-" in Eqs. (60)–(63) are assumed known. They characterize the state before a strong discontinuity. The quantities with the subscript "+" are to be determined. To close the system of equations (60)–(63) they are supplemented with some equations. One of them is the equation of state:

$$P_{i+} = P_i(\rho_{i+}, E_{i+}). \quad (64)$$

The internal specific energy E_{i+} entering into this equation is expressed in terms of ε_{i+} and U_{i+} with the aid of the equation

$$E_{i+} = \varepsilon_{i+} - 0.5 U_{i+}^2. \quad (65)$$

Another two equations are the expressions for the functions of cluster interaction of F_{i+} and Q_{i+} :

$$F_{i+} = -0.5 \rho_{i+} (U_{i+} - U_+)^2, \quad Q_{i+} = 0.5 (U_+ - U_{i+}) (P_{i+} + \rho_{i+} E_{i+}). \quad (66)$$

Equations (66) involve the mixture mass velocity U_+ , which is expressed in terms of the velocities of the components:

$$U_+ = \sum_{i=1}^N \eta_i U_{i+}, \quad (67)$$

where

$$\eta_{i+} = \alpha_{i+} \rho_{i+} / \rho_+, \quad \rho_+ = \sum_{i=1}^N \alpha_{i+} \rho_{i+}. \quad (68)$$

Equations (60)–(68) form a system of $9N+2$ equations to determine $10N+2$ quantities W_i , P_{i+} , ρ_{i+} , E_i , U_{i+} , α_{i+} , ε_{i+} , F_{i+} , Q_{i+} , η_{i+} , U_{i+} , and ρ_{i+} . Equations (60)–(68) are not enough to construct the shock adiabat of the mixture. The fact is that the values of W_i are not interrelated, the more since they are not connected with the velocity of propagation of a strong discontinuity W in a mixture; this velocity is absent in the equations.

Velocity of Propagation of a Shock and the Speed of Sound of a Mixture. In a one-dimensional statement we will consider a quiescent volume Δx that contains N components with known physical characteristics. We will restrict ourselves to the simplest model when all the components are plane layers, having the mass Δm_i , that satisfy the conservation laws

$$\Delta m = \sum_{i=1}^N \Delta m_i. \quad (69)$$

The time of the passage of the layer of mass Δm_i by a shock wave is equal to

$$\Delta t_i = \frac{\Delta m_i}{W_i}.$$

For the successive passage of all N layers by a shock wave the following time will be required:

$$\Delta t = \sum_{i=1}^N \frac{\Delta m_i}{W_i}. \quad (70)$$

We will define the average velocity of the shock wave in the considered layered mixture by the equation

$$W = \frac{\Delta m}{\Delta t}.$$

Substituting the expressions for Δt (70) into the above equation, we will obtain the coupling of W with W_i in the form

$$\frac{1}{W} = \sum_{i=1}^N \frac{\eta_i}{W_i}, \quad (71)$$

where η_i is the mass concentration of the i th component ($\eta_i = \Delta m_i / \Delta m$). By definition

$$W = \rho (D - U), \quad W_i = \rho_i (D_i - U_i).$$

On substitution of W , W_i , and η_i (obtained from (9)) into Eq. (71), we obtain the equation

$$\frac{1}{D - U} = \sum_{i=1}^N \frac{\alpha_i}{D_i - U_i}. \quad (72)$$

The problem of finding the speed of sound of the mixture from the speeds of sound and concentrations of components has been solved by various authors recently on the assumption that the mixture has an equation of state and that the speed of sound can be determined from the classical formula

$$C^2 = \left(\frac{\partial P}{\partial \rho} \right)_S,$$

where ρ , P , and S are the density, pressure, and entropy of the mixture. Moreover, here assumptions were made implicitly that $P_i = P$, α_i and η_i are independent of P and that $S_i = \text{const}$ simultaneously with S [25, 29–31].

We will reject all such implicit assumptions, since, as has been noted above, the mixture has no equation of state. We will proceed from Eq. (72). Acoustic perturbations (infinitely weak shock waves) propagate along the characteristics of the first and second family defined by the equations

$$\frac{dx}{dt} = D = U \pm C, \quad \frac{dx}{dt} = D_i = U_i \pm C_i. \quad (73)$$

Equations (72) and (73) yield the dependence of the mixture speed of sound on the speeds of sound and volume concentrations of the components:

$$\frac{1}{C} = \sum_{i=1}^N \frac{\alpha_i}{C_i}. \quad (74)$$

It can be easily verified that Eq. (74) much more accurately describes experimental data on many multicomponent compositions than other dependences.

Velocity of Propagation of a Shock in a Mixture Component. We will consider the condition on the surface of a strong discontinuity in the i th component in the absence of cluster interaction, with this condition resulting from Eqs. (61)–(63), (65):

$$H_{i+} - H_{i-} = 0.5 W_i^2 (V_{i-}^2 - V_{i+}^2),$$

where $V_i = 1/\rho_i$, $H_i = E_i + P_i V_i$ is the enthalpy. We will add an equation that determines the change of enthalpy along the beam tangential to the isentrope at the point P_{i-} , V_{i-} :

$$H_{i+}^S - H_{i-} = 0.5 (\rho_{i-} C_{i-})^2 (V_{i-}^2 - V_{i+}^2).$$

The ratio

$$\frac{H_{i+} - H_{i-}}{H_{i+}^S - H_{i-}} = \frac{W_i^2}{(\rho_{i-} C_{i-})^2}$$

approximately characterizes the energy dissipation on a strong discontinuity in the i th component. Similarly the following equation obtains:

$$\frac{H_+ - H_-}{H_+^S - H_-} = \frac{W^2}{(\rho_- C_-)^2},$$

which approximately characterizes energy dissipation on a strong discontinuity in a mixture. We will require that the difference between the energy dissipation in all the components and the energy dissipation in the mixture be minimal. For this purpose we will consider the function

$$F = \sum_{i=1}^N \eta_i \left(\frac{W_i^2}{(\rho_{i-} C_{i-})^2} - \frac{W^2}{(\rho_- C_-)^2} \right)^2$$

and we will equate to zero all of its partial derivatives with respect to W_i . As a result, we will obtain N equations that express W_i in terms of W and in terms of the quantities ρ_{i-} , C_{i-} , ρ_- , C_- that characterize the state of the i th component and of the mixture before discontinuity:

$$W_i = W \left(\frac{\rho_{i-} C_{i-}}{\rho_- C_-} \right). \quad (75)$$

Equation (75) adds to the system of equations (60)–(68) N equations more and one quantity W . As a result, the full system of equations (60)–(68), (75) contains $10N+2$ equations and $10N+3$ quantities and is a typical shock adiabat that determines the state behind the surface of a strong discontinuity depending on one parameter W .

Particular Models. Usually, in diffusion models a continuous medium is considered, as well as an impurity having the mass concentration η . The impurity and the carrier medium move with identical velocity \mathbf{U} . In [32], continuity and concentration equations are given in a typical diffusion model:

$$\frac{\partial \rho}{\partial t} + \nabla \rho \mathbf{U} = 0, \quad \rho \frac{\partial \eta}{\partial t} + \nabla \mathbf{J} = 0, \quad (76)$$

where \mathbf{J} is the impurity flux

$$\mathbf{J} = -\rho D_0 \nabla \eta.$$

As noted above, this model contains a fundamental inconsistency. The mass concentration of the impurity η can change with time only when the impurity moves relative to the carrier medium, i.e., when its velocity is not equal to the mixture velocity. But the diffusion models are based on the hypothesis that the impurity velocity is equal to the mixture velocity, i.e., the impurity does not move relative to the carrier component. This is the crux of the inconsistency.

The MCM model considered in the present work contains two continuity equations: for the mixture and for the i th component (impurity):

$$\frac{\partial \rho}{\partial t} + \nabla \rho \mathbf{U} = 0, \quad \frac{\partial \alpha_i \rho_i}{\partial t} + \nabla \alpha_i \rho_i \mathbf{U}_i = 0. \quad (77)$$

With the aid of Eq. (9) we will write the second equation of (77) in the form

$$\frac{\partial \rho \eta_i}{\partial t} + \nabla \eta_i \rho_i \mathbf{U}_i = 0. \quad (78)$$

We will differentiate Eq. (76) termwise and replace $\frac{\partial \rho}{\partial t}$ by $\nabla \rho \mathbf{U}$ with the aid of Eq. (76). As a result we will obtain

$$\rho \frac{\partial \eta_i}{\partial t} + \nabla \eta_i \rho (\mathbf{U}_i - \mathbf{U}) = 0. \quad (79)$$

Equation (79) coincides with the second equation of (76) if

$$J = -\eta_i \rho (\mathbf{U} - \mathbf{U}_i).$$

Thus, if we define the diffusion coefficient by the equation

$$D_0 \nabla \eta_i = -\eta_i (\mathbf{U} - \mathbf{U}_i),$$

then diffusion should be described identically by the MCM model and by the diffusion model [32]. But in reality this is not the case, since in the diffusion models D_0 is usually independent of the difference of velocities.

The Darcy filtration equation [12] results from the model considered on the assumption of the stationarity of the flow. In Eqs. (23) and (24) it is assumed that

$$\frac{\partial \alpha_i \rho_i}{\partial t} = 0, \quad \frac{\partial \alpha_i \rho_i \mathbf{U}_i}{\partial t} = 0.$$

In Eq. (23) it is assumed additionally that

$$\alpha_i = \text{const}, \quad \rho_i = \text{const}, \quad \mathbf{U}_i = \text{const}.$$

After such simplifications Eq. (24) takes the form

$$\nabla P_i = \mathbf{R}_i. \quad (80)$$

Substituting the expression for \mathbf{R}_i (18) into Eq. (80), we arrive at the equation

$$\nabla P_i = \frac{\alpha_{ij}}{\tau_{ij}} (\mathbf{U}_j - \mathbf{U}_i).$$

which is the basic equation of filtration — the so-called Darcy equation.

In the case $N = 1$ Eqs. (23)–(25) transform into the classical equations of a single-component continuous medium. In the case of two components, the model can be applied for modeling nonstationary motion of MCM without widely imposed limitations (incompressibility, the simplest equations of state, etc.).

Properties of the Model. The model of a mixture of ideal media that is set forth in the article admits expansion [1]. To describe the behavior of a solid body, liquid, plasma, and of other states, the deviator of the stress tensor, heat conduction, magnetic pressure, Jole heat and other real properties and processes are included into the equations of momentum and energy of each component.

The components of the deviator of the stress tensor $\mathbf{S}_{ik} = S_{ik1}\mathbf{n}_1 + S_{ik2}\mathbf{n}_2 + S_{ik3}\mathbf{n}_3$ are connected with deformations: elasticity — by Hooke's law, plasticity — by the fluidity conditions, viscosity — by the equation for viscosity. Electric and magnetic fields are determined by the Maxwell equations, chemical reactions — by the equations of chemical kinetics, destruction — by the equation of an increase in microdamage.

The model set forth is the most general and physically most justified MCM model. It contains new forces and energy fluxes that are universal and independent of the physical properties or of the equation of state of the components. The conservation laws in transition from components to a mixture are strictly satisfied. All the equations of a model are invariant with respect to the Galilei transformation. The equations of state of components can be arbitrarily complex and in an equilibrium approximation can describe melting, evaporation, and polymorphic phase transitions [33, 34].

It should be noted that until recently no models of multicomponent media that would account for cluster interaction have been encountered in literature. Without account for cluster interaction in all of such models the conservation laws of a mixture cannot be obtained by summation of the corresponding conservation laws of components [15, 16].

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NOTATION

a_{ij} , b_{ij} , c_{ij} , functions in the equations of pair interaction of the i th and j th components; C , speed of sound; D , velocity of the motion of strong discontinuity; D_0 , coefficient of diffusion; E , internal specific energy of a mixture (per unit mass); f_{ij} , function in the equation of volume concentration; H , nonequilibrium kinetic energy of the mixture; J , impurity flux; \mathbf{K} , momentum; M , mass of a continuous medium; M_i , mass of the i th component; m_v , mass of the v th molecule; N , number of mixture components; n , number of molecules in volume θ ; P , pressure; Q_0 , energy of molecules; \mathbf{Q} , energy exchange in cluster interaction; q , internal energy; R_{ij} , function of momentum exchange in pair inter-

action; S , entropy; S_{ik} , components of stress tensor deviator; T , temperature; t , time; U , velocity; V , specific volume; W , velocity of propagation of strong discontinuity; α , volume concentration; β , γ , parameters of the function of the interaction of components; ε , total specific energy of a mixture (per mass unit); η , mass concentration; θ , volume of a mixture; ρ , density; τ_{ij} , relaxation time; ϕ_{ij} , element of the tensor of the interaction of components; Φ_{ij} , energy exchange between the i th and j th components. Subscripts and superscripts: i, j , numbers of mixture components; v , number of a molecule; l, left; r, right; c.b, contact boundary.

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