

An equation of surface dynamics modeling flame fronts as density discontinuities in potential flows

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A coordinate-free equation modeling the flame front dynamics as propagation of density discontinuity within the framework of the Darreus–Landau hydrodynamical model is derived under the assumption of potential flow. The assumption is based on the observation that for slightly perturbed plane configurations the flow is irrotational if the thermal expansion of the gas is weak. A relationship with an equation obtained earlier for a slightly perturbed plane flame front is established in the case of weak thermal expansion. An invariant equation simultaneously modeling the thermal-diffusional and the hydrodynamical instabilities is suggested, which also can be reduced to earlier results in appropriate limits.

I. INTRODUCTION

In 1977, Sivashinsky¹ introduced an equation describing evolution of a slightly perturbed plane flame front in the limit of a small thermal expansion of gas:

$$\phi_t + \phi_x^2/2 + \epsilon\phi_{xx} + \phi_{xxx} = (\gamma/2)I[\phi]. \quad (1)$$

Here $y = \phi(x, t)$ is a small perturbation of the front, $\gamma \ll 1$ is the thermal expansion parameter (see the definition below), $\epsilon \ll 1$ is a parameter reflecting chemical–physical characteristics of the combustible mixture, and

$$\begin{aligned} I[\phi] &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |k| \phi(x', t) e^{ik(x' - x)} dx' dk \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} |k| e^{-ikx} \vec{\phi}(k, t) dk, \end{aligned} \quad (2)$$

while the overtilde denotes the Fourier transform of ϕ . For simplicity here and following we consider the two-dimensional case, so that the flame front is represented by a curve. The three-dimensional version of the result is discussed in Sec. IV.

Equation (1) describes the development of both the thermal-diffusional instability and the hydrodynamic instability in the flame front. If $\epsilon < 0$ the thermal-diffusional structure stabilizes the front and the corresponding equation is¹

$$\phi_t + \phi_x^2/2 + \epsilon\phi_{xx} = (\gamma/2)I[\phi]. \quad (3)$$

In the long wavelength limit, Eq. (3) can be further reduced to

$$\phi_t + \phi_x^2/2 = (\gamma/2)I[\phi]. \quad (4)$$

Therefore the last equation describes the dynamics of a slightly perturbed plane flame front under the conditions of instability induced by the thermal expansion. Equation (4) was also derived directly² using formal asymptotic expansion in powers of $\gamma \ll 1$ within the framework of a purely hydrodynamic model of flame propagation.

In 1987, Frankel and Sivashinsky³ obtained a strongly nonlinear coordinate-free equation describing the dynamics of the flame fronts within the framework of the thermal-diffusional flame model ($\gamma = 0$). The equation

$$V = -1 + \epsilon\kappa - \kappa_{ss} \quad (5)$$

relates the normal velocity of the surface V to its local geometrical characteristics, such as (in two dimensions) the curvature κ and its second derivative with respect to the arclength s . In particular, for small perturbations of the plane propagating with constant velocity and for near-critical values of parameters, Eq. (5) can be reduced to Eq. (1) with zero right-hand side ($\gamma = 0$). Thus the weakly nonlinear case (1) was traced to its geometrical origin.

In this context it is natural to ask the following question. What is the coordinate-free version of the integral term in Eqs. (1), (3), and (4)? In other words, what is the invariant form of these equations that would model the advance of curved flame fronts as opposed to small perturbations of the plane ones, including the hydrodynamic instability?

Analyzing computations in Ref. 1, one can observe that to the principal order with respect to $\gamma \ll 1$ the gas flow is potential both ahead and behind the flame front. This in turn allows us to cast away a long held belief that Landau instability is necessarily related to the generation of vorticity within the flame structure. This observation was quite clearly stated in the review paper.⁴ Moreover, the purely irrotational model was partly studied in Ref. 2 for weakly perturbed plane flames represented as a density jump propagating at a constant velocity with respect to the gas.

It then seems quite natural to consider the dynamics of arbitrarily shaped fronts within the framework of a purely irrotational flow. Such a study, however, has never been carried out. This is very surprising indeed, since the solution is, in fact, a straightforward exercise in classical potential theory (see the following) and yet it yields a very interesting equation of flame dynamics that, in particular, answers the questions formulated previously.

II. THE EQUATION OF FRONT DYNAMICS

Within the framework of the Darreus–Landau hydrodynamic approximation the flame is regarded as a surface of density discontinuity propagating at a constant velocity relative to the gas.⁵ The flow is assumed to be incompressible and inviscid. We shall further assume that the flow is irrota-

tional in both the unburned (-) and the burned (+) gas.

The latter assumption becomes a correct statement in the principal (nontrivial) order for small value $\gamma \ll 1$ of the thermal expansion constant.² Here we would like to stress the fact that the analyses conducted in Refs. 1 and 2 with or without the potential flow assumption are obviously identical and lead to the same result, i.e., Eq. (4). The derivation we present below, on the other hand, has nothing to do with the condition $\gamma \ll 1$ or asymptotic expansion, once we assume that the gas flow is potential, and is, of course, absolutely rigorous.

Thus the gas flow will be described by a potential function $w(x,y,t)$ such that

$$w_{xx}^{\pm} + w_{yy}^{\pm} = 0, \quad (6)$$

subject to the conditions of continuity, conservation of matter, and, as was mentioned above, a constant (unit) velocity of the front with respect to the gas.

Therefore

$$w^+ = w^-, \quad \left(\frac{\partial w^+}{\partial n} - V \right) \rho^+ = \left(\frac{\partial w^-}{\partial n} - V \right) \rho^-, \quad (7)$$

$$\left(\frac{\partial w^+}{\partial n} - V \right) = 1.$$

Here V is the normal velocity of the flame front, \mathbf{n} is the inward normal vector on the boundary directed toward the burned gas (+), and ρ^{\pm} are the corresponding densities ($\rho^+ = 1$). Using the last of the conditions (7), the second condition can be replaced by

$$\frac{\partial w^+}{\partial n} - \frac{\partial w^-}{\partial n} = \gamma, \quad (8)$$

where γ is defined as $\gamma = 1 - 1/\rho^-$.

The solution of the problem defined by Eqs. (6) and (8) can be found as a single layer potential with constant charge distribution $\gamma/2\pi$ along the curve C corresponding to the instantaneous position of the flame front (Fig. 1):

$$w(\mathbf{r},t) = \frac{\gamma}{2\pi} \int_C \ln|\mathbf{r} - \xi| dl_{\xi}. \quad (9)$$

The dynamics of the front C can be found from the last of the conditions (7) that "overdetermines" the problem. Let $\partial w/\partial \mathbf{n}_0$ denote the line integral of the formal derivative of the logarithmic potential in the direction of the normal vector at the point \mathbf{r} on the curve C :

$$\frac{\partial w}{\partial \mathbf{n}_0}(\mathbf{r},t) = \frac{\gamma}{2\pi} \int_C \frac{\partial}{\partial \mathbf{n}} \Big|_{\mathbf{r}} (\ln|\mathbf{r} - \xi|) dl_{\xi}. \quad (10)$$

Then, the following relationships hold at the interface:

$$\frac{\partial w^-}{\partial \mathbf{n}}(\mathbf{r}) = -\frac{\gamma}{2} + \frac{\partial w}{\partial \mathbf{n}_0}(\mathbf{r}), \quad (11)$$

$$\frac{\partial w^+}{\partial \mathbf{n}}(\mathbf{r}) = \frac{\gamma}{2} + \frac{\partial w}{\partial \mathbf{n}_0}(\mathbf{r}), \quad (12)$$

which is in agreement with the interface condition (8) and, upon substitution of (12) into the last of the conditions (7), leads to the following evolution equation for the flame front:

$$V(\mathbf{r},t) = -1 + \frac{\gamma}{2} \left(1 - \frac{1}{\pi} \int_C \frac{\partial}{\partial \mathbf{n}} \ln|\mathbf{r} - \xi| dl_{\xi} \right). \quad (13)$$

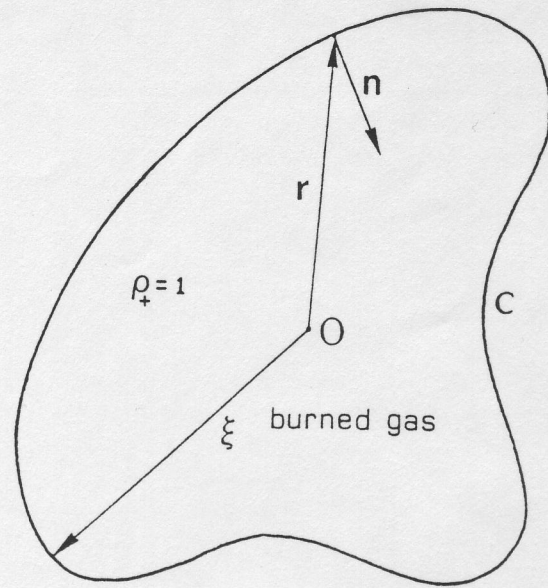


FIG. 1. Curve C represents an instantaneous position of the expanding flame front; normal velocity V in Eq. (14) is evaluated at the point \mathbf{r} ; normal vector \mathbf{n} at \mathbf{r} points toward the burned gas; the integration is performed with respect to ξ .

A more convenient form of Eq. (13) is

$$V(\mathbf{r},t) = -1 + \frac{\gamma}{2} \left(1 + \frac{1}{\pi} \int_C \frac{(\mathbf{r} - \xi) \cdot \mathbf{n}}{|\mathbf{r} - \xi|^2} dl_{\xi} \right) \quad (14a)$$

or

$$V(\mathbf{r},t) = -1 + \frac{\gamma}{2} \left(1 + \frac{1}{\pi} \int_C \frac{\cos \theta}{|\mathbf{r} - \xi|} dl_{\xi} \right), \quad (14b)$$

where θ is the angle between $\mathbf{r} - \xi$ and \mathbf{n} , while \mathbf{n} is the normal to the flame front at \mathbf{r} .

From Eq. (14b) it is obvious that the integrals are regular for a sufficiently smooth boundary. In the form of Eq. (14a), on the other hand, one can easily recognize the normal component of the (burned) gas velocity represented by the superposition of uniformly distributed sources along the boundary C .

Thus we obtain a front dynamics equation that defines the normal propagation velocity at the points of the boundary, which will remain valid until, possibly, the front develops a cusp. Next we shall establish a relationship between the invariant equation (14a) and the corresponding equation (4) for a slightly perturbed plane front.

III. REDUCTION TO EQ. (4)

In this section we assume that $\gamma \ll 1$ and expand in powers of γ as it was done in Refs. 1 and 2 in order to obtain Eqs. (1)-(4). Let us first consider a "near-rectangular" closed contour formed by two vertical lines passing through $x - A$ and $x + A$, a horizontal line $y = d$, and the slightly perturbed boundary $y = 0$ (Fig. 2). Let the perturbed boundary for the points $\mathbf{r} = (x,y)$ and $\xi = (\eta,\zeta)$ be given by the equations

$$y = \phi(x,t) - t \quad \text{and} \quad \zeta = \phi(\eta,t) - t, \quad (15)$$

respectively.

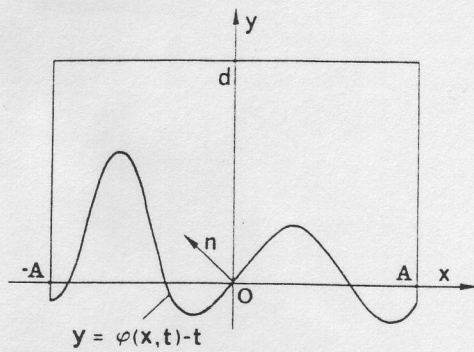


FIG. 2. The contour that is chosen in reduction to Eq. (4) for a weakly perturbed plane front. The perturbed boundary is given by $y = \phi(x, t) - t$. The coordinate frame is translated in such a way that $r = 0$ at $t = 0$.

Following Refs. 1 and 2 again it is known that $\phi \sim \gamma$ and $\phi_t \sim \gamma^2$. Now, we want to compute all the terms in Eq. (14a) up to order γ^2 . Using the above notation we obtain up to order γ

$$n(\mathbf{r}) = [-\phi_x(x), 1] / \sqrt{1 + \phi_x^2} \sim [-\phi_x(x), 1]. \quad (16)$$

Then, the integral along the segment $y = d$ is easily evaluated:

$$\begin{aligned} \int \frac{(\mathbf{r} - \xi) \cdot \mathbf{n}}{|\mathbf{r} - \xi|^2} dl_\xi &= \int_{x-A}^{x+A} \\ &\times \frac{[x - \eta, \phi(x) - d] \cdot [-\phi_x(x), 1]}{[\phi(x) - d]^2 + (x - \eta)^2} d\eta \\ &= -2 \arctan\left(\frac{A}{d - \phi(x)}\right). \end{aligned} \quad (17)$$

Thus the integral along $y = d$ tends to $-\pi$ as $A \rightarrow \infty$.

The integrals along the sides $x \pm A$ tend to zero. Therefore we need only interpret the remaining integral along the perturbed boundary. For the latter we have $|\mathbf{r} - \xi|^2 = (\eta - x)^2$, $dl_\xi = d\eta$ (up to γ) and the integral can be expressed as follows:

$$\begin{aligned} \int \frac{(\mathbf{r} - \xi) \cdot \mathbf{n}}{|\mathbf{r} - \xi|^2} dl_\xi &= - \int_{x-A}^{x+A} \frac{\phi(\eta) - \phi(x) - \phi_x(x)(\eta - x)}{(\eta - x)^2} d\eta \\ &= - \int_{-A}^A \frac{\phi(\chi + x) - \phi(x) - \phi_x(x)\chi}{\chi^2} d\chi. \end{aligned} \quad (18)$$

The integrand in the above integral is obviously a continuous function, and we need not be concerned about convergence at $\chi = 0$. Then it can be evaluated via its principal value (p.v.); the integral of the third term vanishes, whereas the integral of the first term can be reduced in the limit of $A \rightarrow \infty$ as follows:

$$\begin{aligned} - \text{p.v.} \int_{-\infty}^{\infty} \frac{\phi(\chi + x) - \phi(x) - \phi_x(x)\chi}{\chi^2} d\chi \\ = - \left(\frac{1}{\chi^2} : \phi(\chi + x) \right), \end{aligned} \quad (19)$$

where the colon denotes the action of functionals.

Here we used the fact that the principal value of the integral in (19) is the same as the canonical regularization of the singular function $1/\chi^2$, leading to the definition of the corresponding generalized function.⁶ The action of the functional can be expressed in the Fourier transform (overtilde):

$$-\frac{1}{2\pi} \left(\frac{1}{\chi^2} : \phi(\chi + x) \right) = \frac{1}{2} \int_{-\infty}^{\infty} |k| e^{-ikx} \tilde{\phi}(k) dk. \quad (20)$$

Now, recalling that $\phi_t \sim \gamma^2$, for the normal velocity on the left-hand side of Eq. (14a) we obtain up to order γ^2

$$V = (\phi_t - 1) / \sqrt{1 + \phi_x^2} = -1 + \phi_t + \phi_x^2 / 2. \quad (21)$$

Finally, substituting (17), (20), and (21) into the evolution equation (14a) we obtain

$$\phi_t + \frac{\phi_x^2}{2} = \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} |k| e^{-ikx} \tilde{\phi}(k) dk, \quad (22)$$

which is identical to (4).

Several remarks are due concerning the relationship between Eqs. (14a) and (4), in general, and the above reduction in particular. Equation (4) was derived assuming the basic solution to be an infinite linear (plane in three dimensions) interface. One should remember that this is a physical idealization similar to an infinite uniformly charged line (plane), using an analogy from electrostatics, which is an approximation of the field created by a large but finite linear segment near (in a certain sense) its center. We should not be surprised therefore at the necessity of having to choose a (near) symmetrical contour around the point \mathbf{r} in order to handle the integrals in transition to infinity.

The contour can indeed be chosen to be slightly asymmetrical ($x - A, x + B$) with the condition $A/B \rightarrow 1$ as $A, B \rightarrow \infty$. This means that if we consider $(-A, A)$, there is a slower expanding region near zero where the above reduction is valid. However, there is obviously no transition from Eq. (14a) to Eq. (4) for an arbitrarily shaped expanding contour.

We can also carry out a similar reduction of Eq. (14a) to Eq. (4) for another special choice of the contour C : a slightly perturbed circle C_R when its radius R becomes very large. For this purpose we let

$$\begin{aligned} \mathbf{r} &= [R + \phi(0), 0], \\ \xi &= \{ [R + \phi(0)] \cos \theta, [R + \phi(0)] \sin \theta \} \end{aligned} \quad (23)$$

at $t = 0$. Here θ is the polar angle and $\phi(\theta, t) \sim \gamma$ is a small perturbation whose support σ is obtained within an interval $-\delta < \theta < \delta$ and can be assumed to be identical with it. In order to simplify our calculations, we have chosen the point \mathbf{r} to be located on the x axis.

Then up to order γ

$$n = [-1, \phi_\theta(0) / R], \quad dl_\xi = ds = R d\theta, \quad (24)$$

where s is the length along the circular (unperturbed) arc C_R .

After some algebraic and trigonometric manipulations, one can reduce (up to the same order) the line integral in Eq. (14a) to the following form:

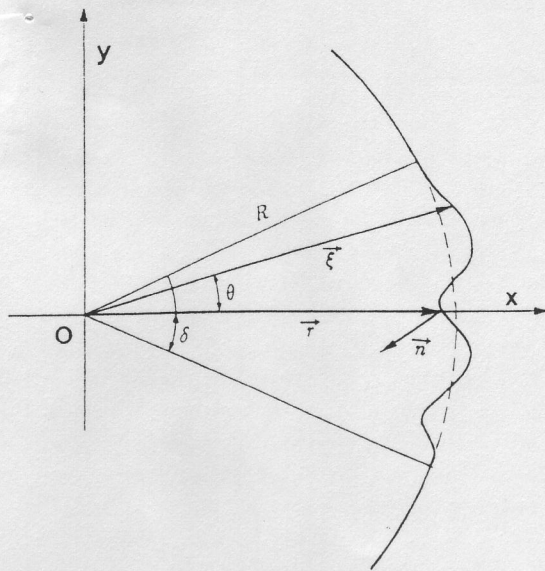


FIG. 3. A slightly perturbed circle $C_R: \mathbf{r} = [R + \phi(0), 0]$, $\xi = \{(R + \phi(\theta)) \cos \theta, [R + \phi(\theta)] \sin \theta\}$. Here θ is the polar angle and $\phi(\theta, t) \sim \gamma$ is a small perturbation whose support σ is contained within an interval $-\delta < \theta < \delta$.

$$\int \frac{(\mathbf{r} - \xi) \cdot \mathbf{n}}{|\mathbf{r} - \xi|^2} dl_\xi = -\pi + \frac{1}{R} \times \int \frac{\phi - \phi(0) \cos \theta - \phi_\theta(0) \sin \theta}{4 \sin^2(\theta/2)} d\theta. \quad (25)$$

The integral on the right-hand side of (25) can be evaluated by partitioning the domain as follows:

$$\int_{C_R} \frac{\phi - \phi(0) \cos \theta - \phi_\theta \eta}{s^2 [4 \sin^2(\theta/2) / \theta^2]} ds = \int_{C_R \setminus \sigma} + \int_\sigma. \quad (26)$$

One can easily check that in absolute value

$$\int_{C_R \setminus \sigma} \leq \frac{|\phi(0)|M}{R\delta}$$

for some constant M independent of R .

Now, we can choose δ small enough for the equalities $\cos \theta = 1$, $\sin \theta / \theta = 1$, and $dy = ds$ to hold with required accuracy inside the support σ . Then up to order γ

$$\int_\sigma = \int_{-R \sin \delta}^{R \sin \delta} \frac{\phi - \phi(0) - \phi_y(0)y}{y^2} dy. \quad (27)$$

Thus as $R \rightarrow \infty$ we obtain the same functional (corresponding to $x = 0$) as in (18). After collecting all the terms we obtain up to order γ^2

$$V = -1 + \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} \tilde{\phi}(k) |k| dk. \quad (28)$$

Finally, expanding as above the normal velocity at $\mathbf{r} = \{[R - t + \phi(\theta, t) \cos \theta], [R - t + \phi(\theta, t) \sin \theta]\}$ and replacing the derivatives with respect to θ by those with respect to y for $t = 0$ and $\theta = 0$, we obtain that up to order γ^2 ,

$$\phi_t + \frac{1}{2} \phi_y^2 = \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} \tilde{\phi}(k) |k| dk, \quad (29)$$

which represents Eq. (14) at $y = 0$. If we choose the point \mathbf{r} in the above argument, which is not situated on the x axis, the calculations become a little more subtle and lengthy but, as one can check, will inevitably reproduce Eq. (4). The remarks concerning the transition to infinite limits made after the previous example are obviously valid in the near circular case.

IV. CONCLUDING REMARKS

The previous examples of the relationship between Eqs. (4) and (14a) do not serve to justify the invariant equation. Indeed, it does not need a "justification" since, on the one hand, the derivation is absolutely rigorous and quite simple once the assumption of the potential character of the flow is made, and since, on the other hand, this assumption is justified in the case of small γ for which Eqs. (1)–(4) were derived. That is, the invariant equation is at least "as correct" as these equations. Moreover, it reflects some desirable features of the realistic physical problem such as zero velocity of the gas at infinity and its invariance.

The front dynamics equation (14a) is obviously invariant with respect to translations and rotations of the coordinate frame as it is expressed in terms of the front velocity in the local normal direction and the distances between the points on the front. The equation can be immediately transferred into three dimensions using Newton's potential instead of the logarithmic one, i.e.,

$$V(\mathbf{r}, t) = -1 + \frac{\gamma}{2} \left(1 + \frac{1}{2\pi} \int_S \frac{(\mathbf{r} - \xi) \cdot \mathbf{n}}{|\mathbf{r} - \xi|^3} dS_\xi \right). \quad (30)$$

In spite of the rather simple form of Eqs. (14) and (30), it is not easy to find any explicit solutions. In fact, we can present only a trivial illustration, namely, that of the expanding circle used in the above example where the integral

$$\int_C \frac{(\mathbf{r} - \xi) \cdot \mathbf{n}}{|\mathbf{r} - \xi|^2} dl_\xi = -\pi \quad (31)$$

can be easily evaluated to yield $V \equiv -1$, which is obviously the case since the burned matter is immobilized. The same result is formally obtained after evaluation of the integral in another trivial case: the initially ignited plane that generates two plane fronts running away from each other with $V \equiv -1$. However, rigorously speaking, this solution is incorrect since Eqs. (9)–(14a) are valid only for closed fronts.

At this stage we cannot present any results of numerical simulation of Eq. (14a), which constitutes our next objective. In view of the similarity between the weak (4) and the invariant (14a) forms, we can expect the development of cusps pointing into the burned matter, as the previous numerical simulation of Eq. (4) has shown.⁷ We should note, however, that the dynamics equation (14a) becomes inconsistent from the very moment of the development of the shock since the normal vector is not defined.

To correct the situation via the introduction of some selection principle on the propagation of discontinuity seems to be a subtle matter at this point. Nevertheless, we have an alternative that may turn out to be more practical from the computational point of view and is interesting in its own

right. Indeed, now we can suggest the invariant form of Eq. (3) as follows:

$$V = -1 + \epsilon\kappa + \frac{\gamma}{2} \left(1 + \frac{1}{\pi} \int_C \frac{(\mathbf{r} - \boldsymbol{\xi}) \cdot \mathbf{n}}{|\mathbf{r} - \boldsymbol{\xi}|^2} dl_{\boldsymbol{\xi}} \right). \quad (32)$$

The curvature in the above evolution equation corresponds to the dissipative term ϕ_{xx} in Eq. (3), and the coefficient ϵ can be chosen sufficiently small in order to simulate the "near shock" behavior of the flame front.

If the similarity to the weakly perturbed plane fronts persists we can expect that a closed curve will develop a number of wrinkles that will gradually merge until only one or two are left, and as the front continues to expand further, we will observe an onset of a secondary, finer pattern of cells.⁸ Equation (32) is not just a lucky guess. Indeed, with only a most insignificant modification, the reduction of Sec. III can be carried out, and then the expansion of the curvature up to γ ,

$$\kappa = \phi_{xx} / (1 + \phi_x^2)^{3/2} \approx \phi_{xx},$$

along with the assumption that $\epsilon \sim \gamma$ will immediately lead to Eq. (3).

Another interesting possibility occurs when the thermal-diffusional instability interacts with the hydrodynamic instability. This can be achieved by combining Eqs. (5) and (14a):

$$V = -1 + \epsilon\kappa - \kappa_{ss} + \frac{\gamma}{2} \left(1 + \frac{1}{\pi} \int_C \frac{(\mathbf{r} - \boldsymbol{\xi}) \cdot \mathbf{n}}{|\mathbf{r} - \boldsymbol{\xi}|^2} dl_{\boldsymbol{\xi}} \right). \quad (33)$$

In this case one can expect the large wrinkles generated by the hydrodynamic instability to occur over a cellular structure corresponding to the thermal-diffusional instability with a smaller characteristic scale. (In three dimensions κ becomes the mean curvature while κ_{ss} is replaced by the surface Laplacian $\Delta\kappa$.³)

Once again Eq. (33) can be reduced to its "near plan" version (1) for $\gamma \ll 1, \epsilon \ll 1$ by using the typical scales for the perturbation: $\phi \sim \epsilon \sim \gamma^{2/3}$, $x \sim 1/\sqrt{\epsilon}$, $t \sim 1/\epsilon^2$ in which Eq. (1) was derived.¹ On the other hand, in the absence of thermal expansion ($\gamma = 0$) the purely thermal-diffusional dynamics equation (5) is recovered.

Thus the surface dynamics equations, (14), (32), and (33), while representing, in our view, very interesting mathematical objects that should generate a variety of nontrivial phenomena, can be expected to model different aspects of the extremely complex dynamics of flame fronts. These equations are "glued" to the earlier results for slightly perturbed plane interfaces and retain additionally the invariant character of the physical problem. We should emphasize, however, that for $\gamma \sim 1$ these equations represent just simplified models that cannot be expected to correctly reflect all the physics of realistic gas combustion.

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