

Numerical study on lateral movements of cellular flames

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The lateral movements of cellular premixed flames for the Lewis number unity or smaller are studied by means of numerical simulation. The numerical model includes compressibility, viscosity, heat conduction, molecular diffusion, body force, chemical reaction, and convection. We superimpose the disturbances with peculiar wavelengths on the plane flames and calculate the evolution of disturbed flames. When the hydrodynamic and body-force instabilities are dominant (the Lewis number is unity), stationary cellular flames are formed. When the diffusive-thermal instability has a great influence (the Lewis number is smaller than unity), laterally moving cellular flames are obtained. The numerical simulation shows that the Lewis number effect and the nonlinear effect of the flame front are the essential factors in the lateral movements of cellular flames. [S1063-651X(97)07009-8]

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I. INTRODUCTION

We know that there are three fundamental effects responsible for the inherent instability of premixed flames [1], i.e., the hydrodynamic effect that is caused by thermal expansion [2–4], the body-force effect, which affects all flames anywhere on earth [5–7], and the diffusive-thermal effect, which is induced by the preferential diffusion of mass versus heat [8–12]. Owing to these effects, either stationary or laterally moving cellular flames are formed.

Cellular flames are steady or unsteady, depending on mixture composition [5,13–15]. To investigate transversely traveling waves on flames, linear analysis was performed using the diffusive-thermal model in which the density change of gases associated with thermal expansion is neglected, i.e., the hydrodynamic effect is disregarded [16,17]. Linear analysis predicted that transversely traveling waves would appear only at the Lewis number (Le) larger than a critical value (>1). However, most cellular flames are usually obtained experimentally at $Le < 1$ and the majority of laterally moving cellular flames are observed under this condition [5]. Linear analysis for $Le < 1$ based on the diffusive-thermal model did not predict transversely traveling waves [9,10]. Subsequently, linear stability analysis taking into account the hydrodynamic effect was performed [7,18–21]. At $Le < 1$, traveling-wave instability will not occur, but cellular instability will. Therefore, the linear analysis did not clarify the lateral movements of cellular flames for small Lewis numbers.

In linear analysis, it is assumed that the disturbances superimposed on flames are infinitesimal, and nonlinear terms are disregarded. To study the behavior of cellular flames taking into account the nonlinear effect, the equation for the nonlinear evolution of the flame front based on the diffusive-thermal model, i.e., the so-called Kuramoto-Sivashinsky (KS) equation, was used. The analysis and the numerical simulation of the KS equation showed the presence of laterally moving cellular flames for small Lewis numbers

[22–30]. From the results, we know that the nonlinear effect is very important to lateral movements.

In the diffusive-thermal model, cellular instability appears only when the Lewis number is smaller than the critical Lewis number (Le_c) and Le_c is less than unity because the activation energy is large but finite. On the other hand, in the hydrodynamic model where the hydrodynamic effect is taken into account, cellular instability appears at $Le = 1$, and $Le < 1$ flames are unstable compared to the $Le = 1$ flame. This denotes that the diffusive-thermal effect has a destabilizing influence on the flames attendant upon thermal expansion not only at $Le < Le_c$ but also at $Le_c < Le < 1$. Thus the stationary or lateral range of cellular flames will shift if one takes into account the hydrodynamic effect.

All flames are attendant upon thermal expansion. Thus the hydrodynamic effect is indispensable to research the behavior of cellular flames. There are successful calculations on flame instability and the formation of cellular flames [31–35] when the hydrodynamic effect is taken into account. Now we can apply the numerical model to cellular flames for the purpose of studying their lateral movements. In this study we calculate the evolution of disturbed premixed flames for $Le \leq 1$. We study the essential factors in the appearance of laterally moving cellular flames.

II. GOVERNING EQUATIONS

We consider two-dimensional single-reactant flames and take the direction tangential to the flame front as the y direction, with the gas velocity in the positive- x direction. To derive the governing equations, the following assumptions are used. (i) Only two species, unburned and burned gases, are present. Both gases are ideal and have the same molecular weights and the same Lewis numbers. (ii) The chemical reaction is an exothermic irreversible one-step reaction and the reaction rate has the Arrhenius form. (iii) The specific heats and the transport coefficients are constant throughout the whole region. (iv) The body force acts only in the x direction. (v) The radiation, bulk viscosity, Soret effects, Dufour effects, and pressure gradient diffusion are negligible

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and the viscous and body-force terms in the energy equation are disregarded.

The flow variables in the equations are nondimensionalized by the characteristic length, the characteristic velocity, and the density of the unburned gas. The characteristic length is 80 times the preheat zone thickness (defined as the thermal diffusivity divided by the burning velocity). The characteristic velocity is the isothermal sound velocity of the unburned gas. The governing equations of two-dimensional reactive flows, including compressibility, viscosity, heat conduction, molecular diffusion, and body force, are written in conservation form as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{S}, \quad (1)$$

where \mathbf{U} , \mathbf{F} , \mathbf{G} , and \mathbf{S} are vectors given by

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho Y \end{pmatrix},$$

$$\mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p - \frac{\text{Pr}}{\text{Pe}} \left(\frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \\ \rho uv - \frac{\text{Pr}}{\text{Pe}} \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \\ (e+p)u - \frac{1}{\text{Pe}} \frac{\gamma}{\gamma-1} \frac{\partial T}{\partial x} \\ \rho Yu - \frac{1}{\text{Pe}} \frac{\partial Y}{\partial x} \end{pmatrix},$$

$$\mathbf{G} = \begin{pmatrix} \rho v \\ \rho uv - \frac{\text{Pr}}{\text{Pe}} \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \\ \rho v^2 + p - \frac{\text{Pr}}{\text{Pe}} \left(\frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right) \\ (e+p)v - \frac{1}{\text{Pe}} \frac{\gamma}{\gamma-1} \frac{\partial T}{\partial y} \\ \rho Yv - \frac{1}{\text{Pe}} \frac{\partial Y}{\partial y} \end{pmatrix},$$

$$\mathbf{S} = \begin{pmatrix} 0 \\ G\rho \\ 0 \\ QB\rho Y \exp(-E/T) \\ -B\rho Y \exp(-E/T) \end{pmatrix},$$

where ρ is the density, u and v are the x and y components of the velocity, p is the pressure, e is the stored energy, T is the temperature, Y is the mass fraction of the unburned gas, Pe is the Péclet number, Pr is the Prandtl number, G is the acceleration, γ is the ratio of specific heats, Q is the heating value, B is the frequency factor, and E is the activation energy. The equation of state is

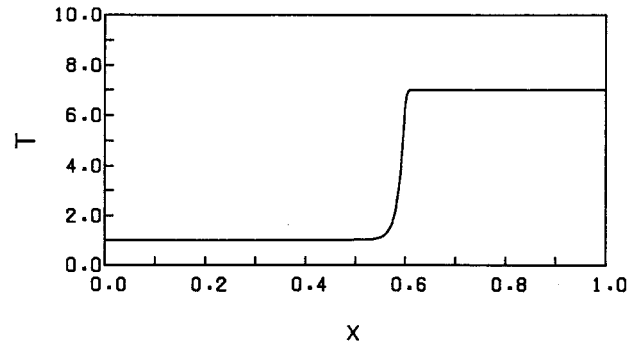


FIG. 1. Temperature distribution of the one-dimensional stationary flame for $\text{Le}=1.0$ and $G=0$.

$$p = \rho T. \quad (2)$$

III. NUMERICAL METHOD

The physical parameters are given to simulate a gas mixture of which the burning velocity is 0.83 m/s and the adiabatic flame temperature is 2086 K at atmospheric pressure and room temperature. Nondimensional burning velocity and adiabatic flame temperature are 2.5×10^{-3} and 7.0, respectively. Nondimensional parameters used in the calculation are $\text{Pe} = 3.2 \times 10^4$, $\text{Pr} = 1.0$, $\gamma = 1.4$, $Q = 21$, and $E = 70$. For the examination of the body-force effect, $G = 0$ and $\pm 1 \times 10^{-4}$ are taken. For the study of the Lewis number effect, $\text{Le} = 0.5, 0.6, 0.8$, and 1.0 are chosen because we are interested only in the lateral movements of cellular flames for $\text{Le} \leq 1$. The frequency factor is determined by the condition under which the burning velocity of the one-dimensional flame is equal to the set burning velocity ($= 2.5 \times 10^{-3}$). The frequency factors are 2.17×10^6 , 1.85×10^6 , 1.44×10^6 , and 1.20×10^6 for $\text{Le} = 0.5, 0.6, 0.8$, and 1.0, respectively.

The explicit MacCormack scheme [36], which has second-order accuracy in both time and space, is adopted for the calculation. A computational domain is 80 times the preheat zone thickness in the x direction and one wavelength of disturbance in the y direction, which is resolved by a 401×65 uniformly spaced grid. The time-step interval is 5×10^{-4} . When the grid size and the time-step interval are halved, no significant differences are observed.

Boundary conditions are as follows. In the x direction, except for the velocity of inlet flow, free-flow conditions are used upstream and downstream and we appropriate one-sided difference approximations with second-order accuracy. The flow velocity upstream is set to the burning velocity of the plane flame so that the flame position will barely move. In the y direction, spatially periodic conditions are used.

Initial conditions for two-dimensional flames are provided with the solutions of one-dimensional flames. The temperature distribution of the one-dimensional stationary flame for $\text{Le} = 1.0$ and $G = 0$ is shown in Fig. 1. On the plane flame, we superimpose the disturbance with the *peculiar* wavelength (the wavelength corresponding to the maximum growth rate) since it was reported that the spacing between cells on the flame is equivalent to the peculiar wavelength [31]. The peculiar wavelength is obtained from the dispersion relation, which is given by the calculation for sufficiently small dis-

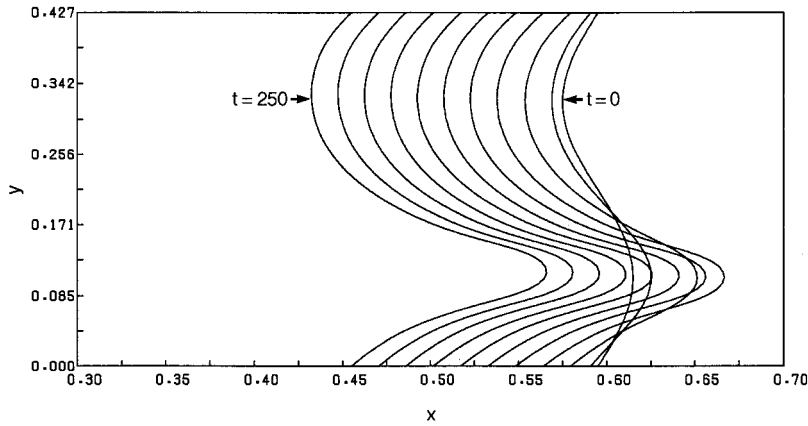


FIG. 2. Evolution of the disturbed flame front for $Le=1.0$, $G=0$, $\lambda=0.427$, and $A_0=0.02$ ($t=0, 25, 50, \dots, 250$).

turbances. The displacement of the flame front in the x direction due to the disturbance is

$$A_0 \sin(2\pi y/\lambda), \quad (3)$$

where A_0 is the initial amplitude of disturbance and λ is the wavelength.

IV. RESULTS AND DISCUSSION

First, to investigate the hydrodynamic effect on the lateral movements of cellular flames, we set $Le=1.0$ and $G=0$. The shapes of the flame front at each time ($t=0, 25, 50, \dots, 250$) for $\lambda=0.427$ and $A_0=0.02$ are illustrated in Fig. 2. The location of the flame front is defined as the position where $T=5$. The unburned gas flows in from the left at the burning velocity of the plane flame and the burned gas flows out to the right. The amplitude of disturbance increases initially with time and eventually reaches a maximum amplitude ($A=0.067$) at $t=90$. The flame front changes from a sinusoidal to a cellular shape. Thereafter, the flame moves upstream, where the amplitude of disturbance and the moving rate of flame are constant, indicating that the burning velocity is increasing. The cell on the flame does not propagate in the y direction. Thus it becomes clear that lateral movements are not generated only by the hydrodynamic effect.

Next, to examine the body-force effect, we take $Le=1.0$ and $G=\pm 1 \times 10^{-4}$. The body-force effect has a destabilizing (stabilizing) influence on the flames at $G>0$ ($G<0$). The evolutions of the disturbed flame fronts are illustrated in Figs. 3 and 4. In both cases, cellular flames are formed and

lateral movements of cells are not observed. Thus we conclude that the body-force effect is not the origin of lateral movements.

As shown in Figs. 2–4, the cellular flames move upstream with time. The moving rates are equal to the increments in the burning velocity, which are 24%, 34%, and 13% for $G=0$, 1×10^{-4} , and -1×10^{-4} , respectively. When the inlet-flow velocities are set to the cellular burning velocities, stationary flames are obtained. The temperature distributions of the stationary cellular flames are shown in Figs. 5–7. The cellular flames hardly move.

Finally, we study the Lewis number effect at $Le<1$. The evolutions of the flames for $Le=0.5, 0.6, 0.8$ and $G=0$ are illustrated in Figs. 8–10. In all cases, the laterally moving cells on the flames are observed. Since the cells move laterally, we do not obtain stationary flames, even though the inlet-flow velocities are set to the cellular burning velocities. The lateral components of velocities of cells are probably constant. The ratios of the lateral velocities of cells to the burning velocity of plane flame are 0.79, 0.41, and 0.03 for $Le=0.5, 0.6$, and 0.8 , respectively. Moreover, the cell on the $Le=0.9$ flame moves slightly in the y direction and lateral movements will occur also at $0.9<Le<1$. Therefore, the Lewis number effect is one of the essential factors in the appearance of laterally moving cellular flames.

At $Le<1$, lateral movements do not occur at the beginning of the calculation, where the amplitude does not reach a maximum amplitude and the disturbance maintains a sinusoidal shape. After the cellular shape of the flame front is formed, lateral movements occur. In addition, the linear analysis did not show traveling-wave instability at $Le<1$.

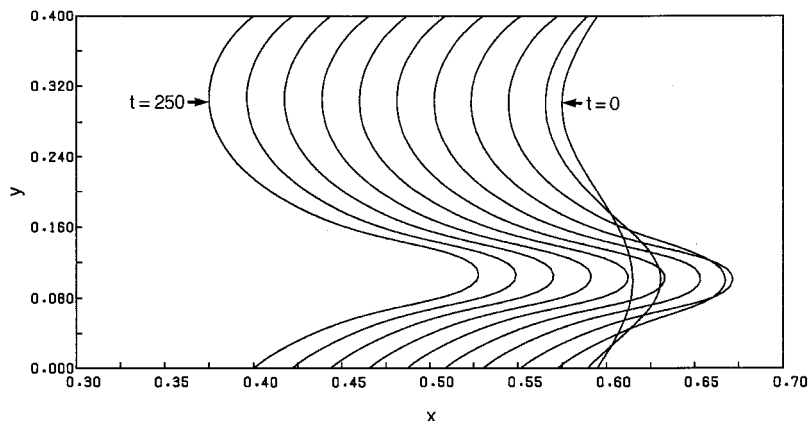


FIG. 3. Evolution of the disturbed flame front for $Le=1.0$, $G=1 \times 10^{-4}$, $\lambda=0.400$, and $A_0=0.02$ ($t=0, 25, 50, \dots, 250$).

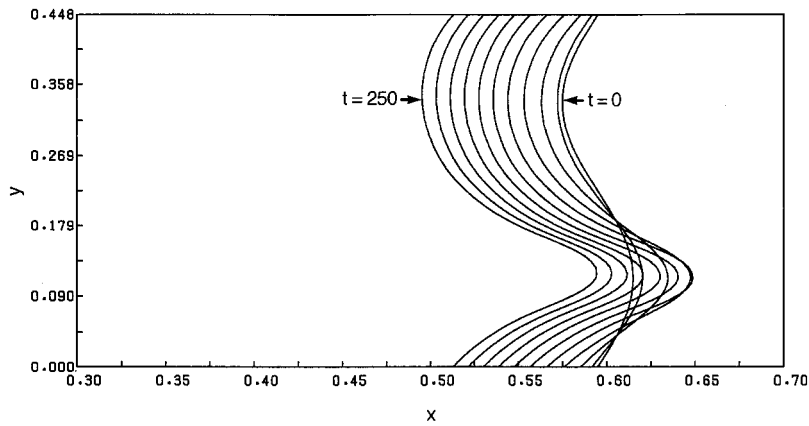


FIG. 4. Evolution of the disturbed flame front for $Le=1.0$, $G=-1 \times 10^{-4}$, $\lambda=0.448$, and $A_0=0.02$ ($t=0, 25, 50, \dots, 250$).

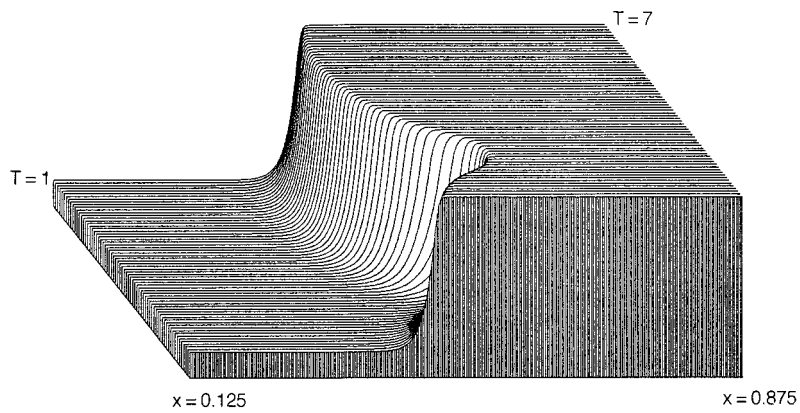


FIG. 5. Temperature distribution of the stationary cellular flame for $Le=1.0$, $G=0$, and $\lambda=0.427$; the inlet-flow velocity is set to 1.24 times the burning velocity of the plane flame.

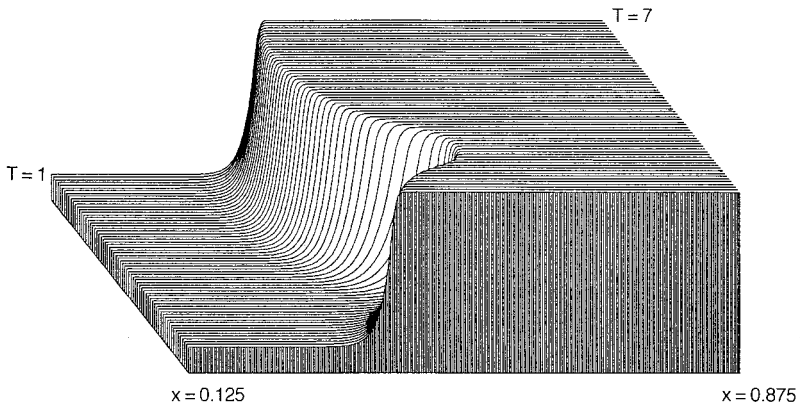


FIG. 6. Temperature distribution of the stationary cellular flame for $Le=1.0$, $G=1 \times 10^{-4}$, and $\lambda=0.400$; the inlet-flow velocity is set to 1.34 times the burning velocity of the plane flame.

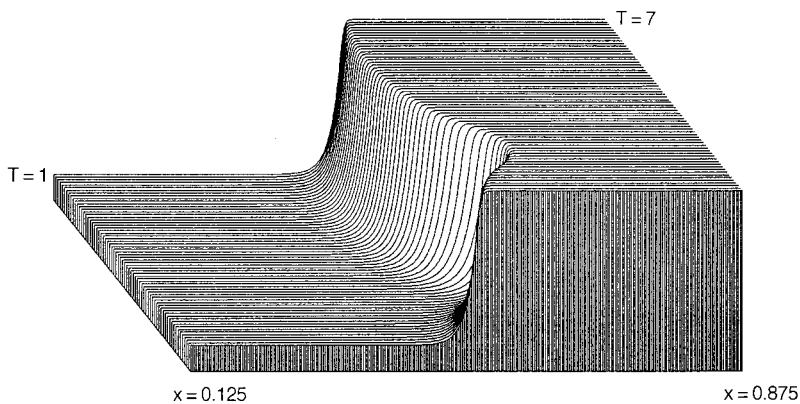


FIG. 7. Temperature distribution of the stationary cellular flame for $Le=1.0$, $G=-1 \times 10^{-4}$, and $\lambda=0.448$; the inlet-flow velocity is set to 1.13 times the burning velocity of the plane flame.

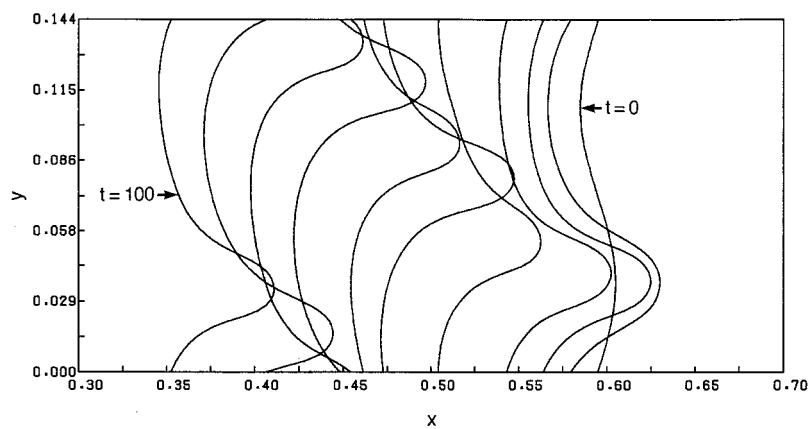


FIG. 8. Evolution of the disturbed flame front for $Le=0.5$, $G=0$, $\lambda=0.144$, and $A_0=0.01$ ($t=0,10,20, \dots, 100$).

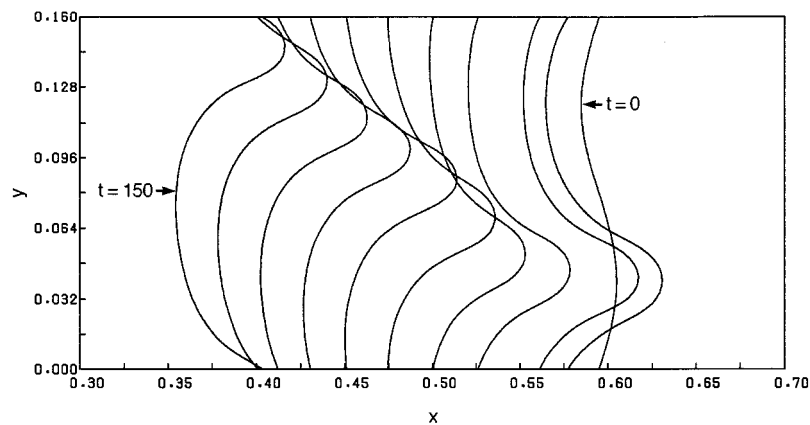


FIG. 9. Evolution of the disturbed flame front for $Le=0.6$, $G=0$, $\lambda=0.160$, and $A_0=0.01$ ($t=0,15,30, \dots, 150$).

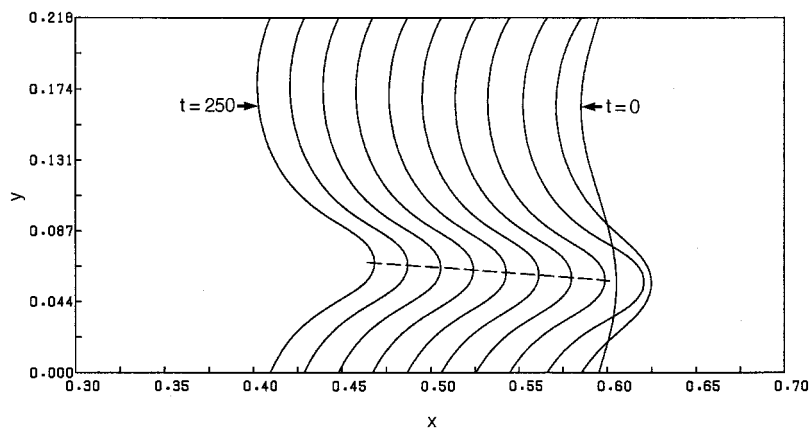


FIG. 10. Evolution of the disturbed flame front for $Le=0.8$, $G=0$, $\lambda=0.218$, and $A_0=0.01$ ($t=0,25,50, \dots, 250$); dashed line denotes the position of the concave flame front toward the unburned gas.

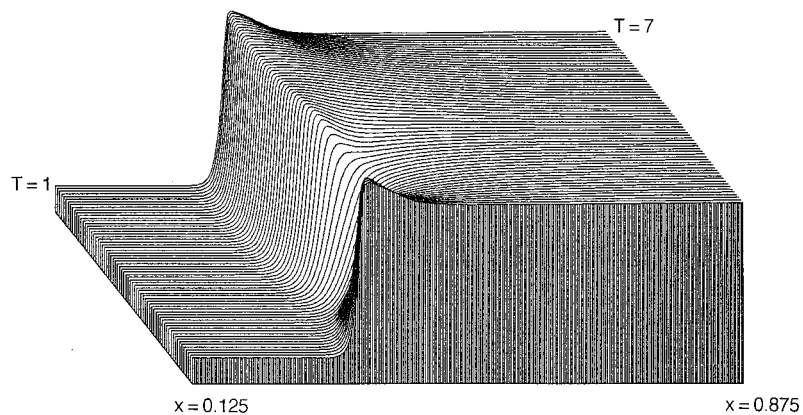


FIG. 11. Temperature distribution of the laterally moving cellular flame for $Le=0.5$, $G=0$, and $\lambda=0.144$ at $t=100$.

Thus it becomes clear that the nonlinear effect of the flame front is prerequisite for the appearance of lateral movements.

We research the mechanism of lateral movements in more detail. It was reported in the diffusive-thermal analysis that lateral movements are introduced with a breaking of the reflection symmetry of cells [28]. We show the temperature distribution of the cellular flame for $Le=0.5$ at $t=100$ in Fig. 11. The temperature has an overshoot at a convex flame front toward the unburned gas, which is not observed when the disturbance is sufficiently small. Similar distributions are found in other cellular flames for $Le<1$, where lateral movements appear. As shown in Figs. 5–7, such an overshoot is not observed in the cellular flames for $Le=1$, where lateral movements do not appear. In general, the physical phenomena associated with the overshoot are not stable. Thus the temperature overshoot induced by the Lewis number effect and by the nonlinear effect of the flame front will cause a breaking of the reflection symmetry of cells and lateral movements appear.

In the diffusive-thermal model, cellular instability does not appear at $Le_c < Le < 1$. When we apply the diffusive-thermal model to the flames used in the present study, we obtain $Le_c=0.767$ because the activation energy is 70 and the adiabatic flame temperature is 7.0 [9]. In the present calculation, the cellular flame moves laterally not only at $Le < Le_c$ but also at $Le_c < Le < 1$. It is due to thermal expansion.

Of course, all flames are attendant upon thermal expansion. Thus we conclude that laterally moving cellular flames are formed at $Le < 1$, which is different from the results of previous investigations based on the diffusive-thermal model.

V. CONCLUDING REMARKS

We have calculated the evolution of disturbed flames for $Le \leq 1$ and studied the essential factors in the appearance of laterally moving cellular flames. The results are summarized as follows.

(i) When the hydrodynamic and body-force instabilities are dominant ($Le=1$), stationary cellular flames are formed.

(ii) When the Lewis number is smaller than unity, laterally moving cellular flames are obtained after the cellular shape of the flame front is formed. The Lewis number effect and the nonlinear effect of the flame front are the essential factors in lateral movements.

(iii) The temperature overshoot found in the cellular flames for $Le < 1$ will cause a breaking of the reflection symmetry of cells and lateral movements appear.

(iv) The lateral movements of cellular flames are obtained not only at $Le < Le_c$ but also at $Le_c < Le < 1$, which is different from the results of previous investigations based on the diffusive-thermal model.

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