

Impact of chemical reactions upon heat transfer

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Abstract

Estimation of some parameters in traditional and new technology requires calculating heat interaction with the surface of fluids and gases which have inside sources of energy and matter. Under laminar flows the problem is generally connected with the development of efficient programmes for solving the systems of conservation equations and with determining the exact values of thermophysical and chemical-kinetic parameters of the matter. Much more difficulties are experienced when analysing the heat and mass transfer with chemical reactions when turbulent flow is being formed. They are due to problems such as exponential dependance of chemical reaction rate on temperature, the necessity of taking into account the characteristic times of chemical reactions and pulsations changing from the frozen to the equilibrium ones. Some examples of successful applications of various models are presented in the paper.

Keywords: Heat transfer; Chemical reaction; Boundary layer; Heat source

1. Introduction

New technologies and technological processes evoked great interest in developing methods of calculating heat transfer between bodies and gas fluxes in the presence of physico-chemical transformations of substance. The main reason of it is the fluid temperature increase (energetics, cosmos, transportation machine-building etc.) and appearance of new chemical technologies as well as devices in which nonequilibrium processes play an important role (atomic energetics, lasers, etc.) [1]. When chemical transformations of substances are not taken into account mistakes in defining various characteristics may result, in particular in the intensity of heat transfer which may be as high as tens and hundreds of percents.

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The impact of chemical reactions, occurring in both free and near-wall flows upon the heat and mass transfer is very important and must be taken into consideration when analysing the flame as well.

Both laminar and turbulent regimes are possible under interaction of gas flows with a body and when they interact among themselves.

2. Laminar flow

There are number of reasons for the interest to the laminar flow. First of all they may occur with small Reynolds number produced by small values of velocity, small specific linear dimensions (close to the front critical point of blunt bodies, porous media, etc.), by low pressures (upper layers of the atmosphere, some processes in chemical industry, technology of drying, etc.) and large values of viscosity.

Secondly, due to the possibility of obtaining solutions that are precise enough they may be used for experimental definition of the important characteristics of the fluid.

As far as the laminar flows with chemical reactions are concerned there exists a closed system of initial conservation equations and of boundary conditions which take into consideration of all parameters, connected with the molecular-kinetic theory of matter both in its general form [2] and in the framework of the boundary layer theory [3]. A system of criteria has been developed which permits to simplify the task in each particular case [4]. As a rule, the particular tasks are solved by using net methods with a computer where the original system of differential equations is substituted by the system of algebraic equations. As a rule in this case some specific difficulties of the calculating character arise, but they are usually solved successfully.

Thus, to obtain solutions which are precise enough it is necessary to have reliable information concerning the dependence of thermo-physical and chemico-kinetical parameters on the temperature, pressure and composition of the fluid. The most difficult problem is determining the rate of chemical transformations. In fact in many cases it is possible to use the limiting values of Damkeller's criterion ($Da = 0$ and $Da \rightarrow \infty$) where in both frozen and equilibrium flows the source members disappear in the initial equations. In case of equilibrium flows, effective values of heat capacity and heat conduction are introduced and the molecular weight dependence on pressure and temperature is taken into consideration. All these relationships are determined from the very accurate tables compiled on the basis of the fundamental laws of thermodynamics for different mixtures of practical interest (air, combustion products of different fuels, etc.). The only point to be closely followed is that diffusion processes would not affect heavily the atomic composition of the mixture.

A number of problems having practical importance were solved in this way. For example, the distribution of velocities, temperatures, and concentrations near a blunt body, moving in the air at the Mach numbers up to 23 and heights up to 70 km were determined and the nonequilibrium processes in a mixture consisting of seven components: O, N, NO, e, NO^+ , O_2 and N_2 were considered [5]. The heat transfer in the flow of dissociating nitrogen oxide in the cluster of heat emitting elements was investigated [6]. Dissociation of N_2O_4 and NO_2 was considered to be equilibrium

and nonequilibrium correpondingly. It is interesting to note that the heat flux experiences significant oscillations, acquiring at some moments negative values. In some cases it is worth while to investigate the distribution of concentrations of some substances which are formed due to reactions with small energy contribution, which does not influence distribution of velocities and temperatures. In such cases the task is significantly simplified.

Thus, distribution of potassium ions in the low-temperature flow of plasma in the channel of magneto-hydrodynamic generator was determined [7]. The solution obtained made it possible to suggest an experimental method for defining kinetic coefficients of recombination processes by means of the ion saturation current which is easy to determine.

The number of examples where solution of the laminar boundary layer equations enables us to develop relatively simple experimental methods for defining the most important properties of the fluids can be extended.

3. Turbulent flow

Defining the impact of chemical reactions in turbulent fluxes is a much more complicated task. There is no closed system of equations even for the flow of inert liquids describing the convective heat transfer. The presence of chemical reactions creates additional problems. Exponential dependence of the rate of chemical reaction on temperature results in the fact that the averaged source member in the conservation equations differs significantly from the real one which may cause changes in the concentration of substances in question by several orders [8]. When determining concentration of nitrogen oxide and electrons in a low-temperature plasma it was accepted that:

$$\overline{Q(T)} = \frac{1}{\sqrt{2\pi(\overline{T'})^2}} \int_A^B Q(T) \exp\left[-\frac{(T')^2}{2(\overline{T'})^2}\right] dT. \quad (1)$$

The intensity of heat transfer in turbulent flow depends, to a great extent, on the relation of time characterizing the speed at which the fluid overflows the body (τ_f), the rate of the chemical reaction (τ_c), and the rate of the turbulent exchange (τ_t). Even in the case of the equilibrium process in the outer flow when $\tau_c \ll \tau_f$ only under $\tau_c \ll \tau_t$ the process of the turbulent mixing will also be equilibrium and its heat capacity will be equal to the effective value $C_p = C_{p\text{ef}}$. If this condition is not observed heat capacity may be much lower and close to its frozen state (C_{p0}):

$$\alpha_{\text{ef}} = \alpha \left[\frac{1}{1 + \tau_c/\tau_t} + \frac{C_{p0}}{C_p} \times \frac{\tau_c/\tau_t}{1 + \tau_c/\tau_t} \right]. \quad (2)$$

Thus, analyses of pulsating processes in the reacting flow must be carried out more thoroughly as compared with those in the inert liquids. In this case the commonly introduced turbulent heat conduction becomes doubtful because the relationship of

the turbulent heat flux and the gradient of the mean temperature is getting more complicated and connected with the gradient of concentration and derivatives of the source function with respect to the temperature and concentration.

Recently, method utilizing statistic moments where the whole empirical information is introduced at the differential level is being widely used when analysing the turbulent heat transfer. It is universal enough as far as different geometrical and physical characteristics of the process are concerned. In such cases additional constants and functions which help to close the original system of equations introduces similar to those used with the flow of a nonreacting liquid. This and the above mentioned problem of averaging the source member oblige one to be very cautious with the results obtained.

Nevertheless in a number of cases the results were fairly satisfactory. The analysis of heat exchange in a turbulent flow of chemically reacting nitrogen oxide overflowing a cluster of rods shows that levelling of temperature occurs due to the reaction [9]. The similar effect was demonstrated with a pipe having longitudinal ribs [10].

High uncertainty with the turbulent energy transfer in the presence of chemical reactions justifies utilizing approximate calculating schemes which in some cases are in good agreement with the experiment.

Common two- or three-layer models of the boundary turbulent layer are used when on their boundaries speed, temperature, concentration of chemical elements, their diffusive flows as well as heat fluxes and friction have been levelled.

The empiric constants in such cases are taken to be equal to their values for the inert gas. As a result chemical reactions affect the profile of speeds and all other parameters mainly due to the changes in the relationship of density and speed. The integral method may also be here of some use. It is based on the system of equations:

$$\frac{dRe_h^*}{dx} + Re_h^* \left(\frac{1}{\Delta h} \times \frac{d\Delta h}{dx} \right) = Re_L St(\psi_c + b_T), \quad (3)$$

$$St = f(Re_h^* \dots), \quad (4)$$

where the first one is the exact integral relation of energy and the second-law of heat transfer, determined in the experimental way, the character of which depends on the chemical transformations.

If it were possible to establish the law of heat transfer for at least some class of reactions, as has been done for the inert liquid, and to represent it in a convenient mathematical form then it would be possible to obtain even the analytical expression for the heat flux distribution along the surface of a body under the arbitrary distribution of the main flow velocity and the temperature of the surface.

And finally, there is one more approximate method which produces satisfactory results both qualitative and quantitative. Characteristics of the turbulent boundary layer depend to a great extent upon the stability of the laminar sublayer which is determined by the near-wall curvature of the speed profile. The criterion of destabilisation, depending, in particular, on the source of heat (Q) distributed within the boundary layer is given in [11].

For the case $Q \sim y^m$ and $u \sim y^{1/p}$ it is possible to get:

$$\frac{St}{St_0} = \frac{C_f}{C_{f0}} - K \frac{\bar{Q} 2h_0}{C_p \Delta T C_{f0}}, \quad (5)$$

where \bar{Q} is mean density of the heat source within the layer, and

$$K = Pr/p(m + 1/p + 1). \quad (6)$$

In spite of the simplified nature of the suppositions made this approach in some cases gives satisfactory results.

4. Conclusion

Development of technology brings about the necessity of developing precise enough methods for calculating heat transfer which take into account chemical transformations of substances. Under laminar flow the main problem is connected with calculation one if thermo-physical and chemical-kinetic parameters of the substance are known.

Solution used for laminar flows may be employed for experimental determination of the important characteristics of substances, including specific nature of chemical processes.

A number of additional problems with the turbulent flow of liquids where chemical reactions take place. These problems are connected with the function of the source, relationship of heat capacity and turbulent characteristics etc., requiring working out physical models of turbulence.

At present we have to use various approximate methods, including modified models of the boundary layer, integral method, differential approximations of various moment method modifications.

The method of destabilizing parameter may be used for the rough approximation of the impact of chemical processes upon heat transfer but it should be done with some caution.

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