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EFFECT OF A HOMOGENEOUS CHEMICAL REACTION ON HEAT TRANSFER

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Heat and mass transfer processes are investigated in the presence of homogeneous physico-chemical conversions of a substance.

The development of engineering technique in various fields (from creation of perfect technological systems to space equipment and perspective nuclear power plants) leads to the necessity to predict thermal interaction with the surface of coolant fluxes, inside of which there are the sources of substance and energy. This is caused, in the first place by the variation of parameters of state up to the limits where chemical reactions and ionization processes begin to play a significant role. In contrast to chemically and physically frozen flows, positive and negative energy and substance sources appear, diffusional energy transfer starts to play a significant role, and, finally, the thermophysical properties of a coolant change. As a result, the heat transfer rate can change several times, which requires greater attention to the phenomena under consideration.

Physicochemical processes are also important in the case of interaction between jets of gases reacting with each other and also in the case of origination of both laminar and turbulent flame fronts, determining the rate of their propagation, the stability in various-kind combustion chambers, and the composition of combustion products, including sulfur and nitric oxides, harmful for the environment, which are formed in power and chemicotechnological plants [1].

The account for physicochemical conversions of a substance is also important for the analysis of nonequilibrium processes of excitation of inner degrees of freedom of molecules and chemical reactions in flows with large gradients of the gas-dynamic parameters. A similar situation arises when designing gas-dynamic [2] and chemical [3] lasers, including gas-dynamic mixing lasers [4].

Similar problems should be solved in the case of mixing of relaxing gases behind the grid of small nozzles [5], allowing one to mix various gases quickly. These and other examples, the number of which can be significantly increased, indicate the importance of creating exact enough engineering methods for designing a great number of apparatus of both traditional and new equipment in which substance and energy sources play an important role.

Heat and mass transfer in the presence of homogeneous physicochemical conversions of a substance can originate both in laminar and in turbulent flow of a coolant. Interest in laminar flow is caused by the fact that it is observed in a number of cases which are of practical interest: small Reynolds numbers and other effects contributing to laminarization (surface suction, negative pressure gradient, increase in the Mach number in hypersonic flows, etc.). Besides, the possibility of obtaining fairly exact solutions enables one to perform experiments on the defining thermophysical and gas-kinetic characteristics of a substance.

Physical problems associated with the determination of heat transfer in homogeneous physicochemical conversions of a substance are relatively simple.

At present a closed system of equations accounting for all phenomena following from the molecular-kinetic theory of a substance exists both in a complete form [6] and within the framework of boundary layer theory [7], and a system of criteria enabling one in separate cases to simplify the initial equations is also known [8]. Thus, the main attention in this field is paid to the study of the dependence of the thermophysical and gas- and chemical-kinetic

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properties on the governing parameters and to the correct definition of the boundary conditions. Computations of that type have been conducted long ago enough and have been fairly successful.

In [9] the flow around blunt bodies of parabolic and elliptical forms at hypersonic velocity ($M_{\infty max} = 27$) were considered, where nonequilibrium chemical reactions and ionization processes play a significant role. The air behind the compression shock consisted of a mixture of O, N, NO, E^-, NO^+, O_2 and N_2. In the results of numerical calculations, the data on the pressure and temperature distribution were obtained with engineering accuracy. Predictions in the region of laminar flows continue up to now.

In [10], the nonstationary conjugate problem of heat and mass transfer in a flow of dissociating nitric oxide in a triangular bundle of fuel elements was solved. The N_2O_4 dissociation was considered to be equilibrium, NO_2 - nonequilibrium, and the initial temperature and concentration distribution at the channel inlet was assumed uniform. It is worth mentioning that, under these conditions, the mean heat flux over the perimeter undergoes significant fluctuations, acquiring at times also negative values.

In spite of the fact that numerical calculation techniques existing at present make it possible to solve the complete system of equations of conservation, a preliminary physical analysis often allows one to simplify the problem and considerably reduce the time of computations.

In [11], in the analysis of the hydrodynamics and heat transfer of a blunt body, instead of the complete equations of conservation, the equations of a viscous shock layer were used, which allowed one to reduce the time of computer calculations by an order, and the results differ from those obtained by a more exact method only by several percent.

Problems of mass transfer can be solved quite easily in cases where the distribution of any reacting component whose concentration is small enough to exert any influence on temperature and velocity profiles is of interest. Here, only the equation of concentration remains, in which the velocity and temperature distributions are considered known.

The solution of laminar boundary layer equations enables one to create the techniques for experimental determination of a number of parameters which are difficult to be defined in some other way. By such a method the kinetic constant of the potassium ion recombination reaction has been determined in the case of analyzing the electrical conductivity of a MHD generator, where the ion saturation current, depending on the recombination kinetics, was the measured value in the laminar flow around a plate [12].

In engineering calculations, prior to the attempt to solve a problem for nonequilibrium reactions, one should estimate the value of the defined characteristics in the limiting cases of frozen and equilibrium flows. In the latter variant, the concept of effective heat capacity and thermal conductivity is introduced, and the source term disappears. At the same time, one should account for the dependence of the mixture molecular weight on temperature and pressure and see to it that the diffusional processes would not strongly affect the atomic composition of the mixture. If the solutions for these limiting variants are slightly different from each other, the case of nonequilibrium reaction can be determined by interpolation.

It is a much more arduous problem to analyze heat and mass transfer with energy and substance sources in the case of formation of a turbulent boundary layer. At present, information about the structure of a nonisotropic turbulence, allowing one to obtain a closed system of equations without empirical coefficients, is not available even for nonreacting liquids. The situation is even more complicated if physicochemical conversions of a substance are present, causing the appearance of a series of additional problems. Let us state some of them.

In spite of the fact that chemical processes in separate globules of turbulent flux are internal, they can exert an effect on their dimensions and the thermophysical properties of the liquid and, therefore, also on the character of the exchange of momentum and energy.

An exponential dependence of the rate of the chemical reaction on the temperature makes the effect of turbulent pulsations on the source term, which can be significantly different from the case of laminar flows, extremely important. Research works exist which show that absence of an account for this phenomenon can change the concentration of components important for the process by several orders of magnitude.

The effective values of heat capacity and thermal conductivity to a great extent depend on the relation between the characteristic times of chemical reactions and pulsations, varying from frozen to equilibrium ones.

It is necessary to thoroughly investigate the process of diffusional energy transfer, which, in the presence of

chemical reactions, can play a fairly significant role. Great attention should be paid to the mixing process of reacting components right down to the molecular level, since only in this case can a reaction take place. These and other additional circumstances markedly complicate the problem of predicting heat and mass transfer in turbulent flows, which is not quite easy itself.

At present, a great number of works exist whose authors try to fit results that have proved their value for the case of nonreacting media to the prediction of heat and mass transfer in chemical processes. Two- and three-layered boundary layer models are employed with joining at their boundaries of velocity, temperature, concentration of chemical elements, their diffusional flows, friction and heat fluxes. Often, the empirical constants characterizing these models are taken equal to those, found for the flow of a nonreating or even incompressible liquid. In this case the effect of chemical conversions reveals itself, in general, through the change in the relation between the density and the velocity in the boundary layer.

In analyzing turbulent processes, a statistical approach with use of statistical moments is wide-spread. All empirical information is introduced on the differential level, which is very convenient for considering different complex flows, whose specific features are determined by appropriate boundary conditions. The system of equations is closed with the aid of additional physical hypotheses and empirical constants and functions. The number of the latter is sufficiently large, what is a disadvantage of such an approach.

The problem of closure, existing also in inert media, in the presence of chemical reactions is complicated by the necessity of averaging the source term and correct account for the influence of the concentration change on transfer processes.

In [13] heat and mass transfer was considered in the turbulent flow of chemically reacting nitric oxide passing over a rod bundle placed in a hexahedral shell. Transport coefficients used in the equations of conservation were defined according to [14].

It is interesting to note that the presence of chemical reactions in a flow leads to temperature leveling over the rod surface; it is caused by the effect of supplementary heat transfer in the asimuthal direction due to concentration diffusion. A similar effect originates in the case of temperature profile production in the channel formed at the surface of a longitudinal finned tube [15].

In the case of heat transfer with complex chemically reacting systems, in which a great number of reactions can occur simultaneously, including chain ones, the prediction of the heat and mass transfer becomes still more complicated. A similar situation occurs during hydrocarbon pyrolysis in a turbulent flow, where, by different models, one accounts for 650-2000 elementary reactions. Here, one has to conduct an analysis of the relations of characteristic times of chemical reactions and hydrodynamic and pulsational ones and employ a series of assumptions associated with the source term [16].

The complexity of the process and, therefore, the great number of assumptions justify the development of fairly approximate calculation techniques, which make it possible in a number of cases to estimate the effect exerted on heat transfer by various factors, including chemical reactions [17].

The turbulent boundary layer characteristics to a considerable degree depend on the stability of a laminar sublayer, which is strongly affected by the near-wall curvature of the velocity profile. Based on this, the destabilization criterion De has been obtained, depending on various characteristics (temperature factor, injection parameter, Mach number, the presence of the heat source distributed over the layer, etc.). The values $De > 0$ or $D < 0$ denote, respectively, the destabilizing or stabilizing effect of the given factor on the boundary layer and, therefore, on the intensity of the interaction between the flow and the circumfluous body.

Processing of a great number of experimental data obtained on the turbulent boundary layer allows one to write down the approximate equality

$$\frac{C_f}{C_{f_0}} = (1 + \mathrm{De})^{-0,55}.$$

If for a qualitative analysis of the effect of chemical reactions on heat transfer we assume that the intensity of a heat source varies by the law $Q = Q_0 y^m$, and the velocity profile is defined by the relation $u \sim y^{1/p}$, then one can obtain

$$\frac{St}{St_0} = \frac{C_f}{C_{f_0}} - K\frac{\bar{Q}2h_0}{C_p\Delta TC_{f_0}},$$

where $\bar{Q}$ is the mean density of the heat source over the layer thickness, and K is a complex parameter allowing for the process peculiar features:

$$K \equiv \frac{Pr}{p\left(m + \frac{1}{p} + 1\right)}.$$

Regardless of the series of strong assumptions, this calculating technique gives satisfactory results in a number of cases, as, for example, in the complex process of carbonaceous acid decomposition in a chemical reactor [18], so that with a certain caution it can be used for estimation calculations. It is possible that the relative efficiency of the technique is attributed to the determination of relative values and the idea of the method of relative correspondence [19].

The enumerated problems and the methods for their solution, associated with the interaction between a chemically reacting flow and a wall, are maintained and even aggravated when analyzing various flames, the methods of overcoming the difficulties being also similar.

In [1] the process of formation of nitric oxides in turbulent flames was investigated, whose simplified scheme was chosen in accordance with [20]. Since NO_x formation occurs significantly more slowly than combustion, the latter was assumed to be equilibrium. For computations the k-ε turbulence model [21] was used with the usual set of nine constants. The source term in the energy equation took account of radiation losses attributed to the presence of CO_2 and H_2O.

The results obtained on the axial and radial distribution of the mean and pulsation temperatures are satisfactorily confirmed by experimental data [22, 23].

It is interesting to note that in spite of the simplified character of the considered chemical processes, the results turned out to be no worse than those of [24], where 33 reactions taking place in reality were taken into account.

The process of origination of a near-wall flame with supply of a coal reagent through porous surface elements is also referred to a singular case of interference of chemical reactions and heat transfer, the flame front being formed inside a specified boundary layer. This problem was investigated in [25-28]. In the latter of them, the set of equations

$$L(\bar{\varphi}) = S_\varphi,$$

was numerically solved, where L is the parabolic operator of turbulent transfer:

$$L(\bar{\varphi}) \equiv \frac{\partial(\bar{\rho}\bar{u}\bar{\varphi})}{\partial x} + \frac{\partial(\bar{\rho}\bar{v}\bar{\varphi})}{\partial y} - \frac{\partial}{\partial y}\left(\frac{\mu_t}{\sigma_\varphi}\frac{\partial\bar{\varphi}}{\partial y}\right),$$

and S_φ is the source term. The k-ε turbulence model was used. The symbol φ denotes any variable defined in the process of calculation: $\bar{u}$, $\bar{v}$, k, ε, etc. As model constants, $\sigma_u = \sigma_v = \sigma_k = 1$; $\sigma_\varepsilon = 1.3$; $\sigma_c = 0.7$ and the constants of the k-ε model $c_{\varepsilon_1} = 1.44$; $c_{\varepsilon_2} = 1.92$ were taken. The turbulent viscosity was defined by the formula

$$\mu_t = 0{,}09\bar{\rho}\bar{k}^2/\varepsilon.$$

Using a series of additional physically justified assumptions, the prediction was performed, comparison of which with experimental data on the velocity and temperature profiles [29] showed satisfactory agreement.

Recently, a great number of predictive and, to a lesser degree, thorough experimental investigations of heat and mass transfer processes in the presence of homogeneous physicochemical conversions of a substance have been published.

The basis of theoretical analysis and the character of the predicted and experimental results in most of the cases do not exceed the limits of the stated above.

Conclusions

1. Development of engineering techniques including modern ones, leads to extended use of processes in which heat and mass transfer is closely connected with physicochemical conversions of a substance.

2. In laminar flows the problem, in general, is reduced to the development of efficient programs for solving a system of equations of conservation and to determination of exact values of the thermophysical and chemico-kinetic parameters of a substance.

3. The solutions obtained for laminar regimes can be efficiently used for experimental determination of substance characteristics.

4. In turbulent flows, it is necessary within the framework of statistical models to deepen the physical analysis of the processes to determine the closing relationships and to widely use precision experiments for verification of introduced hypotheses and determination of the influence of chemical conversions on empirical constants and functions.

5. In considering a particular process, a preliminary evaluating analysis of the phenomena is desirable with the aim to simplify the problem and reduce the time of computer calculations with preservation of reasonable accuracy of the results.

6. On a level with relatively exact computation techniques requiring, as a rule, the use of computers, it is desirable to develop simplified approaches that can give a qualitative and quantitative estimate of the influence of physicochemical reactions on heat transfer.

7. It is desirable to significantly deepen investigations concerning the creation of a physical model of nonisotropic turbulence, including an account for physicochemical substance conversions, in order to minimize the empirical information necessary for closure of the initial system of equations.

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