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NUMERICAL INVESTIGATION OF FLAME PROPAGATION AND EXTINCTION IN A VERTICAL CHANNEL

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One of the most important problems in the theory of combustion limits is the role of natural convection in the extinction process. It is well known that the direction of flame propagation strongly influences the combustion concentration limits: they are narrower in downward propagation than when the flame travels upward.

A hypothesis explaining the mechanism of extinction of a flame as it propagates down through a vessel from the upper wall has been advanced in [1]. The authors suggested that, because of the cooling of hot reaction products by the vessel walls behind the flame front, free-convection flows develop, causing additional heat loss from the combustion zone and extinguishing the flame. Subsequent studies have confirmed the correctness of the hypothesis and led to the creation of approximate theoretical models of this phenomenon [2-6].

The formation of convective vortices behind a combustion front and their influence on flame propagation and shape in ignition from above have been studied in [7, 8]. An experimental study of the influence of gravity on flame propagation in a tube led Strehlov et al. [9] to conclude that extinction in weightlessness and in downward motion of the front is explained by heat transfer to the walls.

A considerable number of papers have been devoted to determining the critical conditions of combustion in ignition from below. Experiments [10] have shown that in a tube, the limiting flame propagation velocity opposite to the gravitational vector is determined by the ascent velocity of hot reaction products, which depends on the tube diameter and the free-fall acceleration; extinction was assumed to occur if the combustion velocity is less than the upwelling velocity of burned gas. In [11], on the basis of a similar extinction hypothesis, the fundamental limiting flame velocity was calculated in the case of ascent of the burning

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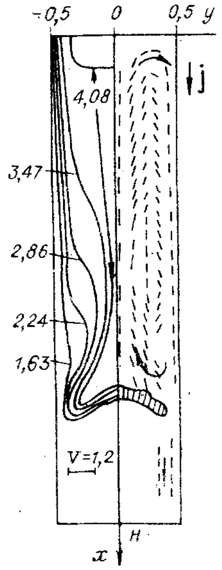

Fig. 1

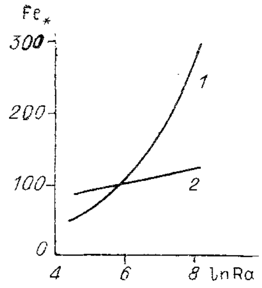

Fig. 2

medium. A mathematical model of extinction of a methane–air flame propagating upward through a cylindrical tube was suggested in [12]. The model is based on ideas advanced in [13]: the cessation of burning is associated with the divergence of streamlines ahead of the flame (the stretch effect), which causes additional heat and mass transfer from the reaction zone. The extinction of an upwelling flame core has also been explained in [9, 14] by "stretching" of the flame by convection flows.

The present paper is a continuation of [15]. The rules of flame propagation and extinction in a flat, closed vertical channel with cold side walls in an external mass-force field are studied by mathematical simulation. A comparison is made with earlier results.

1. Statement of the Problem. Let a stationary fuel mixture fill a flat channel of rectangular cross section, $0 \leqslant x \leqslant H_0$, $-L/2 \leqslant y \leqslant L/2$ (H_0 and L are the channel length and width; the coordinate system is shown in Fig. 1), with rigid impermeable walls. At the initial time the mixture is ignited by hot reaction products that fill a small region near an end wall of the channel. An exothermic, one-stage, irreversible chemical reaction of first order with respect to the deficient component, with an Arrhenius temperature dependence of the reaction rate is assumed to occur in the gas. The thermophysical properties of the combustion products and the initial mixture are assumed to be the same. The end walls of the channel are thermally insulated, and the side walls are maintained at the initial temperature T_0 of the cold gas.

The motion of the reacting mixture is described by a system of two-dimensional nonstationary equations. In introducing the dimensionless variables, the scales of length, velocity, time, temperature, reagent concentration, and gas pressure were chosen to be the channel with L, the velocity u_b of the flame, which propagates from the closed end and is determined from the Zel'dovich–Frank-Kamenetskii equation [16], the time L/u_b, the initial temperature T_0 and concentration a_0 of the deficient reagent in the initial mixture, and the initial gas pressure P_0, respectively. The density scale is expressed in terms of P_0 and T_0 from the equation of state of the gas: $\rho_0 = P_0/RT_0$ (R is the gas constant).

The system of equations in dimensionless variables has the form

$$\frac{\partial\rho}{\partial t} + \operatorname{div}\rho\mathbf{U} = 0,\ \frac{\partial\mathbf{U}}{\partial t} + (\mathbf{U}\cdot\nabla)\,\mathbf{U} = -\frac{1}{\gamma M^2\rho}\nabla P + \frac{1}{\mathrm{Re}\,\rho}\left(\Delta\mathbf{U} + \frac{1}{3}\nabla(\nabla\mathbf{U})\right) + \mathrm{Fr}^{-1}\cdot\mathbf{j},$$

$$\frac{\partial\Theta}{\partial t} + (\mathbf{U}\cdot\nabla)\,\Theta = \frac{\gamma}{\rho\,\mathrm{Re}\,\mathrm{Pr}}\Delta\Theta + (\gamma-1)\,\Theta\operatorname{div}\mathbf{U} + q\,\mathrm{Dm}\,a\Phi(\Theta),\ \frac{\partial a}{\partial t} + (\mathbf{U}\cdot\nabla)\,a = \frac{\mathrm{Le}}{\rho\,\mathrm{Re}\,\mathrm{Pr}}\Delta a - \mathrm{Dm}\,a\Phi(\Theta),\quad P = \rho\Theta,$$

where $\Delta \equiv \partial^2/\partial x^2 + \partial^2/\partial y^2$; $\Phi(\Theta) = \exp\left[E\left(\Theta_a^{-1} - \Theta^{-1}\right)\right]$; $\mathrm{Dm} = \mathrm{Re}\,\mathrm{Pr}\,E^2(\Theta_a - 1)^2/2\Theta_a^5$; t is time, P, ρ, Θ, and a are the gas pressure, density, and temperature and the reagent concentration; $\mathbf{U}(u, v)$ is the gas velocity; $\mathbf{j}$ is the unit vector coinciding in direction with the gravitational force.

The following are the dimensionless complexes: $M^2 = u_b^2/\gamma RT_0$, the square of the Mach number ($\gamma = c_p/c_V$ is the adiabatic index); $Fr = u_b^2/gL$, the Froude number (g is the free-fall acceleration); $Re = Lu_b\rho_0/\eta$, $Pr = c_p\eta/\lambda$, and $Le = \rho_0 Dc_p/\lambda$ are the Reynolds, Prandtl, and Lewis numbers (η, λ, and D are the coefficients of dynamic viscosity, thermal conductivity, and diffusion; the quantities η, λ, and ρD are assumed to be constants); $E = E_0/R_0T_0$; $q = Qa_b/c_VT_0$ (E_0 and Q are the activation energy and caloric effect of the chemical reaction and R_0 is the universal gas constant); $\Theta_a = 1 + q/\gamma$ is the dimensionless adiabatic combustion temperature; $Dm = (L/u_b)k_0 \exp(-E/\Theta_a)$ is the Damköhler number (k_0 is the pre-exponent of the chemical reaction), which, for our means of normalization, is not an independent parameter but is expressed by the above formula.

At the initial time t = 0, a core of hot gas

$$t = 0:\ \Theta = 1 + (\Theta_a - 1)\exp\left(-x^2/r_x^2 - y^2/r_y^2\right),\quad a = (\Theta_a - \Theta)/(\Theta_a - 1)$$

(r_x and r_y are parameters characterizing the initial size of the core) is specified in the stationary gas ($\mathbf{U} = 0$), which is in an equilibrium state (the relationship $\nabla P = \gamma M^2 Fr^{-1} \cdot \mathbf{j}$), is satisfied in the entire region).

Because the gravitational vector is directed along the channel axis (y = 0), the problem is symmetrical relative to y = 0 and the solution was sought in half of the region, $0 \leqslant x \leqslant H$, $0 \leqslant y \leqslant 0.5$ (H is the dimensionless length of the channel), with symmetry conditions specified at the boundary y = 0:

$$y = 0:\ \partial u/\partial y = v = \partial\Theta/\partial y = \partial a/\partial y = 0.$$

The attachment condition $\mathbf{U} = 0$ was specified for the velocity at the rigid boundaries. The walls were assumed to be impermeable to the reagent, and a constant temperature, equal to the initial temperature of the cold gas, was maintained at the side wall, while the end walls were assumed to be thermally insulated:

$$x = 0, H: \partial\Theta/\partial x = \partial a/\partial x = 0;\ y = 0.5: \Theta = 1,\ \partial a/\partial y = 0.$$

The formulated problem was integrated numerically using a finite-difference method [17]. The main calculations were carried out in a uniform grid with a spatial step size h = 1/20 and a time step corresponding to the value of the Courant number, determined from the speed of sound in the hot gas, about 4 or 5.

2. Ignition from Above. The influence of convection on combustion for this means of ignition was investigated for $\gamma = 1.4$, $M^2 = 0.01$, Re = 50-300, $Fr^{-1} = 1$-10, Pr = Le = 1, q = 5, H = 4, and $r_x = r_y = 0.2$.

The general rules of development of convection and of its influence on downward flame propagation are the following. The hot reaction products begin to cool due to their interaction with the cold side walls. Free-convection flows develop in the unevenly heated gas in the gravitational field in the presence of horizontal temperature gradients. The gas near the walls cools faster than at the center of the channel, becomes heavier, and descends. At the same time, on the other hand, the hot reaction products being formed at the flame front ascend. As a result, circulation flow develops behind the combustion front: near the cold side walls the gas descends, then near the flame front it turns around, and it ascends at the center of the channel up to the end wall, along which it flows out towards the side walls. For a given dimensionless calorific effect q, the flow intensity depends on Re and the Froude number, which characterizes the external force.

The calculations showed that at Fr = 1, the flame propagates over the entire channel length in the entire investigated range of Re. For Re = 50-100, the pattern of flame propagation resembles combustion in weightlessness, the only difference being that the combustion front becomes flatter than in the case of $Fe^{-1} = 0$ because descending flow develops near the side walls. An increase in Re leads to the development of more intense flows in the combustion products, so that for Re = 200 and especially for Re = 300 one observes a very pronounced influence of convection flows on combustion. In Fig. 1 we show the flame structure formed at t = 11.1 for Re = 300 and Fr = 1. The velocity field and the combustion zone (the hatched region, in which $\psi = a\Phi(\Theta) \geqslant 0.01$ and $\psi_{max} = 0.05$) are shown on the right, and isotherms with the indicated temperatures on the left. The formation of a convection eddy results in the edge of the flame near the side walls traveling ahead, while the core lags behind. Such a flame shape has been observed experimentally [6].

A decrease in Fr leads to intensification of convection flows and hence to their greater influence on the flame. Extinction of the flame is observed at $Fr^{-1} \geqslant 3$ for all analyzed values of Re. The eddy flow behind the flame front rapidly cools the hot reaction products and the zone of chemical conversion, which gradually shrinks and ultimately disappears at the center of the channel.

Thus, in downward propagation of the flame, free-convection flows develop in the combustion products, which strongly affect the development of the combustion process. A flame that is capable of propagating in the absence of an external force may, for fairly small Fr, go out because the convection eddies in the combustion products, the intensity of which depends on Fr, contribute to cooling the reaction zone.

Let us compare the results of the numerical calculations with published estimates. Equations for the critical Péclet number Pe_* in the presence of conductive and convective heat loss have been derived in [3, 4]. For a fairly long channel

$$Pe_* = \frac{0{,}07\Delta}{4} Ra^{1/3} + \left[\left(\frac{0{,}07\Delta}{4} Ra^{1/3}\right)^2 + 2\nu Nu\Delta\right]^{1/2}, \quad (2.1)$$

where $Pe_* = \rho_b u_* c_p L/\lambda$; $Ra = Fr^{-1}Pe^2(T_b - T_0)/PrT_b$ is the Rayleigh number; $\Delta = (T_a - T_0) E_0/R_0 T_a^2$; $Nu = \alpha L/\lambda$ is the Nusselt number; ρ_b is the density of the combustion products; u_* is the critical combustion velocity; T_a and T_b are the combustion temperature under adiabatic conditions and at the limit; α is the heat-transfer coefficient; ν characterizes the symmetry of the problem ($\nu = 2$ for a flat channel and $\nu = 4$ for a tube).

The numerical calculations showed that in the entire investigated range of Re, the flame propagates over the entire channel length at Fr = 1 and is extinguished at $Fr^{-1} = 3$. The critical conditions thus correspond to Fr = 1 and Re = 50-300. Calculating the corresponding Rayleigh numbers, we compare the values of Pe_* obtained from (2.1) and from the numerical calculations [the Pe_* from (2.1) were converted to Péclet numbers constructed from u_b and ρ_0]. In Fig. 2 we show the dependence of $Pe_* = \rho_0 u_b c_p L/\lambda$ on Ra, determined by numerical calculation and from Eq. (2.1) (curves 1 and 2, respectively; the extinction region lies below the curves). These data indicate a considerable difference between the results. This is because Eq. (2.1) was derived in a one-dimensional approximation, which cannot yield very good results, naturally, when used to describe multidimensional convective heat transfer between the combustion front and the cooling reaction products.

Since the formation of asymmetrical convection eddies behind the flame front has been observed experimentally [7, 8], we also carried out calculations in a complete channel (without using the symmetry conditions) with weakly asymmetrical initial conditions (the center of the hot gas core was set at x = 0 and y = 0.05 and 0.1). It was found that in the range Re = 50-500 and $Fr^{-1} = 1$-10 two slightly asymmetrical eddies are formed behind the flame front; this flow structure was stable and remained to the end. It is quite possible that the channel length was insufficient for a system of asymmetrical eddies to form.

Thus, in flame propagation in a channel in the direction of the gravitational vector, the developing convection flows considerably affect the flame structure and shape. They increase heat transfer from the combustion zone to the reaction products, which narrows the combustion limits in comparison with weightlessness. The numerical calculations showed that published equations for Pe_* as a function of Ra, which characterizes the convection intensity, are unreliable in the investigated range of the parameters. It should also be noted that combustion with ignition from above in a channel with cold side walls differs considerably from the analogous process in a thermally insulated channel, in which the rules of flame propagation resemble those of combustion in weightlessness [18].

3. Ignition from Below. As noted earlier, the combustion limits are wider for ascending flames than in other cases. The point is that in this kind of ignition, convection flow develops, increasing the flame velocity, which is comprised of the normal combustion velocity and the velocity of the ascending gas. The higher flame velocity weakens the influence of heat transfer to the cold walls on the propagation of the combustion front, since the characteristic time of the heat-conduction process usually is considerably longer than the characteristic convection time. The increase in flame velocity also increases the surface area at which the chemical conversion occurs, which increases the amount of heat released in comparison with the case of a planar flame front. These two factors (the decrease in the influence of the cold walls and the increase in heat release) mean that mixtures that are incapable of burning in weightlessness or in ignition from above will burn in ignition from below.

To clarify the rules of flame propagation for ignition from below, we carried out numerical calculations for Re = 20-70, Fr^{-1} = 1-70, q = 5, and $r_x = r_y = 0.2$, which showed that combustion was observed in a wider range of Re. It was found that even for Re = 30, when rapid extinction occurs in weightlessness (in $t \approx 1.2$), at $Fr^{-1} = 10$ the flame is able to propagate over the entire channel length. For Re = 20, no combustion was observed for any Fr from the above range because of the large heat loss to the cold walls.

The following is a typical pattern of flame propagation: hot reaction products ascend due to the Archimedes force, with a symmetrical pair of cylindrical eddies being formed near the side combustion zone; their analog for the axisymmetric problem is the annular eddy. By setting the surrounding gas into motion, these eddies deform the combustion surface. The smaller Fr, the higher the velocity of the flame front.

Extinction of the flame was observed for sufficiently small Fr, even in the range of Re in which the combustion front propagates over the entire channel length in weightlessness. Here extinction is associated with the formation of strong convection eddies, which so intensify heat transfer between the reaction zone and the cold gas that the flame is extinguished. In Fig. 3 we show how this process occurs for Re = 70 and Fr^{-1} = 70 (a-c for t = 0.2, 0.4, and 0.6; the velocity field and isotherms are shown in the left half of the channel and the combustion zone in the right half, where $\psi = a\Phi(\Theta) \geqslant 0.02$ and $\psi_{max} = 0.06$). It is clearly seen that the transverse size of the combustion zone decreases rapidly and the flame is extinguished at the axis of symmetry.

Let us discuss the extinction mechanism in more detail. For this it is convenient to change to a coordinate system moving with the combustion core. The hydrodynamic flow pattern resembles flow over a cylinder by a liquid stream. We estimate the velocity of the oncoming stream, which in the laboratory coordinate system equals the ascent velocity of the core. Using the approach suggested in [19] (the only difference is that here we are considering a flat channel, and hence the flow is over a cylinder rather than a sphere), for the velocity of the oncoming stream we obtain $V = 0.5\sqrt{gR}$ (R is the radius of the core). Taking $R \approx L/2$ for the estimates, we find $V = 0.354\sqrt{gL}$ or, in dimensionless form,

$$V = 0{,}354/\sqrt{\mathrm{Fr}}. \tag{3.1}$$

Equation (3.1) is most applicable under almost limiting conditions, when the normal combustion velocity is considerably lower than the gas velocity. The critical parameters were found in the numerical calculations: with Re fixed, Fe^{-1} was increased with a step size of 5; the maximum values at which the core propagated over the entire channel length were taken as the critical parameters. The velocities calculated from Eq. (3.1) agree well with the core ascent velocities obtained in the numerical calculations at the critical parameters.

As noted above, during extinction the combustion core gradually shrinks from the walls toward the center; the combustion region located at the axis of symmetry of the channel is extinguished last (see Fig. 3). This means that the primary heat transfer from the combustion zone occurs from the side surfaces of the ascending core. The reason for the heat loss is the flow of cold gas over the combustion zone, and the higher the flow velocity, the greater the heat loss.

To estimate the conditions for extinction at the side surface of a flame over which a cold gas stream flows, we compare the characteristic time of heating in the Michelson zone ahead of the combustion front, $\tau_f \approx \delta/u_n$ ($\delta = \varkappa/u_n$ is the width of the heating zone, u_n is the normal flame velocity, and $\varkappa$ is the thermal diffusivity coefficient), and the characteristic time of heat transfer due to the stream of cold gas, $\tau_c \approx r/V$ (r is the length of the side surface; for the estimates we take r = L). It is obvious that if $\tau_c < \tau_f$, the flame must go out, since the convection flows are able to remove heat from the reaction zone. From the condition $\tau_f \approx \tau_c$, we find $\varkappa/u_n^2 = L/V$. This equation, obtained from simple physical considerations, agrees to within $\pi/2$ with the equation from the stretch-effect theory [16]. Substituting V from (3.1) yields

$$\mathrm{Fr}_*^{-1} = (\mathrm{Re}\,\mathrm{Pr}/0{,}354T_a^2)^2. \tag{3.2}$$

Flameout occurs at $Fr < Fr_*$.

The main reason for extinction of the flame is thus the flow of a stream of cold gas over the hot core – the stretch effect.

To establish how significantly the cold side walls affect extinction for the given orientation of the gravitational force, we made numerical calculations of flame propagation in a

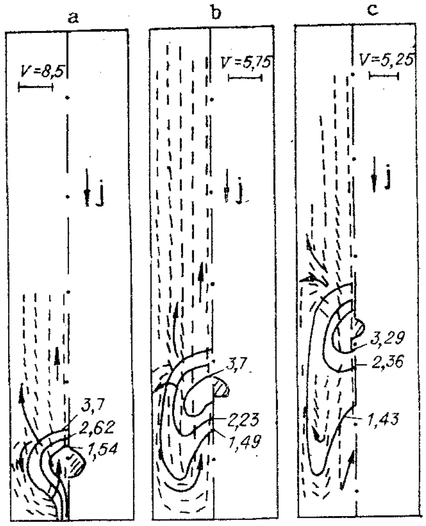

Fig. 3

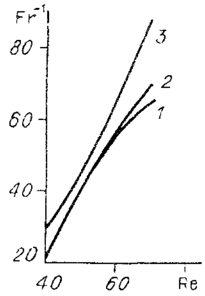

Fig. 4

channel with thermally insulated side walls, which showed that in the range of parameters under consideration, flame propagation and extinction in a fully adiabatic channel resemble, both qualitatively and quantitatively, the analogous process in a channel with cold side walls.

In Fig. 4 we show the critical Fr as a function of Re for flame propagation in channels with cold and with thermally insulated side walls (curves 1 and 2), as well as calculations made from Eq. (3.2) (curve 3). It is seen from Fig. 4 that the change in boundary conditions has almost no effect on the limiting conditions (the slight divergence between curves 1 and 2 is explained by the fact that the critical values were determined by varying Fr^{-1} with a discrete step size of 5). This fact confirms that the main heat loss from the combustion zone is due to convective gas motion rather than the presence of the cold wall. It is also seen that Eq. (3.2) yields fairly good estimates (within ~20%) of the critical parameters.

The shape and structure of a flame propagating upward in a channel thus depend on Fr. Flameout was found to occur for fairly small Fr. Intense convective gas motion is the cause of the extinction. The cold side walls are found to have almost no effect on extinction. The critical values of the parameters were found.

In conclusion, let us illustrate our results with a concrete example. The combustion of lean mixtures of carbon monoxide and air can be described using the general kinetic equation [20]

$$\frac{d\,[\mathrm{CO}]}{dt} = -1{,}04\cdot 10^{12}\frac{[\mathrm{CO}]}{C}[\mathrm{O_2}]^{0,25}[\mathrm{H_2O}]^{0,5}T^{-2,5}\exp(-32000/R_0T).$$

Here the quantities inside the brackets are the relative molar concentrations of the respective substances; C is the total molar concentration, mole/cm^3; t, sec; E_0 = 32,000 cal/mole is the activation energy.

On the basis of data [13] on the combustion temperature of a mixture of carbon monoxide and air, we can estimate the calorific effect of the reaction. We find that a 13% CO + air + 1% H_2O mixture having an initial temperature T_0 = 360 K and a combustion temperature T_a = 1645 K corresponds to the dimensionless parameters E = 33 and q = 5, used in the numerical calculations. Changing from the relative molar concentration of CO to its mass concentration in the kinetic law, and replacing the power-law temperature function by an exponential law at the reference temperature T_a [16], from the Zel'dovich–Frank-Kamenetskii equation for the normal flame velocity we find u_n = 3.44 cm/sec and u_b = 15.7 cm/sec. Using thermophysical data for air from [21], we determine, in particular, a kinematic viscosity η/ρ_0 = 0.77 cm^2/sec. Modeling with respect to the Mach number is unnecessary, since it has no significant influence in the given range of parameters, as seen from a detailed investigation of its influence on the solution in [22].

The numerical calculations for ignition from above yielded the critical conditions Fr = 1 and Re = 50-300, which for the mixture under consideration correspond to a channel width L = 2.5-15 cm; for L = 2.5 cm extinction occurs at g > 99.8 cm/sec^2 = 0.1g_0, and for L = 15 cm it occurs at $g > 16.6\ cm/sec^2 = 1.7 \cdot 10^{-2} g_0$, where $g_0 = 9.8 \cdot 10^2\ cm/sec^2$. Extinction thus occurs at normal free-fall acceleration for ignition from above.

For ignition from below, the critical conditions correspond to Re = 40-70 and Fr^{-1} = 20-65. Those values correspond to a channel width L = 2-3.5 cm. Extinction for L = 2 cm occurs at $g > 2.5 g_0$, and for L = 4.5 cm it occurs at $g > 4.7 g_0$. The extinction of a given mixture ignited from below thus requires the creation of an overload in comparison with earth gravity.

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