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HEAT AND MASS TRANSFER IN A DISSOCIATED
LAMINAR BOUNDARY LAYER OF AIR WITH CONSIDERATION
OF THE FINITE RATE OF CHEMICAL REACTION

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16. Abstract A numerical investigation of heat and mass transfer in a dissociated laminar boundary layer of air ^{on} an isothermal flat plate is carried out for different degrees of cooling of the wall. A finite-difference chemical model is used to study elementary reactions involving NO ₂ and N ₂ O. The analysis is based on equations of continuity, momentum, energy, conservation and state for the two-dimensional viscous flow of a reacting multicomponent mixture. Attention is given to the effect of both catalyticity and non-catalyticity of the wall.			
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HEAT AND MASS TRANSFER IN A DISSOCIATED
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A. O. Oyegbesan, J. Algermissen

INTRODUCTION

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Processes of heat- and mass transfer during gas flow play an important role in many types of equipment. For example, because of the development of hypersonic engine systems, it is important to know the interaction between chemical reactions and diffusion phenomena in the boundary layer to define the process of heat exchange at walls. Processes of energy and mass transfer in boundary layers are very complex, especially at hypersonic speeds. Although significant progress has been made in describing the phenomena which occur, the role of chemical kinetics in precise calculation of energy and mass transfer processes in boundary layers and, consequently, flows toward a wall is still of major interest to researchers.

Theoretical research on flows must be conducted to obtain data on the progress of basic processes. Because a few experimental studies cannot provide all the required information about basic aspects of boundary layer phenomena, Stuttgart University's Institute for Thermodynamics of Air and Space Flight is conducting extensive numerical analysis of complex energy and mass transfer processes in chemically reactive boundary layer flows, including chemical reactions at finite rates, since boundary layer variables, as stated in [1], are subject to the effect of a flow's nonequilibrium properties.

This report presents a numerical study of the processes of energy and mass transfer in a laminar flow of dissociated air

*Numbers in the margin indicate pagination in the foreign text.

in a boundary layer at a flat isothermic plate for various degrees of wall cooling with regard for a chemical model of elemental reactions in the presence of chemical components NO₂ and N₂O.

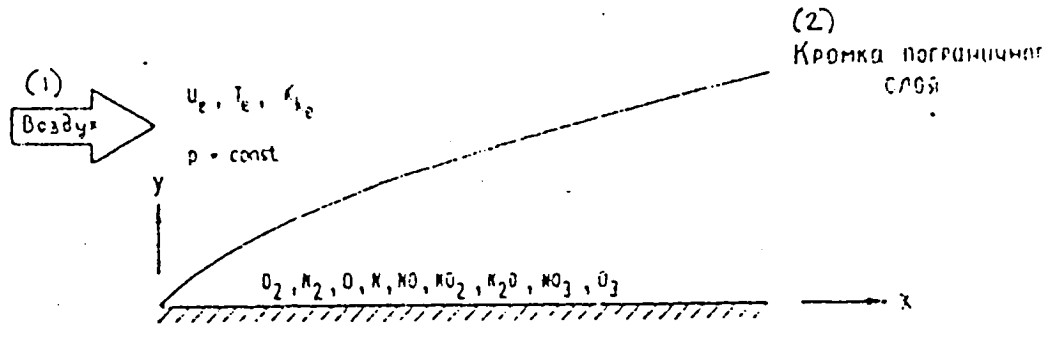


Fig. 1. Diagram of a boundary layer.

Key: (1) Air; (2) Edge of boundary layer.

The effect of wall material as a catalyst is studied. The analyzed flow is a boundary layer at inlet to the combustion chamber of a supersonic rocket. Figure 1 is a diagram of the flow.

ANALYSIS

With regard for standard approximations of the boundary conditions, the following equations were written for a two-dimensional viscous flow of a chemically reactive multi-ingredient mixture:

- Continuity
$$\frac{\partial}{\partial X}(\rho u) + \frac{\partial}{\partial Y}(\rho v) = 0, \tag{1}$$

- ~~Amount of motion~~ Momentum
$$\rho u \frac{\partial u}{\partial X} + \rho v \frac{\partial u}{\partial Y} = \frac{\partial}{\partial Y} \left(\mu \frac{\partial u}{\partial Y} \right) - \frac{\partial p}{\partial X}, \tag{2}$$

- Energy
$$\rho u \frac{\partial H_T}{\partial X} + \rho v \frac{\partial H_T}{\partial Y} = \frac{\partial}{\partial Y} \left[\mu \frac{\partial (u^2/2)}{\partial Y} + \frac{\partial \Gamma}{\partial Y} - \sum_k j_k h_k - \frac{RT}{\rho} \sum_k \sum_l \frac{K_l M D_k^T}{M_l M_k D_{kl}} \left(\frac{j_k}{K_k} - \frac{j_l}{K_l} \right) \right], \tag{3}$$

- Conservation
 • ~~Preservation~~ of mixture components

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$$\rho u \frac{\partial K_k}{\partial X} + \rho v \frac{\partial K_k}{\partial Y} = \frac{\partial}{\partial Y} (-j_k) + W_k, \quad (4)$$

- Condition

$$p = \rho \frac{R}{M} T. \quad (5)$$

Boundary conditions for solving the equation in partial derivatives were defined by conditions at the wall and at the edge of the boundary layer. At the edge of the boundary layer ($y \rightarrow \infty$):

$$u = u_e, \quad (6)$$

$$T = T_e, \quad (7)$$

$$K_k = K_{k_e}. \quad (8)$$

At the wall ($y = 0$):

$$u = 0 \quad (\text{Condition of adhesion}) \quad (9)$$

$$T = T_w \quad (\text{Isothermic wall}) \quad (10)$$

$$\sum_k a_{lk} j_{k_w} = 0. \quad (\text{Nonporosity condition}) \quad (11)$$

Mass concentrations on sample surfaces were determined by the catalytic capacity of the wall material. Cases of manifestation of a wall's lack of catalytic capacity and of total catalytic capacity were considered. In the first case, mass concentrations were obtained by solving a series of equations:

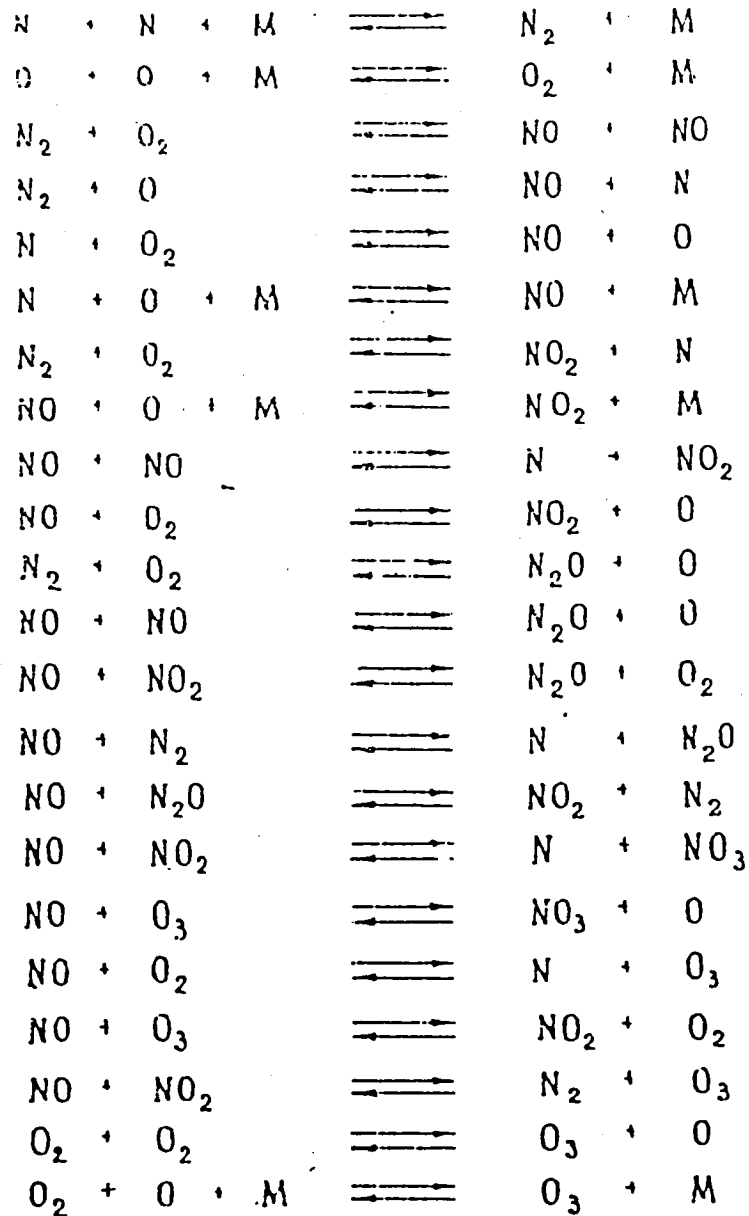
$$j_{k_w} = 0. \quad (12)$$

In the second case, when chemical reactions at the wall are so rapid that chemical equilibrium predominates, we have

$$K_k = K_{k_{eq}}. \quad (13)$$

Transfer processes are studied by using the approximation proposed by Bird [2]. A detailed evaluation of transfer properties can be found in [3] and [4].

The finite-difference chemical model studied is that used by the authors in [1]. It describes the following elementary reactions:



In these reactions, M symbolizes some third substance. Rate constants derived in [5] were used in the calculations. Equations for calculating the rate of chemical substance formation and rates of elementary processes can be found in [5].

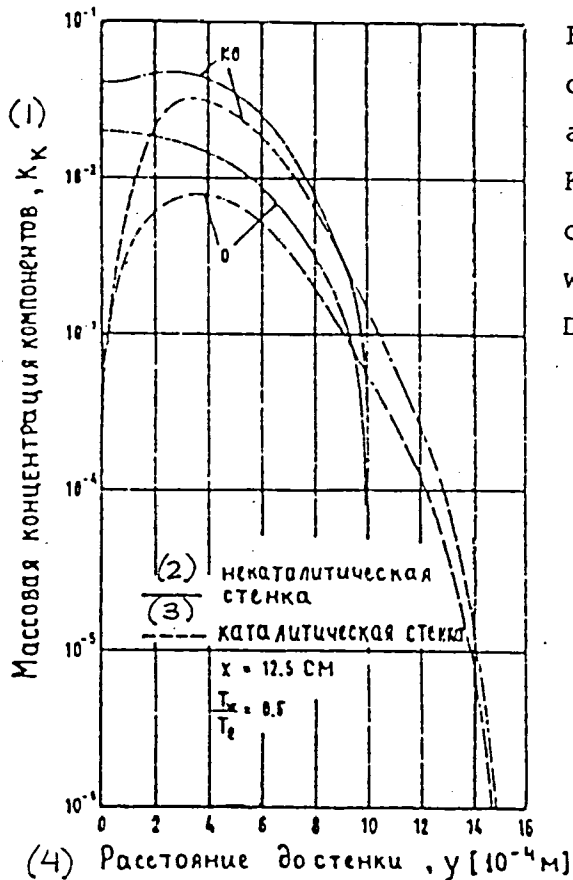


Fig. 2. Profiles of mass concentrations of nitrous oxide and atomic oxygen.

Key: (1) Mass concentration of components; (2) Non-catalytic wall; (3) Catalytic wall; (4) Distance to wall.

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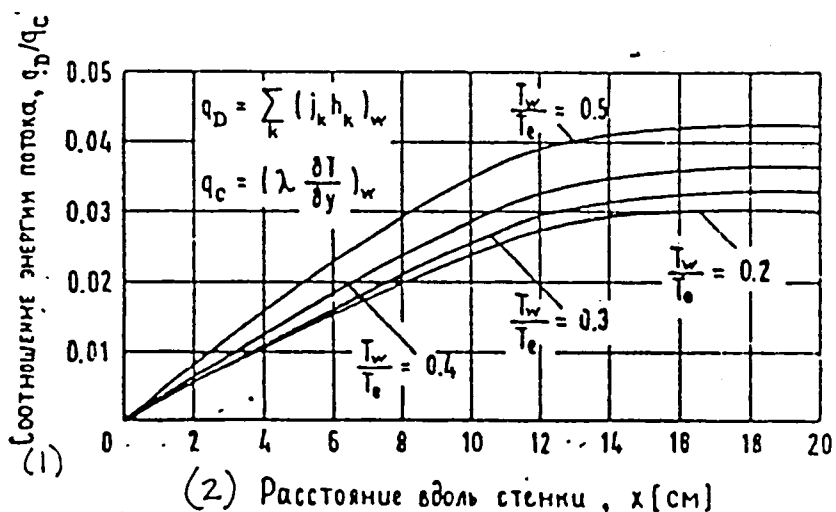


Fig. 3. Profile of energy ratio along a wall.

Key: (1) Flow energy ratio; (2) Distance along wall.

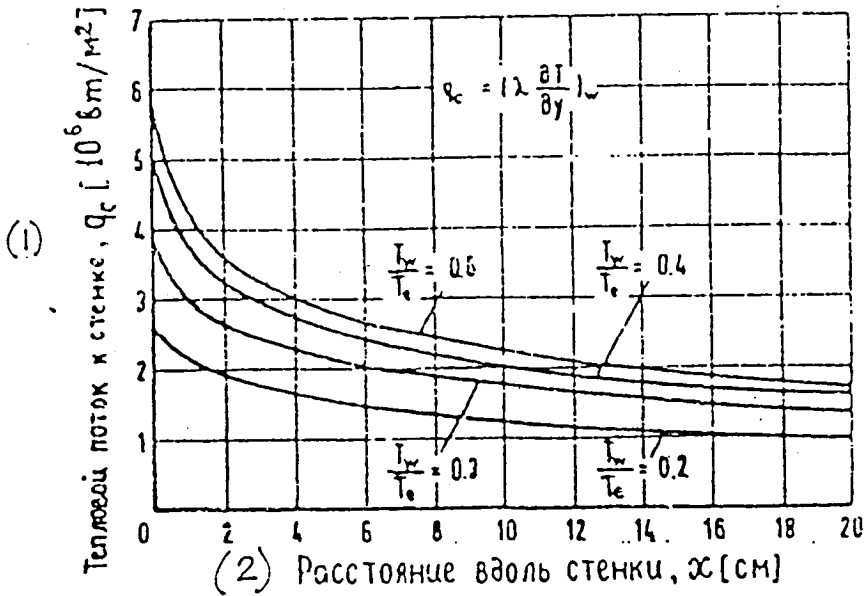


Fig 4. Thermal flow along a wall. Key: (1) Thermal flow toward wall, q_c [10^6 W/m²]; (2) Distance along wall.

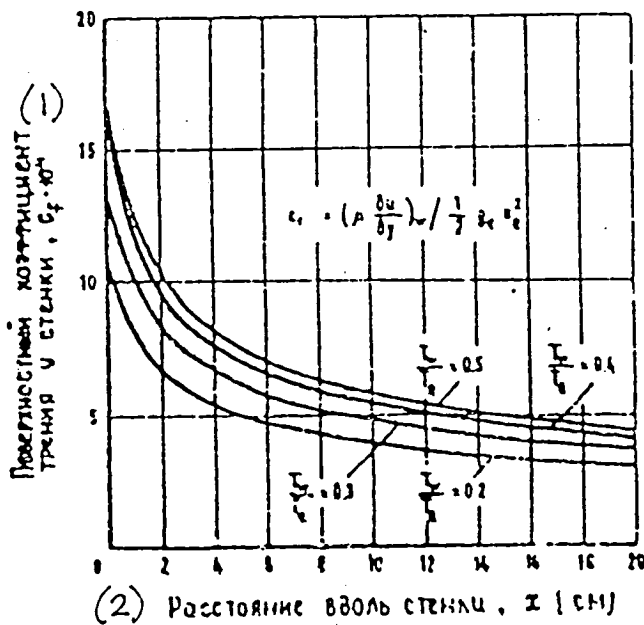


Fig. 5. Surface friction coefficient at a wall toward the axis. Key: (1) Surface friction coefficient at wall, $C_F \cdot 10^4$; (2) Distance along wall.

A similar procedure was used in [7] to study nonreactive turbulent boundary layers. Finite-difference diagrams for equations in partial derivatives were given in [1].

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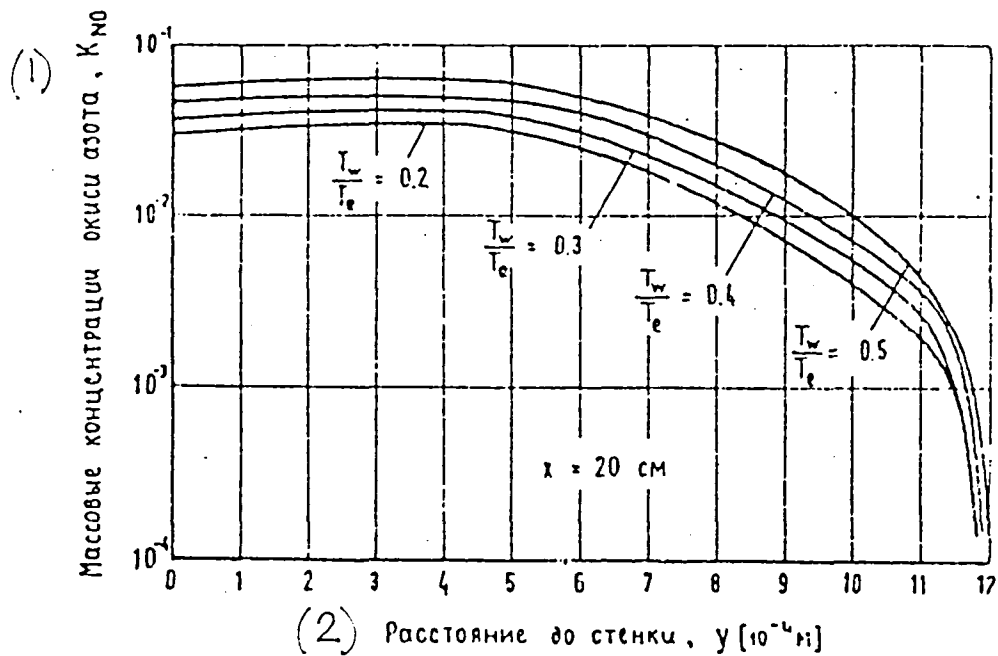


Fig. 6. Profiles of mass concentration of nitrous oxide for various degrees of wall cooling.

Key: (1) Mass concentration of nitrous oxide; (2) Distance to wall.

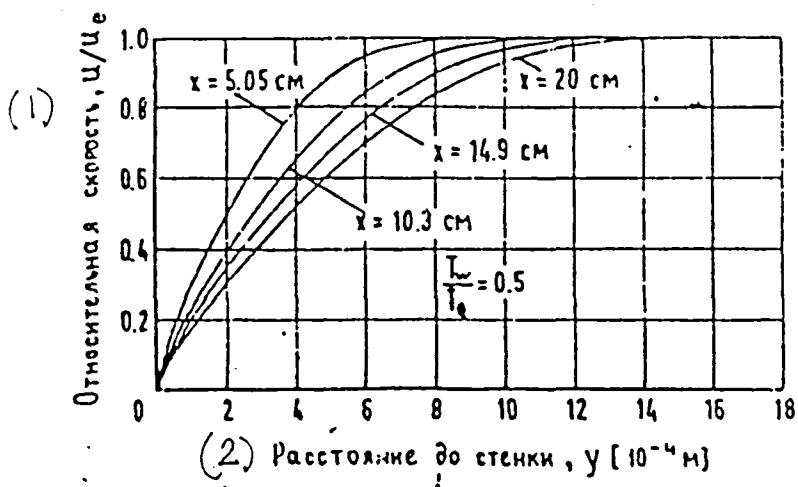


Fig. 7 Profiles of speeds in the boundary layer.

Key: (1) Relative speed; (2) Distance to wall.

Numerical calculations on the SD 6600 at Stuttgart University for boundary conditions at inlet to a supersonic rocket's combustion chamber:

$$\begin{aligned}
 p_e &= 0.4882 \text{ bar} \\
 T_e &= 2575 \text{ K} \\
 u_e &= 6320 \text{ m/sec } (Ma_e = 6.45), \\
 K_{O_2e} &= 0.21 \\
 K_{N_2e} &= 0.79
 \end{aligned}$$

were obtained for different levels of wall cooling.

CONCLUSIONS

Preliminary calculations of boundary variables were done for cases of catalytic and non-catalytic walls. Results show that a wall's lack of catalytic capacity has little effect on profiles for speed and temperature in the boundary, while catalytic near-wall recombination has a significant impact on profiles for mass concentration of chemical samples, as shown in fig. 2 for profiles of the mass concentration of atomic oxygen and nitrous oxides.

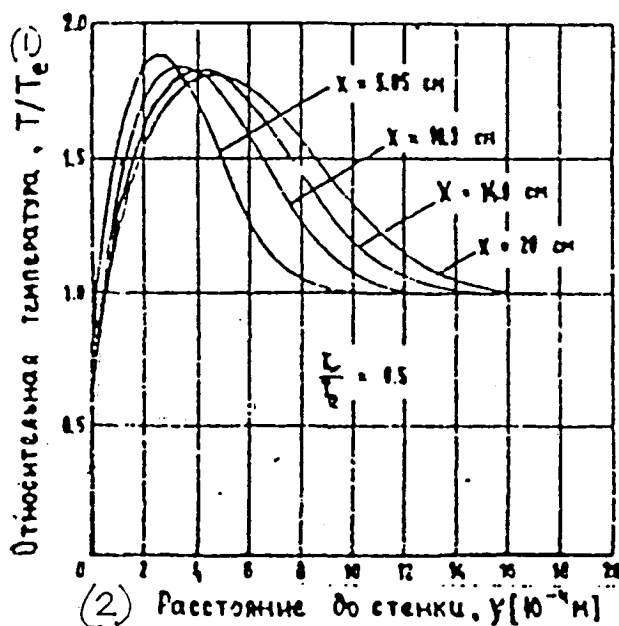


Fig. 8. Profile of temperature distribution in the boundary layer.
Key: (1) Relative temperature; (2) Distance to wall.

In the case of lack of catalytic capacity, energy flow toward the wall depends on conductance; for a completely catalytic wall, since mass diffusion flows are not related, an additional member dependent on convection appears. To show the effect of convection of energy flow toward a wall, fig. 3 gives the ratio of convective energy flow toward a wall due to multicomponent diffusion to conductive thermal flow for different levels of wall cooling. It was noted that, as wall temperature rises, convective transfer of energy to the wall by means of diffusion increases.

The results of the study show that the magnitude of convective energy transfer to a wall increases in the direction of flow, since chemical reactions predominate in the boundary layer. Nonetheless, thermal flow to the wall usually depends on thermal conductivity, which is a function of the temperature gradient near the wall. However, on the other hand, energy processes affect temperature distribution in the layer because of chemical reactions, and in this sense chemical kinetics

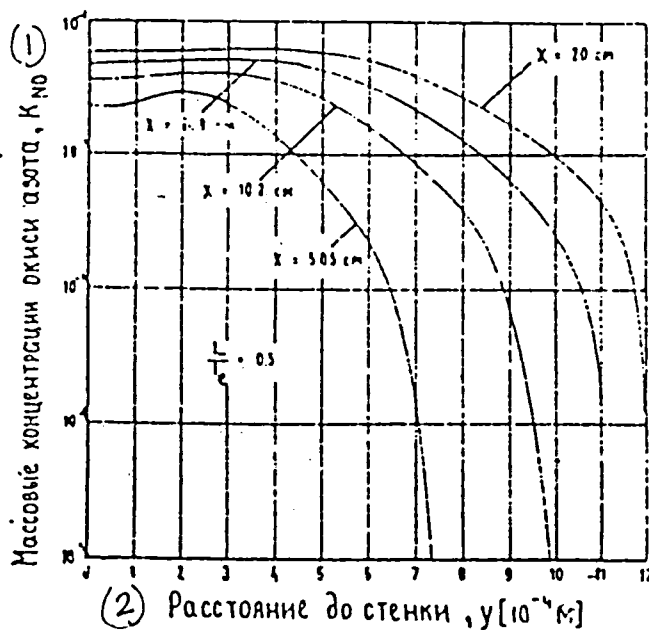


Fig. 9. Profiles of the mass concentration of nitrous oxides for a non-catalytic wall. Key: (1) Mass concentrations of nitrous oxide; (2) Distance to wall.

plays a key role, as shown by the authors in [7]. Proposed levels of thermal flow to the wall are shown in fig. 4 for various degrees of wall cooling. Figure 5 shows the effect of wall cooling on the surface friction factor.

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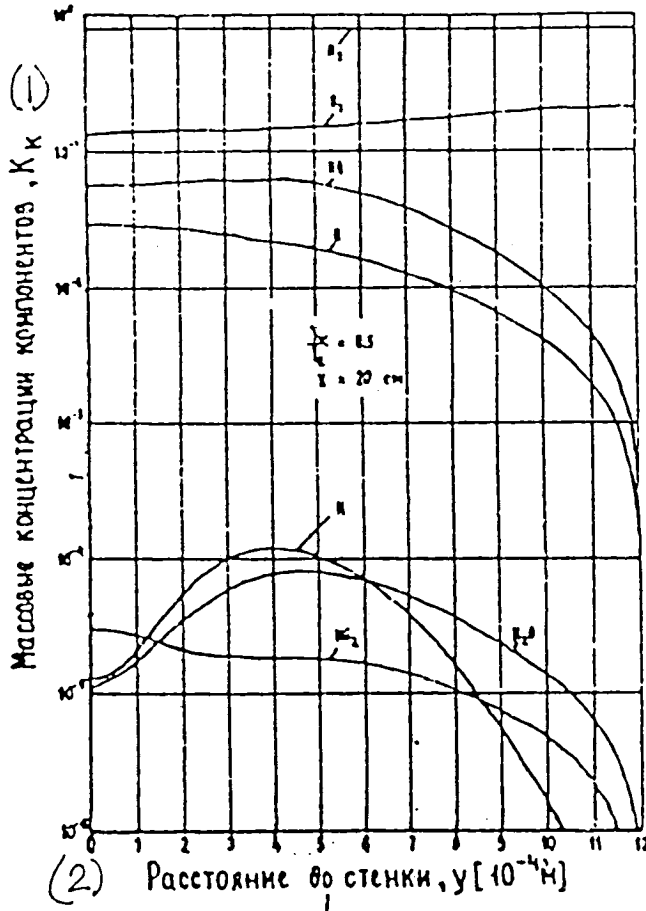


Fig. 10. Chemical composition of the gas mixture for a non-catalytic wall.

Key: (1) Mass concentrations; (2) Distance to wall.

The primary substance obtained as a result of chemical reaction in the boundary layer is nitrous oxide, which is a major polluting product in jet engine systems. Figure 6 shows that the concentration of nitrous oxide in the boundary layer may be diminished by reducing wall temperature. Figure 7 presents a profile of speeds in the boundary layer; figure 8, a graph of the corresponding temperature distribution. Profiles of the boundary layer show that it thickens toward the flow. Mass concentration profiles for nitrous oxide, one of the primary substances formed during chemical reactions, appear in fig. 9.

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SYMBOLS

D_k^T - multicomponent factor for thermodiffusion for component k ; D_{kl} - binary diffusion coefficients for components k and l ; h_k - enthalpy of component k ; H_T - total enthalpy; J_k - diffusion flow of component k ; K_k - mass concentration of component k ; M - molecular weight of the gas mixture; M_k - molecular weight of component k ; p - local static pressure; R - universal gas constant; T - local static temperature; u - longitudinal speed; v - transverse speed; W_k - speed at which component k forms due to chemical reactions; X - coordinate along the axis; Y - radial coordinate; α_{lk} - mass concentration of element l in component k ; λ - specific thermal conductivity; μ - dynamic viscosity; ρ - gas mixture density; e - values at the edge of the boundary layer; e_q - equilibrium value; k - component; l - component or element; W - wall.

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