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EFFECT OF MEMORY ON DISSIPATIVE STRUCTURES FORMING IN DISTRIBUTED KINETIC SYSTEMS

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Integrodifferential equations which include memory effects are proposed for describing the formation of dissipative structures in distributed kinetic systems.

Quite thorough studies have been made in recent years concerning dissipative structures in distributed kinetic systems describable by parabolic equations of transfer [1-5], these equations being derived from the conditions of balance and from phenomenological laws which express instantaneous and local relations between thermodynamic fluxes and forces on the assumption that local equilibrium prevails in every small element of the medium. The local state of the medium is, moreover, completely described by an equation which does not contain any gradients. In most models the kinetic transfer coefficients are assumed to be constant [1-3]. Equations of the parabolic kind with constant transfer coefficients admit solutions (not physically realistic) which yield infinitely large fluxes at time zero [6-8]. Despite these singularities in the solutions, the latter rather accurately describe experimental data obtained in studies of structurization during low-intensity transient processes. Singularities in the solutions to parabolic equations cause difficulties of theoretical nature, however, in description of experimental data obtained about dissipative structures in distributed active systems during fast nonequilibrium processes. In such processes the gradients are large and dispersion effects become significant so that it becomes necessary to include nonlocality and memory effects in the relations between thermodynamic fluxes and forces. It is then incorrect to describe the formation of structures with parabolic equations derived in accordance with conventional nonequilibrium thermodynamics, and equations of far-from-equilibrium thermodynamics are required instead.

Methods of nonlinear thermomechanics of continuous media yield the equations

$$\alpha_n(0)\frac{\partial^2 z_n(x,\,t)}{\partial t^2}+\beta_n(0)\frac{\partial z_n(x,\,t)}{\partial t}+\int_0^\infty \beta_n'(\theta)\frac{\partial z_n(x,\,t-\theta)}{\partial t}\,d\theta=$$

$$=k_n(0)\nabla^2 z_n(x,\,t)+\int_0^\infty k_n'(\theta)\nabla^2 z_n(x,\,t-\theta)\,d\theta+$$

$$+\sum_r \nu_{nr}\dot{W}_r'+\Phi(x,\,t),$$

$$C_V\frac{\partial^2 T(x,\,t)}{\partial t^2}+\beta(0)\frac{\partial T(x,\,t)}{\partial t}+\int_0^\infty \beta'(\theta)\frac{\partial T(x,\,t-\theta)}{\partial t}\,d\theta=\qquad (1)$$

$$=k(0)\nabla^2 T(x,\,t)+\int_0^\infty k'(\theta)\nabla^2 T(x,\,t-\theta)\,d\theta=$$

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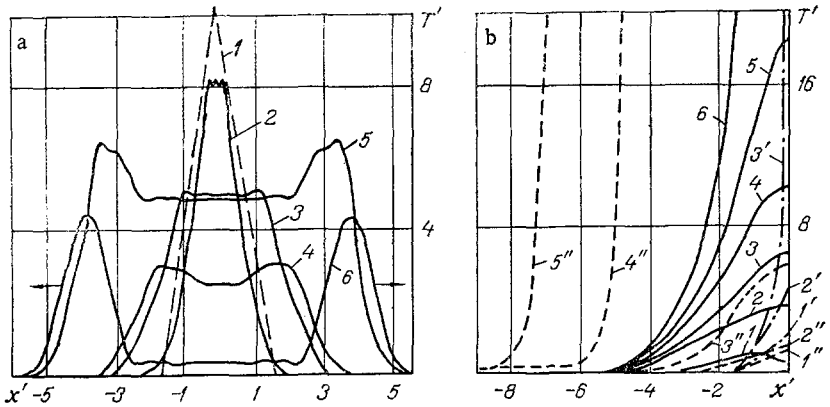

Fig. 1. Space–time distribution of temperature (T) during combustion with evolution of dissipative structures from initial temperature fluctuation: (a) formation of two dissipative structures during decay of one initial temperature fluctuation [formation time $t_2' = 120$; $m = l = 10$; $\tau_n = \tau_n' = 10^3$; $\psi = 0$; 1) $t' = 0$; 2) $t' = 0.19$; 3) $t' = 0.99$; 4) $t' = 1.99$; 5) $t' = 99.9$; 6) $t' = 120$]; (b) formation of structures in peaking and localization mode (only halves of symmetric profiles shown), solid lines representing structure with temperature profile whose half-width increases at first instant [$m = l = 10$; $\tau_n = \tau_n' = 10^2$; 1) $t' = 13.9$; 2) $t' = 31.7$; 3) $t' = 35.7$; 4) $t' = 37.7$; 5) $t' = 39.7$; 6) $t' = 41.7$]; dash-dot lines representing structure with temperature profile whose half-width decreases with time [$m = 7$; $l = 2$; $\tau_n = \tau_n' = 10^9$; $\psi = 100\phi$; 1') $t' = 0.01$; 2') $t' = 0.1$; 3') $t' = 0.2$]; dash lines representing structure formed in process with infinitesimally short memory [$m = 7$; $l = 2$; $\tau_n \to 0$; $\tau_n' \to 0$; $\psi = 0$; 1") $t' = 0.2$; 2") $t' = 0.3$; 3") $t' = 1.9$; 4") $t' = 2.9$, 5") $t' = 4.3$]; memory length τ_n in units of time $\tau' = a\beta(0)/k(0)$; $t' = t/\tau'$, $x' = x/(\tau' a)^{1/2}$; $T' = T/T_0$.

$$= -\sum_r \sum_n \nu_{nr} H_n \dot{W}_r',$$

$$\frac{d}{dt}(W')_r = -\sum_{s=1}^{R}\sum_{n=1}^{N} \nu_{ns}\left(a_{rs}(0)\,\mu_n + \int_0^\infty a_{rs}'(\theta) \times \right.$$

$$\left. \times \frac{d}{dt}\,\mu_n(x,\ t-\theta)\,d\theta\right),\ n = 1, 2, \ldots, N,\ r,\ s = 1, 2, \ldots, R,$$

$$a_{rs}(0) = a_{sr}(0),\ a_{rs}'(\theta) = a_{sr}'(\theta)$$

describing the structurization process with memory effects without convection [9]. The memory effects are described by kinetic kernels, the latter being time correlation functions for fluxes with various lengths of correlation decay time (various lengths of memory persistence). These kernels account only for the role of equilibration processes faster than the thermodynamic ones. Functions characterizing kernels in the phenomenological formulation are either determined experimentally or stipulated so as to satisfy thermodynamic constraints based on the Second Law [10]. Functions describing kernels which depend on the intermolecular interaction potentials, on the temperature, the density, etc. can be derived directly by methods of statistical nonequilibrium thermodynamics [11]. The appearance of integral terms in Eqs. (1) is a consequence of an abridged system description at the level of thermodynamic quantities. When the gradients of fluxes do not vary appreciably over the correlation decay time and distance, then the delay terms in integrodifferential Eqs. (1) become negligible and differential equations of transfer are obtained as a result. Differential equations of various kinds are obtained, depending on the form of functions which describe the kinetic kernels. With constant kinetic coefficients in kernels characterizing an infinitesimally short memory, for instance, we have the parabolic equations on which the modern

theory of dissipative structues has been constructed [1-5]. For kernels describing processes with infinitely long memory, on the other hand, Eqs. (1) yield wave equations. In the intermediate case with a memory of finite length in a process with Maxwell—Cattaneo kernels, finally, Eqs. (1) yield telegrapher's equations: hyperbolic equations including the simplest form of memory, namely a finite velocity of matter propagation.

The graph in Fig. 1 depicts results of numerical solution of Eqs. (1) and illustrates the formation of structures during combustion initiated by a temperature fluctuation in a distributed one-component (N = 1) kinetic system. The profiles of initial fluctuations from which structures shown here evolve are the same. The system of Eqs. (1) was solved numerically for kernels and source functions

$$k'(\theta) = \frac{k(0)}{\tau_n}\exp\left(-\frac{\theta}{\tau_n}\right),\ \beta'(\theta) = 0,\ \beta(0) = \text{const} > 0,$$

$$a'_{rs}(\theta) = \frac{a_{rs}(0)}{\tau'_n}\exp\left(-\frac{\theta}{\tau'_n}\right),$$

$$\dot{W}'_r = T^l(1 - T^{m-l}) + \int_0^\infty a'_{rs}(\theta)\,T^l(\theta)\,d\theta,$$

$$n = r = s = 1$$

with initial and boundary conditions

$$T(x,\ 0) = \varphi(x),\ \frac{\partial T}{\partial t}(x,\ 0) = \psi(x),$$

$$T|_{\partial\Omega} = \omega(x),\ t > 0,\ \Omega : \{x \in [-x_0,\ x_0]\},$$

$$\varphi(x) = \begin{cases} b(x - l_1)/(l_2 - l_1),\ l_1 \leqslant x \leqslant l_2, \\ b(l_3 - x)/(l_3 - l_2),\ l_2 \leqslant x \leqslant l_3, \end{cases}$$

$$\psi(x) = N\varphi(x),\ N = 100,\ \omega(x) = 0,\ b = 1,$$

$$l_3 - l_2 = 2.8,\ l_2 - l_1 = 1.4.$$

The algorithms of solution of Eqs. (1) and the difference scheme used for the solution, also a validation of these calculations, are all given in earlier reports [9, 12, 13].

The graph in Fig. 1a depicts dissipative structures evolving from one initial temperature fluctuation. These structures spread in opposite directions (as indicated by arrows) and pulsate periodically. The length of time taken by formation of two structures depends on length τ_n' of the memory. Also the type and the characteristics of structures which form in the peaking and localization mode (Fig. 1b) depend on length τ_n' of the memory (with φ, ψ, m, l remaining invariable). When the memory length is equal to t_1':

$$\tau'_n = t'_1 = \frac{[(\varphi,\ \varphi) + (\varphi,\ \psi)]^{1/2} + [(\varphi,\ \varphi) + (\varphi,\ \psi) + 10(m-1)/(l+1) + 2(\varphi,\ \psi) + (16/(m-1))(\varphi,\ \varphi)(\varphi,\ \psi)]^{1/2}}{+ [(\varphi,\ \varphi) + (\varphi,\ \psi)]^{1/2}},\ \varphi > 0,\ \psi > 0,$$

$$(\varphi,\ \varphi) = \int_\Omega \varphi(x)\,\varphi(x)\,dx,\ (\varphi,\ \psi) = \int_\Omega \varphi(x)\,\psi(x)\,dx,$$

then the release of heat during the combustion process becomes localized within a structure whose half-width remains constant in time. The length of time t_2' taken by formation of such a structure depends on τ_n', namely,

$$t'_2 = \frac{2\tau'_n}{\beta_n(0)}\ln\left\{\frac{[(m-1)/4]\,\tau'_n(\varphi,\ \psi) + \frac{l}{4}(\psi,\ \psi)}{[(m-1)/4]\,\tau'_n(\varphi,\ \psi) - \frac{\beta_n(0)}{2}(\varphi,\ \varphi)}\right\},$$

$$\psi > 0,\ \varphi > 0.$$

As the memory becomes infinitely long $\tau_n' \to \infty$, $\tau_n \gg t_1'$, the structure in the peaking and localization mode forms with a half-width which decreases in time and a length of time taken by its formation which does not depend on τ_n':

$$t_2' = [4(\varphi, \varphi)/(m-1)](\varphi, \psi), \ \psi > 0, \ \varphi > 0.$$

As the memory becomes shorter than t_1', structures in the peaking mode appear in the medium with a combustion zone whose half-width increases at the first instant and which subsequently localizes within a definite width.

Evidently, therefore, the conditions of structurization in the peaking and localization mode depend on the length of the memory. It is to be noted that the processes under consideration here occur in one-component systems according to Eqs. (1) with constant coefficients. In earlier studies formation of structures in the peaking and localization mode in one-component systems was tracked on the basis of parabolic equations with power-law temperature-dependent transfer coefficients, considering in that case definite relations between the power exponents of these coefficients and the power exponents in the source function [4, 5].

When Eqs. (1) have Maxwell—Cattaneo kernels and functions $\dot{W}_r' = T - T^3$, $\dot{W}_r' = -T + T^3$, then they have soliton solutions for high-temperature combustion. When they have kernels corresponding to processes with infinitely long memory and functions $\dot{W}_r' = \xi \exp(T)$, which characterize high-temperature ignition, then Eqs. (1) have three soliton solutions with one of them an unstable one. When

$$\dot{W}_r' = T^l + \int_0^\infty a_{rs}'(\theta) T^l(\theta) d\theta, \ l > 3,$$

then Eqs. (1) describe self-localized long-wave oscillations during combustion. According to today's prevailing theory of combustion and dissipative structures, based on parabolic equations of transfer, there should not exist any solitons [1-5]. Solutions to those parabolic equations can be obtained from the solutions to Eqs. (1) by letting the length of the memory approach zero.

NOTATION

z_n, molar volume concentration of a substance; T, temperature of a substance; $\beta_n(0)$, $k_n(0)$, $a_{rs}(0)$, $\alpha_n(0)$, $\beta(0)$, $k(0)$, kinetic coefficients; $k'(\theta)$, $a_{rs}'(\theta)$, $\beta_n(\theta)$, $k_n'(\theta)$, $\beta'(\theta)$, kinetic kernels of the memory; $\dot{W}_r$, rate of a reaction referred to unit volume; ν_{ns}, stoichiometric coefficient for n-kind particles in a chemical reaction s; μ_n, chemical potential of n-kind particles; H_n, partial molar enthalpy of substance n; $\Phi(x, t)$, function of external sources; θ, t, time; x, space coordinate; τ_n, τ_n', relaxation times in Maxwell—Cattaneo kernels; C_V, thermal capacity at constant volume; λ, thermal conductivity in state of equilibrium; a, thermal diffusivity; D, diffusion coefficient; m, l, power exponents in the source function; $\psi(x)$, $\varphi(x)$, functions characterizing the initial temperature distribution; $\omega(x)$, function characterizing the temperature distribution over boundary $\partial\Omega$ of region Ω.

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THERMAL STRESSES IN A HEAT-SENSITIVE SPHERE

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A solution is obtained for the quasistatic problem of thermoelasticity for a heat-sensitive sphere heated by a heat flux. Thermal stresses are investigated in a steel sphere.

Let us examine an isotropic elastic sphere of radius R, free from external load but subjected to sudden heating by a heat flux of constant density q. The initial temperature of the sphere is zero. All the physicomechanical characteristics of the material except the coefficient ν are functions of the temperature.

For many materials [1] the temperature dependences of the heat conduction $\lambda_t(t)$ and volume specific heat $c_v(t)$ coefficients are identical in nature, whereupon their coefficient of thermal diffusivity is $a = \lambda t(t)/c_v(t) = \text{const}$. Then by using the Kirchhoff variable

$$\vartheta^*(t^*) = \int_0^{t^*} \lambda_t^*(\xi)\, a\xi \tag{1}$$

the nonlinear heat-conduction problem is linearized. We consequently arrive at a boundary-value problem for the Kirchhoff variable:

$$\rho^{-2}\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial\vartheta^*}{\partial\rho}\right) = \frac{\partial\vartheta^*}{\partial \mathrm{Fo}}\,, \tag{2}$$

$$\left.\frac{\partial\vartheta^*}{\partial\varsigma}\right|_{\rho=0} = 0, \quad \left.\frac{\partial\vartheta^*}{\partial\rho}\right|_{\rho=1} = \mathrm{Ki}\, S_+(\mathrm{Fo}), \tag{3}$$

$$\vartheta^*(\rho,\ 0) = 0, \tag{4}$$

whose solution has the form [2]

$$\vartheta^* = \mathrm{Ki}\left[\ 3\mathrm{Fo} - \frac{3-5\rho^2}{10} - \sum_{n=1}^{\infty}\frac{2\sin\mu_n\rho}{\mu_n^3\rho\cos\mu_n}\exp\left(-\mu_n^2\ \mathrm{Fo}\right)\ \right], \tag{5}$$

where $t^* = t/t_0$; $\rho = r/R$; $\mathrm{Fo} = a\tau/R^2$; $\lambda_t^*(t^*) = \lambda_t(t)/\lambda_t^{(o)}$; $\mathrm{Ki} = qR/\lambda_t^{(o)}t_0$ is the Kirpichev criterion; μ_n are the roots of the characteristic equation $\tan\mu = \mu$.

Knowing the expression for the Kirchhoff variable and the temperature dependence of the heat-conduction coefficient, we can determine the temperature field in the sphere from the relationship (1).

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