Variational calculations for thermal combustion waves

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We use a variational principle for reaction diffusion equations which enables us to obtain simple analytical estimates for the speed of a flame valid into the region where the rate of heat release is not localized.

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I. INTRODUCTION

It is well known in the theory of thermal propagation of flames that in simple cases the problem can be modeled by a simple one-dimensional reaction diffusion equation [1,2]

$$\theta_t = \theta_{xx} + \omega(\theta), \tag{1}$$

where the reaction term is given by the Arrhenius law, which in a reduced version is of the form

$$\omega(\theta) = (1-\theta)^r \left[e^{\beta(\theta-1)} - e^{-\beta}\right], \tag{2}$$

where the term $e^{-\beta}$ is introduced to remedy the cold boundary problem [3,4]. Other formulas for reaction terms have been considered [4,5], and they all share similar qualitative features. For simplicity we consider only one case; the results given here can be applied to those cases as well. The degree of localization of the reaction zone is measured by the Zeldovich number β. For very large β, the width of the reaction zone is narrow and the speed of the flame is given by the Zeldovich-Frank-Kamenetskii (ZFK) formula [1]

$$c_{\rm ZFK} = \left(2\int_0^1 \omega(\theta)\, d\theta\right)^{1/2} \tag{3}$$

which is the exact value in the limit $\beta \to \infty$. For values of $\beta < 2$ the reaction term is concave and the speed is given by the Kolmogorov-Petrovski-Piskunov (KPP) value [6]

$$c_{\rm KPP} = 2\sqrt{\omega'(0)}. \tag{4}$$

Realistic values of β lie between these two extremes. The transition between these two regimes has been studied numerically and in cases where the reaction function ω adopts a simple form that allows the exact solution of the problem [3,4]. Corrections to the ZFK formula have been obtained by means of asymptotic expansions in the parameter $1/\beta$ [4]. The prescription has been [3] to take the larger value between $c_{\rm ZFK}$ (or its corrections) and $c_{\rm KPP}$ as the best approximation to the correct value of the speed. We have shown recently that the value of the speed for arbitrary ω derives from a variational principle [7],

$$c = \sup\left(2\frac{\int_0^1 \sqrt{-\omega g g'}\, d\theta}{\int_0^1 g\, d\theta}\right), \tag{5}$$

where g is a positive monotonically decreasing function. The purpose of this work is to analyze the connection between this exact result and the $c_{\rm ZFK}$ value and to show that by making use of the variational principle it is possible to obtain simple analytical formulas that reproduce the numerical values of the speed in a wide range of β. In Sec. II we obtain results valid for arbitrary ω and in Sec. III these results are applied to the case in study. We obtain simple analytical formulas and compare them with numerical results from integration of the partial differential equation.

II. APPROXIMATIONS FOR ARBITRARY ω

We are interested in estimating the speed of monotonic fronts $\theta(x-ct)$ of Eq. (1). These fronts satisfy

$$\theta_{zz} + c\theta_z + \omega(\theta) = 0, \qquad \lim_{z\to-\infty}\theta = 1, \quad \lim_{z\to\infty}\theta = 0, \tag{6}$$

where $z = x - ct$ and we assume that c is positive. Defining $p = -d\theta/dz$ one finds that monotonic fronts satisfy

$$p(\theta)\frac{dp}{d\theta} - cp(\theta) + \omega(\theta) = 0,$$

with

$$p(0) = p(1) = 0 \qquad \text{with } p > 0.$$

The variational principle Eq. (5) can be deduced from the equation for p. It follows that

$$c \geq 2\frac{\int_0^1 \sqrt{-\omega g g'}\, d\theta}{\int_0^1 g\, d\theta}. \tag{7}$$

As a first step we shall show that the ZFK value for the speed is a lower bound for all ω (a different proof has been given directly from the ordinary differential equation elsewhere [8]). To do so, choose as a trial function

$$g = \sqrt{2\int_x^1 \omega\, d\theta}. \tag{8}$$

With this choice we obtain

$$\int_0^1 \sqrt{-\omega g g'}\, d\theta = \int_0^1 \omega\, d\theta \tag{9}$$

and we have that

$$\int_0^1 g\, d\theta = -\int_0^1 g'\theta\, d\theta \le -\int_0^1 g'\, d\theta = g(0), \tag{10}$$

where we have used the fact that $g(1) = 0$. Replacing these results in Eq. (7) we obtain

$$c \ge 2\frac{\int_0^1 \omega\, d\theta}{g(0)} = \sqrt{2\int_0^1 \omega\, d\theta} = c_{\mathrm{ZFK}}, \tag{11}$$

that is, the speed is always greater than the ZFK value. Next we construct a set of functions g for which the bound can be expressed in terms of simple integrals of ω. Define

$$\phi(x) = \int_x^1 \omega\, d\theta \tag{12}$$

and let

$$g(x) = [\phi(x)]^n. \tag{13}$$

Then $g' = -n\omega\phi^{n-1}$. With this choice the integrals can be performed readily. For the numerator we obtain

$$N = 2\int_0^1 \sqrt{-\omega g g'}\, d\theta = \frac{4\sqrt{n}}{2n+1}\phi^{n+1/2}(0)$$

with $1/2 < n < 1$. For the denominator we may approximate

$$D = \int_0^1 g\, d\theta = \int_0^1 \phi^n\, dx \le \left(\int_0^1 \phi(x)\, dx\right)^n = \left(\int_0^1 \theta\omega(\theta)\, d\theta\right)^n.$$

Therefore the speed satisfies

$$c \ge \frac{4\sqrt{n}}{2n+1}\frac{\left(\int_0^1 \omega\, d\theta\right)^{n+1/2}}{\left(\int_0^1 \theta\omega\, d\theta\right)^n}. \tag{14}$$

This bound is valid for $1/2 < n < 1$ and for arbitrary ω such that $\omega(0) = \omega(1) = 0$ and $\omega \ge 0$ in $(0,1)$. In addition one can maximize with respect to n. The best n is given by

$$n = \frac{1 - \ln(\gamma) - \sqrt{[\ln(\gamma) - 1]^2 - 4\ln(\gamma)}}{4\ln(\gamma)},$$

where

$$\gamma = \frac{\phi(0)}{\int_0^1 \theta\omega(\theta)\, d\theta}.$$

When there is no real solution for n, the best choice is $n = 1$.

III. BOUNDS FOR THE COMBUSTION CASE

In this section we shall apply the above results to the case

$$\omega_r(\theta) = (1-\theta)^r \left[e^{\beta(\theta-1)} - e^{-\beta}\right] \tag{15}$$

for $r = 1$ and $r = 2$ as examples. As a first step we have performed numerical integrations of the reaction diffusion equation taking sufficiently localized initial conditions that guarantee the asymptotic approach to the monotonic front [9]. For the time evolution operator we have used a Trotter product formula. The time evolution was made by means of alternate application of propagators associated with the diffusion and nonlinear terms. A semi-implicit finite-difference algorithm for partial parabolic equations was used for the diffusion generator. A fourth order Runge-Kutta applicated through every point in the discrete lattice was used for the nonlinear generator. The method was tested in cases for which an exact solution is known. The error never exceeded three-tenths of a percentile.

For the value of ω above with $r = 1$ we have that

$$c_{\mathrm{KPP}} = 2\sqrt{\beta e^{-\beta}}, \tag{16}$$

$$A = \int_0^1 \theta\omega\, d\theta = \frac{1}{\beta^3}\left[\beta - 2 + e^{-\beta}\left(2 + \beta - \frac{\beta^3}{6}\right)\right], \tag{17}$$

$$B = \int_0^1 \omega\, d\theta = \frac{1}{\beta^2}\left[1 - e^{-\beta}\left(1 + \beta + \frac{\beta^2}{2}\right)\right], \tag{18}$$

and

$$c_{\mathrm{ZFK}} = \sqrt{2B}. \tag{19}$$

The results of the calculations are shown in Fig. 1. The results of the numerical integration of the PDE are shown with a solid line, and the dashed lines correspond to the KPP and ZFK values whereas the dot-dashed line is the result of the variational bound obtained using the expression (14) given above. For large β the best value for

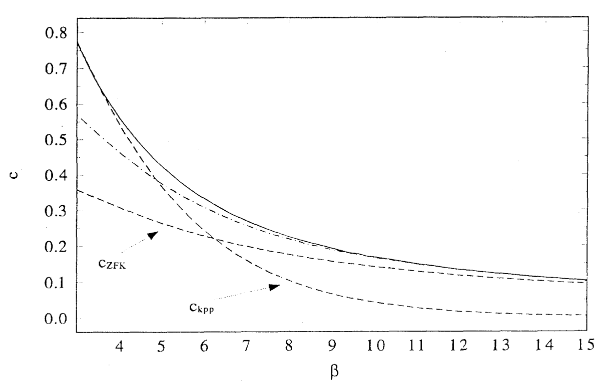

FIG. 1. Speed of the fronts as a function of the Zeldovich parameter β obtained from the integration of the PDE for ω_1 is shown with a solid line. The linear KPP value and the ZFK values predict the speed in the low and large β regime, respectively. For large and intermediate values of β a closer estimate is obtained from the variational principle.

the variational parameter is the $n = 1/2$ value which increases with decreasing β. For $\beta < 13$ the best result is obtained with $n = 1$. As shown in the graph, this variational bound approximates closely the numerical results for β larger than ≈ 6. Due to the form chosen for the trial function g it is possible to give a simple approximate expression for this curve.

For large β,

$$A \approx \frac{\beta - 2}{\beta^3},$$

$$B \approx \frac{1}{\beta^2},$$

and

$$c_{\mathrm{ZFK}} \approx \frac{2}{\sqrt{\beta}}. \tag{20}$$

With $n = 1/2$ we obtain

$$c_{1/2} \approx \sqrt{\frac{2}{\beta(\beta - 2)}} \tag{21}$$

and with $n = 1$ we have

$$c_1 \approx \frac{4}{3}\frac{1}{\beta - 2}. \tag{22}$$

In Fig. 2 we show again the results of the numerical calculation together with the ZFK value and these approximate expressions for large β. For very large values of β, exactly $\beta > 18$ the value $c_{1/2}$ is a closer approximation and tends to the ZFK value for $\beta \to \infty$ but for $5.5 < \beta < 18$ a much better approximation is obtained with c_1. We notice that the approximate value c_1 gives a good approximation even beyond the region where it is strictly valid, as it departs from the bound shown in Fig. 1. As an example, at $\beta = 7$, the value obtained from c_{ZFK} is 35% below the exact value, the bound obtained from (8) is 5% below, and the approximate formula c_1 is less than 1% below. At larger β the error diminishes.

Similar simple approximations can be obtained for other choices of ω provided that the integrals of ω and $\theta\omega$ can be calculated. Notice that the simple expressions (21) and (22) above cannot be obtained by perturbation theory. For lower values of β the approximations made are no longer valid and the full expression for A and B must be used. If one is interested in the transition from the linear or KPP regime to the nonlinear one, a simple trial function of the form $g = \exp(-sx)$ with s as a variational parameter gives a closer approximation to the speed for low β. In the present case this trial function predicts the transition at $\beta \approx 4.1$ whereas the numerical integrations set it at $\beta \approx 3.1$ in agreement with previous work [2]. The exact transition point from the linear or KPP regime can be predicted using the variational principle as accurately as desired by judicious choice of trial function.

For $r = 2$ similar results hold. We do not give the details which are straightforward. For large values of β we obtain

$$c_{\mathrm{ZFK}} = \frac{2}{\beta^{3/2}} \tag{23}$$

and a good approximation to the bound given in Eq. (14) for large β is given by

$$c_1 \approx \frac{4\sqrt{2}}{3}\frac{1}{\sqrt{\beta}(\beta - 3)} \tag{24}$$

if we take the variational parameter $n = 1$ and

$$c_{1/2} \approx \frac{2}{\beta\sqrt{\beta - 3}} \tag{25}$$

for the variational parameter $n = 1/2$. As in the previous case, for very large β, $n = 1/2$ yields a better approximation and $n = 1$ is a better approximation for moderate values of β. These results are shown in Fig. 3. The solid line corresponds to the results of the numerical integration of the PDE, and the dashed lines correspond to the ZFK and KPP values. The dotted line is the bound Eq.

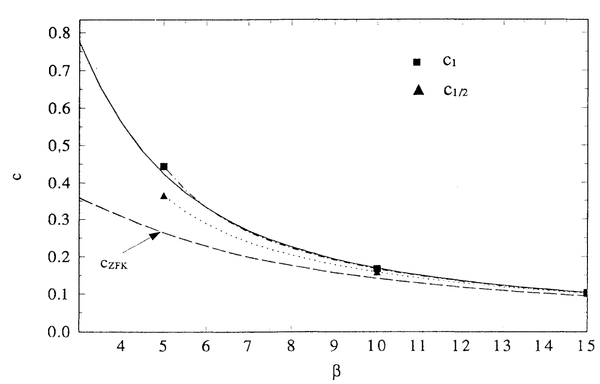

FIG. 2. As in the previous graph the solid line depicts the speed obtained from the numerical integration of the PDE. The approximate analytical formulas c_1 and $c_{1/2}$ approximate the correct value of the speed in a wide region.

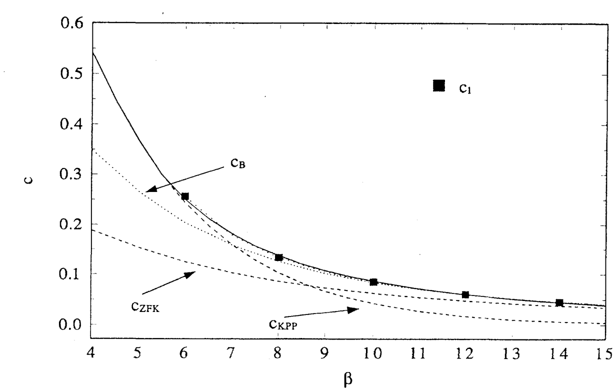

FIG. 3. Numerical and approximate results are shown for ω_2. The solid line corresponds to the speed obtained from the numerical integration of the PDE. The KPP, ZFK, and the bound c_B are shown. The approximate formula c_1 reproduces the numerical results in a wide range.

(14). The dot-dashed line corresponds to the approximate expression c_1 for large β.

IV. CONCLUSION

We have studied the problem of the velocity selection for the reaction diffusion equation in a case relevant to combustion theory, namely very localized reaction terms. Starting from a variational principle which yields the exact speed in principle, we have shown that the ZFK formula is a lower bound for the speed. We derive an approximate result for the speed valid for arbitrary reaction functions, which, when applied to a case of relevance in combustion, is seen to give a better analytical simple approximation than the ZFK value. These approximate formulas are not obtainable from a perturbative approach. The method used here can be extended to other cases such as θ_i models or to density dependent diffusion coefficients [10,11] to obtain simple approximate analytical expressions in other cases as well.

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