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NUMERICAL ANALYSIS OF COMBUSTION IN SUPERSONIC FLOWS

by

P. I. Chushkin, Computing Centre of the USSR
Academy of Sciences, Moscow, USSR

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P.I.Chushkin
Computing Centre of the USSR Academy
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Abstract

The numerical investigation of combustion in supersonic stationary flows of hydrogen-air mixture past bodies is carried out. A two-component model with direct and inverse reaction is assumed for kinetics. The numerical method using characteristic compatibility relations is applied for computations. The structure of combustion zone and the distributions of physical parameters in a flow-field are studied in various cases (cone at zero and non-zero angle of attack, point-nose cylinder, nozzle).

1. Introduction

The investigation of supersonic stationary flow of a combustible gas mixture is of interest in the connection with the problem of fuel burning in supersonic streams. Crossing the bow shock wave formed ahead of a body the combustible mixture can be heated to the temperature of ignition and then exothermal reactions start to run. In general, these reactions proceed with finite rates, and therefore a flow in shock layer is essentially nonequilibrium.

The analysis of such flows may be carried out with the aid of numerical methods. However, the kinetics of combustion in gases is characterized by a considerable complication, including chain-branching mechanism with a great number of elementary chemical reactions, which is often not sufficiently studied. Hence a numerical calculation of combustion taking into account a complete kinetics is a very difficult problem especially in three-dimensional case. Some authors confining themselves to several basic reactions have computed the combustion of hydrogen-oxygen or hydrogen-air mixtures in a one-dimensional stream [1] or in a axisymmetrical shock layer on nose part of a sphere [2-4].

The process of combustion for the mixtures mentioned has the following general behavior. At first, within certain distance behind the shock wave during the induction period mesured by the induction delay time t_i, the reactions run without any thermal effect. Subsequently a zone of reactions with heat energy release takes place. There are the sharp changes of concentration and temperature at the front boundary of this region(the ignition boundary), but further a relatively slow transition to an equilibrium state occurs. Such a regime is typical one for a certain range of temperatures and pressures. In this case it is possible to consider some simplified models of combustion kinetics, which prove to be enough reliable for the investigation of general properties of supersonic flows of combustible gas mixtures [(5)].

The simplest model of such a type is the well-known model of detonation wave while crossing which the momentary heat release is assumed. The two-front model was applied to treat the flow past nose part of a sphere; here all the heat is discharged on a combustion front closing the induction zone downstream of the bow shock wave [(6)]. Calculating two-dimensional and axisymmetrical flows, the author has considered an model with an exothermal reaction proceeding immediately behind the shock wave and obeying the Arrhenius law [(7)]. The author has also developed a model with direct and inverse reactions after an induction delay time [(8)]. In the present paper this model is used for the numerical investigation of plane, axisymmetrical and three-dimensional supersonic streams with combustion past various bodies and in nozzles. It should be mentioned that a non-stationary one-dimensional propagation of blast wave in a combustible gas mixture has computed on the base of similar model [(9)].

2. Governing equations and method of solution

Let us consider the problem of supersonic stationary stream of combustible gas mixture flowing past a body of the given shape. We suppose that behind bow shock wave the internal degrees of freedom are in local equilibrium, but chemical reactions run with finite rates. All the transport effects such as viscosity, thermal conduction, radiation, diffusion are neglected. The chemical kinetics in the model will be described by a single variable - the total mass cocentration C of unreacted molecules. The direct reaction (combustion) and the inverse reaction (recombination) start to run in a time interval t_i after crossing the shock wave by a gas particle. The initial mixture and the products of combustion are assumed to be perfect gases with different molecular weight μ and ratio of specific heats γ. Each moment the gas mixture is also supposed to be an uniform perfect gas with averaged thermodynamical properties.

In the case under consideration the system of gas dynamics equations has the form

$$\left.\operatorname{div}\rho\bar{V}=0\ ,\ \rho\frac{d\bar{V}}{dt}+\operatorname{grad}p=0\ ,\ \right\}(1)$$

$$\left.\begin{aligned} &\frac{dp}{dt}-\frac{\gamma p}{\rho}\frac{d\rho}{dt}+(\gamma-1)\rho q\frac{dc}{dt}=0\,, \\ &p=\frac{R}{\mu}\rho T\;, \end{aligned}\right\} \quad (1)$$

where $\bar{V}, p, \rho, T$ denote the velocity vector, the pressure, the density and the temperature, respectively; R is the universal gas constant, q is the total heat release per unit mass of combustible mixture.

The induction delay time, depending on local values of flow parameters, will be determined for the hydrogen-air mixture by the formula

$$t_i=\frac{k_i}{p^{m-1}}\exp\left(\frac{E_i}{RT}\right)\,, \quad (2)$$

where E_i is the activation energy, k_i is the positive constant, $m=2$. We introduce the fraction of induction delay time φ which is defined by the equation

$$\frac{d\varphi}{dt}=\frac{1}{t_i}\,. \quad (3)$$

The equation for concentration C is taken in the form of Arrhenius relation describing a variation of this function due to direct and inverse reactions

$$\begin{aligned} \frac{dc}{dt} = &-k_1 c^m p^\ell \exp\left(-\frac{E}{RT}\right)+ \\ &+k_2(1-c)^m p^n \exp\left(-\frac{E+q}{RT}\right), \end{aligned} \quad (4)$$

where k_1 and k_2 are the constants of reaction rate, E is the activation energy, ℓ and n are the exponents.

Therefore, the present model takes into account the interaction of flow-field and chemical processes in a particle. Indeed, the heat release in the equations (1) is determined by the total concentration, while the kinetic equations (2) - (4) include local values of gasdynamic functions.

The boundary conditions are as follows. The normal velocity component must vanish on the body surface. The usual Rankine-Hugoniot relations should be satisfied on the shock wave being an adiabatic surface of strong discontinuity; here, $\varphi=0$ and $C=1$. The ignition boundary is defined by condition $\varphi=1$. Obviously within the induction region $C=1$, $q=0$ and there is the adiabatic flow which allows to set initial data at some small value of time t in comparison with the induction delay time t_i .

The system of governing equations in general three-dimensional supersonic case will be integrated by the numerical method using two-dimensional characteristic compatibility relations. This method was worked out for the computations of flows in presence of non-equilibrium physical-chemical processes [10-12]. The system of equations (1) - (4) is taken in cylindrical coordinates x , τ , ψ connected with the body. The flow region between the body surface $\tau=\tau_B(x,\psi)$ and the shock wave $\tau=\tau_w(x,\psi)$ is straightened out by the introducing a normalized variable $\xi=(\tau-\tau_B)/(\tau_w-\tau_B)$ instead of τ . The derivatives with respect to ψ are eliminated from the governing system (rewritten in the variables x , ξ , ψ) with the aid of the trigonometrical polynomials with interpolation nodes on a number of meridional planes $\psi = \text{const}$. As a result we obtain the approximating system of differential equations in the variables x and ξ , which define the values of basic unknown functions on all the meridional planes of interpolation. This system is of hyperbolic type(under the certain supersonic conditions) and has two families of wave characteristics and one family of analogues of stream lines in each plane of interpolation. Hence, a characteristic computational scheme of the second order approximation may be constructed. In this scheme the solution is calculated on successive planes $x = \text{const}$ and characteristic lines are projected from the fixed nodal points on the plane to be calculated towards the previous plane. This computational scheme is also suitable in particular cases of two-dimensional and axisymmetrical flows.

3. Analysis of numerical results

The numerical solution of the problem was carried out for various bodies in supersonic stream of stoichiometrical hydrogen-air mixture. Now some numerical results will be presented considering all the functions in dimensionless form and using as reference quantities the certain value of induction delay time t_i , the critical velocity of sound a_{cr} and the free-stream density ρ_∞ .

At the beginning, we discuss the results obtained for a circular cone with semi-apex angle $\omega = 30^\circ$, when the undisturbed stream has the following parameters: the Mach number $M_\infty = 5$, the angle of attack $\alpha = 0^\circ$, the temperature $T_\infty = 685^\circ K$ and the pressure $p_\infty = 1\,atm$; in this case the reference quantities are the induction delay time $t_i = 0.52 \times 10^{-6}$ sec and the critical velocity of sound $a_{cr} = 1380$ m/sec.

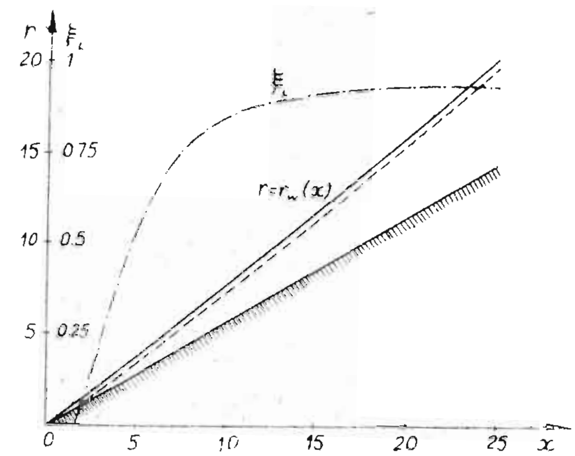

Fig.1. The shock wave and the ignition boundary for the cone at zero angle of attack.

The bow shock wave (solid line) and the ignition boundary (dashed line) are shown for this flow in Fig.1 ; the relative coordinate ξ_i of ignition boundary is here depicted by dash-dotted line. During the combustion process the thickness of shock layer increases due to the decreasing of density. Thus, the slope of shock wave rises, the pressure and the temperature behind the shock wave become higher, the induction delay time diminishes and, as the result, the boundary of ingnition approches the shock wave.

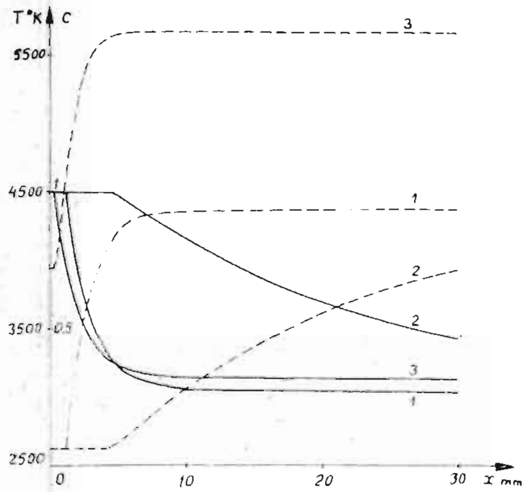

Fig.2. The distributions of concentration and temperature along the cone at various free-stream conditions.

The distribution of temperature T (dashed line) and the distribution of concentration C (solid line) along the cone surface are drawn in Fig.2. Here in addition to the curves 1 for the basic variant of calculation ($T_\infty = 685°K$, $P_\infty = 1$ atm) we also present the curves 2 ($T_\infty = 1000°K$, $P_\infty = 1$ atm) and the curves 3 ($T_\infty = 685°K$, $P_\infty = 0.25$ atm) for other cases. To illustrate the influence of free-stream parameters this graph is given with respect to dimensional quantities. After the induction period the combustion process develops intensively being accompanied by a sharp increase of temperature, but later on it slows down. The concentration drops rapidly along the stream lines approaching to a value corresponding to the equilibrium of direct and inverse reactions, that is the complete burning and the complete heat release do not achieve in this case. When the free-stream pressure decreases ($P_\infty = 0.25$ atm), the combustion proceeds less fastly, but the temperature and the concentration on the body at large distance x tend to the same equilibrium values as in the case with $P_\infty = 1$ atm. As concernes the pressure, it somewhat increases along the surface of cone having a slight maximum. At further distances x usually some oscillations have been observed in the flow-field, and their character depends, mainly, on the activation energy.

The structure of combustion zone for the basic variant of calculation is illustrated by the distributions of concentration, temperature and density across the layer between the shock wave ($\xi = 1$) and the cone surface($\xi = 0$). In Figs.3-5 these functions are plotted versus the variable ξ for a series of planes x =const.

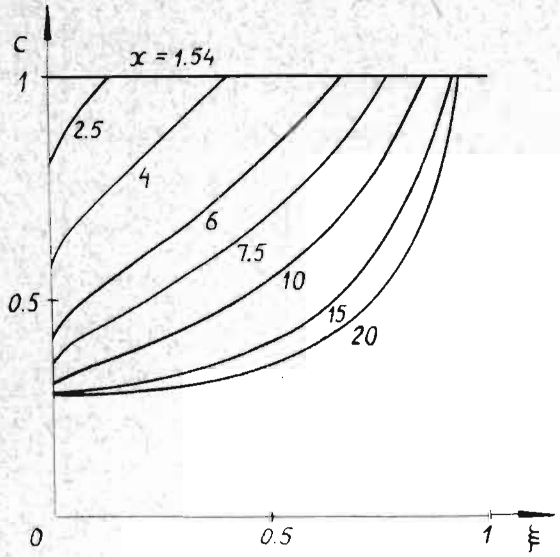

Fig.3. The shock layer distribution of concentration on the cone.

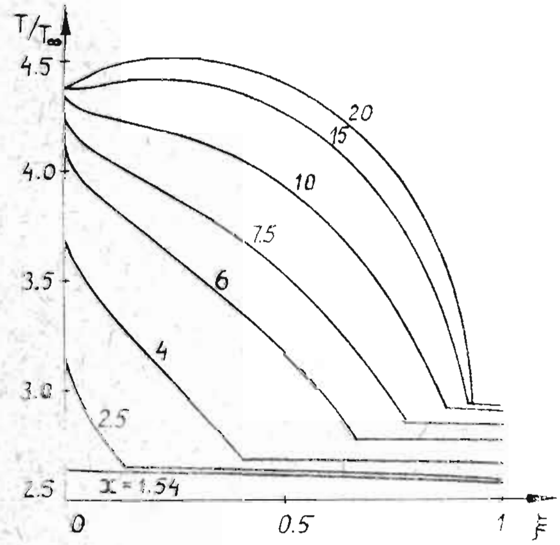

Fig.4. The shock layer distribution of temperature on the cone.

in the induction zone (at $x \leq 1.54$) all the functions change as in the adiabatic flow, and they have discontinuities of their derivatives at the ignition boundary. The field of concentration is presented in Fig.3. The graph of temperature (Fig.4.) demonstrates an interesting effect - the maximal temperature before the equilibrium takes place on the body surface, and subsequently it occurs inside the flow-field. The profiles of density in shock layer (Fig.5), as the profiles of pressure, have a complicated form with peak at the ignition boundary.

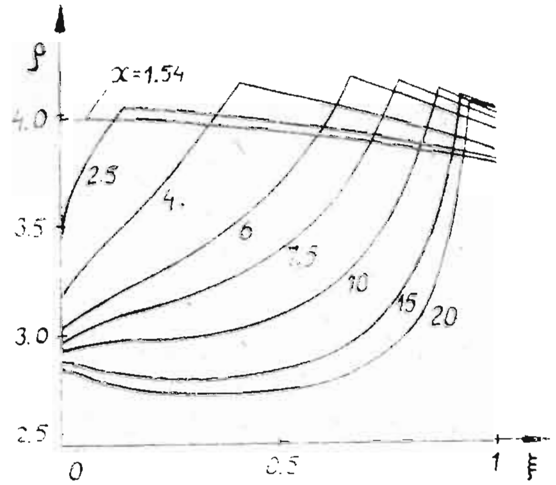

Fig.5. The shock layer distribution of density on the cone.

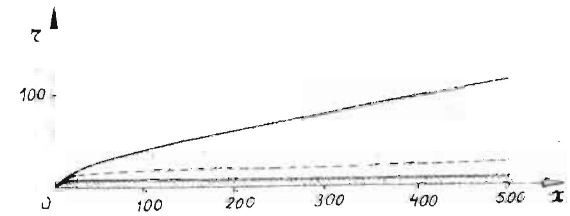

Fig.6.The shock wave and the ignition boundary for the pointed cylinder.

Now we consider the case of supersonic axisymmetrical flow (M_∞ =7, T_∞ =288°K, p_∞ =1 atm) past a long circular cylinder with pointed ogive nose part which has the form shown by a dash-dotted line in Fig.7. Here the flow-field pattern and distributions of parameters in the combustion zone have different features, than in the preceding example of cone. The induction delay time is much more in this case through the decay of shock wave (Fig.6). The ignition boundary (dashed line) is situated close to the body surface, where there is a narrow layer of burned gas with the thickness depending on the intensity of reaction behind the shock wave.

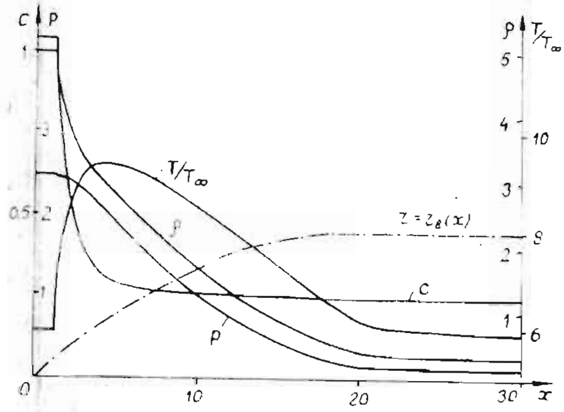

Fig.7. The distribution of physical parameters along the pointed cylinder.

The distribution of various parameters on the nose part of the pointed body is given in Fig.7. The interaction between the heat release in exothermal reaction and the acceleration of flow around the ogive nose body surface causes the non-monotonic behavior of temperature. The density and the pressure signiticantly decrease on the nose part of the body, but they change only slightly on the cylindrical part.

It should be noted that the combustion process for the supersonic flow past a wedge proceeds in the same manner as in the case of cone. However, the shock wave in front of a wedge (for the same free-stream conditions and the same apex angle) is stronger, therefore the combustion in the two-dimensional case runs more intensively than in the axisymmetrical one.

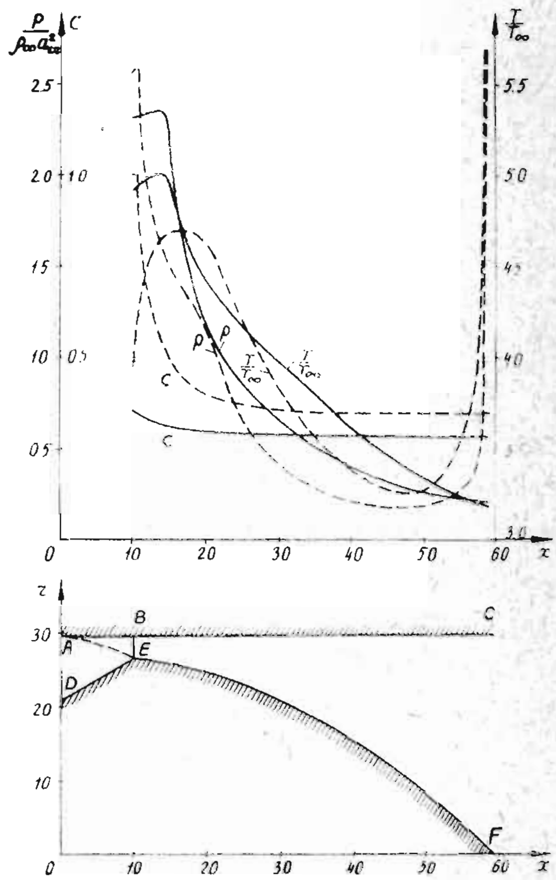

Fig.8. The distribution of physical parameters in the axisymmetrical nozzle and the form of nozzle.

We have also computed the combustion of a hydrogen-air mixture in supersonic two-dimensional and axisymmetrical nozzles with a inner body of various shape. Along the head part DE of the inner body (see the bottom part of Fig.8) the supersonic stream with the Mach number M_∞ impinges the external wall ABC of nozzle. The shock wave AE, behind which the combustion is initiated, passes from the leading edge A of external wall to the angle point E on the contour of inner body. The inclination of inner body profile in the point E is chosen so that any other shock waves do not arise in the narrow section BE of nozzle.

As an example we present in Fig.8 the flow inside the short axisymmetrical nozzle with the following parameters of the impinging stream - $M_\infty=5$, $T_\infty=685°K$, $P_\infty=1$ atm. This graph gives the distributions of concentration C, temperature T/T_∞, density ρ and pressure p along the external wall (solid lines) and along the inner body (dashed lines) behind the narrow section of nozzle ($x=10$). The exothermal reaction on the inner body starts to run immediately after the point E and results in the rapid alteration of flow parameters. The combustion process on the external wall develops fastly along the portion AB (the corresponding data do not present in Fig.8), but it gets weaker after the narrow section. When the equilibrium of direct and inverse reactions is achieved, the rarefaction of gas in a channel begins to play a principal role, resulting to the drop of temperature and pressure. The very sharp growth of temperature and pressure takes place near the end point F of inner body in axisymmetrical nozzle (in contrast to two-dimensional one), and a rear compression shock must arise there.

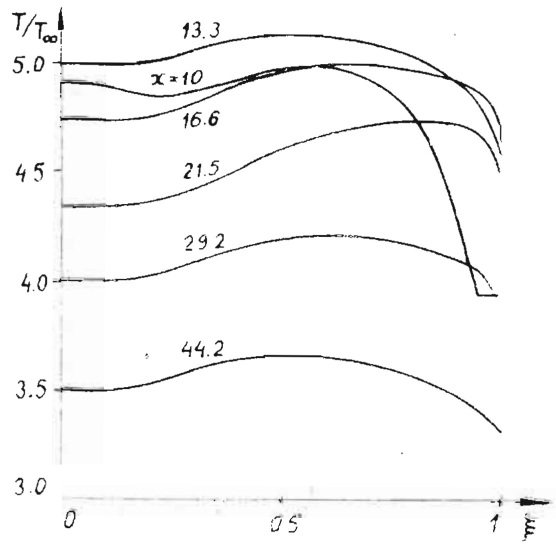

Fig.9. The temperature variation in cross-sections of nozzle.

Fig.9 and 10 show the variations of temperature and pressure as a function of the variable ξ (with on the external wall $\xi=0$ and on the inner body $\xi=1$) for a series of cross-sections of nozzle. These curves illustrate the flow smoothening with respect to the nozzle length. The differences of parameters on the wall and on the inner body at large values x are, naturally, smaller for longer nozzles.

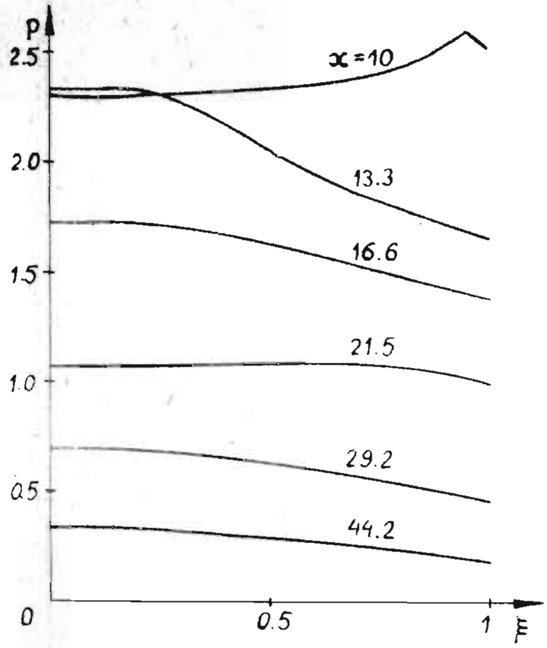

Fig.10. The pressure variation in cross-sections of nozzle.

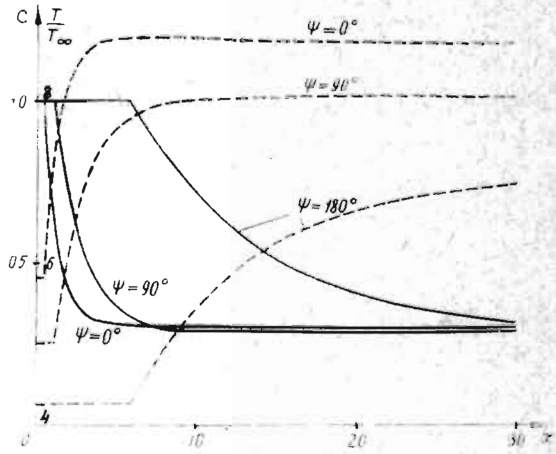

Fig.11.The distributions of concentration and temperature along three generators of the cone at angle of attack.

The analysis of three-dimensional supersonic flow with combustion past a body set at an angle of attack is a very interesting problem. We treat some numerical results for a cone with semi-apex angle $\omega = 30^{\circ}$ in the stream of stoichiometric hydrogen-air mixture at Mach number $M_{\infty}=7$, angle of attack $\alpha = 10^{\circ}$, temperature $T_{\infty} = 400^{\circ}K$ and pressure $p_{\infty} = 1$ atm. In this case the reference quantities are the induction delay time $t_i = 0.6 \times \times 10^{-6}$ sec and the critical velocity of sound $a_{cr} = 1410$ m/sec.

The distributions of concentration (solid line) and temperature (dashed line) along three generators of cone $\psi = 0^{\circ}$ (windward side), $\psi = 90^{\circ}$ and $\psi = 180^{\circ}$ (leeward side) are plotted in Fig.11. The temperature and the pressure on the windward side are higher, the induction delay time is significantly less than one on the leeward side, by this reason the combustion proceeds there intensively. The variation of concentration and of temperature are essentially smaller on the leeward side at the same distances from the cone apex. It should be noted that the pressure varies rather weakly along the body.

The relative coordinate ξ_i of ignition boundary is depicted in Fig.12 with respect to variable ψ for different planes x = const. At large values of x the ignition boundary is situated

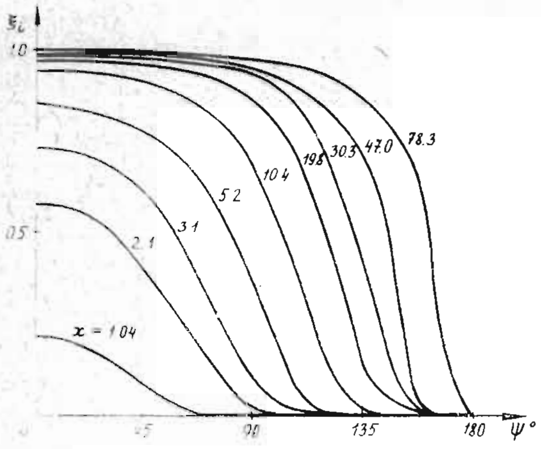

Fig.12. The position of ignition boundary in the shock layer on the cone at angle of attack.

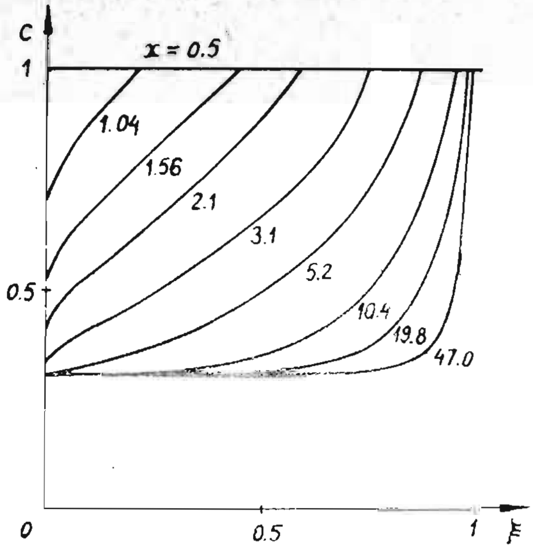

Fig.13. The distribution of concentration in the windward plane for the cone at angle of attack.

on the windward side near the shock wave and on the leeward side near the body. This fact, naturally, defines a different behavior of physical parameters across the shock layer in different meridional planes. For example the profiles of concentration and of temperature in the windward plane $\psi = 0^\circ$ are given in Fig.13 and 14; they are similar to the corresponding graphes for the case of cone at zero angle of attack.

An interesting effect concerning the form of shock wave is found in the three-dimensional case of flow around the cone. The variation of shock wave radius z_w versus the angle ψ is plotted in Fig.15 for a series of values of x.

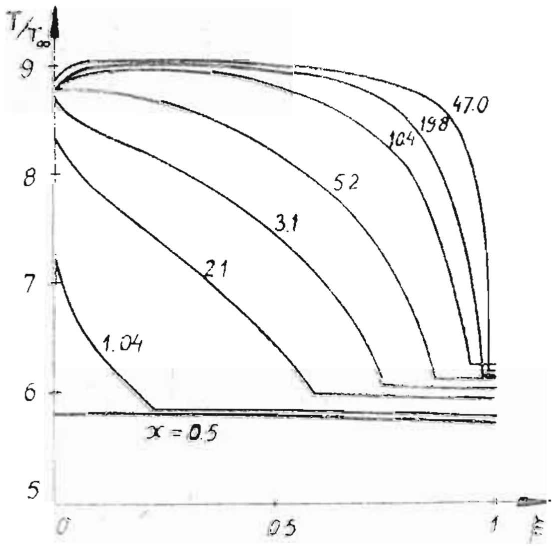

Fig.14. The distribution of temperature in the windward plane for the cone at angle of attack.

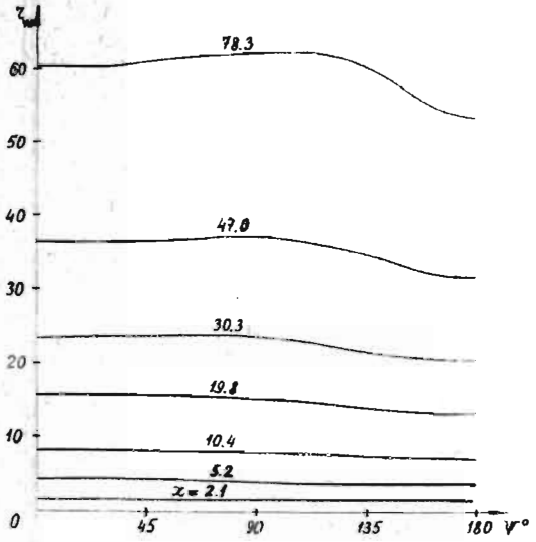

Fig.15. The shape of shock wave for the cone at angle of attack.

The cross-section of shock wave for the corresponding adiabatic flow past the cone at angle of attack represents a curve very close to a circle. Due to non-uniform heating and cross gas flow the deformation of shock wave appears. The shock layer becomes the most thick inside the region $0^\circ < \psi < 180^\circ$. When the coordinate x grows, the magnitude of this maximum increases, and its position moves towards greater values of ψ. The shock wave on windward side is set closer to the body, than on leeward side. The remarked effect is also observed in an adiabatic flow past a cone, when an angle of attack increases [see the tables (13)]. Thus, the exothermal reaction intensities the three-dimensional structure of stream past a cone at angle of attack.

The numerical computations based on the model, approximating the kinetics of combustion, have given a possibility to study the structure of combustion zone and the physical features of supersonic flow past various bodies and for various conditions. The model has taken into account the inverse reaction which is important; this conclusion is maintained by comparison with work(7) where the inverse reaction was not consider. Some new physical effects were found by calculations of plane, axisymmetrical and three-dimensional supersonic streams of combustible gas mixtures. However, it should be remarked that numerical computations with more complete kinetics of combustion would be very interesting.

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