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THE ROLE OF EFFECTS DUE TO NONLOCALITY AND DELAY IN TRANSFER PROCESSES IN MICROSTRUCTURED MEDIA

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The role of effects due to nonlocality and delay in irreversible transfer processes, which arise after taking into account nonequilibrium phenomena in the medium structure is studied. By an example of the isothermal response of the medium to an instantaneous perturbation of shear velocity, the evolution of stress-tensor components is studied. It is shown that, in a medium of constant density, its strained state is determined by the tangent shear stress, by the first and second differences of normal stresses, and by the relaxation of these differences to their equilibrium values in an oscillatory process with a decaying amplitude. In this case, thermodynamic variables of state (pressure tensor and internal energy) are functions of shear velocity and time. It is found that the approximation of locally equilibrium thermodynamics is valid for microstructured media if their relaxation times are an order of magnitude shorter than the characteristic time of the problem.

There are many types of liquid flows for which adequate modeling of thermomechanical transfer processes is possible only with allowance for the actual number of microstructure states.

A model for closing the conservation laws for matter and momentum in chemically active microstructured media was proposed in [1]. This model includes evolution of a continuous internal parameter of the medium due to the change in its microstate, or, more specifically, in the first moments of the local distribution function of the microscopic probability density of some kinetic elements of the flow during a nonlocal interaction between shear, entropy, and diffusion forces. The microstate of the medium has an equilibrium scale of order $æD$, and the thermodynamic functions that depend on the initial value of the internal parameter are governed by the behavior of this parameter in the course of medium relaxation to its equilibrium state over a certain time scale $æ/\tau_*$ ($æ$ is the characteristic relaxation time, D is the diffusivity, and τ_* is the characteristic time of the nonequilibrium macroscopic process).

The microstructure of the medium is treated as a system of uniform Brownian effective friction nodes connected together by elastic subchains immersed into a structureless liquid. This choice of the medium structure is motivated by the fact that, under shear conditions, this structure displays such characteristic macroscopic properties as viscosity and elasticity.

The relaxation of the internal parameter to its equilibrium value determines the character of nonequilibrium transfer and the corresponding flows in the system as a whole.

In the approach where the thermodynamic theory of irreversible processes describes not only nonequilibrium transfer processes but also such nonequilibrium phenomena as medium-microstructure variability, including configurational changes and distortions, the principle of local thermodynamic equilibrium is abandoned.

It is known that this principle, normally used to describe sufficiently slow flows, although admits nonequilibrium [2] (dependence of macroscopic variables of state on the time-space point coordinate, but in small space scales for which conservation laws are written), restricts possible interrelations between these variables to equilibrium-thermodynamics relations of the form $f(P, \rho, T) = 0$. A typical feature of microstructured media is a nonlocal mechanism of interfield interactions: the pressure, temperature, and deformation velocity at a time-space point de-

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pend on an internal parameter that relaxes in a vicinity of this point. For this reason, the thermodynamic variables even in the small are not the same function of state as in the equilibrium state: the microstructure has not enough time to adapt itself to the new equilibrium state. In studying the dynamics of such systems, the time dependence between thermodynamic variables must be taken into account. The nonlocality of thermodynamic variables is responsible for the transition of the macroscopic system into the new equilibrium state with different relaxation times unique for each individual variable. For this reason, the delayed processes in momentum, heat, and mass transfer or, in other words, in mechanical and heat- and mass-transfer processes, manifest themselves in some "delay" of fluidity, elasticity, thermal conductivity, or give rise to elastic or inertial turbulence.

Below, an example of the isothermal response of a constant-density medium to its instantaneous perturbation from the state at rest to a state with $\dot{v}_{ij} = G = \text{const}$ is considered (G is the shear-velocity gradient). Dependences for components that characterize the change in the microstate of the medium are derived, and the evolution of the experimentally measurable component of the shear-stress tensor $\tau_{12}(t) = \tau_{21}(t)$, the evolution of differences between normal stresses $\sigma_1(t) = P_{11} - P_{22}$ (the first difference) and $\sigma_2(t) = P_{22} - P_{33}$ (the second difference), and also the change in the heat content of the unit volume of the medium in time, are studied.

In contrast to [1], variations of dynamic variables of the system are considered with allowance for kinetic rigidity of the medium microstructure [3]. In this case, a force in the form $f_4 = \alpha\zeta x_j \dot{e}_{ij}$ is introduced in addition to the above-listed forces. Here α is the kinetic rigidity (the resistance of the microstructure to shear strains), $\dot{e}_{ij} = 0.5G$ is the symmetrical part of the shear-velocity gradient tensor, $x_j \dot{e}_{ij}$ is the shear-velocity vector, and ζ is the viscous friction of the nodes (effective kinetic elements) with the structureless liquid.

In the problem of interest, the dynamic equation, the total-stress tensor under an assumption that $\tau_{ij} \gg 2\mu\dot{e}_{ij}$ (τ_{ij} is the nondeviatoric excess pressure, $2\mu\dot{e}_{ij}$ is the viscous-stress tensor, and μ is the medium viscosity, which can be determined based on the known kinematics), and the rheokinetic expression for a nonreacting medium have the form [3, 4]:

$$\partial_j P_{ij} = 0 \qquad (P_{ij} = -p^*\delta_{ij} + \tau_{ij}); \tag{1}$$

$$P_{ij} = -p^*\delta_{ij} + \varepsilon(\langle x_i x_j\rangle - \delta_{ij}) + \eta(\langle x_i x_k\rangle \dot{e}_{kj} + \dot{e}_{ik}\langle x_k x_j\rangle); \tag{2}$$

$$d_t\langle x_i x_j\rangle = \langle x_j x_k\rangle(\dot{v}_{ki} - \alpha\dot{e}_{ki}) + \langle x_k x_i\rangle(\dot{v}_{kj} - \alpha\dot{e}_{kj}) - 2æ^{-1}(\langle x_i x_j\rangle - \delta_{ij}). \tag{3}$$

Here P_{ij} is the total-stress tensor, p^* is an arbitrary scalar, $\langle x_i x_j\rangle = \displaystyle\int x_i x_j W(\boldsymbol{x}, t)\, dv$ is the moment of $W(\boldsymbol{x}, t)$, $W(\boldsymbol{x}, t)$ is the law of the probability-density distribution of friction nodes in the configuration space at the time t (the local microscopic probability density that characterizes the medium structure), δ_{ij} is the Kronecker delta, $\eta = 0.5\alpha\varepsilon æ$ is the internal viscosity, which depends on the kinetic rigidity of structural elements, $æ$ is the relaxation time (duration of internal structural transformations after strain application/removal), and ε is the elasticity modulus of the medium.

System (1)–(3) contains nondeviatoric excess stresses τ_{ij}, or, in other words, the spur of the tensor τ_{ij} is not zero. Owing to this, the quantity p^* here, unlike the case of classical thermodynamics, is not an independent variable of state. In fact, this quantity should be considered as an independent mechanical variable to be determined depending on problem conditions. That is why, we have $p^*(G, t) = p + \tau_{ii}/3$ in Eqs. (1) and (2) [5]. Here p is the hydrostatic pressure that defines the total-stress tensor through the deviatoric tensor and $\tau_{ii}/3$ is the spur of the tensor τ_{ij}.

For a medium of constant density under adiabatic conditions of deformation, the relation for the rate of conversion of mechanical energy into thermal energy can be represented in the form

$$\rho C_p\, d_t T = \tau^1_{ij}\dot{v}_{ij}, \tag{4}$$

where $\tau^1_{ij} = \tau_{ij} - \tau_{ii}/3$ is the deviatoric stress, T is the temperature that corresponds to the mean kinetic energy and varies in proportion to squared diffusion velocity [1], ρ is the density, and C_p is the specific heat.

Normal stresses arise due to the fact that the medium accumulates internal energy in some elastic form of a thermal nature. Due to this, the right-hand term in Eq. (4) is, generally speaking, the sum of dissipation and accumulated elastic energy, for instance, in the form of some difference between normal stresses.

For the type of flows under consideration, it follows from relation (3) that the system of equations for $\langle x_i x_j\rangle$ is

$$\begin{gathered}
d_t\langle x_1^2\rangle + 2æ^{-1}(\langle x_1^2\rangle - 1) = 2\langle x_1 x_2\rangle G(1 - 0.5\alpha), \quad d_t\langle x_2^2\rangle + 2æ^{-1}(\langle x_2^2\rangle - 1) = -\langle x_1 x_2\rangle \alpha G,\\
d_t\langle x_3^2\rangle + 2æ^{-1}(\langle x_3^2\rangle - 1) = 0, \quad d_t\langle x_1 x_2\rangle + 2æ^{-1}\langle x_1 x_2\rangle = \langle x_2^2\rangle G(1 - 0.5\alpha) - 0.5\alpha G\langle x_1^2\rangle,\\
d_t\langle x_2 x_3\rangle + 2æ^{-1}\langle x_2 x_3\rangle = -0.5\alpha G\langle x_1 x_3\rangle, \quad d_t\langle x_1 x_3\rangle + 2æ^{-1}\langle x_1 x_3\rangle = \langle x_2 x_3\rangle G(1 - 0.5\alpha).
\end{gathered} \tag{5}$$

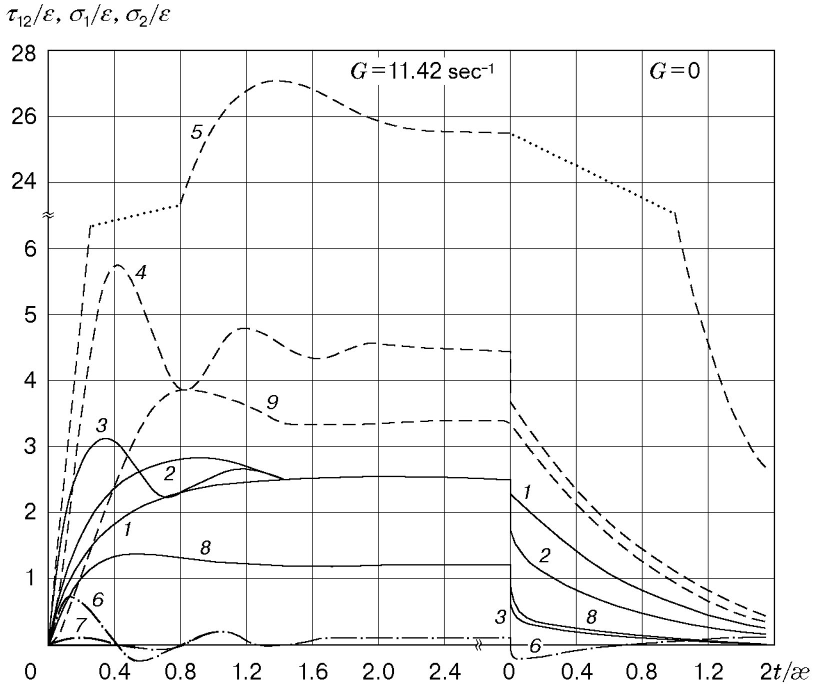

Fig. 1. Dependences of τ_{12}/ε (1, 2, 3, and 8), σ_1/ε (4, 5, and 9), and σ_2/ε (6 and 7) on the parameter $2t/æ$, calculated by formulas (8) for the case of an instantaneously applied (on the left) and then removed (on the right) constant shear-velocity gradient: 1) $æ = 0.8$ and $\alpha = 10^{-3}$; 2) $æ = 0.8$ and $\alpha = 10^{-2}$; 3) $æ = 0.8$ and $\alpha = 10^{-1}$; 4) $æ = 0.8$ and $\alpha = 10^{-1}$; 5) $æ = 0.8$ and $\alpha = 10^{-2}$; 6) $æ = 0.8$ and $\alpha = 10^{-1}$; 7) $æ = 0.8$ and $\alpha = 10^{-2}$; 8) $æ = 0.4$ and $\alpha = 10^{-1}$; 9) $æ = 0.4$ and $\alpha = 10^{-1}$.

Under the conditions $\langle x_i x_i\rangle = 1$ and $\langle x_i x_j\rangle = 0$ at $t = 0$, from the system of inhomogeneous differential equations we find the components of the distribution-function moment matrix $\|\langle x_i x_j\rangle\|$ using the method of variation of arbitrary constants [4]:

$$\begin{gathered}
\langle x_1^2\rangle = 0.5b^{-1}(A + 2æ^{-1}B - a + b), \quad \langle x_2^2\rangle = 0.5a^{-1}(A + 2æ^{-1}B + a - b), \quad \langle x_3^2\rangle = 1, \\
\langle x_2x_3\rangle = \langle x_3x_2\rangle = \langle x_1x_3\rangle = \langle x_3x_1\rangle = 0, \qquad \langle x_1x_2\rangle = B, \\
A = \gamma r_1 \exp(r_1 t) + \beta r_2 \exp(r_2 t), \quad B = 2(a+b)/(r_1 r_2 æ) + \gamma \exp(r_1 t) + \beta \exp(r_2 t), \\
r_{1,2} = -2æ^{-1} \pm 2(ab)^{0.5}, \quad \gamma = -(a+b)(1 + 2/(æ r_1))/(r_2 - r_1), \\
\beta = (a+b)(1 + 2/(æ r_2))/(r_2 - r_1), \quad a = G(1 - 0.5\alpha), \quad b = -0.5\alpha G.
\end{gathered} \tag{6}$$

Relations (6) characterize the distortions of the medium microstructure in time due to its instantaneous perturbation with a uniform shear velocity. The shear affects the microstructure of the liquid and, correspondingly, the macroscopic transfer characteristics.

In accordance with (2), the stress-tensor components $\|P_{ij}\|$ acquire the form

$$\begin{gathered}
P_{11} = -p^* + \varepsilon(\langle x_1^2\rangle - 1) - æ\varepsilon b\langle x_1x_2\rangle, \quad P_{22} = -p^* + \varepsilon(\langle x_2^2\rangle - 1) - æ\varepsilon b\langle x_1x_2\rangle, \\
P_{33} = -p^*, \quad P_{12} = \varepsilon\langle x_1x_2\rangle - 0.5æ\varepsilon b(\langle x_1^2\rangle - \langle x_2^2\rangle), \quad P_{23} = P_{13} = 0.
\end{gathered} \tag{7}$$

In experiments, the normal-stress differences $\sigma_1 = P_{11} - P_{22}$ (first) and $\sigma_2 = P_{22} - P_{33}$ (second) are usually measured, as well as the tangent shear stress τ_{12}:

$$\begin{gathered}
P_{11} - P_{22} = \varepsilon(\langle x_1^2\rangle - \langle x_2^2\rangle), \quad P_{22} - P_{33} = \varepsilon[(\langle x_2^2\rangle - 1) - æb\langle x_1x_2\rangle], \\
P_{12} \equiv \tau_{12} = \varepsilon[\langle x_1x_2\rangle - 0.5æb(\langle x_1^2\rangle - \langle x_2^2\rangle)].
\end{gathered} \tag{8}$$

Figure 1 shows the calculation results obtained by formulas (8) for the case of an instantaneously applied and then removed constant shear-velocity gradient $G = 11.42$ sec^{-1}. Is it seen that the mechanical characteristics of the

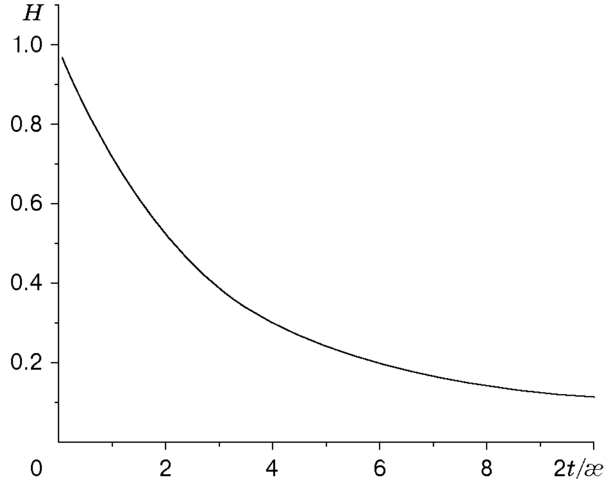

Fig. 2. Nonlinear time dependence between thermodynamic variables.

system approach their equilibrium values with their own relaxation times. The oscillatory transition regime with decaying amplitude points to the existence of near-order correlation moments, which is typical of microstructured fluid media.

An analysis of the results shows that the value of σ_1 depends on the deviation of the medium microstructure from its equilibrium state, whereas the value of σ_2 is determined by the deviation rate. The second difference between normal stresses depends on the kinetic rigidity of the chains; the influence of this difference is observed at the unsteady stage of deformation only.

The introduction of an additional force f_4, dependent on the rigidity of the elastic microstructure, into the rheokinetic model exerts no effect on the most probable equilibrium state: only the rate of transition from one configuration state into the other changes under the action of the constant shear-velocity gradient G. Thus, with rigidity introduced into the microstructure, the entropy of its most probable state remains unchanged, and only the rate of configuration transformations undergoes changes.

The rate of irreversible conversion of mechanical energy of the medium into its internal energy can be found from relations (2)–(7) with $\alpha = 0$.

For $\dot{v}_{ij} \equiv G$, $t = 0$, and $T = T_0$ (T_0 is the initial temperature), it follows from (4) that

$$4\rho C_p(T - T_0)/(\varepsilon æ^2 G^2) = 2t/æ + \exp(-2t/æ) - 1.$$

Figure 2 shows the dependence between thermodynamic variables in the form

$$H \equiv 1.5(p^* - p)/(\rho C_p(T - T_0)) = [1 - \exp(-2t/æ) - (2t/æ)\exp(-2t/æ)][2t/æ + \exp(-2t/æ) - 1]^{-1}.$$

It is seen that, as the system undergoes an instantaneous perturbation with a uniform shear velocity, a nonlinear time dependence between thermodynamic variables is observed. The response of the considered macrosystem to mechanical and thermal perturbations depends on the time of internal structural transformations. In the region $2t/æ > 10$, approximations of locally equilibrium thermodynamics are valid.

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