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Low vorticity and small gas expansion in premixed flames

Bruno Denet\textsuperscript{1} and Vitaly Bychkov\textsuperscript{2}

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\textsuperscript{1}IRPHE 49 rue Joliot Curie BP 146 Technopole de Chateau Gombert 13384 Marseille Cedex 13 France

\textsuperscript{2}Institute of Physics, Umeå University, SE 901 87, Umeå, Sweden

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Abstract

Different approaches to the nonlinear dynamics of premixed flames exist in the literature: equations based on developments in a gas expansion parameter, weak nonlinearity approximation, potential model equation in a coordinate-free form. However the relation between these different equations is often unclear. Starting here with the low vorticity approximation proposed recently by one of the authors, we are
able to recover from this formulation the dynamical equations usually obtained at the lowest orders in gas expansion for plane on average flames, as well as obtain a new second order coordinate-free equation extending the potential flow model known as the Frankel equation. It is also common to modify gas expansion theories into phenomenological equations, which agree quantitatively better with numerical simulations. We discuss here what are the restrictions imposed by the gas expansion development results on this process.

1 Introduction

The nonlinear description of the Darrieus-Landau (DL) instability of premixed flames began twenty-five years ago, when Sivashinsky obtained, as a first-order development in powers of a gas expansion parameter, a nonlinear equation known today as the Sivashinsky equation (Sivashinsky 1977). Starting with the first simulations of Michelson (see for instance (Michelson and Sivashinsky 1982)) and with the analytical solution of Thual with coauthors (Thual, Frisch and Henon 1985), this equation has shown a surprising qualitative agreement with experiments and direct numerical simulations (Denet and Haldenwang 1995, Bychkov, Golberg, Liberman and Eriksson 1996, Kadowaki 1999, Travnikov, Bychkov and Liberman 2000). The only nonlinear term of the Sivashinsky equation has a purely geometrical origin and is not related to the usual nonlinearity of the Navier-Stokes equations. Challenged by Clavin about the fact that the Navier-Stokes nonlinearity should induce
modifications of the flame equation, particularly for realistic gas expansion, Sivashinsky went on to show, in a joint paper with Clavin (Sivashinsky and Clavin 1987), that even at the second order in gas expansion, the equation obtained was still an equation with the same terms, only with modified coefficients. Today various methods try to improve on these equations by using the approximation of weak nonlinearity or next orders in gas expansion (Zhdanov and Trubnikov 1989, Joulin 1991, Bychkov 1998a, Kazakov and Liberman 2002b, Boury 2003). On the other hand, similar to the original Sivashinsky equation, all these equations have been derived for the planar on average flame front, and are valid only when the slope is not too large. Actually, different variations of the Sivashinsky equation have been constructed for different geometries like expanding flames (Filyand, Sivashinsky and Frankel 1994, D’Angelo, Joulin and Boury 2000) or oblique flames (Boury and Joulin 2002), when the flame shape departs slightly from the unperturbed case.

A different equation was introduced in the theoretical community by Frankel (Frankel 1990) in 1990, although parts of this approach were anticipated by numerical studies, see for instance (Ghoniem, Chorin and Oppenheim 1982). The Frankel equation was derived in a coordinate-free form (in two or three dimensions) using similarities between electrostatics and the flame-generated flow. Constructing his theory Frankel assumed that the flow is potential everywhere and neglected vorticity generated by the flame in the burnt gas. As a matter of fact, such an assumption originated in the analy-
sis by Sivashinsky (Sivashinsky 1977). Numerical simulations demonstrated that the Frankel equation describes qualitatively well the nonlinear evolution of expanding flames (Frankel and Sivashinsky 1995, Blinnikov and Sasorov 1996, Ashurst 1997, Denet 1997) and oblique flames (Denet 2002) (even recently in three dimensions (Denet 2004)). The Frankel equation became especially popular in the studies of fractal flames developing because of the DL instability on large scales (Blinnikov and Sasorov 1996, Denet 1997).

From a theoretical point of view, the relationship between the Frankel and Sivashinsky equations was put forward from the very beginning, since the original paper (Frankel 1990) showed that the Frankel equation reduces to the Sivashinsky equation for plane on average flames (with lateral boundaries at infinity) and for expanding flames. However, validity of the Frankel equation has been questioned rather often because of the assumption of the potential flow, which, in principle, violates hydrodynamic conservation laws of the flame front. The original analysis (Frankel 1990) did not demonstrate if the Frankel equation follows from the hydrodynamic equations in the limit of small gas expansion, as it was done for the Sivashinsky equation (Sivashinsky 1977).

Recently, however, one of us (Bychkov, Zaytsev and Akkerman 2003) reconsidered the problem and introduced a low vorticity approximation (compared to the Frankel case, where the vorticity is strictly zero), which was justified by the previous analysis of curved flames (Bychkov 1998a). The approximation of low vorticity enabled to derive a system of coordinate-free
equations describing the evolution of the front even for realistically large thermal expansion of the burning matter. This system of equations is rather complex and has not been successfully solved numerically for the moment. In the present paper, we develop this system up to the second order in gas expansion, which is equivalent to developing the hydrodynamical equations at this order. Such calculation proves the Frankel equation at the first order in gas expansion, and leads to a second order form of the equation (we will however insist on some difficulties specific to the oblique flame geometry). This form in turn can be demonstrated to contain the Sivashinsky-Clavin equation in the planar on average case.

In Section 2 we obtain this second order form. In Section 3 this equation will be reduced to the Sivashinsky-Clavin equation. In Section 4 we discuss some basic problems related to the Sivashinsky-Clavin equation and expansion in powers of a small parameter in general. Finally, Section 5 contains a conclusion.

2 Derivation of the second order Frankel equation

Let us start this section by summarizing the main points of the low vorticity approximation of (Bychkov et al. 2003) (the reader is invited to read this article for more details). This approximation is derived from the hydrodynamical equations:
\[ \nabla \cdot \mathbf{u} = 0, \]

\[ \frac{\partial \mathbf{u}}{\partial \tau} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\vartheta \nabla \Pi, \]

where the equations written are made non-dimensional with the use of the laminar flame velocity \( U_f \) and a reference length \( R \). The non-dimensional velocity is noted \( \mathbf{u} \) and the pressure \( \Pi = (P - P_f)/\rho_f U_f^2 \), \( \vartheta = 1 \) in the fresh mixtures and \( \vartheta = \Theta \) in the burnt gases. The flame is considered as a discontinuity, \( \Theta = \rho_f/\rho_b \) is the ratio of density in fresh and burnt gases. The parameter \( (\Theta - 1) \) will be the parameter of the expansion. The boundary conditions of the flame can be classically shown to lead to

\[ \mathbf{u}_+ = \mathbf{u}_- + (\Theta - 1) \mathbf{n}, \]

\[ \Pi_+ = \Pi_- + 1 - \Theta, \]

where \( \mathbf{n} \) is the normal vector to the flame surface, directed towards the burnt gases. The first boundary condition accounts for both the jump of normal velocity and conservation of tangential velocity at the front. We introduce the velocity potentials in fresh (−) and burnt (+) matter \( \phi_\pm \), which satisfy
the Laplace equation and are defined by

\[ u_- = \nabla \phi_-, \]

\[ u_+ = u_{p+} + u_{v+} = \nabla \phi_+ + u_{v+}, \quad (1) \]

where \( u_{p+} \) and \( u_{v+} \) are the potential and vortical parts of the velocity field in the burnt gases.

We work in a local system of coordinates moving with the flame front at the velocity \(-V_s \mathbf{n}\) such as \( \nabla_s = \mathbf{e}_t \cdot \nabla \), where \( \mathbf{e}_t \) is the unit tangential vector, and

\[ \frac{\partial}{\partial \tau_s} = \frac{\partial}{\partial \tau} - V_s \frac{\partial}{\partial \mathbf{n}}. \]

Using basic properties of Green functions of the Laplace equation, Bernoulli integrals, and boundary conditions at the front, the following system of equations (low vorticity limit) is obtained

\[ \frac{\partial}{\partial \tau_s} (\phi_+ - \phi_- + \phi_- (1 - \Theta)) = \frac{\Theta - 1}{2} u_-^2 - (\Theta - 1) V_s^2 + (\Theta - 1) V_s + V_s u_{v+} + f; \]

\[ \frac{\partial u_v}{\partial \tau} + (u_{p+} \cdot \nabla) u_v = 0. \]

Note that the form given here is not the final form of (Bychkov et al. 2003), here we do not incorporate \( \Theta \) into the variables in order to make the development in \( (\Theta - 1) \) easier. Equation (2) comes from the Bernoulli integral;
$f$ is generally a function of time appearing in the Bernoulli integrals (unlike (Bychkov et al. 2003) we have included a constant term $(\Theta - 1)^2/2$ into $f$). We will choose however not to include any additive terms containing a function of time in the potentials, so that $f$ has to be considered as a constant. Furthermore, strictly speaking, we could add a constant in $u_{v+}$ and subtract it from $u_{p+}$ but naturally $u_{v+}$ has to be taken as small as possible, which makes the Bernoulli integral a good approximation of the Navier-Stokes equation in the burnt gases. A non-zero value of $f$ would lead to a constant value of $u_{vm+}$ at infinity (convected by the potential velocity) for a plane or oblique geometry, so that we must have in this case $f = 0$. Similarly, in the case of the expanding geometry, a non-zero value of $f$ would leave a constant value of $u_{vm+}$ behind the front, which is not possible because there is no source or sink present inside the expanding flame.

Equation (3) expresses the fact that the vortical part of the velocity field is convected by the potential part (it will create a shear flow at infinity in the plane configuration that would disappear far from the flame if viscosity was included). Note that this equation is different from the equivalent one given in (Bychkov et al. 2003), which included only the time derivative. As formulated in (Bychkov et al. 2003), the approach of low vorticity takes into account only convection by the uniform component of the velocity field. In the geometry of planar (on average) flame front propagating along $z$-axis this corresponds to the drift term $\Theta \partial u_v/\partial z$. In the case of expanding flames there is no uniform velocity in the burnt matter and the vorticity created at
the flame surface is simply left behind as the flame radius increases; by this reason the drift term was omitted in (Bychkov et al. 2003). In the present paper we are interested in small gas expansion of the flame equations, which allows to consider a more general form of equation (3). Note also that at the dominating order in gas expansion, the convection by the potential velocity is simply equivalent to the convection by the injection velocity. Developing equation (3) and using the continuity equation (n is the normal, s represents the tangential coordinates)

\[ \frac{\partial u_{vn+}}{\partial n} + \nabla_s \cdot u_{st+} = 0 \]

and \( u_{st+} = \nabla_s (\phi_+ - \phi_-) \), we obtain

\[ \frac{\partial u_v}{\partial r_s} \cdot \mathbf{n} + ((u_{pt+} \cdot \nabla_s) u_v) \cdot \mathbf{n} = (V_s + u_{pn+}) \nabla^2_s (\phi_- - \phi_+), \quad (4) \]

where \( V_s = 1 - u_{n-} \). Compared to (Bychkov et al. 2003), we have two supplementary terms coming from the convection by the potential flow field. The first term of equation (4) (the term with the time derivative) is also slightly corrected compared to this paper.

The Laplace equation leads to an equation with a different form in two and three dimensions:

\[ 3D : \quad \phi_+ + \phi_- = -\frac{1}{2\pi} \int \left( \frac{\Theta - 1 - u_{vn+}}{|\mathbf{r}_s - \mathbf{r}|} + (\phi_+ - \phi_-) \mathbf{n} \cdot \frac{\mathbf{r}_s - \mathbf{r}}{|\mathbf{r}_s - \mathbf{r}|^3} \right) dS(\mathbf{r}_s), \quad (5) \]
or

\[ 2D : \quad \phi_+ + \phi_- = -\frac{1}{\pi} \int \left( (\Theta - 1 - u_{vn+}) \ln |r_s - r| - (\phi_+ - \phi_-) \mathbf{n} \cdot \frac{r_s - r}{|r_s - r|^2} \right) dl(r_s). \]

(6)

Now let us expand all variables in powers of \((\Theta - 1)\):

\[
\begin{align*}
\phi_\pm &= \phi^{(1)}_\pm + \phi^{(2)}_\pm + \cdots \\
u_- &= u^{(1)}_- + u^{(2)}_- + \cdots \\
V_s &= V_s^{(0)} + V_s^{(1)} + V_s^{(2)} + \cdots \\
u_{vn+} &= u^{(1)}_{vn+} + u^{(2)}_{vn+} + \cdots \\
\frac{\partial}{\partial r_s} &= O(\Theta - 1),
\end{align*}
\]

where the subscript \((i)\) means that the term is of order \((\Theta - 1)^i\). Note also that we do not expand the positions \(r\) in powers of \((\Theta - 1)\); this can be done only in particular geometries, when the difference between the actual and the unperturbed positions is of order \(O(\Theta - 1)\). To reduce the equation obtained to the Sivashinsky-Clavin equation in the planar geometry, we will have to consider the fact (see section 3) that the vertical coordinate is of order \((\Theta - 1)\), but this order of magnitude estimate is not geometry-independent.

First, using the relation \(V_s = 1 - u_{n-}\) we find that \(V_s^{(0)} = 1\). Note that at this zeroth order, we can have a term \(V_{boundary}^{(0)} \equiv V_{inj}\) (a constant injection velocity, for instance) that has to be added to the velocity field in order to satisfy the boundary conditions at infinity. At each order, we will encounter a \(V_{boundary}\) term, so let us define it properly. \(V_{boundary}\) is a velocity field obeying the Laplace equation, without jumps on the flame surface, which
helps satisfying the boundary conditions at infinity. Although we will perform
the calculations in a reference frame without injection velocity, let us note
that with an injection velocity we would have $V_s^0 = 1 - V_{inj}$. Obviously,
the Bernoulli relation is Galilean invariant, so we choose the reference frame
where the calculations are simpler, knowing that at the end, the injection
velocity (if present) may be added to the final formula.

By developing equation (2) we have at the $O(1)$ order

$$- (\Theta - 1) V_s^{(0)2} + (\Theta - 1) V_s^{(0)} + V_s^{(0)} u_{vn+}^{(1)} = 0,$$

which, with $V_s^{(0)} = 1$, leads to $u_{vn+}^{(1)} = 0$. We also have, according to equation
(4)

$$0 = \nabla_s^2 \left( \phi_{-}^{(1)} - \phi_{+}^{(1)} \right),$$

which implies in three dimensions, using equation (5) and the value of $u_{vn+}^{(1)}$

$$\phi_{-}^{(1)} = \phi_{+}^{(1)} = - \frac{1}{4\pi} \int \frac{\Theta - 1}{|r_s - r|} dS(r_s). \quad (7)$$

This is the potential of a uniformly charged surface. Apart from multiplica-
tive factors we will call $(\Theta - 1)$ the surface charge (or line charge for the cor-
responding two dimensional equation). The reader is referred to (Denet 2002)
for a simple presentation of this electrostatic analogy. This potential leads
to the corresponding velocity

\[ V_s^{(1)} = -u_n^{(1)} = \frac{(\Theta - 1)}{2} \left( 1 + \frac{1}{2\pi} \int \frac{n \cdot (r_s - r)}{|r_s - r|^3} dS(r_s) \right) - V_{boundary} \cdot n. \] (8)

Up to the first order, \( V_s = 1 + V_s^{(1)} \), which is exactly the Frankel equation in three dimensions (when the flame front is a surface).

Now let us consider the \( O(2) \) terms. At this order, we have from equation (2)

\[ -2(\Theta - 1) V_s^{(0)} V_s^{(1)} + (\Theta - 1) V_s^{(1)} + V_s^{(0)} u_{vn+}^{(2)} + V_s^{(1)} u_{vn+}^{(1)} = 0. \]

With the previous computed values \( V_s^{(0)} = 1 \) and \( u_{vn+}^{(1)} = 0 \), it reduces to

\[ u_{vn+}^{(2)} = (\Theta - 1) V_s^{(1)}. \] (9)

Taking into account that \( \phi_-^{(1)} = \phi_+^{(1)} \) equation (4) gives

\[ \nabla_s^2 \left( \phi_-^{(2)} - \phi_+^{(2)} \right) = \left[ (u_{inj} \cdot \nabla_s) u_{vn+}^{(2)} \right] \cdot n, \] (10)

so we obtain from (5) in three dimensions with the previous value of \( u_{vn+}^{(2)} \)

\[ \phi_{\pm}^{(2)} = -\frac{1}{4\pi} \int \left( \frac{-(\Theta - 1) V_s^{(1)}}{|r_s - r|^3} - \left( \phi_-^{(2)} - \phi_+^{(2)} \right) \frac{n \cdot \frac{r_s - r}{|r_s - r|^3}}{dS(r_s)} \right) (\phi_{\pm}^{(2)})/2 \]

with \( (\phi_-^{(2)} - \phi_+^{(2)}) \) determined by equation (10). Let us note however that
this term exists only when there is a strong tangential velocity field (i.e. for oblique flames). In the plane and expanding flame cases, the tangential velocity field can be neglected, so that \( \phi_+^{(2)} - \phi_-^{(2)} \) is also negligible in the previous formula. In the rest of the article, we will only write the formulas with this term neglected, but let us insist on the fact that by doing so, we neglect a dipolar contribution to the potential, which could be important in oblique cases.

Summing the first and second order terms, we have

\[
\phi_+^{(1)} + \phi_-^{(2)} = \phi_+^{(1)} + \phi_+^{(2)} = -\frac{1}{4\pi} \int \frac{(\Theta - 1) - (\Theta - 1) V_s^{(1)}}{|r_s - r|} dS(r_s), \tag{11}
\]

which can be interpreted as a local surface charge modified from \( \Theta - 1 \) to

\[
\Theta - 1 - (\Theta - 1) V_s^{(1)}. \tag{12}
\]

Then the total velocity field up to the second order is

\[
V_s^{(0)} + V_s^{(1)} + V_s^{(2)} = 1 - u_n^{(1)} - u_n^{(2)}
\]

\[
= 1 + \frac{\Theta - 1 - (\Theta - 1) V_s^{(1)}}{2} \left( 1 + \frac{1}{2\pi} \int \frac{n \cdot (r_s - r)}{|r_s - r|^3} dS(r_s) \right)
\]

\[-V_{\text{boundary}} \cdot n - V_{\text{boundary}}^{(1)} \cdot n - V_{\text{boundary}}^{(2)} \cdot n, \tag{13}\]
or using $V_s^{(1)} = V_s - 1 + O(\Theta - 1)$ we find the equivalent formulation

$$V_s = 1 + \frac{\Theta - 1}{2} (2 - V_s) \left( 1 + \frac{1}{2\pi} \int \frac{n \cdot (r_s - r)}{|r_s - r|^3} dS(r_s) \right) - V_{\text{boundary}} \cdot n. \quad (14)$$

Formula (13) is the coordinate-free equation for the flame front velocity obtained within the second order in gas expansion; the first order gives the Frankel equation. We recall that $V_s$ is the normal velocity of the front propagation, including laminar flame speed and induced velocity field. Curvature and strain effects are not included, see (Bychkov et al. 2003). In two dimensions, the equation, obtained by similar calculations is

$$V_s^{(0)} + V_s^{(1)} + V_s^{(2)} = 1 - u_{n-}^{(1)} - u_{n-}^{(2)}$$

$$= 1 + \frac{\Theta - 1 - (\Theta - 1) V_s^{(1)}}{2} \left( 1 + \frac{1}{\pi} \int \frac{n \cdot (r_s - r)}{|r_s - r|^3} dl(r_s) \right)$$

$$- V_{\text{boundary}}^{(0)} \cdot n - V_{\text{boundary}}^{(1)} \cdot n - V_{\text{boundary}}^{(2)} \cdot n. \quad (15)$$

or

$$V_s = 1 + \frac{\Theta - 1}{2} (2 - V_s) \left( 1 + \frac{1}{\pi} \int \frac{n \cdot (r_s - r)}{|r_s - r|^2} dl(r_s) \right) - V_{\text{boundary}} \cdot n. \quad (16)$$

In order to solve this equation numerically, the front would have to be described with marker particles moving according to the equation

$$\frac{d\mathbf{r}}{dt} = -V_s \mathbf{n}. \quad (17)$$
Numerical solution to equation (17) may involve reconnections in two and three dimensions; possible ways to overcome these difficulties are described in (Denet 2002, Denet 2004).

3 Reduction to the Sivashinsky-Clavin equation

We have previously said that equation (15) obtained in the coordinate-free case is supposed to be the equivalent of the Sivashinsky-Clavin equation in the plane case. Indeed, this last equation is derived by a development which is one order higher than the Sivashinsky equation, while equation (15) is one order higher than the Frankel equation. However, transition from one case to the other is not obvious at all. The Sivashinsky-Clavin equation contains the same terms with different coefficients, but our modified Frankel equation contains a surface (or line) charge, which is not apparently constant at every position on the front. Furthermore, the order of magnitude of the flame front position makes another problem, since the position is supposed to be of order $O(\Theta - 1)$ for the planar case and $O(1)$ in the coordinate-free case. So, is it possible to recover the Sivashinsky-Clavin equation from equation (15)? Naturally, we have the help of the original Frankel article (Frankel 1990), where it was shown for the planar (on average) case with lateral boundaries at infinity and for the circular expanding case that the Frankel equation reduces to the Sivashinsky equation. Let us start by repeating this reasoning
before going to the next order. In two dimensions, the Frankel equation gives:

\[ V_s = 1 + \frac{\Theta - 1}{2} \left( 1 + \frac{1}{\pi} \int \frac{n \cdot (r_s - r)}{|r_s - r|^2} dl(r_s) \right) - V_{\text{boundary}}^{(0)} \cdot n - V_{\text{boundary}}^{(1)} \cdot n. \]

In the planar case, the normal vector is

\[ n(r) = \left[ -\alpha_y, 1 \right] / \sqrt{1 + \alpha_y^2}, \]

where \( y \) is the lateral coordinate, \( \alpha \) is the vertical position of the front, the vertical \( z \) coordinate is positive towards the burnt gases, \( \alpha_y \) is a notation for the \( y \) derivative. Then equation (17) gives

\[ \frac{\alpha_t}{\sqrt{1 + \alpha_y^2}} = -V_s. \]  

(18)

In order to recover the Sivashinsky equation, we have to develop the square root, so we suppose \( \alpha = O(\Theta - 1) \) and \( y = O(1) \). We have

\[ \alpha_t = -1 - \frac{\alpha_y^2}{2} - \frac{\Theta - 1}{2} \cdot \frac{\Theta - 1}{2} \cdot p.v. \int_{-\infty}^{+\infty} \frac{\alpha(\chi + y) - \alpha_y(\chi) - \alpha_y(y) \chi}{\chi^2} d\chi + V_{\text{boundary}}^{(0)} + V_{\text{boundary}}^{(1)}. \]

Frankel has shown that the principal value in this formula is

\[ \frac{\Theta - 1}{2} I(\alpha), \]

where \( I(\alpha) \) is the Landau operator (multiplication by \(|k|\) in Fourier space,
see (Frankel 1990) for details).

Let us take as usual the hypothesis that the injection velocity is parallel to the $z$ direction and has the value $V_{boundary}^{(0)} = V_{inj} = [0, 1]$. This term simplifies itself with the $-1$ of the previous equation. All the following terms of the boundary velocity are obtained by saying that they do not change the injection velocity. If this velocity is imposed at a finite distance, then this is simply obtained by the same integral as in the Frankel equation, with the same charge, but for the mirror image of the front relative to the injection location (see (Denet 2002) for an example). If the injection is moved to infinity, then the velocity field, according to the Gauss theorem, will be the same as the velocity generated by a plane front, but with a charge multiplied by the ratio of the front surface to the surface of an equivalent plane front $V_{z}^{(1)}_{boundary} = \frac{\Theta - 1}{2} \langle \sqrt{1 + \alpha^2 y} \rangle = \frac{\Theta - 1}{2}$, where $\langle \rangle$ is a lateral mean value. Higher orders will be obtained by developing the square root and replacing $\Theta - 1$ by $\Theta - 1 - (\Theta - 1) V_{s}^{(1)}$, as discussed in the previous section. For the time being however, the boundary term only leads to suppress the term $- (\Theta - 1) / 2$. We thus obtain the Sivashinsky equation (without curvature terms)

$$\alpha_t + \frac{\alpha^2}{2} = \frac{\Theta - 1}{2} I(\alpha).$$

(19)

Note that with $\alpha = O(\Theta - 1)$ and $\frac{\partial}{\partial t} = O(\Theta - 1)$ all the terms of the equation are of the second order.

Let us now perform the same calculation at the next order starting from
the two-dimensional equation (15)

\[ V_s = 1 + \frac{\Theta - 1 - (\Theta - 1) V_s^{(1)}}{2} \left( 1 + \frac{1}{\pi} \int \frac{\mathbf{n} \cdot (\mathbf{r}_s - \mathbf{r})}{|\mathbf{r}_s - \mathbf{r}|^2} dl(\mathbf{r}_s) \right). \]

Equation (18) is still valid. We have, retaining terms up to the third order

\[ \alpha_t = -1 - \frac{\alpha_y^2}{2} \frac{\Theta - 1 - (\Theta - 1) V_s^{(1)}}{2} - \frac{\Theta - 1}{4} \frac{\alpha_y^2 + (\Theta - 1) V_s^{(1)}}{2} I(\alpha). \]

As before, the constant terms (not depending on \( y \)) are eliminated by introducing the boundary velocity terms, but what do we do about \( V_s^{(1)} \), given in equation (8), which depends on position? The answer is simple: since now we have \( \alpha = O(\Theta - 1) \), then we obtain a product of \( \Theta - 1 \) and \( \alpha \) in \( V_s^{(1)} \).

This term is not of the first order anymore, it is now of the second order and can be neglected (note that this is not necessarily the case in all geometries).

The constant terms in \( V_s^{(1)} \) are as usual suppressed by the boundary velocity, and we find

\[ \alpha_t = -1 - \frac{\alpha_y^2}{2} \frac{\Theta - 1 - (\Theta - 1) V_s^{(1)}}{2} - \frac{\Theta - 1}{4} \frac{\alpha_y^2 + (\Theta - 1) V_s^{(1)}}{2} I(\alpha). \]

Finally, adding the effects of the boundary terms, and disregarding terms of higher orders we obtain

\[ \alpha_t + \frac{\alpha_y^2}{2} \left( 1 + \frac{\Theta - 1}{2} \right) - \frac{\Theta - 1}{2} \frac{\alpha_y^2}{2} = \frac{\Theta - 1}{2} \left( 1 - \frac{\Theta - 1}{2} \right) I(\alpha). \quad (20) \]
This is the Sivashinsky-Clavin equation, written in units of laminar flame speed (relative to the fresh gases). The lateral mean value term comes from the boundary velocity and was absent in the original article. It was later added by Joulin, who used it in a number of papers, the first one being probably (Joulin and Cambray 1992) and called it a counter-term. In Sivashinsky-Clavin units the value \( \gamma = \frac{\Theta - 1}{\Theta} \) was used to characterize gas expansion and all velocities were scaled by the laminar flame speed relative to burnt gases \( U_b = \Theta U_f = U_f/(1 - \gamma) \). In such units equation (20) would be written as

\[
\alpha_t + \frac{\alpha_y^2}{2} \left( 1 - \frac{\gamma}{2} \right) - \frac{\gamma}{2} \left( \frac{\alpha_y^2}{2} \right) = \frac{\gamma}{2} \left( 1 - \frac{\gamma}{2} \right) I(\alpha).
\]

In units of laminar flame speed relative to fresh gases \( U_f \), but using \( \gamma \) as a parameter the equation takes the form

\[
\alpha_t + \frac{\alpha_y^2}{2} \left( 1 + \frac{\gamma}{2} \right) - \frac{\gamma}{2} \left( \frac{\alpha_y^2}{2} \right) = \frac{\gamma}{2} \left( 1 + \frac{\gamma}{2} \right) I(\alpha).
\]

4 Do we have the first or second time-derivative in the flame equations?

One more question concerns the order of time-derivative in the Sivashinsky-Clavin equation, which also affects the structure of nonlinear terms in the equation. The original DL dispersion relation (Landau and Lifshitz 1989) is of the second order describing two independent linear modes of the flame
front perturbation: one mode is growing and one is decaying. Unlike this, the Sivashinsky equation is of the first order in time capturing the growing mode only; the Sivashinsky-Clavin equation has the same property. When investigating development of the DL instability, the growing mode dominates over the decaying one and the first-order derivative looks quite sufficient. However, the second-order time derivative proved to be of principal importance in many adjacent problems of flame dynamics: propagation of tulip flames (Dold and Joulin 1995), flame interaction with sound (Searby and Rochwerger 1991, Bychkov 1999), with shocks (Bychkov 1998b) and with external turbulence (Searby and Clavin 1986, Aldredge and Williams 1991, Akkerman and Bychkov 2003). In all these cases some external force redistributes energy between growing and decaying modes, and it is incorrect to exclude the decaying mode out of consideration. Besides, as we said above, changing the order of the time derivative we also modify the nonlinear terms of the equation. At this point, following comments of one of the referees, we would like to add that, in general, even a first-order time derivative may produce a complicated spectrum with many stable and unstable modes. However, in the particular case of the linear DL instability for an infinitely thin planar flame front and a fixed wave number of perturbations the number of modes is unambiguously related to the order of time derivative. The first order time-derivative of the Sivashinsky equation provides only one mode (growing), while the original DL dispersion relation with the second order derivative has two modes (one is growing and one is decaying).
Let us consider how the Sivashinsky-Clavin equation should be modified to take into account the second time derivative. Within the accuracy of the Sivashinsky-Clavin approach we can substitute (19) into the second-order terms of (20) and find

\[
\frac{\Theta - 1}{2} \alpha_t + \alpha_t + \frac{\Theta}{2} \alpha_y^2 + \left\langle \frac{\alpha_y^2}{2} \right\rangle = \frac{\Theta - 1}{2} I(\alpha) \tag{21}
\]

or

\[
I^{-1}(\alpha_{tt}) + \alpha_t + I^{-1} \left( \frac{\partial}{\partial t} \frac{\alpha_y^2}{2} \right) + \frac{\Theta}{2} \alpha_y^2 - \frac{\Theta - 1}{2} \left\langle \alpha_y^2 \right\rangle = \frac{\Theta - 1}{2} I(\alpha). \tag{22}
\]

The operator \( I^{-1} \) has a meaning of an integral, and it is defined with the accuracy of a constant. Still, this constant is included already into the counter-terms. One more trouble with this operator concerns \( I^{-1} \) acting on a constant. However, in the case of equation (22), a constant under \( I^{-1} \) would imply physically meaningless solutions like a planar accelerating flame front, which may be obviously ruled out. One can easily see that the linear terms of equation (22) coincide with the DL dispersion relation written in the limit of \( \Theta - 1 \ll 1 \)

\[
\frac{\Theta + 1}{2\Theta} I^{-1}(\alpha_{tt}) + \alpha_t = \frac{\Theta - 1}{2} I(\alpha). \tag{23}
\]

Equation (22) contains only one counter-term, because the time-dependent nonlinear term involves the complete time derivative and gives zero after averaging. Though equations (20) and (22) are mathematically equivalent...
within the expansion in $\Theta - 1 \ll 1$, they may lead to somewhat different conclusions about properties of curved flames. For example, one of the most important questions in the nonlinear theory of the DL instability is the velocity increase of curved stationary flames. Let us consider propagation of such a flame $\alpha(t, y) = -\Omega t + \alpha(y)$. In that case equations (20) and (22) reduce to

$$-\Omega + \frac{\alpha_y^2}{2} \left( 1 + \frac{\Theta - 1}{2} \right) - \frac{\Theta - 1}{2} \left( \frac{\alpha_y^2}{2} \right) = \frac{\Theta - 1}{2} \left( 1 - \frac{\Theta - 1}{2} \right) I(\alpha)$$

and

$$-\Omega + \frac{\Theta}{2} \alpha_y^2 - \frac{\Theta - 1}{2} \left\langle \alpha_y^2 \right\rangle = \frac{\Theta - 1}{2} I(\alpha).$$

As we can see, equations (24) and (25) are different. It is interesting that equation (25) is consistent with the stationary theory (Bychkov 1998a) within the accuracy of $(\Theta - 1)\alpha_y^2$, while (24) is not. The above calculations illustrate the fact that any rigorous expansion in power series leaves plenty of freedom for mathematical manipulations, which may lead to ambiguous physical conclusions. Unfortunately, almost always people use expansion in power series of a small parameter to obtain physical results beyond the validity limits of the expansion. As a simple illustration, suppose that we calculated some value $a$ using expansion in power series of $\varepsilon \ll 1$, and found $a = b$ in the zero order approximation with $a = b(1 - c\varepsilon)$ for the first order. The same expression may be written in an infinite number of equivalent mathematical forms like $a = b(1 - [c + b - a]\varepsilon)$, $a = b(1 - 2c\varepsilon)^{1/2}$, $a = b/(1 + c\varepsilon)$, etc.
Though these forms are equivalent within the first order in $\varepsilon \ll 1$, we come
to different conclusions when investigating zero points of $a$ with the help of
these expressions. In the above four versions of the same formula we find
$a = 0$ at $\varepsilon = 1/c$, $\varepsilon = 1/(c + b)$, $\varepsilon = 1/2c$ and $\varepsilon = \infty$, respectively. One
encounters a similar trouble within both linear and nonlinear theories of the
DL instability. For example, the linear theories (Pelcé and Clavin 1982) and
(Matalon and Matkowsky 1982) lead to noticeably different expressions for
the cut off wavelength of the DL instability, though both theories are math-
ematically correct and equivalent within the same accuracy of small wave
numbers. Performing manipulations similar to those described above, we
can actually obtain infinite number of absolutely different formulas for the
cut off wavelength in scope of the theory (Pelcé and Clavin 1982) keeping
the same accuracy. So in the case of the linear DL instability the simple
example $a = b(1 - c\varepsilon)$ is sufficient to explain the discrepancy between the
analytical values for the cut-off wavenumber obtained by different authors,
as this formula is a simplified version of the dispersion relations obtained in
the two previously mentioned articles.

What does it mean if one tries to derive a non linear equation for the
DL instability using perturbation methods? In that case, as pointed out by
one of the referees, the perturbations concern operators instead of functions,
which is a much subtler subject. Of course, in this case, the example with
$a = b(1 - c\varepsilon)$ is ultimately simplified, still it gives a rough idea why the non linear
approaches like (Zhdanov and Trubnikov 1989, Joulin 1991, Bychkov 1998a,
Kazakov and Liberman 2002b, Kazakov and Liberman 2002a) may lead to different equations for a flame front even if all mathematical calculations are performed correctly. Singular perturbation methods for partial differential operators are much more sophisticated than for functions, and can involve a large number of new phenomena, boundary layers being of course the most well-known example. However singular layers can also occur during the time evolution, for instance initial layers for times close to the initial conditions. See below for a discussion of the difficulties that could happen in formal manipulations of second order in time equations.

When one uses expansion in powers of a small parameter, the nonlinear equation for a flame front may be presented in an infinite number of forms. For example, suppose that we have derived a time-dependent nonlinear equation within the approach of weak nonlinearity as it was done in (Zhdanov and Trubnikov 1989, Kazakov and Liberman 2002b). Within the same accuracy of calculations one can take square of the DL dispersion relation (23) with any coefficient and add it to the equation obtained. However, when we use the new version of the nonlinear equation to study curved stationary flames, square of the right-hand side of (23) makes a non-zero contribution, while square of the left-hand side becomes zero (the first term gives zero exactly, and the second term provides nonlinearity of the fourth-order). Making such manipulations one comes to a stationary equation like

\[-\Omega + \left(\frac{1}{2} + C_1\right) \alpha_y^2 + C_2 [I(\alpha)]^2 - C_1 \left\langle \alpha_y^2 \right\rangle - C_2 \left\langle [I(\alpha)]^2 \right\rangle = \frac{\Theta - 1}{2} I(\alpha). \quad (26)\]
with almost arbitrary coefficients $C_1$ and $C_2$. The only restriction on the factors $C_1$ and $C_2$ is that they should tend to zero sufficiently fast as $\Theta \to 1$, and that the development in $\Theta - 1$ of the stationary solution is the same as the original (25). It gives $C_1 = (\Theta - 1)/2 + O(\Theta - 1)^2$ and $C_2 = O(\Theta - 1)^2$ for small $(\Theta - 1)$, but it must be admitted that these restrictions are too loose taking into account realistically large values of $\Theta = 5 - 8$ (also, it must be remembered that curvature-related terms have to be added to (26) in agreement with the linear theory of the DL instability). This result is rather discouraging, because it leaves no hope to obtain an unambiguous formula for the flame velocity by using perturbation theories. As an illustration of this fact, the authors of the two companion papers (Kazakov and Liberman 2002b) and (Kazakov and Liberman 2002a) have produced two different formulas for the flame velocity. The first-order approximation in (Zhdanov and Trubnikov 1989, Kazakov and Liberman 2002b, Boury 2003), contrary to the reasoning used above to obtain equation (26), employed the DL-dispersion relation for the growing mode only

$$ \frac{\partial \alpha}{\partial t} = \frac{\Theta}{\Theta + 1} \left( [\Theta + 1 - 1/\Theta]^{1/2} - 1 \right) I (\alpha). $$

Using (27) within the second-order approximation one can always convert time-dependent nonlinear terms into time-independent terms and vice versa. We would like to stress that manipulations with the time-derivatives is not something that we have invented in the present paper. They have been
performed already in a number of papers on flame dynamics, leading to ambiguous physical results. In the present paper, we just clarify the ambiguity and point out the danger of such manipulations.

At this point one of the referees asks, if it is not safer to transform second-order time derivatives into space-derivatives. Unfortunately, even in that case some ambiguity remains in the non linear terms. Besides, as we pointed out above, by getting rid of the second-order derivatives one loses the possibility to study a large number of effects like tulip flames, flame interaction with shocks and many other phenomena. At present, we do not know how to avoid the ambiguity in the perturbation theory of the non linear equation for a flame front. In the present section we rather formulate a question than give an answer. We hope to insist here on the fact that an infinite number of different non linear equations for a flame front can be obtained by high order formal perturbation methods. Among these formally equivalent equations, some will give bad quantitative results (particularly if the development parameter is not small, which is unfortunately the case for flame fronts). Some will even give bad qualitative results, for instance we could have second order in time equations which, without forcing, do not approach a first order in time dynamics (which is well known to attract the dynamics for a flame without forcing). Even worse, we could have equations with pathological mathematical properties (this is particularly possible with time derivatives in the non linear terms). Although in the rest of the paper, we insist on the quantitative agreement on the flame velocity, it must be kept in mind
that at some point, the time evolution of the proposed models must also be compared with direct numerical simulations and found satisfactory.

On the other hand, without using perturbation methods one comes to a rather complex set of equations (Bychkov et al. 2003) with almost zero hope to solve it analytically, and also very difficult to solve numerically. Luckily, in the case of curved stationary flames the problem of flame velocity has been solved with the help of direct numerical simulations (Bychkov et al. 1996); later calculations (Kadowaki 1999, Travnikov et al. 2000) confirmed the original results.

The uncertainty in the rigorous perturbation nonlinear theories of the DL instability increases the role of simple phenomenological models like that proposed in (Joulin and Cambray 1992). Using the models one can obtain qualitative or even semi-quantitative understanding of flame dynamics, which may be checked and corrected quantitatively in direct numerical simulations. The model (Joulin and Cambray 1992) included first-order time-derivative similar to the Sivashinsky equation (19). When second-order derivatives are important, similar model can be constructed on the basis of equation (22). Comparing equations (22) and (23) we can easily extrapolate (22) to the case of realistic \( \Theta \) as

\[
\frac{\Theta}{2\Theta} I^{-1}(\alpha_t) + \alpha_t + I^{-1}\left(\frac{\partial}{\partial t} \frac{\alpha_y^2}{2}\right) + \left(\frac{1}{2} + C_1\right) \alpha_y^2 - C_1 \langle \alpha_y^2 \rangle = \frac{\Theta - 1}{2} I(\alpha).
\]

(28)

Similar equation was proposed in Boury’s thesis (Boury 2003), in the spirit
of the phenomenological theory used in (Dold and Joulin 1995) to study tulip flames. The linear part of (28) is a well-known DL dispersion relation. Let us note however that including curvature effects in this type of equation may be non trivial, because actually the Markstein lengths are frequency-dependent (see (Joulin 1994, Clavin and Joulin 1997, Denet and Toma 1995)). The unknown coefficient $C_1$ may be adjusted by using direct numerical simulations of curved stationary flames. In (Boury 2003) the coefficient was chosen to provide the same stationary amplitude as either a third order gas expansion theory or direct numerical simulations. However, we believe that fitting direct numerical simulations is a better idea. As explained before, a high order perturbation theory can be written in several equivalent ways, with different quantitative results for large $\Theta$ (see for instance, equations (24) and (25)). Below, we illustrate that this kind of fit can actually be used to obtain almost any curved flame velocity, with only some restrictions for small gas expansion. The stationary version of (28) is

$$-\Omega + \left( \frac{1}{2} + C_1 \right) \alpha_y^2 - C_1 \langle \alpha_y^2 \rangle = \frac{\Theta - 1}{2} I(\alpha).$$

Equation (29) may be solved analytically (Thual et al. 1985, Joulin and Cambray 1992), which leads to the maximal velocity increase

$$\Omega_{\max} = \frac{(\Theta - 1)^2}{8 (1 + 2C_1)^2}.$$ 

The maximal velocity increase obtained in direct numerical simulations (Bychkov
et al. 1996, Kadowaki 1999, Travnikov et al. 2000) is plotted in figure 1 by markers. The curves of figure 1 show the analytical formulas for the velocity increase, which follow from the theories (Zhdanov and Trubnikov 1989, Bychkov 1998a, Kazakov and Liberman 2002b, Joulin and Cambray 1992). As we can see, the formulas (Zhdanov and Trubnikov 1989, Kazakov and Liberman 2002b, Joulin and Cambray 1992) overestimate the velocity increase noticeably, especially for $\Theta = 8$ corresponding to stoichiometric methane and propane flames. So far, the formula proposed in (Bychkov 1998a)

$$\Omega_{max} = \frac{\Theta - 1}{2} \frac{\Theta^3 + \Theta^2 + 3\Theta - 1}{\Theta^3 + \Theta^2 + 3\Theta - 1}$$

(31) provides the best analytical fit for the numerical results. At this point we have to note that, as was remarked in (Boury 2003), neither of the papers (Zhdanov and Trubnikov 1989, Bychkov 1998a, Kazakov and Liberman 2002b, Kazakov and Liberman 2002a) included Joulin counter-terms (see again (Joulin and Cambray 1992)), which would lead to considerable quantitative corrections to all these results including equation (31). However, one can obtain almost any velocity increase in scope of the perturbation approaches, and the formula (31) of (Bychkov 1998a) as well as other formulas of (Zhdanov and Trubnikov 1989, Kazakov and Liberman 2002b, Kazakov and Liberman 2002a) may be equally treated as analytical guesses rather than unambiguous results. Taking (31) as the estimate for the velocity in-
crease we find

\[ C_1 = \frac{(\Theta - 1)}{4(2\Omega_{\text{max}})^{1/2}} - \frac{1}{2} = \frac{1}{4} \left( \Theta^2 + \Theta + 3 - 1/\Theta \right)^{1/2} - \frac{1}{2}. \]  

(32)

The model equation (28) involves also time-dependent nonlinear terms, which cannot be adjusted with the help of direct numerical simulations for stationary flames. However, studies of curved flame stability (Bychkov, Kovalev and Liberman 1999, Petchenko and Bychkov 2004) indicate that time-dependent nonlinear terms are of minor importance. For simplicity, when constructing a qualitative model the time-dependent nonlinear term may be omitted. Still, there is another problem with formula (31), namely, equation (32) does not reproduce correct asymptotics for \( C_1 \) at \( \Theta \to 1 \). Making slight modifications of (31) we can remedy this trouble, since, as we have pointed out above, the stationary flame velocity is almost a free parameter in the nonlinear perturbation theories. For example, we can choose

\[ \Omega_{\text{max}} = \frac{\Theta}{2} \frac{(\Theta - 1)^2}{\Theta^3 + 2\Theta^2 + 5\Theta - 4} \]  

(33)

with respective corrections to the coefficient \( C_1 \)

\[ C_1 = \frac{(\Theta - 1)}{4(2\Omega_{\text{max}})^{1/2}} - \frac{1}{2} = \frac{1}{4} \left( \Theta^2 + 2\Theta + 5 - 4/\Theta \right)^{1/2} - \frac{1}{2}. \]  

(34)

The velocity increase (33) is shown in figure 1 by the dashed line. As we can see, it provides even better agreement with direct numerical simulations.
than (31).

Of course, the above calculations is not the way to construct an unambiguous rigorous equation to calculate the flame propagation velocity. Particularly, one of the referees points out that the second order time derivative is useless, if the ultimate goal is only to compute the flame velocity. But we recall that the non linear theory of the DL instability in an inevitable starting point for many other problems like oblique flames, tulip flames, flame interaction with turbulence, with acoustics or shock waves, burning in tubes with heat losses. As an example, the non linear equations (see for instance (Joulin and Cambray 1992, Bychkov 1998a)) developed to describe the DL instability were later used with some modifications to study turbulent flames in (Cambray and Joulin 1992, Denet 1997, Bychkov 2000, Zaytsev and Bychkov 2002, Akkerman and Bychkov 2003). In the same way, equation ((28)) can also be modified to get an understanding of other, much more complicated phenomena.

5 Conclusion

In this article, starting from a low vorticity approach (Bychkov et al. 2003) proposed to describe premixed flames in a coordinate-free way, we have developed this formulation in powers of the gas expansion parameter. It appears that at the lowest order in gas expansion, the Frankel equation (equivalent of the Sivashinsky equation for the coordinate-free case) is recovered. At the
second order, we have shown that complications arise in the case of oblique
flames. On the contrary, if the tangential velocity is small (planar on aver-
age and expanding flames), we have obtained a modified form of the Frankel
equation, with a correction of the surface charge. In the planar case, we have
shown that this modified equation reduces to the Sivashinsky-Clavin equa-
tion (a second order in gas expansion correction to the original Sivashinsky
equation). We have thus shown that the small vorticity formulation contains
the Sivashinsky-Clavin equation as a particular case. A direct numerical so-
lution of this formulation, although difficult, could describe both the slow
dynamics of a flame without external forcing, and the rapid evolution that
takes place under some conditions (acoustic forcing, interaction with shock
waves). On the contrary, the equations obtained here as the lowest orders of
a development in gas expansion are inherently limited to a slow, first order
in time dynamics. Although potentially easier to solve than the full small
vorticity equations (at least without tangential blowing) it must be recalled
that in the planar case, in order to obtain good quantitative agreement with
numerical simulations, Joulin and Cambray (Joulin and Cambray 1992) have
been obliged to perform some empirical modifications of the coefficients of the
Sivashinsky-Clavin equation. The purpose of these new coefficients was to
describe better the instability growth rates and the amplitude of stationary
cellular flames. We suggest different ways to construct similar phenomenolog-
ical equations, particularly taking into account second-order time derivatives
inherent to the DL dispersion relation. We also discuss the best way of ad-
justing the numerical coefficients of the model equation using recent results of direct numerical simulations for the velocity increase because of the DL instability (Bychkov et al. 1996, Kadowaki 1999, Travnikov et al. 2000). It remains to be seen if the same type of modification has to be used in the coordinate-free case, both for the small vorticity equations and its small gas expansion, low frequency limit. In any event, we hope that the present article has served to explain the relations between different existing approaches to the problem of nonlinear premixed flames dynamics.

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References


Figure 1: Maximal velocity increase for curved stationary flames scaled by the planar flame velocity versus the thermal expansion $\Theta$. The markers show results of direct numerical simulations (Bychkov et al. 1996, Travnikov et al. 2000) (circles) and (Kadowaki 1999) (crosses). The solid lines correspond to the analytical results of (Zhdanov and Trubnikov 1989, Bychkov 1998a, Kazakov and Liberman 2002b, Joulin and Cambray 1992). The dashed line presents equation (33).