HYDRODYNAMICS HARMFUL EMISSIONS AMONG THE METHODS OF NONEQUILIBRIUM THERMODYNAMICS

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Study of hydrodynamics of harmful emissions into the environment by means of mathematical modeling is an urgent problem.

The purpose of research - to formulate a mathematical model of anthropogenic emissions by non-equilibrium thermodynamics.

Materials and methods of research. The linear non-equilibrium thermodynamics as defining (rheology) relationships that complement the system of hydrodynamic equations of conservation, applied the phenomenological relations of irreversible processes (Onsager relations):

$$J_k = \sum_{k=1}^{Q} L_{kl} \cdot X_l \,; \quad (k = 1,2 \ldots Q), \tag{1}$$

where K - the number of independent physical processes; Lkl - phenomenological matrix (kinetic) coefficients linking the flow of Jk and thermodynamic forces Xl. First match the rate of change of extensive quantities (such as mass, energy), for which there are conservation laws, or portable units (such as heat) which are associated with the flow in the conservation laws; the second is proportional to the gradients of intensive parameters, deflection from equilibrium thermodynamic system. Fluxes and thermodynamic forces in (1) are, in general, of any rank tensor quantities. As mentioned above, in the framework of the phenomenological theory of the explicit form of the kinetic coefficients in (1) is not deciphered, but their physical meaning can be clarified within the framework of molecular - kinetic theory. The number of non-zero kinetic coefficients in (1) is limited by the Curie principle according to which, by virtue of the symmetry properties of the considered material environment, the components (where components of the vectors along the coordinate axes) flows will depend not on all components of the thermodynamic forces. In particular isotropic system (the properties of which in the equilibrium condition the same in all directions), processes different tensor dimensions do not interact with each other. In addition, when the axiomatic approach is accepted as an independent postulate symmetry relations Onsager - Casimir (reciprocity)

$$L_{kl} = (B, \Omega) = \varepsilon_k \varepsilon_l \cdot L_{lk}(-B, -\Omega), \tag{2}$$

which allows to minimize the number of phenomenological coefficients in the linear equation (1). Where B - magnetic induction, W - the angular velocity of rotation of the system, and for the even (energy concentration) and odd (pulse density) macroscopic parameters (even or odd function of the velocity of the particles). For an isotropic non-rotating system in the absence of an external magnetic field symmetry relations (2) acquire a simpler form:

$$L_{kl} = L_{lk}\,, \tag{3}$$

где L_{kl} – скалярные величины.

The symmetry relations (2) may be regarded as an axiom is empirically stable, regardless of the evidence in the framework of statistical mechanics. Experimental confirmation of the principle of reciprocity is as convincing as confirmation of 1st, 2nd and 3rd law of thermodynamics. This gives reason to erect a postulate (2) the status of a paradigm shift, and used as a basis to describe a wide range of phenomena.

To determine the flows and their conjugate thermodynamic forces are usually used concrete representation of the rate of production (power density) of the entropy within the system in this irreversible process in the form of a bilinear form.

$$T\sigma_{(S)} = \sum_{k=1}^{Q} J_k X_k \geq 0, \tag{4}$$

and, after a defined flow Jk, their associated forces are uniquely Xk, the coefficients corresponding to the flow in this expression.

The results of research. We apply the provisions set out in the analysis of dissipative function and entropy production in a two-phase medium.

Assume the assumption of local thermodynamic equilibrium in phase, as well as assumption of additive mixture of internal energy and entropy of the mixture from the masses of the mixture of phases.

$$\rho u = \sum_{i=1}^{N} \rho_i u_i\left(\rho_i^o, T_i\right), \;\; \rho s = \sum_{i=1}^{N} \rho_i s_i\left(\rho_i^o, T_i\right), \qquad (5)$$

where ρ - density of the mixture; u - internal energy; T - absolute temperature; and - the entropy; N - number of phases; - True density of the i-th phase; i - the index represents the number of phases.

Consider dissipative function for a heterogeneous environment, ie function that gives the entropy production mix for a fixed mass media through internal processes. Substantial derivative of entropy along the lines of the current phase is given.

$$\rho \frac{D_S}{Dt} = \sum_{i=1}^{N} \left\{ \rho_i \frac{d_i s_i}{dt} + \sum_{j=1}^{i=1} J_{ij}\left(s_i - s_j\right) \right\}. \qquad (6)$$

where ρ - density of the mixture; u - internal energy; T - In contrast to the change in the total energy of the medium E described derivative, the change in entropy of the mixture described, due not only to external influence, but also to internal processes (between phases and in phase) in a selected volume of the medium. As well as, the value is not associated with the inflow and outflow of the substance from the phase of the selected volume.

In this case, the heterogeneous mixture can be considered as consisting of two phases. The dissipative function is represented by the following thermodynamic forces:

$$X_1^k = \frac{e_1^k}{T_1};\; X_2^k = \frac{e_2^k}{T_2};\;\; X_{q1}^k = \nabla^k\left(\frac{1}{T_1}\right);\;\; X_{q2}^k = \nabla^k\left(\frac{1}{T_2}\right);$$

$$X_F^k = \left(\upsilon_1^k - \upsilon_1^k\right)\left(\frac{\chi_{21}}{T_1} + \frac{\chi_{12}}{T_2}\right);\; X_Q = \frac{1}{T_2} - \frac{1}{T_1}; \qquad (7)$$

$$X = \frac{Z_1}{T_1} - \frac{Z_2}{T_2} + i_{12}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) + \frac{\left(V_{12} - V_2\right)^2}{2T_2} - \frac{\left(V_{21} - V_1\right)^2}{2T_1};$$

and thermodynamic flows:

$$J_1^k = \tau_1^k;\; J_2^k = \tau_2^k;\; J_{q1}^k = q_1^k;$$

$$J_{q2}^k = q_2^k;\; J_Q = Q_{12}. \qquad (8)$$

In accordance with the thermodynamics of nonequilibrium dissipative function is a sum of products of thermodynamic forces on the thermodynamic flows.

$$\begin{aligned} D_S^{(\mathrm{int})} &= \sum J_0 X_0 = \tau_1^k \frac{e_1^k}{T_1} + \tau_2^k \frac{e_2^k}{T_2} + q_1^k \nabla^k \left(\frac{1}{T_1}\right) + q_2^k \nabla^k \left(\frac{1}{T_2}\right) + \\ &+ F_{12}^k \left(\upsilon_1^k - \upsilon_2^k\right)\left(\frac{\chi_{21}}{T_1} + \frac{\chi_{12}}{T_2}\right) + Q_{12}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) + \\ &+ J_{12}\left[\frac{z_1}{T_1} - \frac{z_2}{T_2} + i\left(\frac{1}{T_2} - \frac{1}{T_1}\right) + \frac{\left(V_{12} - V_2\right)^2}{T_2} - \frac{\left(V_{21} - V_1\right)^2}{2T_1}\right]. \end{aligned} \tag{9}$$

In the formulas (6) - (9), the values of: τk - tensor shear directions; Jij - the intensity of an array of phase transitions per unit volume of the mixture; - The strain rate tensor; - The diffusion coefficient; zi - thermodynamic potential; - Tensor of heat flow; χ - polytropic exponent; vji - the rate of weight due to phase transition; i, j - the index represents the number of phases; superscript k - number of Cartesian coordinates.