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CALCULATION OF THE EFFECT OF A CONSTANT ELECTRIC FIELD ON THE GAS DYNAMICS AND NITROGEN OXIDE EMISSION IN A LAMINAR DIFFUSION FLAME

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A laminar methane diffusion flame in a constant electric field whose direction is opposite to that of the velocity of the gas flow from the burner nozzle is considered. The mathematical model used includes the complete system of Navier-Stokes equations for the velocity and passive admixture concentration fields, the charge transport equation, together with the Poisson equation for the self-consistent electric field, and the chemical kinetic equations for a thin combustion zone. The calculations show that the flame shortens and its thickness increases in the root zone when an electric field is imposed. This effect is accompanied by a reduction in the nitrogen oxide emission, while is consistent with the experimental data.

The effect of an electric field on the characteristics of hydrocarbon flames has been studied for a long time. An extensive review of the results obtained cab be found, for example, in [1, 2]. A much smaller number of studies has been devoted to the direct effect of an electric field on the emissive characteristics of the flame. These studies include an investigation of premixed-hydrocarbon combustion [3] in which the change in CH concentration distribution following the imposition of an electric field was determined.

In the pioneering experiments on the effect of a uniform electric field on nitrogen oxide emission in a propane flame [4] it was observed that applying a negative potential to the burner leads to a decrease of 30% in the nitrogen oxide emission factor. In this case strong flame deformation, expressed as shortening and widening in the root zone, was observed.

However, the reasons for the decrease in nitrogen oxide emission observed experimentally remained unclear. One of the possible mechanisms suggested was a decrease in the temperature of the flame as a consequence of an increase in the carbon black fraction and an increase in heat losses due to radiation. Experiments carried out later with methane as the fuel, in which carbon black production was an order less, led to similar results [5]. Thus, the question arises: can this phenomenon be explained without allowance for the effects associated with carbon black radiation? The present investigation makes it possible to answer this question in the affirmative.

1. QUALITATIVE DESCRIPTION OF THE PROCESSES AND GENERAL CHARACTERIZATION OF THE MODEL

Positive ions and electrons are the principal charged particles in flames since at flame temperatures negative ions are unstable and rapidly disintegrate into an electron and a neutral molecule [1]. These particles are formed as a result of chemo-ionization reactions in a narrow zone in the neighborhood of the maximum flame temperature. The shape of this zone coincides closely with the observed shape of the flame. Most of the other chemical reactions of oxidation of the fuel and atmospheric nitrogen also take place in this zone.

In the absence of an external field in the combustion zone the plasma is quasineutral so that the total rate of charged particle formation is equal to the total recombination rate. The application of an external field leads to charge separation and an electrogasdynamic (EGD) body force exerted on the gas, as well as to an electric current in the discharge gap. As a result of the equality of the total ion and electron currents and the high mobility of the electrons, in the main zone of the flame outside the narrow combustion zone the electron concentration is much less than the ion concentration and the entire flame acquires a positive charge, being "attracted" to the negative electrode. The corresponding change in the hydrodynamics of the flow inside the flame and its deformation lead to change in the fuel-oxidizer diffusion mixing rate. This is directly associated with the intensity of the combustion process and, consequently, may affect the nitrogen oxide formation.

To analyze these effects we need a physico-mathematical model of the laminar diffusion flame in an external electric field. This model must include hydrodynamic equations for describing the flow field in the presence of electric body forces, transport equations for the components of the mixture with allowance for chemical reactions, and equations for the ion concentrations and electric fields.

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The problem of a multicomponent reacting-mixture flow which describes the laminar diffusion flame is fairly complex even without taking the electric effects into account. So far, there have been few studies (for example, [6]) in which this problem is solved in the general formulation, which involves heavy computing costs. In the present paper we propose the following simplified model which makes it possible to divide the problem into two parts: "hydrodynamic" and "burning". As distinct from premixed-gas flames, in laminar diffusion flames the fuel combustion rate is limited by the fuel-oxidizer mixing process and in the first approximation the composition of the mixture can be determined from the chemical equilibrium condition. Since at the combustion temperature the equilibrium is displaced in the direction of the combustion products, the combustion process can be approximated by a single-stage irreversible reaction: fuel (f) + oxidizer (o)=products, and the chemical equilibrium condition can be written in the form $c_o c_f=0$, where c are the mass fractions of the components. This approximation corresponds to an infinitely narrow combustion zone, on one side of which there is only fuel and combustion products and on the other only oxidizer and combustion products. On this combustion surface the fuel and oxidizer concentrations vanish simultaneously, and their normal derivatives are discontinuous and in stoichiometric proportion and determine the surface fuel combustion rate [7]. The shape of the combustion surface, which coincides closely with the visible shape of the flame, is not known in advance and must be found in the course of solving the problem.

Under a series of simplifying assumptions the basic parameters of the mixture: the temperature, the fuel, oxidizer, and combustion product concentrations are functions of a single scalar variable z, usually called the passive admixture concentration, which satisfies the transport equation for the component not involved in the chemical reactions and the boundary conditions for the fuel concentration (the Bourke-Schumann model). In this case the above-mentioned combustion surface is an isoscalar surface $z=z_s$=const. Using this approach, we can find the velocity fields and the flame shape.

After finding the flame shape, in order to take the finite thickness into account and consider the structure of the narrow laminar combustion zone we employ the model used in [8]. This yields the rates of formation of the components with low concentrations, namely, nitrogen oxides and positive ions.

Thus, the model proposed makes it possible to solve the hydrodynamic and chemical kinetics equations separately.

The ion formation rate found on the basis of the solution of the problem of the structure of the laminar combustion zone is used to find the volume charge and electric field distributions. This makes it possible to find the electric body forces exerted on the gas which are included in the hydrodynamic equations used to find the flame shape. This closes the problem.

2. FORMULATION OF THE PROBLEM

We will consider a vertical laminar diffusion methane flame issuing from a burner nozzle of radius R_0. Assuming that the problem is axisymmetric, we choose the calculation domain and the directions of the coordinate axes as shown in Fig. 1. Here, the x axis (axial coordinate) is directed vertically upward, the origin is located at the centre of the burner nozzle, the fuels flows out from the burner nozzle in the direction of the x axis, and the radius of the supply tube is equal to the radius of the outlet R_0. At x=0 (segment AE) and on the right boundary (segment FG) there are assumed to be metal grids for establishing the electric boundary conditions.

The need to consider the solution downstream from the plane of the edge of the burner nozzle is associated with the possibility of the onset of reverse current zones under the action of the EGD forces directed opposite to the gas flow velocity. The flow velocities and the flame shape can be found from the axisymmetric system of Navier-Stokes equations written in stream function-vorticity variables (ψ, ω) [6] with allowance for the action on the of the body forces gas due to the electric field. The basic equations of the system have the form:

$$\frac{\partial}{\partial x}\left(\frac{1}{y\rho}\frac{\partial \psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{1}{y\rho}\frac{\partial \psi}{\partial y}\right)+2\omega=0$$

$$\frac{\partial}{\partial x}(\rho u\omega)+\frac{\partial}{\partial y}(\rho v\omega)-\frac{1}{y^2}\left\{\frac{\partial}{\partial x}\left(y^3\frac{\partial}{\partial x}\left(\frac{\mu}{y}\omega\right)\right)-\frac{\partial}{\partial y}\left(y^3\frac{\partial}{\partial y}\left(\frac{\mu}{y}\omega\right)\right)\right\}-$$

$$g\frac{\partial \rho}{\partial y}-e\left(\frac{\partial nE_y}{\partial x}-\frac{\partial nE_x}{\partial y}\right)-\frac{1}{2}\left\{\frac{\partial(u^2+v^2)}{\partial x}\frac{\partial \rho}{\partial y}-\frac{\partial(u^2+v^2)}{\partial y}\frac{\partial \rho}{\partial x}\right\}=0$$

$$\rho u\frac{\partial z}{\partial x}+\rho v\frac{\partial z}{\partial y}-\frac{1}{y}\frac{\partial}{\partial y}\left(y\frac{\mu}{Sc}\frac{\partial z}{\partial y}\right)-\frac{\partial}{\partial x}\left(\frac{\mu}{Sc}\frac{\partial z}{\partial x}\right)=0$$

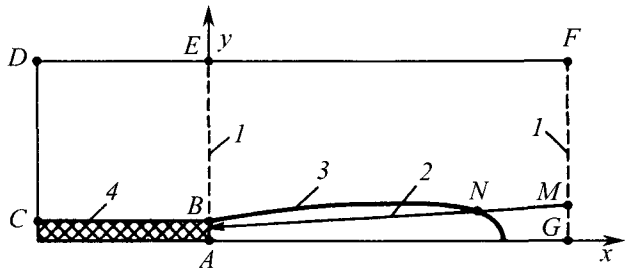

Fig. 1. Calculation domain: electrode-grids *1*, combustion surface *2*, trajectory of a positive ion *3*, supply tube *4*.

$$\operatorname{div}(n(u + bE))=0, \qquad \Delta\varphi=-(e/\varepsilon_0)n \tag{2.1}$$

$$2y\rho u=\partial\psi/\partial y; \quad 2y\rho v=-\partial\psi/dx; \quad E_x=-\partial\varphi/\partial x; \quad E_y=-\partial\varphi/\partial y; \quad \omega=\partial v/\partial x - \partial u/\partial y$$

Here, ψ and ω are the stream function and the vorticity, μ and ρ are the dynamic viscosity and the density of the mixture ($\mu=\mu(z)$ and $\rho=\rho(z)$); u and v are the flow velocity components, n and b are the ion mobility and concentration, E and φ are the electric field strength and the electric potential, g is the acceleration of free fall, and Sc is the laminar Schmidt number.

This system must be supplemented with the corresponding boundary conditions. For the hydrodynamic and transport equations the usual conditions are imposed. The distribution of the velocity u, the vanishing of v, and the condition $z=1$ are specified at the nozzle edge (segment AB), the no-slip condition and the vanishing of the normal derivative of z on the segment BC, the symmetry condition on the segment AG, the vanishing of the normal derivatives of the quantities ψ, ω, and z (soft boundary conditions) on the segments CD and FG, and the vanishing of the normal derivatives of the quantities ψ and ω and the vanishing of z on the segment DF. Equations (2.1) are solved only for positive x (in the region bounded by the grids). On the segments AE and FG we specify the values of the electric potential corresponding to a given potential difference between the grids, on the segment EF a linear potential distribution, and on the segment AG the symmetry condition.

The charge transport equation is an hyperbolic first-order equation whose characteristics coincide with the trajectories of positive ions in the electric field. These characteristics depart from the boundary of the region and can intersect the combustion surface as shown in Fig. 1. By virtue of the condition of absence of a particle flow from the boundary of the region the zero ion concentration is conserved along the characteristic from the point of departure from the boundary (point M) to intersection with the combustion surface (point N). On the surface itself the equation is not fulfilled as a result of the charge formation. In order to obtain a relation between the charged particle concentrations on different sides of the combustion surface we will consider the charge conservation law for a thin volume surrounding a surface element. Neglecting the particle flow across the lateral surface of the volume considered, whose area is proportional to the volume thickness, we can write

$$en_2(u_n + bE_{n2}) - en_1(u_n + bE_{n1})=q_e$$

Here, the symbols with the subscript n denote the components of the corresponding quantities normal to the combustion surface, the subscripts 1 and 2 denote the values of the quantities on different sides of the surface, and q_e denotes the rate of formation of the surface charge. Here we assume that the gasdynamic velocity on the surface is continuous. An analysis of the structure of the chemo-ionization zone shows that there is no surface charge on the combustion surface, i.e., $E_{n1}=E_{n2}=E_n$. Hence we obtain

$$\Delta n=n_2 - n_1=\frac{q_e}{be|E_n + u_n/b|}$$

The value of n_2 is the boundary condition for the fragment of the characteristic from the point N to its intersection with the boundary of the region, as shown in Fig. 1, or to the intersection of the characteristic with another point on the combustion surface.

The quantity q_e can be found from the solution of the problem of the structure of the combustion zone with allowance for ion formation under the assumption that the reactions of ion formation from neutral components are irreversible and there

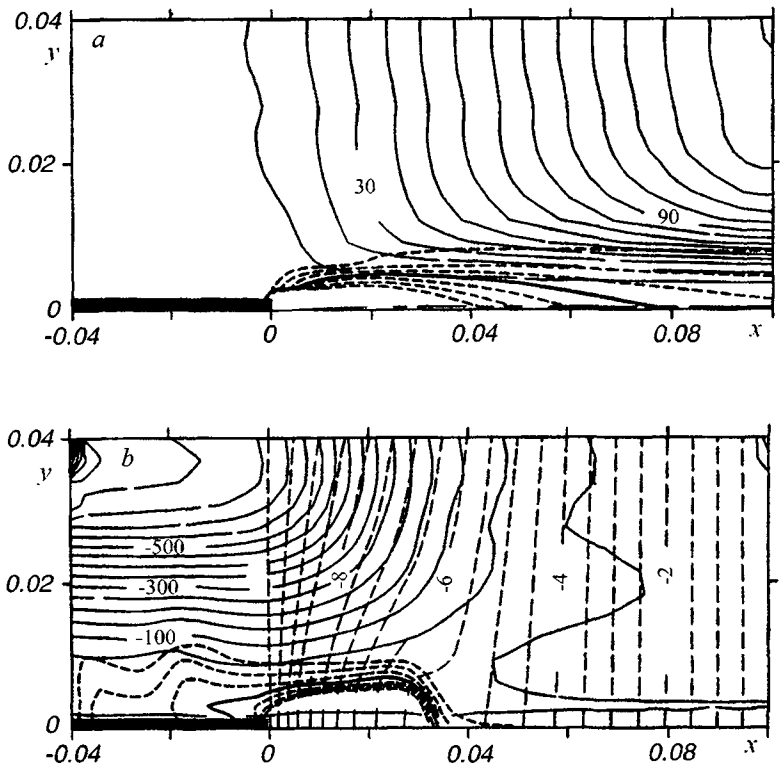

Fig. 2. Laminar diffusion flame for zero (*a*) and negative (*b*) burner polarity. The streamlines are plotted as thin continuous curves, the isoscalar lines z=const as broken curves, the lines φ=const as dashed curves, and the shape of the flame $z=z_s=0.055$ as a bold continuous curve. The passive admixture concentration isolines are plotted with a step $\Delta z=0.015$. The stream function is divided by the fuel mass flow rate, the geometric dimensions are indicated in meters, the potential in kilovolts, and the tube supplying the fuel is represented schematically by the heavy black line at the bottom left of the calculation domain.

is no charged particle recombination. In accordance with the conclusions of [9] the volume rate of charge formation in the flame is assumed to be proportional to the rate of the following chemical reaction:

$$CH + O \rightarrow CHO^+ + e^-$$

As a result of ion-molecular reactions the initial ion CHO^+ is transformed into other positive ions. This does not affect the total volume positive-charge density. In the calculations we used the chemical kinetics from [10, 11].

3. CALCULATION RESULTS

The methane flame was simulated numerically for a gas mass flow rate Q=2 mg/s, the burner radius R_0=0.4 mm, and potential differences between the lower and upper grids $\Delta\varphi$=0 and −10 kV. The average velocity of the flow from the burner nozzle was 6.6 m/s. This corresponds to the Reynolds and Froude number values Re=98 and Fr=10^4. The ion mobility was kept constant and equal to 10 $cm^2/V \cdot s$. The possibility of choosing the calculation conditions was limited, first, by the flame length which, as shown by numerous investigations, is proportional to the fuel mass flow rate and, second, by the fact that for large burner diameters, and, hence, lower fuel flow velocities, when a negative potential is imposed on the burner the pattern observed is unsteady and, more over, in the numerical calculations a steady-state solution cannot be established.

In the absence of an external electric field our calculations agree with experiment to within ~10% with respect to both the flame length and the nitrogen oxide emission for any burner diameter. For the above-mentioned values of Q and R_0 it is possible to obtain a stable steady-state flow pattern for a negative burner potential both experimentally and in the calculations.

We have reproduced the calculation results in Fig. 2. In this figure we can see the deformation of the flame and the formation of a reverse current zone. For the given parameters, calculation of the emission characteristics yields a 29% decrease in nitrogen oxide production in the methane flame with respect to the corresponding value for zero potential difference. The calculation overestimates the deformation of the flame and the decrease in NO_x production, but nevertheless yields qualitatively correct results. The calculation inaccuracies are attributable to inaccurate knowledge of the ion mobility and the possible formation of negative ions in the relatively cold zones of the jet. The calculated value of the current in the interelectrode gap, which is equal to the integral rate of charge formation in the volume considered amounts to 11.7 μA. This agrees with the experimental data to within 10%.

From Fig. 2 we can see that for a negative burner potential in the neighborhood of the curve $z=z_s$ corresponding to the combustion surface the spacing of the isoscalar curves z=const is perceptibly denser. This corresponds to an increase in the fuel and oxidizer concentration gradients and their mixing rate. The increase in the fuel-oxidizer diffusion mixing rate is accompanied by a decrease in the combustion zone thickness and, hence, in the volume in which nitrogen oxides are formed and by a decrease in the maximum temperature in the combustion zone. Both these factors lead to a decrease in NO_x production.

Summary. The proposed physical and mathematical models of a laminar diffusion flame in an external electric field make it possible to explain the decrease in nitrogen oxide production in the flame described in [4], which arises when a negative potential is applied to the burner due to the change in the flame hydrodynamics and the associated change in the fuel-oxidizer diffusion mixing rate.

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