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Diffusive-thermal instabilities in premixed flames: Stepwise ignition-temperature kinetics

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This study is motivated by the observation that in combustion of hydrogen–oxygen/air and ethylene–oxygen mixtures the global activation energy appears to be high at low enough temperatures and low at high enough temperatures, reflecting the complex nature of the underlying chemistry. Stability analysis of a uniformly propagating planar premixed flame controlled by a stepwise ignition-temperature kinetics (representing the activation energy temperature-dependence) is carried out. It is shown that, for all its schematic nature, the diffusive-thermal model based on the ignition-temperature kinetics reproduces quite successfully the basic features of both cellular and pulsating instabilities typical of low and high Lewis number mixtures.

1. Introduction

Considerable progress has recently been achieved in understanding the flammability characteristics of hydrogen–oxygen/air and hydrocarbon–oxygen mixtures. In particular, theoretical/numerical studies based on the detailed chemistry mechanisms revealed that the global activation energy E_g of the hydrogen–oxygen/air and ethylene–oxygen mixtures appears to be high at low enough temperatures and low at high enough temperatures (Lutz [1], Kuznetsov et al. [2], Sánchez and Williams [3]). These findings suggest that in an improved description of combustion waves one may, as is often done, employ the global one-step kinetics but with an appropriately modified Arrhenius exponent. Moreover, to sharpen the physical pictures one may consider the extreme situation where $E_g = \infty$ at $T < T_i$ and $E_g = 0$ at $T > T_i$, with T_i being the effective ignition temperature. The concept of ignition temperature has been known in combustion theory since the pioneering work of Mallard and Le Chatelier [4], and is occasionally still used for mathematical tractability [5–8]. However, in view of the above observations the stepwise ignition-temperature kinetics may well acquire a new lease of life, but this time on entirely physical grounds. One of the immediate implications of the ignition-temperature kinetics is formation of the realistically wide reaction zone. Within conventional one-step Arrhenius kinetics this may be attained only by adopting an unduly low activation energy.

The model based on the ignition-temperature kinetics appears to be rich enough to reproduce the basic features of counter-flow flames [6] as well as deflagration-to-detonation transition in smooth-walled channels [9]. In the present study the ignition-temperature kinetics is applied to the problem of diffusion-driven instability in premixed flames - one of the most fascinating phenomena in reactive systems [3,10–15]. For all its long and rich history the topic is still an active area of experimental and theoretical research both in combustion and in general physics of pattern formation [16–22]. As shown in the present study, despite its utter simplicity, the ignition-temperature kinetics captures quite successfully the basic features of both cellular and pulsating instabilities. Moreover, the diffusion-driven instabilities based on the ignition-temperature kinetics challenge the importance of the reaction-rate temperature-dependence, which is occasionally used in physical interpretation of the phenomena.

It has been brought to our attention by Dr. Kurdyumov that the oscillatory instability governed by the stepwise kinetics was previously studied also by Berman et al. [23].

2. Formulation

Our point of departure is the constant density model, which ignores thermal expansion of the gas and hence the impact of

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combustion on the underlying flow-field [24–26]. In this model a flame spreading through a motionless gas may be described by a system consisting merely of the heat equation for the gaseous mixture and diffusion equation for the deficient reactant which is completely consumed in the course of the reaction. In suitably chosen units the set of governing equations thus reads,

heat,

$$\Theta_t = \nabla^2\Theta + W(\Theta,\Phi), \tag{1}$$

diffusion,

$$\Phi_t = \mathrm{Le}^{-1}\nabla^2\Phi - W(\Theta,\Phi). \tag{2}$$

Here $\Theta = (T - T_0)/(T_b - T_0)$ is the reduced temperature, T_0 and T_b being the unburned and burned gas temperatures, respectively; $\Phi = C/C_0$, scaled mass fraction of the deficient reactant in units of its initial value, C_0; Le, Lewis number, the ratio between thermal and molecular diffusivities D_{th} and D_{mol}; The reference spatio-temporal scales are specified as $D_{th}/U_b,\ D_{th}/U_b^2$, respectively, where U_b is the velocity of the planar flame, regarded as a prescribed parameter. W is the scaled reaction rate specified as follows.

For the first-order stepwise kinetics,

$$W(\Theta,\Phi) = \begin{cases} A\Phi & \text{at} \quad \Theta \geqslant \Theta_i, \\ 0 & \text{at} \quad \Theta < \Theta_i \end{cases} \tag{3}$$

For the zero-order stepwise kinetics,

$$W(\Theta,\Phi) = \begin{cases} A & \text{at} \quad \Theta \geqslant \Theta_i \quad \text{and} \quad \Phi > 0, \\ 0 & \text{at} \quad \Theta < \Theta_i \quad \text{and/or} \quad \Phi = 0 \end{cases} \tag{4}$$

Here $\Theta_i = (T_i - T_0)/(T_b - T_0)$ is the reduced ignition temperature, and A is the normalizing factor to ensure that for the undisturbed planar flame its scaled propagation velocity is set at *unity*.

Eqs. (1)–(4) are considered over a plane (x, y) jointly with the boundary conditions,

$$\Theta(+\infty,y,t) = 0, \qquad \Theta(-\infty,y,t) = 1, \tag{5}$$
$$\Phi(+\infty,y,t) = 1, \qquad \Phi(-\infty,y,t) = 0. \tag{6}$$

The flame front $x = F(y,t)$ is defined by the ignition interface,

$$\Theta(F(y,t),y,t) = \Theta_i. \tag{7}$$

At the flame front, apart from Eq. (7), the following continuity conditions are held,

$$[\Theta] = 0, \qquad [\Phi] = 0, \tag{8}$$
$$[\nabla\Theta\cdot\mathbf{N}] = 0, \qquad [\nabla\Phi\cdot\mathbf{N}] = 0, \tag{9}$$

where

$$\mathbf{N} = (\mathbf{i} - F_y\mathbf{j})/\sqrt{1+F_y^2} \tag{10}$$

is the normal to the front and $[\cdot]$ denotes a jump across the interface.

For the zero-order kinetics (4) the problem involves the second (trailing) interface, $x = G(y,t)$, of the vanishing mass fraction/reaction rate,

$$\Phi(G(y,t),y,t) = 0. \tag{11}$$

Apart from (11), at the trailing interface the following continuity conditions should be met,

$$[\Theta] = 0, \qquad [\Phi] = 0, \tag{12}$$
$$[\nabla\Theta\cdot\mathbf{M}] = 0, \quad [\nabla\Phi\cdot\mathbf{M}] = 0, \tag{13}$$

where

$$\mathbf{M} = (\mathbf{i} - G_y\mathbf{j})/\sqrt{1+G_y^2}, \tag{14}$$

is the normal to the trailing interface.

3. Planar flame solution for the first-order kinetics and its linear stability

The problem formulated in the previous section allows for the planar traveling wave solution corresponding to the planar front, $x = F = t$ (Fig. 1). Introducing a moving frame coordinate $\xi = x - t$ and substituting traveling wave ansatz $(\Theta,\Phi)(x,y,t) = (\Theta^{(0)},\ \Phi^{(0)})(\xi)$ into (1)–(3), (5)–(9) after some algebra we have

$$\Theta^{(0)}(\xi) = \begin{cases} \Theta_i\exp(-\xi), & \xi > 0, \\ 1 - (1-\Theta_i)\exp\left(\frac{\Theta_i}{1-\Theta_i}\xi\right), & \xi < 0, \end{cases} \tag{15}$$

$$\Phi^{(0)}(\xi) = \begin{cases} 1 - \frac{\Theta_i}{\Theta_i + \mathrm{Le}(1-\Theta_i)}\exp(-\mathrm{Le}\,\xi), & \xi > 0, \\ \frac{\mathrm{Le}(1-\Theta_i)}{\Theta_i+\mathrm{Le}(1-\Theta_i)}\exp\left(\frac{\Theta_i}{1-\Theta_i}\xi\right), & \xi < 0 \end{cases} \tag{16}$$

and

$$A = \frac{\Theta_i}{1-\Theta_i}\left(1 + \frac{\Theta_i}{\mathrm{Le}(1-\Theta_i)}\right). \tag{17}$$

Prior to its normalization the propagation velocity V is described by the relation,

$$V^2 = \frac{A\mathrm{Le}(1-\Theta_i)}{\Theta_i[\Theta_i + \mathrm{Le}(1-\Theta_i)]}. \tag{18}$$

As one would expect, $V \to 0$ at $\Theta_i \to 1$, and $V \to \infty$ at $\Theta_i \to 0$.

Now we present results of the conventional linear stability analysis of the planar wave solution given by (15) and (16). Thus we set,

$$\Theta(x,y,t) = \Theta^{(0)}(\xi) + \vartheta(\xi,y,t), \tag{19}$$
$$\Phi(x,y,t) = \Phi^{(0)}(\xi) + \varphi(\xi,y,t), \tag{20}$$
$$F(y,t) = t + f(y,t), \tag{21}$$

where $\vartheta,\ \varphi$ and f are small perturbations proportional to $\exp(\omega t + iky)$, ω and k being the instability growth rate and transverse wave number. Perturbations $\vartheta,\ \varphi$ are required to meet the boundary conditions,

$$\vartheta(\pm\infty,y,t) = \varphi(\pm\infty,y,t) = 0. \tag{22}$$

Then upon some straightforward but rather lengthy algebra one ends up with the following dispersion relation between ω and k (see Appendix A),

$$\Delta(\omega,k,\mathrm{Le},\Theta_i) = (q-l)[\Theta_i - 2(1-\Theta_i)p][(1-\mathrm{Le})(\omega - l) - A\mathrm{Le}] + A\mathrm{Le}(p-l) = 0, \tag{23}$$

where

$$p = \frac{1}{2}\left(\sqrt{1+4\omega+4k^2} - 1\right), \tag{24}$$
$$q = -\frac{1}{2}\left(\sqrt{\mathrm{Le}^2 + 4\mathrm{Le}\,\omega + 4k^2} + \mathrm{Le}\right), \tag{25}$$
$$l = \frac{1}{2}\left(\sqrt{\mathrm{Le}^2 + 4\mathrm{Le}(A+\omega) + 4k^2} - \mathrm{Le}\right). \tag{26}$$

To meet the boundary conditions (22) p, q, l should obey the restrictions,

$$\mathrm{Re}\ p > 0, \quad \mathrm{Re}\ q < 0, \quad \mathrm{Re}\ l > 0. \tag{27}$$