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FLAME FLASHBACK AND PROPAGATION OF PREMIXED FLAMES NEAR A WALL

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The flashback or propagation of premixed flames along the near-wall low-velocity region at the base of a laminar boundary layer of a reactive mixture has been studied numerically. The analysis, carried out using the constant density approximation for an Arrhenius overall reaction, accounts for the effects of the Lewis number of the fuel. The flow field, as seen by an observer moving with the front, includes the unknown flame front velocity U relative to the wall and the linear velocity gradient A at the base of the boundary layer. Due to this gradient, the flame front is curved with a radius of curvature $l_F = S_L/A$, proportional to the planar flame velocity S_L. The front velocity is changed from S_L by a factor which depends on the Karlovitz number, or non-dimensional wall velocity gradient, defined as the ratio between the thickness of the planar flame and the front curvature l_F. The front velocity has been calculated in the limiting cases of adiabatic and isothermal walls. The front velocity changes from negative to positive when the Karlovitz number decreases below a critical value, determining the onset of flashback. This critical value, which decreases when the Lewis number of the fuel increases, is smaller for isothermal than for adiabatic walls. In this second case, when the flame is not quenched close to the wall, flashback is prevented by flame stretch associated with flame curvature.

Introduction

In order to reduce the current levels of NO_x emissions from gas turbine engines, different alternatives have been proposed. One of the most promising schemes corresponds to the LP (lean premixed) or the LPP (lean premixed prevaporized) combustors, where combustion takes place with premixed flames, in contrast with the traditional turbojet combustors based on diffusion flames. In LP or LPP burners, a lean mixture is generated without combustion, in a premixing tube. The reaction should take place only downstream, in the combustion chamber, in the mixing layer between the premixed stream and the hot recirculating products of combustion. These burners are prone to combustion instabilities and flashback, or upstream propagation of the flame in the premixing tubes. The mean flow velocity in such tubes is large when compared with the velocity of the planar flame of the gaseous mixture; therefore, flame flashback can occur only in the low-velocity region of the boundary layers near the wall.

Two different limiting cases are considered in this paper. In the first one, the wall is assumed to be adiabatic. In this case, the flame reaches the wall of the tube without quenching. In the second—more realistic—limiting case, the temperature of the wall is assumed to be fixed, equal to that of the unburned mixture upstream; then, the reaction quenches near the wall because of the lower temperatures due to heat losses, and the flame does not reach the wall. Although flashback has been the subject of a number of experimental, analytical, and numerical studies in the past [1–10], there is renewed interest in these problems because they are encountered in the development new technologies.

A criterion of a critical wall velocity gradient, below which flashback is possible, was put forward by Lewis and von Elbe [1,5]. The criterion, stating that flashback will occur if the gas velocity gradient at the wall is less than the ratio of the flame speed and the quenching distance, was supported by a number of experimental results (see, for example, Ref. [7]). Nevertheless, this criterion, essentially correct qualitatively in the case of isothermal walls, is not quantitatively predictive unless the quenching distance is directly related to the thickness of the premixed flame. In the adiabatic case, when no quench layer is found near the wall, this criterion is not applicable at all. We give in this paper a description of the flame front regime for flashback that provides the critical value of the Karlovitz number.

A pioneering numerical analysis of flame flashback in a tube with isothermal walls and Poiseuille flow was given by Lee and Tien [9], who based the study on the steady Navier-Stokes energy and species equations. They addressed the analysis to both the quenching of flame propagation for small tube diameters and to the determination of the critical velocity gradient for flashback for large tubes.

In the present paper, using the thermodiffusive approximation, we analyze in detail the structure of the leading edge region of flames near the wall, which determines the speed of propagation. This constant density approximation is not drastic for LP burners, because the ratio of the flame temperature to the initial temperature is not very high. On the other hand, we account for the important effects of the Lewis number of the fuel on the flashback phenomena.

Consideration is given to the cases in which the radius of the premixing tube is much larger than the preheated flame layer thickness, and the gas velocity in the central part of the tube is also large compared with the planar flame velocity, thus preventing the upstream flame propagation in the bulk of the flow. Under these conditions, flashback may occur only near the wall, in the region of the boundary layer, which is considered herein to be laminar, where the gas velocity has a linear profile.

For small values of the velocity gradient, A, the flame thickness, δ_L, will be small compared with the characteristic radius of curvature, or size, l_F, of the flame front region. This is determined, in terms of the premixed flame speed, S_L, by the relation $S_L = Al_F$, based on the assumption that the local flame front velocity relative to the fluid is S_L.

The parameter δ_L/l_F, which can be written in the form $A\alpha/S_L^2$ in terms of the thermal diffusivity, α, of the mixture, is the Karlovitz number which plays an important role in the flashback phenomena. For small values of δ_L/l_F, flashback is possible; although the flame front, which approaches the wall in a normal direction, is quenched, as shown first in the analysis of Millán and von Karman [10], at a distance of order δ_L from the wall.

When δ_L/l_F grows to values of order unity, the quench layer becomes of the order of l_F, and in addition, there are strong effects of flame curvature on the local flame front speed of propagation, if the Lewis number is different from unity. The propagation of the flame front may be prevented either by near-wall quenching or by flame stretch.

The main purpose of this work is to identify the parameters that define the critical conditions for flashback. After posing the problem in non-dimensional form, the numerical method is described, and the results and conclusions are given. Then, we discuss the possible use of these results of the analysis when the flow in the boundary layer is turbulent.

Mathematical Formulation

As indicated, we base the analysis of the flame flashback process on what is called the thermal diffusive approximation, for which the values of the density, ρ, thermal conductivity, λ, heat capacity, c_p, and diffusion coefficient, D, are assumed to be constant. The chemical reaction is modeled by a one-step, irreversible reaction with Arrhenius kinetics, for which the mass of the deficient component consumed per unit volume and unit time is

$$\Omega = \rho BY \exp(-E/RT) \quad (1)$$

Here B, Y, T, and E/R denote the pre-exponential factor, the mass fraction of the deficient reactant, and the local and activation temperatures, respectively.

By neglecting the variations in density and viscosity of the gas, the velocity field is no longer affected by the temperature variation due to the release of heat. In the base of the laminar boundary layer near the wall, where flashback may occur, the velocity of the fluid is $u = Ay$, $v = 0$, where x and y are distances along and normal to the wall and A is the constant velocity gradient at the wall.

To formulate the problem in a non-dimensional form, the following scales for the length, time, and velocity are defined

$$l_N = \sqrt{\alpha/A},\ t_N = A^{-1},\ U_N = \sqrt{\alpha A} \quad (2)$$

where $\alpha = \lambda/\rho c_p$ is the thermal diffusivity. These values correspond to the near-wall region where the local Peclet number is of order unity, and therefore, upstream conduction and diffusion is possible. The non-dimensional steady equations for the temperature and deficient reactant concentration, written in a reference frame traveling with the flame front with a speed U relative to the solid wall, take the form

$$(V + y)\frac{\partial\theta}{\partial x} = \frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} + Da\ k(\theta)Y \quad (3)$$

$$(V + y)\frac{\partial Y}{\partial x} = \frac{1}{Le}\left(\frac{\partial^2 Y}{\partial x^2} + \frac{\partial^2 Y}{\partial y^2}\right) - Da\,k(\theta)Y \quad (4)$$

where

$$k(\theta) = \frac{1}{2} Le^{-1}\beta^2 \exp(\beta(\theta - 1)/\{1 + \gamma(\theta - 1)\}) \quad (5)$$

Here, $\theta = (T - T_0)/(T_e - T_0)$ is the non-dimensional temperature rise, and Y is the mass fraction of the deficient reactant scaled with its value in the fresh mixture Y_0. T_0 is the initial temperature of the gas, and $T_e = T_0 + QY_0/c_p$ is the adiabatic flame temperature resulting from the heat release Q per unit mass of the reactant. The non-dimensional flame speed relative to the wall, $V = U/U_N$, is determined in the course of the solution of the problem. The flames which are analyzed correspond to upstream propagation fronts (flashback) if $V > 0$, or receding flame fronts if $V < 0$.

The following non-dimensional parameters remain: the Lewis number, $Le = \alpha/D$, the Zeldovich number, $\beta = E(T_e - T_0)/RT_e^2$, assumed to be large compared with unity, the heat release parameter, $\gamma = (T_e - T_0)/T_e$, and the modified Damköhler number, $Da = (U_L/U_N)^2 = U_L^2/\alpha A$. Here, $U_L = \sqrt{2BLe\beta^{-2}\alpha} \exp(-E/2RT_e)$ is the asymptotic value of the velocity of the planar flame, calculated in the limit $\beta \gg 1$ (see Zeldovich et al. [16]). In what follows, anticipating that in the region where the chemical reaction term is important, $\beta(\theta - 1)$ is of order unity, the factor $\{1 + \gamma(\theta - 1)\}$ in equation 5 is be replaced by 1, thus reducing the number of non-dimensional parameters.

By defining the Damköhler number in term of the planar flame speed, we may expect the results not to be affected strongly by the Arrhenius simplification in the reaction mechanism.

Two limiting cases are considered in this paper. In the first, the wall is considered adiabatic. In the second, the temperature of the wall is fixed equal to that of the unburned mixture, T_0. Thus, the wall boundary conditions are

$$\text{at } y = 0\text{: } \partial Y/\partial y = 0, \quad \text{and } \partial\theta/\partial y = 0, \text{ or } \theta = 0 \qquad (6)$$

Far upstream and downstream of the flame front we require

$$x \to -\infty\text{: } \theta = 0,\ Y = 1;\ x \to \infty\text{: } \quad \partial\theta/\partial x = 0,\ \partial Y/\partial x = 0 \qquad (7)$$

More accurately, the solution downstream should evolve to the solution of the boundary layer form of equations 3 and 4. The stretching of the flame by the flow with the velocity gradient, A, is measured by the Damköhler number, $Da = (U_L/U_N)^2$, or, following Ref. [5], by the Karlovitz number, defined as

$$K = \delta_T A/S_L = \alpha A/S_L^2 = (U_N/S_L)^2 \qquad (8)$$

where S_L is the dimensional velocity propagation of the planar flame, and $\delta_T = \alpha/S_L$ is the preheat zone thickness. The non-dimensional parameter K was first introduced in Ref. [11].

For the Karlovitz number, we need a more accurate value of the velocity of the planar premixed flame than the first term, U_L, of the asymptotic expansion given above. For large β, the ratio S_L/U_L is, according to [12], of the form

$$S_L/U_L = f(\beta, Le) = 1 + \Lambda_1/\beta + \ldots \qquad (9)$$

For more accurate results, the factor $f(\beta, Le)$ was calculated numerically instead of using this asymptotic formula. Notice that for large activation energies, $K = 1/Da$.

Numerical Method

For the numerical treatment, equations 3–7, with the time derivative retained was discretized using finite differences and solved with a transient method, proceeding in time until a steady solution was attained. Second-order, three-point approximations, for space derivatives and a first-order, explicit approximation for the time derivative were used. The non-dimensional velocity, V, of the frame relative to the solid wall was determined by imposing the temperature to be constant, equal to a value $\theta_* < 1$ and chosen arbitrarily at a reference point (x_*, y_*),

$$V\text{: } \theta(x_*, y_*, t) = \theta_* \qquad (10)$$

The velocity so obtained determines motion of the frame of reference which follows the flame front. If after an initial transient period the flame propagates with a constant velocity, the temperature distribution becomes steady in the frame of reference attached to the flame front, and V gives the velocity of the flame propagation relative to the wall. In the case of the adiabatic wall, the position of the reference point (x_*, y_*) was chosen where the flame reaches the wall, at $y_* = 0$. For an isothermal wall, the value of the transverse coordinate y_* was chosen so that the reference point lies outside the quenching layer.

Taking into account that the temperature in the reference point does not vary, the finite difference temperature equation written in this point (x_*, y_*) becomes

$$(x_*, y_*)\text{: } (V + y_*)L_x\theta = L_{xx}\theta + L_{yy}\theta + Da\ k(\theta_*)Y_* \qquad (11)$$

Here, Y_* is the concentration at the reference point; L_x, L_{xx}, and L_{yy} are the finite-difference representations of space derivatives where four grid points around (x_*, y_*) are involved.

Calculations were performed in two different ways: in the first, the modified Damköhler number, Da, was fixed and equation 11 was used to calculate the velocity, V. Then, the value of the velocity so obtained was used to compute the variables in the rest of the grid points at the next time level. This gives the real time-dependent development of the combustion process (with first-order accuracy in time), when transient distributions have a physical sense. Only stable solutions can be obtained using this method, not the unstable steady solutions. The second way to use equation 11 is to calculate the modified Damköhler number, Da, for a given value of V. Then, this value is used to calculate variables in the rest of the grid points at the next time level. In this way, the value of Da changes with time, although transient distributions of variables are artificial. Only the terminal, steady distributions have a

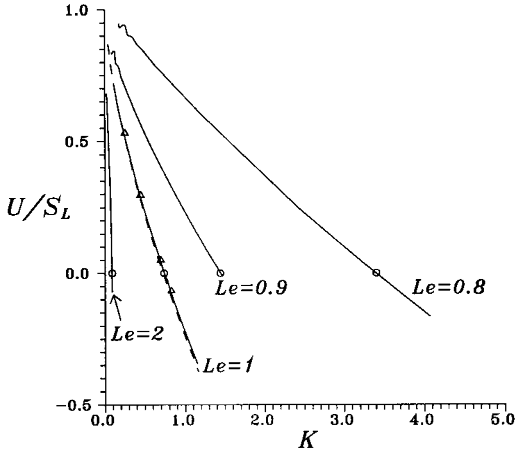

FIG. 1. Curved flame front velocity, U, measured with the planar stoichiometric premixed flame velocity, S_L, as a function of Karlovitz number for different Lewis numbers. Solid lines, calculations with $\beta = 15$; dashed line, $\beta = 12$; triangles, $\beta = \infty$; circles, critical points for flashback.

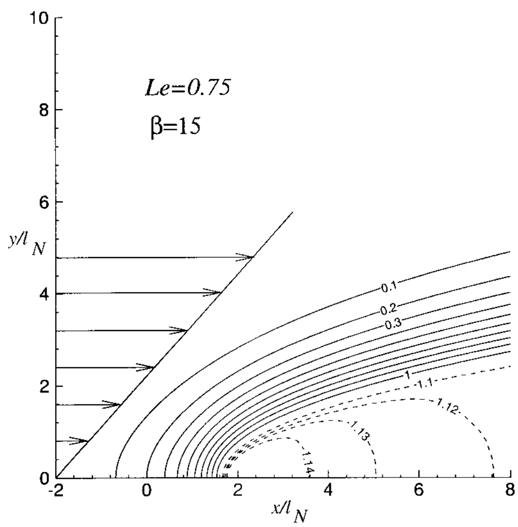

FIG. 2. Sketch of the velocity field and typical isotherms at the onset of flashback near an adiabatic wall for Lewis number smaller than unity. Solid lines, temperatures less or equal to the adiabatic flame temperature; dashed lines, temperatures larger than the adiabatic flame temperature.

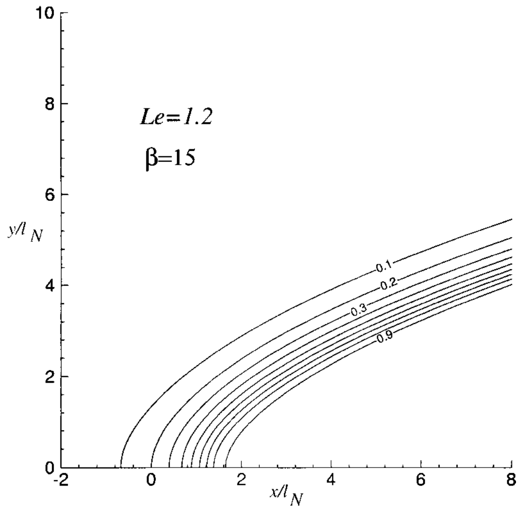

FIG. 3. Isotherms for a Lewis number larger than unity.

physical sense. As shown below, when using this method we can obtain the steady unstable branches of solutions. The two methods give the same results for the stable solutions.

The calculations were carried out in a finite computational domain, with typical outer boundaries at $x_{min} = -10$, $x_{max} = 10$, and $y_{max} = 10$. The reference point was arbitrarily located at $x_* = 0$. The boundary conditions $\partial\theta/\partial y = \partial Y/\partial y = 0$ were used at $y = y_{max}$. The numerical calculations show that the value of y_{max}, where these boundary conditions are posed, does not influence the value of the velocity propagation if y_{max} is large enough. To test the grid independence, calculations were carried out using 301 × 151 and 401 × 201 grids, and the variation of the flame propagation velocity was found to be typically less than 1.5%. It was also found that qualitative aspects of the solution (stability and multiplicity) did not change in any of the cases. Only time-independent, steady solutions (which may be unstable, see below) were obtained; therefore, the first-order approximation of the time derivatives does not affect the accuracy of results. The criterion for a steady distribution was $\max_{i,j}|\hat{f}_{i,j} - f_{i,j}|/\tau < 10^{-5}$, where $\hat{f}$ and f are the values of the temperature at the current and previous time levels, respectively, and τ is the time step.

Results

Adiabatic Wall

In this section, we present the numerical results obtained for the flame propagation near adiabatic walls. In these cases, the flame reaches the wall without quenching. Shown in Fig. 1 are the resulting values of the flame velocity, V, measured with the planar flame velocity, S_L, plotted as a function of the Karlovitz number for different values of the Lewis number. Upstream flame propagation occurs for values of $K < K_c$, and the critical values corresponding to $V = 0$ are shown in this figure with circles.

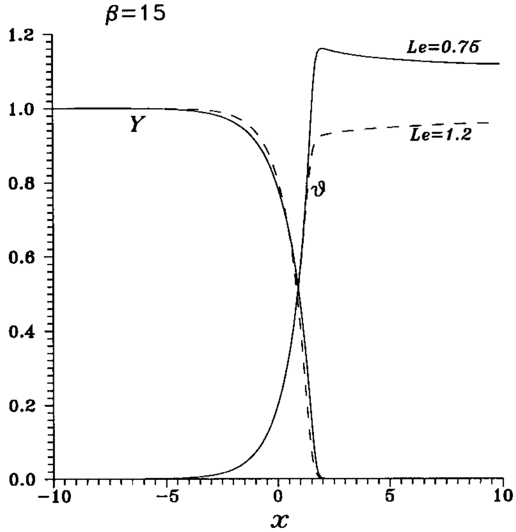

FIG. 4. Mass fraction and temperature profiles along the wall. Solid lines, $Le = 0.75$; dashed lines, $Le = 1.2$.

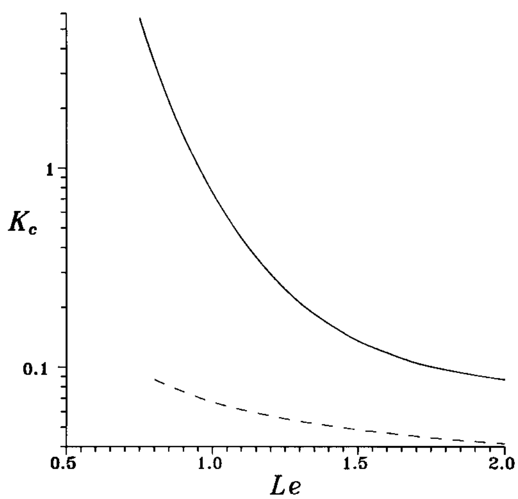

FIG. 5. Critical Karlovitz number, giving the onset of flashback, as a function of Lewis number. Solid line, adiabatic wall; dashed line, isothermal wall. There is flashback for smaller values of K.

Figure 1 reveals a substantial influence of the Lewis number on flashback. When $Le < 1$, differential diffusion effects, associated with flame curvature, result in an increase of the flame temperature, which leads to an increase of the flame propagation velocity. If $Le > 1$, we encounter the opposite effect. Figs. 2 and 3 give examples of isotherms calculated for different values of the Lewis number in the critical case of onset of flashback, when $V = 0$. The distributions of temperature and concentration along the wall are presented in Fig. 4. An overheated region, due to the effect of curvature, can be observed behind the flame in these figures for $Le = 0.75$.

Shown in Fig. 1 with a dashed line and triangles are the flame velocities calculated for $\beta = 12$ and $\beta = \infty$, respectively, and $Le = 1$. One can see that the influence of the Zeldovich number on the propagation velocity is weak. For $Le \geq 1$, the non-dimensional flame velocity, U, measured with S_L, monotonically tends to unity as $K \to 0$ (or $Da \to \infty$) and the effects produced by the velocity gradient decrease. Propagation of the planar flame becomes oscillatory for these values of parameters, but no oscillations were found in our calculations. Presumably, the enhancement in the flame stability is caused by its curvature and the downstream traveling of the disturbances, leading to flame stabilization, as shown in Ref. [13].

The dependence V/S_L on K becomes more complicated at small Karlovitz numbers if the Lewis number is below 1. It is well known that a small Lewis-number deflagration is subject to instabilities that lead to a cellular flame structure (see, for example, Ref. [14] and Ref. [15]). For $Le < 1$, this effect appears reflected in the oscillation of the flame speed versus K when $K \ll 1$. No details are given in this paper regarding the interaction between cellular structured flames and flows with velocity gradients.

Shown in Fig. 5 with a solid line are the critical values of the Karlovitz number in terms of Le for $\beta = 15$. Below this curve, for $K < K_c$, flame flashback occurs. For $K > K_c$, the flame front velocity is negative, and the flame is swept downstream. Observe the influence of the Lewis number on the onset of

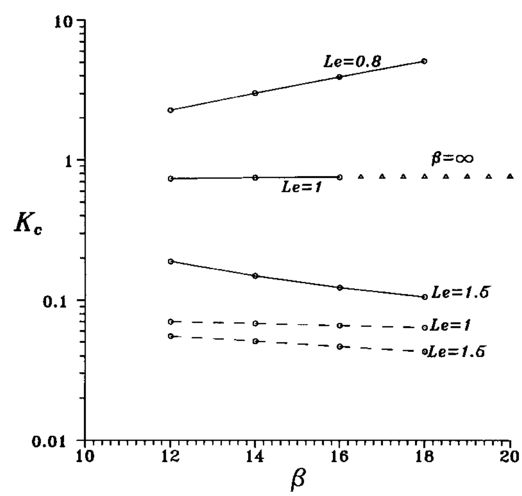

FIG. 6. Critical Karlovitz number for flashback as a function of β for different Lewis numbers. Solid line, adiabatic wall; dashed line, isothermal wall; triangles, asymptotic limit $\beta = \infty$.

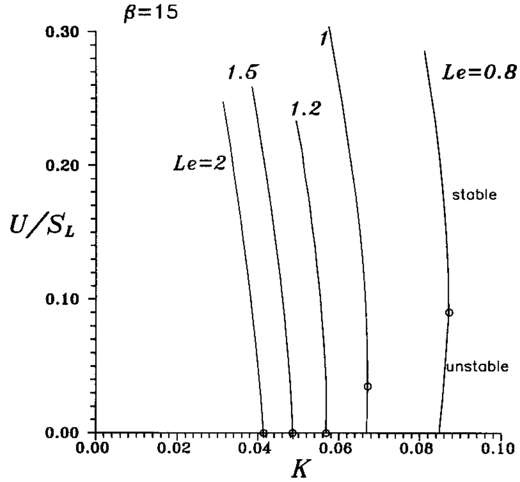

FIG. 7. Flame front velocity, U, along an isothermal wall, measured with the planar stoichiometric premixed flame velocity, S_L, as a function of Karlovitz number for different Lewis numbers. Circles, critical point for flashback.

flashback. The values of K_c are plotted versus β in Fig. 6 with solid lines. One can see that the changes with the activation energy are weak, so the main effects of the kinetics are incorporated through S_L.

Isothermal Wall

In this section, we present the numerical results for realistic cases when the temperature of the wall is the same as that of unburned mixture upstream. The presence of a cold layer near the isothermal wall, where the flame is quenched, makes propagation possible only outside without a velocity gradient, as first analyzed by Millán and von Karman [10]. When we account for the velocity gradient, the increased values of the gas velocity, where the edge of the flame lies, leads to an increase of the critical Karlovitz number for the onset of flashback when compared with the adiabatic case.

Shown in Fig. 7 with solid lines are the values of the flame front velocity, U, measured with the velocity of the planar flame, S_L, plotted in terms of the Karlovitz number for different values of the Lewis numbers. Observe that some of the curves, including the curve calculated for $Le = 1$, are double valued. The points for onset of flashback are shown in this figure with circles. The stable solutions correspond to the points above the circles. The unstable solutions, below the circles, were calculated using the second method described above. The value of the Lewis number, Le_c, below which multiplicity is observed, is about 1.1. The multiplicity of solutions found for $Le < Le_c$ means that when the Karlovitz number is below its threshold value and flashback occurs, the flame velocity undergoes a jump and takes a finite value.

Examples of isotherms and reaction rate contours, calculated at the onset of flashback, are shown in Fig. 8. One can see that the quenching distance near the wall is of order l_N. Curvature effects lead to an increase in the flame temperature for Lewis numbers below 1. However, they are not so strongly mani-

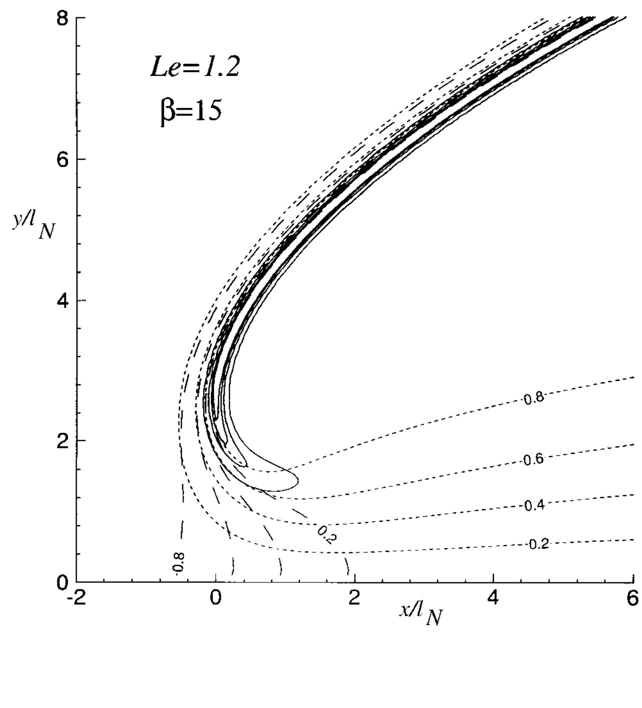

FIG. 8. Isotherms (small dashes), fuel mass fraction contour lines (large dashes) and reaction rate contour lines (solid) calculated at the ouset of flashback ($K = 0.057$) for an isothermal wall.

fested here in comparison with the adiabatic case, due to the heat losses to the wall, which reduce the flame temperature.

The critical values of the Karlovitz number, K_c, for onset of flashback are shown in Figs. 5 and 6 with dashed lines, plotted as functions of the Lewis and Zeldovich numbers, respectively. One can see that the dependence on the Lewis number, shown in Fig. 5, is weaker as compared with the adiabatic case.

Conclusions

An analysis has been presented for the description of flashback along the low-velocity region of the boundary layer in the flow of a reacting mixture in a duct. The results lead to a critical value, of order unity, of the Karlovitz number, $\alpha A/S_L^2$, based on the planar flame speed below which flashback occurs. This onset value for flashback decreases with the Lewis number of the limiting component of the mixture. At the onset of flashback, the thickness of the premixed flame is of the order of $l_N = \sqrt{\alpha/A}$, and S_L is also of the order of $U_N = \sqrt{\alpha}$.

The velocity U_N and length l_N are defined so that $U_N l_N/\alpha = 1$, allowing for upstream heat conduction in the domain of size l_N when reaction takes place there.

Although the analysis has been carried out for a laminar flow, we may conjecture that results are applicable, at least qualitatively, to turbulent flows. In these, the wall velocity gradient determines the thickness of the viscous sublayer, our l_N, and the friction velocity, which is our U_N. The analysis would be directly applicable if there were not fluctuations, in time and space of the wall velocity gradient. Then the leading curved flame front, which determines its propagation speed, should lie entirely in the viscous sublayer.

Acknowledgment

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