Analytical Determination of One-dimensional Cellular Structures in Flame Fronts

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Abstract
The purpose of the present paper is to calculate, using modal decomposition, constant-speed, space-periodic solutions of the Michelson-Sivashinsky equation. We thus determine secondary bifurcation points and the relationship between the flame velocity and the wave number.

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1 Introduction

Body-force, hydrodynamic and thermal-diffusive effects are the three main phenomena determining intrinsic instabilities of premixed, plane flame fronts.

An stability analysis, in which body-forces are neglected and the flame front is treated as a discontinuity in density propagating with constant velocity normal to itself, leads to the well known result of unconditional instability [1]. The influence of thermal-diffusive effects seem to have been first addressed by Zel’dovich[2]. It is now a well established fact that when the Lewis Number $L_e$ is less than one, i.e., the reactant is strongly diffusive, thermal-diffusive instability occurs.

Let $l_d$, the width of the thermal structure of the flame, $V_b$ the normal velocity of the flame relative to the burnt gas, $T_b$ the adiabatic temperature of the combustion products, $\sigma$ the coefficient of thermal expansion of the gas ($\sigma < 1$) and $R$ the universal gas constant, then, the behavior of hydrodynamic instabilities caused by thermal expansion of the gas and transport effects is characterized by the solution of the Michelson-Sivashinsky equation [3]

$$\frac{\partial F}{\partial t} + 4(1 + \sigma)^2 \nabla^4 F + \varepsilon \nabla^2 F + \frac{1}{2} (\nabla F)^2 = (1 - \sigma) I[F]$$

where

$$I[F] = \frac{1}{8\pi^2} \int_{-\infty}^{\infty} |k| F(\xi, \tau) \exp i k \cdot (\xi - \xi) d\xi dk,$$

$F = F(\xi, \tau)$ is the dimensionless perturbation
of the flame front, $\zeta$ is the dimensionless space coordinates vector, both measured in units of $l_{th}$, $\tau$ is dimensionless time in units of $l_{th}/V_b$ and
\[\epsilon = \left( L_{e_0} - L_e \right) / \left( 1 - L_{e_0} \right),\]
being $L_{e_0}$ the critical Lewis Number defined by
\[L_{e_0} = 1 - 2/E(1 - \sigma).\]
$E$ is here the dimensionless activation energy in units of $R^0T_b$.

Numerical integration suggests that, under suitable conditions, equation (1) possesses space-periodic solutions travelling with constant, non-zero velocity[4]. Several analytical works also show that this is so in the particular case of the Kuramoto-Sivashinsky equation ($\sigma = 1$) [5, 6, 7, 8, 9]. The purpose of the present paper is to calculate constant-speed, space-periodic solutions of the one-dimension form of (1) using modal decomposition. In this way, we determine the relationship existing between the flame velocity, wave-number and a physical parameter $\lambda$ to be defined below.

Existence of constant-speed, space - periodic solutions

Let us consider the one-dimension form of (1), and let
\[F = \epsilon f, \quad \tau = \left[ \frac{2\left(1 + \epsilon \right)}{\epsilon} \right]^2 t,\]
\[\zeta = \frac{2\left|1 + \epsilon \right|}{\sqrt{|\epsilon|}} z \quad (\epsilon \neq 0, -1)\]
then, equation (1) is transformed into the pair of one-parameter equations:
\[\frac{\partial f}{\partial t} + \frac{\partial^4 f}{\partial x^4} + \text{sgn}(\epsilon) \frac{\partial^2 f}{\partial x^2} + \left( \frac{\partial f}{\partial z} \right)^2 = \frac{\lambda}{\pi} I[f] \quad (2)\]
where
\[\lambda = 2\left|1 + \epsilon \right| \left(1 - \sigma \right) / |\epsilon|^{3/2},\]
sgn is the signum function and $f(x, t)$ is the function obtained from $\tilde{f}$ after the change of variables. It is interesting to observe that $\lambda^{-2/3}$ is the scaling factor of $L_{e_0} - L_e$ in the derivation of (1) under the conditions $E \to \infty$ and $\sigma \to 1$ while $E(1 - \sigma)$ remains finite.

Let us now seek constant-speed, $2\pi$-space-periodic solutions of (2). In this case the integral in it can be replaced by the series
\[I[f] = \frac{\pi}{2l} \sum_{n=1}^{\infty} n \left( b_n \cos \frac{n\pi}{l} z + c_n \sin \frac{n\pi}{l} z \right),\]
where
\[b_n = b_n(f, l) = \frac{1}{l} \int_{-l}^{l} f(\xi, t) \cos \frac{n\pi}{l} \xi d\xi,\]
\[c_n = c_n(f, l) = \frac{1}{l} \int_{-l}^{l} f(\xi, t) \sin \frac{n\pi}{l} \xi d\xi.\]
The period of the sought solution can be fixed equal to $2\pi$ setting $\kappa z = x$, where $\kappa = \pi/l$. We thus obtain from (2)
\[\frac{\partial g}{\partial t} + \kappa^4 \frac{\partial^4 g}{\partial x^4} + \text{sgn}(\epsilon) \kappa^2 \frac{\partial^2 g}{\partial x^2} + \left( \frac{\partial g}{\partial x} \right)^2 = \lambda \kappa I[g] \quad (3)\]
with $g(x) = f(kx)$, $b_n = b_n(g, \pi)$, $c_n = c_n(g, \pi)$.

It is evident that $g \equiv 0$ is a solution of (3) for all $\lambda$ and $\kappa$. Linearizing the equation around this solution we have
\[\frac{\partial \tilde{g}}{\partial t} + \kappa^4 \frac{\partial^4 \tilde{g}}{\partial x^4} + \text{sgn}(\epsilon) \kappa^2 \frac{\partial^2 \tilde{g}}{\partial x^2} = \lambda \kappa I[\tilde{g}]\]
where the dots on $b_n$ and $c_n$ indicate the coefficients corresponding to $\dot{y}$. Setting $\dot{y} = \exp(\omega t + i x)$ we get

$$
\dot{b}_n = \frac{1}{\pi} \int_{-\pi}^{\pi} \cos x \cos nx \, dx \\
+ \frac{i}{\pi} \int_{-\pi}^{\pi} \sin x \cos nx \, dx = \delta_{n1}
$$

$$
\dot{c}_n = \frac{1}{\pi} \int_{-\pi}^{\pi} \cos x \sin nx \, dx \\
+ \frac{i}{\pi} \int_{-\pi}^{\pi} \sin x \sin nx \, dx = i \delta_{n1}.
$$

Hence,

$$
\omega = -\kappa^4 + \text{sgn}(\epsilon) \kappa^2 + \kappa \lambda. \tag{4}
$$

One must observe in (4) that $\omega = 0$ implies that either $\kappa = 0$ or

$$
-\kappa^3 + \text{sgn}(\epsilon) \kappa + \lambda = 0. \tag{5}
$$

Let us analyze this last case. Simple algebraic manipulation of equations (4,5) shows that (4) always possesses one and only one non-zero, positive root. At it,

$$
\lambda = \lambda_0(\kappa) = \kappa^3 - \text{sgn}(\epsilon) \kappa \\
= \kappa(\kappa^2 - \text{sgn}(\epsilon)).
$$

The root of (4) for $\epsilon > 0$ occurs only for $\kappa \geq 1$.

Since $\kappa$ and $\lambda$ are real so is $\omega$, therefore for fixed $\lambda$, $u \equiv 0$ is unstable if $\kappa < \kappa_0^2(\lambda)$, where $\kappa_0^2(\lambda)$ are the roots of equation (5), corresponding the plus and minus signs to $\epsilon > 0$ and $\epsilon < 0$ respectively. One can then expect a non-trivial, constant-speed, space-periodic solution of (3) only in the unstable region. In order to determine it we set

$$
g(x,t) = -\mu t + u(x),
$$

$$
u(x + 2\pi) = u(x) \forall x.
$$

which yields

$$
\kappa^4 u^{iv} + \text{sgn}(\epsilon) \kappa^2 u'' \\
+ \frac{1}{2} \kappa^2 (u')^2 = \mu + \lambda \kappa I[u]. \tag{6}
$$

an equation which has a $2\pi$-periodic solution guaranteed by the bifurcation theorem [10]. We can thus expand it in its Fourier Series

$$
u(x) = \sum_{p=1}^{\infty} \hat{u}(p) \cos px. \tag{7}
$$

with, so far, unknown coefficients $\hat{u}(p)$. We must observe that

$$
b_n = b_n(\cos px) = \delta_{np},
$$

$$
c_n = c_n(\cos px) = 0,
$$

hence, using (7) in (6),

$$
\sum_{n=1}^{\infty} \left[ (n \kappa)^4 - \text{sgn}(\epsilon) (n \kappa)^2 \right] \hat{u}(n) \cos nx \\
+ \frac{1}{2} \kappa^2 \left( \sum_{p=1}^{\infty} p \hat{u}(p) \sin px \right)^2
$$

$$
= \mu + \lambda \kappa \sum_{n=1}^{\infty} n \hat{u}(n) \cos nx \tag{8}
$$

Expanding the square and collecting harmonics, we obtain the infinite system of algebraic equations valid for $n = 1, 2, \ldots$:

$$
[(n \kappa)^4 - \text{sgn}(\epsilon) (n \kappa)^2 - n \kappa \lambda] \hat{u}(n) \\
+ \frac{1}{2} \kappa^2 \{ 2 \sum_{p=1}^{\infty} n(n+p) \hat{u}(p) \hat{u}(n+p) \\
- \sum_{p=1}^{n-1} p(n-p) \hat{u}(p) \hat{u}(n-p) \} = 0 \tag{9}
$$

Summation with $p$ from 1 to $n - 1$ in (9) must be understood as zero when $n = 1$. 

Once (9) has been solved, \( \mu \) is determined by the formula

\[
\mu = \frac{1}{4} \kappa^2 \sum_{p=1}^{\infty} p^2 \hat{u}^2(p),
\]

corresponding to the constant term of (8), which can also be obtained by direct integration of both terms of equation (6) using the periodicity of \( u(x) \) and Parseval's equality, i.e., the velocity is the square of the \( L^2 \) norm of the solution's gradient.

Any numerical method for solving a finite truncation of (9) would require a, not at all obvious, initial guess. However, one must observe that \( \hat{u}(n) = 0 \) \( \forall n \) is a solution of (9) for all \( \kappa \) and \( \lambda \). Linearizing around it we have also for \( n = 1, 2, \ldots \):

\[
[(n \kappa)^4 - \text{sgn}(\varepsilon)(n \kappa)^2 - \kappa \lambda] \hat{u}(n) = 0
\]

Since we want a fundamental period \( 2\pi \), then either \( \hat{u}(n) = 0 \) \( \forall n \), or equation (5) must be satisfied. Using regular perturbation methods and bifurcation theory, one can seek solutions of (9) in the form \( \lambda = \lambda(\nu) \), \( \lambda(0) = \lambda_0(\kappa) = \kappa^3 - \text{sgn}(\varepsilon) \kappa \), \( \kappa \) fixed. Up to terms of order \( o(\nu^3) \), this procedure yields:

\[
\hat{u}^\pm(n) \approx \delta_{n1} \nu + \frac{\delta_{n2} \nu^2}{8[7\kappa^2 - \text{sgn}(\varepsilon)]} + \frac{\delta_{n3} \nu^3}{48[7\kappa^2 - \text{sgn}(\varepsilon)][13\kappa^2 - \text{sgn}(\varepsilon)]}
\]

\[
\lambda^\pm \approx \kappa^3 - \text{sgn}(\varepsilon) \kappa + \frac{\kappa \nu^2}{8[7\kappa^2 - \text{sgn}(\varepsilon)]}
\]

\[
\mu^\pm \approx \frac{\kappa^2 \nu^2}{4} \left\{ 1 + \frac{\nu}{16[7\kappa^2 - \text{sgn}(\varepsilon)]} \right\}
\]

Discussion of results and conclusions

We have implemented the algorithm described in the previous section using ten modes, obtaining results for both \( \varepsilon \) positive and negative, varying \( k \) from, respectively, 1.1 and 0.5 to 2.0. The procedure, started with an approximation obtained using a combination of power series and Fourier series [9], converges for each fixed \( k \) up to a maximum value of \( \lambda \), which we shall denote by \( \lambda_\ast(k) \), as shown in Figure 1. At this maximum, \( \lambda_\ast(k) = \lambda(2k) \) and \( \mu(\lambda_\ast(k)) = \mu(\lambda(2k)) \) (Figure 2), while the shapes of the flames fronts agree, resulting in a secondary bifurcation point, as exemplified in Figure 3, where we show the shapes of the flames fronts for three different values of \( \lambda \) between the primary bifurcation point of \( 2k \) and \( \lambda_\ast(k) \). The inner maximum of the \( 2\pi/k \)-periodic solution appears at a value of \( \lambda \) smaller than the one where the flame velocity \( \mu \) attains its maximum, evolving with increasing \( \lambda \) toward the same value of them. At this point, the shapes of the \( \pi/k \) and \( 2\pi/k \)-periodic solutions coincide when the former is considered over two full periods.

Comparing Figures 2 and 3 one must observe that if a gas is such that its constant \( \lambda \) is at the critical value \( \lambda_\ast(k) \) for some \( k \), a variation in its physical properties, in such a way that \( \lambda \) varies to a value slightly lesser than \( \lambda_\ast(k) \) will make the flame to have one of two different configurations, travelling with different velocities.

Whether the flame will present one or the other configuration depends on the stability of these solutions, an analysis that will be presented elsewhere. Euristically, one should expect that the slower, and less corrugated flame (the \( \pi/k \)-periodic solution has two maxima and one minimum over a period and the \( 2\pi/k \)-periodic one has three maxima and two min-
ima over its period) will be the stable one and therefore, the only one of possible physical realization.

We have introduced in this paper a parameter $\lambda$ which summarizes the physical properties of a gas mixture, and determined the dependence of the periodic solutions of the one dimensional Michelson-Sivashinsky equation on $\lambda$, as well as the dependence of the primary, secondary bifurcation points and the flame velocity on this parameter. Although, as said before, the physical properties of the gas mixture are summarized by $\lambda$, it is not enough to fully describe the periodic solutions of (3) because they are quantitatively and qualitatively different for positive and negative $\epsilon$, a fact that should be expected, since they correspond to Lewis numbers greater and smaller than the critical Lewis Number.

We have not exhausted in this article all the possible investigations on the one dimensional Michelson-Sivashinsky equation and much work remains to be done. For example, the relationships between the findings here and the stretching and curvature of the flame remains to be studied, a research for which, we believe, the algorithm of modal decompositions will be suitable.

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Figure 3: Flame shapes for $k = 1.5$ and $k = 3.0$, positive $\varepsilon$. Of both curves with the same symbol, the upper one corresponds to $k = 1.5$.

References


