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A physical model is proposed as are integral dependences of the friction coefficient and Stanton number on the chemical reaction rate in a gas flow.

The general problem of the interaction of physicochemical processes with turbulence has not yet been solved completely, however, some of its aspects have been studied in sufficient detail. The significant influence of turbulent fluctuations on the mean chemical reaction rate has been shown, certain mechanisms have been established for the influence of nonequilibrium physicochemical processes on the coefficients of turbulent substance and energy transfer, and mathematical models of a number of processes have been developed [1-3].

Studied least is the mechanism of the influence of nonequilibrium processes on hydrodynamic turbulence, qualitative models have not been developed for turbulent friction and heat transfer, there are practically no necessary integral regularities.

To solve these problems we turn to an analysis of the structure of a nonequilibrium turbulent boundary layer. According to standard representations, turbulent friction is due to the exchange of momentum of elementary turbulent formations performing chaotic motion between two adjacent fluid or gas layers. Any internal process, including a chemical reaction, cannot change the momentum of a moving mole.

The influence of bulk sources of substance and energy can appear only in a change of the thermophysical properties of a medium. Therefore, the problem of describing hydrodynamic turbulence in reacting gases reduces substantially to a problem of turbulent heat and mass transfer in inhomogeneous media. A qualitative solution of the question of the influence of a bulk source on the regularities of turbulent transfer can be obtained by analyzing the general problem of a turbulent boundary layer.

Attention has been turned to the substantial influence of laminar sublayer stability on the general turbulent flow and heat transfer characteristics [4, 5] in many recent experimental investigations. However, the results of studying the friction, heat and mass transfer coefficients are represented, as a rule, as a function of different derivatives of the stability factor: the temperature factor, the stream Mach number, etc. [6]. At the same time, a general stability criterion exists for a definite circle of flows, the curvature of the gas velocity profile at a wall [7]. It is determined in an inhomogeneous thermal field by the change in dynamic viscosity of the gas [7]

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{up} = -\frac{1}{\mu_e} \left(\frac{\partial \mu}{\partial y} \frac{\partial u}{\partial y}\right)_{up}.$$

Converting the expression to a normal form, we obtain the flow destabilization criterion under nonequilibrium heat and mass transfer conditions

$$\mathrm{De} = -n \; \frac{\mu_w}{\mu_e \theta_w} \left(\frac{\partial \theta}{\partial u}\right)_w - \frac{\mu_2 - \mu_1}{\mu_e} \left(\frac{\partial c_2}{\partial u}\right)_w,$$

where θ is the relative gas temperature, c is the relative concentration of the reacting component of a binary mixture, u is the relative velocity, and μ_1 , μ_2 are the viscosity coefficients of a binary mixture of gases.

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Fig. 1. Dependence of the friction coefficient on the destabilization factor De (generalization of experimental data [6, 8]).

Positive values of the criterion correspond to the destabilizing influence on the thermophysical actions and the negative to stabilizing influence. A criterion of analogous form can be formulated also for the action of blowing or acceleration on the hydrodynamic flow.

Utilization of a criterion of general form permits the description of turbulent friction regularities by one equation under conditions of both heat transfer and internal heat liberation that is characteristic for reacting gas flows. The hydrodynamics of nonequilibrium flows has been investigated inadequately. Consequently, to determine the turbulent friction we use experimental data on flows with external heating and supersonic flows [6, 8]. Any particular regularity converted identically to a form containing the stability criterion can be used as the mode of the general friction law. Utilizing the extensively used powerlaw dependence of the relative friction coefficient on the temperature factor we obtain

$$\frac{C_f}{C_{f_0}} = (1 + \mathrm{De})^{-0.55} \,. \tag{1}$$

The regularity (1) is compared in Fig. 1 with experimental data obtained under heat transfer and compressibility conditions of a medium [6, 8]. The satisfactory description of the different experimental data by one equation is seen. In the nature of derivation, the regularity (1) is universal for actions whose influence is manifest in velocity profile stabilization or destabilization. The definition of the stability parameter is common and based on calculations of the second derivative of the gas velocity near the wall here for flows with blowing, a pressure gradient, heat and mass transfer. Shown for comparison in Fig. 1 are experimental data on blowing converted by using the destabilization factor [6]. A further search for a common stability criterion is needed for other actions.

We use the law (1) to describe the nonequilibrium physicochemical processes in a boundary layer. Let us examine the qualitative solution for an inhomogeneous source of particles of the form $Q = Q_0 y^m$. A change in the exponent m permits simulation of different reaction rate distributions encountered in practical problems.

Determination of the stability criterion of a nonequilibrium flow requires knowledge of the gas concentration and temperature distribution in the boundary layer. A sufficiently exact description for the purposes of the present analysis can be obtained for the stream parameters by using the method of local self-similarity [9]. The transport differential equations corresponding to this approach have the form

$$\frac{\partial}{\partial y} \left(\frac{\tau c_p \partial T}{\Pr \partial u} \right) = Q h_0, \tag{2}$$

$$\frac{\partial}{\partial y} \left(\frac{\tau}{\mathrm{Sc}} \frac{\partial c}{\partial u} \right) = -Q, \tag{3}$$

 $h_{\ensuremath{\text{0}}}$ is the enthalpy of reaction product formation, and y is the coordinate normal to the surface.

The condition $Pr \simeq Sc$ used extensively in the theory of the nonequilibrium boundary layer is applied in writing (2) and (3).

For definiteness we assume that the surface of the apparatus is not catalytic

$$y=0; \quad \frac{\partial c}{\partial u}=0; \ T=T_w; \ y \to \infty; \ c=c_\infty; \ T=T_e.$$



As a result of the double integration of (2) and (3) under the conditions τ = $\tau_W,$ u ~ $y^{1/p}$ we obtain

$$\frac{\mathrm{St}}{\mathrm{St}_0} = \frac{C_f}{C_{f_0}} - K \frac{\overline{Q}2h_0}{c_p\Delta TC_{f_0}}, \ c_w = c_e + K \frac{\overline{Q}2\,\mathrm{Sc}}{C_f\,\mathrm{Pr}},$$

where $\bar{Q} = \int_{0}^{R} \frac{Q}{\rho_0} dy$ is the mean source density.

A feature of the solution obtained is the dependence on a single complex that includes all the parameters undetermined in this formulation of the problem

$$K = \frac{\Pr}{p(m+1/p+1)}.$$

Analysis of the known data indicates a definite conservativity of the parameter K in nonequilibrium flows [2]. The exponent m of the source exerts great influence on the solution. The reaction whose rate decreases with distance from the wall m < 0 exerts the greatest influence on the concentration and temperature field K ~ Pr. A very much smaller influence K ~ Pr/p corresponds to a homogeneous source m = 0. A source concentrated far from the wall m \gg 1 has practically no effect on the heat and mass transfer.

After substituting the solution obtained into (1) and simple manipulation, we obtain a dependence of the friction coefficient on the chemical reaction rate:

$$\frac{C_f}{C_{f_0}} = \left(\theta_w - \frac{KZ(\theta_w - 1)}{1 + KZ}\right)^{-0.55} .$$
(4)

The expression

$$Z = \frac{\overline{Q}h_0}{c_p \Delta T \,\mathrm{St}}$$

is used here as the chemical reaction rate parameter. In its physical meaning it is the ratio between the quantity of heat being liberated because of the chemical reaction and the heat supplied. By definition the quantity Z is bounded: $|Z| \leq 1$. In cases of dissociating gas heating and cooling of practical importance, Z is a negative quantity under recombination conditions.

According to the result obtained, the influence of the reaction on the turbulent friction is insignificant in chemical decomposition reactors. A somewhat greater influence of the particle recombination reaction on friction can be expected. However, the growth of turbulent friction corresponding to this kind of flow cannot be unlimited in the domain of negative values of the stability parameter. Flow stabilization results in the long run in laminarization accompanied by a diminution in the friction.

On the whole the relative influence of the chemical reaction on turbulent friction turns out to be small and, according to estimates performed, restricted to several tenths of the quantity. This can explain the satisfactory description of numerous experimental results by theoretical models without taking account of the singularities of the turbulence of the reacting gases [3]. A completely different situation turns up when analyzing the influence of volume physicochemical sources on turbulent heat transfer. The solution of the boundary layer problem obtained above permits determination of the relative heat transfer law for a reacting gas

$$\frac{St}{St_0} = \frac{C_f / C_{f_0}}{1 + KZ} \,.$$
(5)

According to (5), turbulent heat transfer grows in both the cases considered above of a flow particle dissociation and recombination. This result is also confirmed by experimental data [3, 10].

As a practical application of the model we compute a chemical carboxylic acid decomposition reactor for which there are experimental data [10]. Using the integral regularities of turbulent friction and heat transfer of a reacting gas (4) and (5), we limit ourselves to a one-dimensional description of the flow in the apparatus channel:

$$G\frac{R}{2}\frac{du}{dx} = \tau_w - \frac{dP}{dx}\frac{R}{2}, \qquad (6)$$

$$G\frac{R}{2}c_{\rm p}\frac{dT}{dx} = q_w - h_0 \int_0^R Q\frac{y}{R} \, dy, \tag{7}$$

$$G\frac{R}{2}\frac{dc}{dx} = \int_{0}^{R}Q\frac{y}{R}\,dy,\tag{8}$$

where G is the gas specific mass flow rate, u, c, T are the mean value of the velocity, the product concentration, and the temperature, and τ_W , q_W are the friction stress and heat flux on the reactor walls.

The carboxylic acid vapors dissociate effectively in a complex chain of transformations during heating in the reactor. As a first approximation we use the effective description of a dissociation reaction of the form

$$A_2 \approx 2A, \ Q = Q_0 \exp(-T_E/T) \left(\frac{1-c}{2} - \frac{2P}{K_p} \frac{c^2}{1+c} \right),$$

where ${\tt T}_{\tt E}$ is the effective value of the activation energy and ${\tt K}_p$ is the equilibrium constant.

Utilization of the equation of state

$$P = \rho RT (c+1)$$

and the approximate coupling equations

$$G = K_1 \rho u; \int_0^R \rho u^2 \frac{y}{R} \, dy = K_2 G u \frac{R}{2}$$

is necessary for a closed description of the problem, where K_1 and K_2 are weak functions of the velocity profile [11].

In conjunction with the closing relationships (4) and (5) as well as the known laws of friction and heat transfer of an inert gas, the system (6)-(8) describes the behavior of a reactor in the form of a Cauchy problem. Methods to solve this problem are well known.

Shown in Fig. 2 is a comparison between certain computed reactor parameters and experimental data [10]. The experiments were performed in a tube of 10 mm inner diameter and 1400 mm length. The pressure was 10^5 Pa at the entrance to the channel, the supplied heat density was $q_W = 1.6 \cdot 10^4$ W/m², and the stream Reynolds number was Re = $2 \cdot 10^4$. The best agreement of the data on the heat transfer coefficient is obtained for the value K = 1.08 of the model parameter. Both the computed and experimental results show that the vapor flow is almost equilibrium. Precisely under these conditions is a dropping law of the heat transfer coefficient observed along the tube. Although the tendency of the change in the heat transfer coefficient is characterized by diminution, its absolute value exceeds the "frozen" many times in complete conformity with the law (5). The results of direct measurements of flow hydrodynamics in a decomposition reactor are not represented [10]. Consequently, by the agreement of the reactor thermophysical parameters it is possible to speak about the indirect confirmation of turbulent friction model of a reacting gas.

NOTATION

c, relative concentration; C_f, friction coefficient; c_p, specific heat; G, gas flow rate; h₀, enthalpy of substance formation; De, destabilization factor; p, static pressure; Q, density of the particle source; q_w, density of the heat flux; R, channel radius; St, Sc, Pr, Stanton, Schmidt, and Prandtl numbers; T, gas temperature; u, gas velocity; x, y, longitudinal and transverse coordinates; μ , viscosity; ρ , density; θ , relative temperature; τ , friction stress. Subscripts: e, flow and w, wall.

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