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## THE STRUCTURE OF MULTICOMPONENT NONEOUILIBRIUM VISCOUS SHOCK LAYERS

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## Abstract

This article presents a numerical study to investigate the main regularities of the structure of multicomponent nonequilibrium thin viscous shock layers under hypersonic vehicle flight conditions at altitudes from 60 to 110 km. The results focus on the chemical, diffusion and heat transfer processes in the layers near catalytic body surface. The structure of the catalytically influenced zone of the flow near the surface is analyzed. The analysis demonstrates that in order to increase the accuracy of the determination of heat flux values, it is necessary to utilize more reliable information on transfer properties of multicomponent gas mixture and the constants of chemical reaction rates. The main characteristics of the catalytically influenced zone fits width. temperature, and concentrations of species on the external boundary of the zone) can be useful for creation of new approximation methods for prediction of heat fluxes at catalytic surface materials of a vehicle.

### Nomenclature

C, = heat-transfer coefficient

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H	= total enthalpy
h	= altitude
q	= heat flux
R	= vehicle nose radius
$\mathrm{Re}_{\mathrm{of}}$	= $\rho_{\infty} U_{\infty} R/\mu(T_{of})$ , Reynolds number
Sc <sub>i</sub>	= Schmidt number of the i-component
St	= $q/(\rho_{\infty}U_{\infty}(H_{o} - H_{w}))$ , Stanton number
Т	= temperature
T <sub>of</sub>	= stagnation temperature
U.	= free streem velocity
$lpha_{ m i}$	= mass concentration of the i-component
δ	= width of the catalytically influenced zone
ε	= degree of body darkness
μ	= viscosity coefficient
ρ	= density
σ	= constant of Stephan-Boltzmann
χ	= the sweep angle of the leading edge
subscripts	
e	= equilibrium conditions
f	= "frozen" conditions
i	= air component
s	= parameters at the boundary of the TVSL
w	= wall conditions

- = wall conditions
- = boundary conditions at the catalytically influenced zone

= freestream conditions œ

= stagnation conditions

## Introduction

The areas of aerodynamic heating and heat protecting techniques have brought renewed interests in the design of

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modern hypersonic vehicles.<sup>1-3</sup> To analyze the structure of the flows of a chemical nonequilibrium multicomponent gas (air) near a blunt body, one of the approximations of the Navier-Stokes equations was used, i.e., a model of a thin viscous shock layer (TVSL) developed by Cheng,<sup>1,4</sup> Moss,<sup>5</sup> Miner and Lewis,<sup>6</sup> Anderson,<sup>7</sup> and Gusev et al.<sup>8</sup> Using this model of the TVSL, study of streamlining of blunt bodies (with spherical and cylindrical nose shapes) by hypersonic air flow under re-entry conditions were conducted at the altitudes from 110 to 60 km. The influence of different approximation models of the mass diffusion flux, heat flux and the value of the chemical reaction rates was researched. The results of the calculations of the flow characteristics in the viscous shock layer around blunting surfaces are received for different degree of catalytic activity on the vehicle surface. Studies were conducted on the characteristics of the catalytically influenced zone of the flow near the catalytic surface of the body. It is the catalytic properties of the body surface, as well as diffusion gas characteristics, that define the features of this specific zone. The present results are the development of the research conducted by Gusev et al.,8 Provotorov and Riabov,<sup>9-12</sup> and Botin et al.<sup>13</sup>

## Approximation of a Thin Viscous Shock Layer

A detailed exposition and formulation of the corresponding boundary-value problem in terms of the TVSL, as well as the system of differential equations and boundary conditions have been developed by many researchers.<sup>4-13</sup> And for the sake of brevity there are not discussed in this study.

The conditions of adhesion and nonpenetration are assumed to be specified at the surface of the body, as are the conditions of equilibrium-radiation heat exchange and mass component balances with consideration of various catalytic properties of the surface material. The generalized Rankine-Hugoniot conditions are assumed to be satisfied at the external boundary of the thin viscous shock layer.

In the numerical solution of the two-dimensional boundary-value problem describing the flow in a nonequilibrium thin shock layer, a numerical procedure was used for the solution of nonlinear partially differential equations with a small parameter for the higher derivatives, in which approximations of the differential equations with respect to the two-point second-order Keller scheme were realized. The procedure and physical flow model were described by Provotorov and Riabov<sup>9.12</sup> in detail.

The mass diffusion flux, viscosity, and heat conductivity of multicomponent gas mixture were calculated by the approximation method of Riabov<sup>14</sup>.

#### Calculation Results

Calculations of the Stanton number  $St = q/(\rho_{\infty}U_{\infty}(H_{0} -$ H<sub>m</sub>)) in the critical point of the spherical one meter radius body, with dependency on the Reynolds number  $Re_{ef}$  =  $\rho_{\infty} U_{\infty} R/\mu(T_{cf})$  along the Space Shuttle trajectory,<sup>15</sup> are displayed in Fig. 1. The viscosity coefficient  $\mu$  is calculated at the stagnation temperature T<sub>of</sub> and "frozen" conditions.<sup>8</sup> The degree of catalytic activity of the body's surface material significantly influences the value of heat flux q. The greater the difference of the value q between the absolutely noncatalytic (empty squares) and ideally catalytic (filled squares) surface indicated decreasing velocity with decreasing re-entry flight altitudes, h (or increasing Re<sub>of</sub>). The altitude h ranged between 110 and 60 km, and the direct relationship was noticed below the 80 km range ( $Re_{of} = 230$ ). The values of the heat flux under the flight conditions at this altitude differ by factor of three for various catalytic vehicle surfaces. These significant differences point to the nonequilibrium character of physical and chemical processes in the thin viscous shock layer under the considered conditions of vehicle flight.

The flight velocity  $U_{\infty}$  is one of the defining parameters of the flow around the vehicle.<sup>12</sup> In the case of the flight altitude of h = 80 km with constant velocity  $U_{\infty}$ = 7.9 km/sec, a significant decrease of the Stanton number St is noticed between the noncatalytic surface and calculated value. At the altitude of h = 67.5 km this difference reaches 240%. Concurrently the degree of influence of this parameter in the case of ideally catalytic surfaces is insignificantly small.<sup>12</sup>

A certain pattern in the values of q for the ideal

catalytic surface material is observed in a number of publications<sup>1-17</sup> at different flight conditions and different models of physical and chemical processes in the TVSL. The results of the calculations of the nonequilibrium layer near the catalytic surface at high level of accuracy correlate with the data<sup>11</sup> obtained for equilibrium viscous shock layer displayed in Fig.1 (marker x).

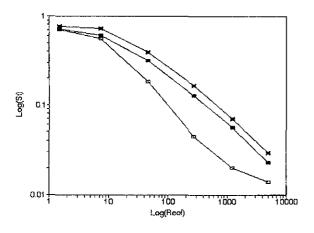


Fig 1. The values of the Stanton number St vs the Reynolds number  $\text{Re}_{of}$ : empty squares - the data for absolutely noncatalytic surface; filled squares - the data for ideally catalytic surface; x - the data for equilibrium conditions.

As it was mentioned in previous publications,  $^{8-10,12}$  the degree of catalytic surface activity doesn't noticeably influence such values as pressure, thickness of the shock layer and coefficient of friction. The research done in this study for altitudes of 60 - 110 km confirmed this conclusion.

The degree by which the nonequilibrium physical and chemical processes influenced the flow in the TVSL at small magnitudes of the Reynolds number  $1 \le \text{Re}_{of} \le 49$ was analyzed by Gusev et al.,<sup>8</sup> and Provotorov and Riabov.<sup>9,10</sup> The results of the calculations for the conditions of the flight at higher Reynolds numbers (and lower altitudes) are displayed in Figs. 2-7.

The distribution of the mass concentration of the air components  $\alpha_i = \rho_i / \rho_i$  at the Reynolds number  $\text{Re}_{of} = 230$  and the flight conditions at altitude h = 80 km is displayed at Figs. 2.

The degree of catalytic surface activity influences significantly the component distributions in the viscous

shock layer. The specific measure of this influence is the width of the catalytically influenced zone  $\delta$ , which is characterized by the significant difference in the component distributions  $\alpha_i$  for two extreme cases: ideally catalytic (dash lines) and absolutely noncatalytic (solid lines) surfaces. Thus, the flight conditions at these altitudes fully define the degree of dissociation of molecules  $O_2$ , NO,  $N_2$ , and concentrations of O and N atoms as well as the catalytically influenced zone  $\delta$ . As it was mentioned in the studies of Gusev et al.<sup>8</sup>, and Provotorov and Riabov<sup>9-10</sup> this influence was distributed through the thickness of the viscous shock layer, under the above mentioned conditions at h = 90 - 110 km.

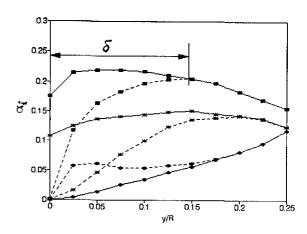


Fig 2. The mass concentration  $\alpha_i$  of the air components in the TVSL at  $\text{Re}_{of} = 230$ : • - O, + - NO, asterisk -N; dash lines - ideally catalytic surface; solid lines absolutely noncatalytic surface.

Figure 3 displays the distribution of the mass component concentrations  $\alpha_i$  of the dissociating air (molecules of oxygen (empty squares), nitrogen (triangles), and nitric oxide (plus), as well as atoms of oxygen (filled squares) and nitrogen (asterick)) on the external boundary of the thin viscous shock layer at the values of the Reynolds number  $1.49 \leq \text{Re}_{of} \leq 5130$ . The offered data suggests that the catalytically active surface influences the full width of the viscous shock layer at the flight altitudes above 85 km. In the range of considered models of the TVSL under the terms of decreasing altitude (or the increase of the Reynolds number  $\text{Re}_{of}$ ), concentration  $\alpha_i$  on the external boundary of the layer reaches its value in upstream equilibrium flow.<sup>H-12</sup> Under the conditions corresponding to the flight at the altitudes of  $H \le 60$  km, instead of modified conditions of Rankine-Hugoniot, it is better, with acceptable accuracy, to use standard boundary conditions at the shock wave.

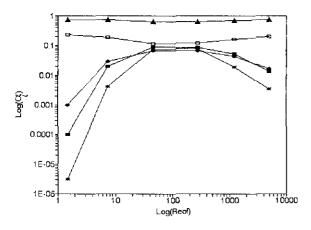


Fig.3 The values of the mass concentrations  $\alpha_i$  of the dissociated air components on the external boundary of the TVSL as a function of the Reynolds number Re<sub>of</sub>:  $\Box - O_2$ ,  $\bullet - O_2$ ,  $\bullet - O_2$ ,  $\bullet - N_2$ .

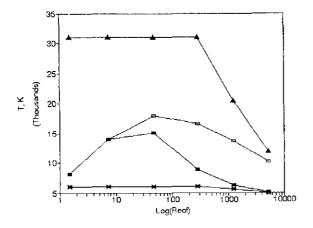


Fig. 4 The values of temperature  $T_s$  (°),  $T_{\delta}$  (\*),  $T_{of}$  ( $\bigstar$ ),  $T_{of}$  ( $\bigstar$ ),  $T_{oe}$  (marker x) as functions of Reynolds number  $Re_{of}$ .

The distributions of the temperature values  $T_s$  along the external boundary of TVSL (empty squares) and the stagnation temperature values  $T_{of}$  (triangles) are shown in Fig. 4. The distribution of  $T_s$  has a number of specific features in the different sections of the flight trajectory. As the Reynolds number  $Re_{of}$  increases,  $T_s$  rises at the range of altitudes from 110 to 90 km. As the altitude falls to 80 km, a relative stabilization of  $T_s$  occurs. Then a sudden monotonous decrease of  $T_s$  is observed. This phenomena is due to significant inhibition<sup>15</sup> of the vehicle in layers of high density atmosphere and to decrease of  $T_{of}$  (see Fig. 4). In the case of relatively large values of Reynolds number  $Re_{of} \ge 230$ , the regular boundary layer begins to be formed inside the TVSL. The width of the catalytically influenced zone  $\delta$  is its specific characteristic (see Fig. 2).

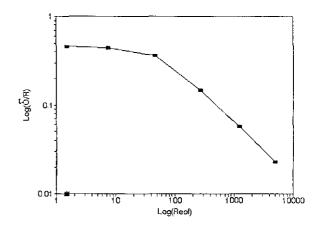


Fig. 5 The values of the width of the catalytically influenced zone  $\delta$  as a function of Reynolds number Re<sub>of</sub>.

We used the distribution of the mass concentration of oxygen atoms for the determination of  $\delta$  because of the significant sensitivity of the atoms to the catalysis at the vehicle surface. The other correlations of the parameter  $\delta$  could be done if the other components are taken into consideration. The difference between the component distributions and the appropriate parameters  $\delta$  can be explained by different transport properties of the components.14 As presented in Fig. 5, the results of calculations show, the value  $\delta$  correlates with the parameter Re<sub>of</sub> according to the exponential law in the broad range of the Reynolds number  $230 \le \text{Re}_{of} \le 5130$ and under the flight conditions at altitudes from 90 to 60 km. In Fig. 4 the distribution of the gas temperature value  $T_{\delta}$  (filled squares) on the conditionally introduced boundary  $\delta$  is shown. As the altitude falls (from 90 km), a significant decrease of temperature  $T_{\phi}$  is observed on the assumed boundary of the catalytically influenced zone and the values  $T_{\delta}$  merge with the values<sup>11</sup> of the stagnation

temperature  $T_{oe}$  corresponding to equilibrium dissociated air behind the shock wave (see Fig. 4, markers x).

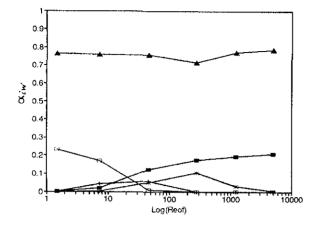


Fig. 6 Air component mass concentrations  $\alpha_{iw}$  on the noncatalytic vehicle surface:  $\Box - O_2$ ,  $\blacksquare - O_2$ ,  $= - O_1 + - NO_2$ , asterisk - N,  $\blacktriangle - N_2$ .

Decrease of typical temperature in the TVSL with the decreasing flight altitude leads to the significant redistribution of the component concentrations (see Fig. 2). As a matter of fact, this phenomena appears in the distribution of air component concentrations on the noncatalytic surface according to the changing flight altitude conditions. These correlations are shown in Fig. 6. The above mentioned results point to the critical character of the flow at the altitude H = 80 km. The process of dissociation of molecules of oxygen and nitrogen is fully completed at this altitude. As a result, there is maximum presence of oxygen and nitrogen atoms.

Consequently, there was conducted an additional analysis of the characteristics of the flow in the TVSL at the altitude of 80 km. In particular, the influence of different models of description of the diffusional fluxes were researched. It appears that if thermodiffusion is considered, it leads to minor adjustments (no more than 2%) of the heat flux value and of distribution of component concentration values (about 4%). In the case of the absolutely noncatalytic surface, it is noticed, that using the approximation method<sup>12,14</sup> of description of diffusion with the help of the Fick law (Schmidt numbers Sc<sub>i</sub> = 0.5) leads to certain inaccuracies in the values of diffusional fluxes (up to 25%).

Moss,<sup>5</sup> Miner and Lewis,<sup>6</sup> Gusev et al.,<sup>8</sup> Provotorov

and Riabov,<sup>9-12</sup> Schexnayder and Evans,<sup>16</sup> and Blottner<sup>17</sup> have used different expressions of the rates of chemical reactions as functions of temperature. The influence of this factor on the characteristics of thermal and mass transfer in the viscous shock layer may turn out to be very significant.<sup>12</sup> The following data confirms the above statement. The value of the heat-transfer coefficient  $C_{h} =$  $2q/(\rho_{\infty}U_{\infty}^{3})$  received while using the constants<sup>9</sup> of chemical reactions considering the reaction  $O_2 + N_2 \rightleftharpoons$ 2NO, turns to be 0.04305. While using the constants<sup>16</sup> without considering the reaction, the value  $C_{\rm b}$  is 0.03804. If the above reaction is taken into consideration the heat transfer coefficient becomes 0.03806. While the value based on the reaction rates by Blottner<sup>17</sup> is 0.03685. Using the constants<sup>16</sup> of the reactions leads to the decrease of the heat flux towards the absolutely noncatalytic wall by 12% at the altitude of 80 km, but the constants recommended by Blottner<sup>17</sup> leads to the decrease of C<sub>h</sub> by 14%. The greatest difference in the values of backward reaction constants, which are considered as functions of temperature, occurs in the dissociation-recombination reactions with participation of atoms of oxygen and nitrogen. The role of exchange reaction  $O_2 + N_2 \neq 2NO$ is insignificant. In the case of ideally catalytic surface the usage of other values of the chemical reaction rates as the functions of temperature leads to minor changes (about 1-2%) in the values of the heat flux  $C_h$  or the Stanton number St.12

This analysis demonstrates that in order to increase the accuracy of the determination of the heat flux characteristics in nonequilibrium viscous shock layer, it is recommended to utilize more reliable information on transfer properties<sup>14</sup> of multicomponent gas mixture and the constants<sup>2</sup> of chemical reaction rates.

The present study showed that the binary similitude law<sup>8</sup> is satisfied in all the researched conditions of streaming of blunt bodies.

## Equilibrium temperature of the vehicle surface.

Large values of the heat flux towards the surface of the spherical body under flight conditions at high altitudes lead to high level of equilibrium temperature  $T_{we} = (q/\epsilon\sigma)^{4}$  ( $\epsilon$  - degree of darkness;  $\sigma$  - the constant of Stephan-Boltzmann) of the surface of the body. In Figs. 7 and 8, as an example, the values  $T_{we}$  with  $\varepsilon = 0.85$  are shown, for axial symmetrical critical point of the body with the blunt radius R = 1 m and on the critical line of cylinder having R = 0.1 m for two extreme cases of catalytic activity of the vehicle surface. Using noncatalytic surface material (empty squares) leads to a significant decrease in the equilibrium temperature.

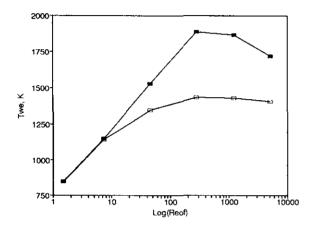


Fig. 7 Equilibrium temperature  $T_{we}$  of the spherical surface ( $\mathbf{R} = 1 \text{ m}$ ) at different values of the Reynolds number  $\text{Re}_{ol}$ : • - catalytic surface; • - noncatalytic surface.

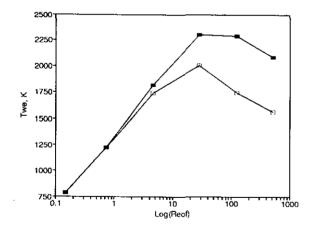


Fig. 8 Equilibrium temperature  $T_{we}$  of the cylindrical surface (R = 0.1 m) at different values of the Reynolds number  $\text{Re}_{of}$ : • - catalytic surface; • - noncatalytic surface.

Fig. 9 demonstrates the influence of the sliding angle  $\chi$  on the equilibrium temperature  $T_{we}$  along the critical

line of the cylinder surface (R = 1 m) for two extreme cases of the process of heterogeneous reactions (on three points of the trajectory<sup>15</sup>): solid lines correspond to noncatalytic, and dash lines - to the ideally catalytic wall of the vehicle.

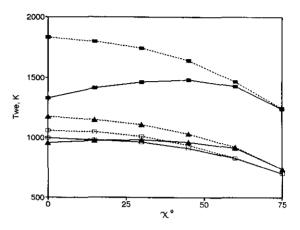


Fig. 9 Equilibrium temperature  $T_{we}$  as a function of the sweep angle  $\chi$  for different values of the Reynolds number  $Re_{of}$  and flight altitudes: dash curves catalytic surface; solid curves - noncatalytic surface;  $\Box$ -  $Re_{of} = 6.97$ ,  $\blacksquare$  -  $Re_{of} = 230$ ,  $\blacktriangle$  -  $Re_{of} = 5130$ .

The calculations indicate that the equilibrium temperature of the surface monotonously decreases as the angle  $\chi$  increases and only slightly depends on the mechanism of the process of the reactions on the surface. The degree of the dissociation of the gas is significant under the conditions of maximum heat fluxes ( $Re_{of}$  = 230, H = 80 km), hence leading to the substantial difference of the value  $T_{we}(\chi)$  for different materials of the surface.<sup>12</sup> As for the absolutely noncatalytic wall, this value carries nonmonotonous character, and in the point of maximum T<sub>we</sub> the value of equilibrium temperature is approximately 150K higher then of the corresponding value when  $\chi = 0$ . As the further decrease of the altitude occurs, these differences decrease. The explanation of this effect is: as the sweep angle gets bigger, the degree of dissociation of gas decreases in the viscous shock layer.<sup>18</sup> This consequence leads to the decrease of the part of energy of the free upstream flow which is directed towards the dissociation of the molecules and to the decrease of influence of noncatalytic surface on the heat flux. As a result, the equilibrium temperature T<sub>we</sub>

approaches the value corresponding to the ideally catalytic surface.

Under considered flight conditions the behavior of the heat flux depending on the sweep angle fully corresponds to the changes of the equilibrium temperature of the surface.

## Concluding Remarks

The computational tests for this study were designed specifically as a model problem for heat protection systems of hypersonic vehicles such as the Space Shuttle. The computed results presented in this study further validate the TVSL method for calculating nonequilibrium multicomponent gas flow near blunt bodies. The understanding of the main characteristics of the catalytically influenced zone can be useful for creation of new approximation methods of describing heat flux at a catalytic surface of a vehicle.

#### Acknowledgment

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