Finite flame thickness effects on Kolmogorov-Petrovsky-Piskunov turbulent burning velocities

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KPP (Kolmogorov-Petrovsky-Piskunov) solutions of the reaction-diffusion equation have application in various physical phenomena occurring in biology, ecology, and reacting flows. In particular, these solutions are commonly used in turbulent combustion to scale turbulent burning velocities. Subject to certain conditions on reaction rate profile through the flame brush and turbulent diffusivity, this theory relates the turbulent burning velocity to the derivative of the reaction rate ($\tilde{\omega}$) at the leading edge of the flame brush ($d\tilde{\omega}/d\tilde{c}|_{\tilde{c}=0}$). Such waves are often referred to as "pulled fronts." However, turbulent flames never actually satisfy the KPP conditions for a pulled front, as the turbulent flame brush, parametrized here by the thickness δ_t, consists of an ensemble of laminar flamelets of thickness δ, where $\epsilon = \delta/\delta_t \ll 1$ is very small, but nonzero, and $d\tilde{\omega}/d\tilde{c}$ tends to zero at the brush leading edge for high activation energy, combustion-type kinetics. This paper analyzes these effects on KPP wave solutions, parametrized by $\epsilon = \delta/\delta_t$ and Zeldovich number Ze focusing on whether turbulent flames retain their pulled front character and what the correction to the KPP wave speed is. Variational solutions of the reaction-diffusion equation show that the solution can be expanded in powers of $1/|\ln\epsilon|$. Both numerical and asymptotic results are presented, showing that the wave still exhibits pulled front solutions but with significant corrections to the KPP result. The leading order correction is of the form $|\ln\epsilon|^{-2}$ and independent of Ze. Higher order corrections are function of both ϵ and Ze. However, the dominant factor influencing the wave speed correction is due to the finite ϵ, with Ze exhibiting a weaker effect.

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I. INTRODUCTION

Kolmogorov, Petrovsky, and Piskunov analyzed traveling wave solutions to the reaction-diffusion equation, generalizing Fisher's nonlinearity [1], to describe population dynamics [2]. These solutions have subsequently been used to model a host of phenomenon, including applications in biology [3], combustion [4], and plasma physics [5]. In this article, we focus on its application to the turbulent flame speed and Arrhenius modification to the Kolmogorov-Petrovsky-Piskunov (KPP) type nonlinearities. Although we present the analysis using turbulent combustion terminology, it can be applied in general where similar functional forms occur for nonlinearities.

A fundamental observation of the turbulent burning velocity is that it increases with increasing turbulence intensity in the approach flow, at least over a range of turbulence intensities. Formal mathematical analyses of this problem lead to at least two approaches for addressing this causal relationship. Damköhler's first hypothesis, which can be thought of as a "global" description, emphasizes the augmentation of flame surface area by turbulent disturbances, leading to a higher turbulent velocity [6]. In contrast, a "local" description follows from the Kolmogorov-Petrovsky-Piskunov (KPP) theorem [2], which relates the turbulent burning velocity to conditions at the leading edge of the turbulent flame brush [7]. These two descriptions have fundamentally different answers to questions around causality. In the global description, a flame area increase "causes" the increase in burning velocity, whereas the flame area increase is an "effect" of increasing burning velocity with the local description. Analyses of deterministic solutions of the G equation have shown that both descriptions are the formally appropriate ones in different limiting circumstances [8].

The objective of this study is to analyze KPP wave solutions [2], specifically the steady state wave speeds of a reaction diffusion equation. We specifically consider a statistically stationary, one-dimensional front [9,10], given by

$$v d\tilde{c}/d\zeta = d^2\tilde{c}/d\zeta^2 + \tilde{\omega}(\tilde{c}), \tag{1}$$

where $\tilde{c}$ and $\tilde{\omega}$ are the Favre-averaged progress variable and reaction rate respectively and v is the wave speed. Note that we absorb D_T (turbulent diffusion coefficient) into the definition of the spatial coordinate by defining $\zeta - \zeta_0 = \int_{x_0}^{x} 1/[\bar{\rho} D_T(x')]dx'$, $v = \bar{\rho} S_T$ (where S_T is the turbulent flame speed and $\bar{\rho}$ is the average unburned gas density) and $\tilde{\omega} = \bar{\rho}^2 D_T W$ (where W is the reaction rate. Note that $\tilde{c} = 0$ and $\tilde{c} = 1$ represent unburned and burned gases respectively. Reaction rates are assumed to be zero at both limits, i.e., $\tilde{\omega}(\tilde{c} = 0) = \tilde{\omega}(\tilde{c} = 1) = 0$.

Our interest in this paper is particularly around the dependence of the solution upon the functional nature of the reaction rate term. The reader is referred to work from Lipatnikov and Sabelnikov [11–13] on solution characteristics with various diffusivity forms, including countergradient diffusion, where $D_T < 0$ in part of the flame. Consequently, we assume that $D_T > 0$ for this analysis. Two limiting forms of solution exist to this equation (which turn out to closely approximate

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that found in a laminar and turbulent flame) depending upon whether $\tilde{\omega}(\tilde{c})$ is concave or not. If $\tilde{\omega}(\tilde{c})$ is not concave, the solution asymptotes to the following equation which, as shown by Zeldovich and Frank-Kamenetskii [7,14], is valid when the reaction rate is negligible except near ($\tilde{c} \to 1$), a profile that approximates laminar premixed flames with high activation rate kinetics [7,15]:

$$v = \sqrt{2 \int_0^1 \tilde{\omega}(\tilde{c}) d\tilde{c}}. \tag{2}$$

In this case, note that v is controlled by the integral of the reaction rate profile and is independent of any particular local values. These are sometimes referred to as "pushed fronts."

A completely different solution form exists when the reaction rate profile is concave in [0, 1] or more precisely

$$\tilde{\omega}(0 \leqslant \tilde{c} \leqslant 1) \geqslant 0, \tag{3a}$$

$$d\tilde{\omega}/d\tilde{c}|_{\tilde{c}\to 0} > \max d\tilde{\omega}/d\tilde{c}|_{0<\tilde{c}\leqslant 1}, \tag{3b}$$

then the reaction diffusion equation admits a family of uniformly traveling wave solutions for all flame speeds (v) greater than a minimum speed, v_{KPP} given by [2]

$$v \geqslant v_{\mathrm{KPP}} = 2\sqrt{(d\tilde{\omega}/d\tilde{c}|_{\tilde{c}\to 0})}. \tag{4}$$

The equality holds for sufficiently localized initial conditions and for initial condition such that $\tilde{c}(x < 0, t = 0) = 0$ and $\tilde{c}(x \geqslant 0, t = 0) = 1$ [2,16]. These fronts are referred to as "pulled fronts" since the flame speed depends only on the leading edge of the turbulent flame brush ($\tilde{c} \to 0$).

Most turbulent flame reaction rate closure models in the literature satisfy KPP constraints given by Eq. (3) [10]; e.g., the eddy break up model [17], Magnussen model [18], and Bray-Moss-Libby model [19]. For example, the Bray-Moss-Libby model in conjunction with the flamelet crossing model [20] uses a reaction rate term of the form $\tilde{\omega}(\tilde{c}) \sim \tilde{c}(1-\tilde{c})$, plotted in Fig. 2. For this reason, it is common in turbulent combustion studies to use the KPP solution to approximate the turbulent flame speed [4,21–23].

This study is motivated by the fact that no real turbulent flame (with flame brush thickness δ_t), which is composed of finite thickness flamelets of thickness δ, satisfies the constraint given by Eq. (3). First, due to Arrhenius kinetics, in the region $O(\delta/\delta_t)$ close to the leading edge, i.e., near $\tilde{c} \to 0$, $d\omega/d\tilde{c} \to 0$ [24–27]: this is sketched in Fig. 1. Second, it is possible for the leading edge of the laminar flamelet to be slightly endothermic, due to fuel decomposition. This leads to the following asympotic problem: "What is the nature of the solutions in the limit of $\delta/\delta_t \to 0$, where $\tilde{\omega}(\tilde{c})$ does not formally satisfy Eq. (3), even while being asymptotically close to it (e.g., see Fig. 2)?" For such source functions, it is not clear whether the front is still a pulled front, perhaps with a small correction, or exhibits completely different characteristics altogether.

Some insight into this question was developed by Brunet and Derrida [28] in the context of a Fisher-Kolmogorov equation. In particular, they looked at finite size effects of microscopic stochastic model of directed polymers. They similarly considered a small deviation to the $\tilde{\omega}(\tilde{c})$ function, in a small region close to the leading edge ($\tilde{c} \to 0$) by multiplying

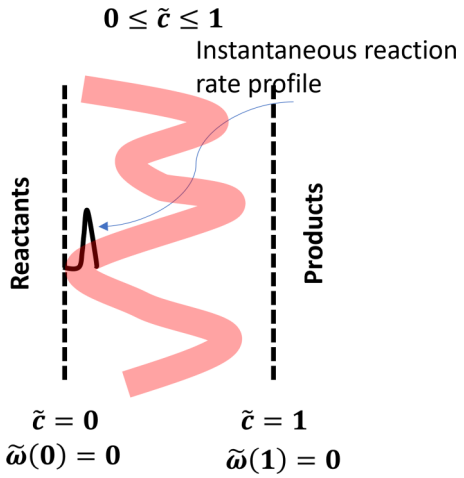

FIG. 1. Schematic of 1D statistically stationary flame indicating progress variable and boundary conditions.

a leading-edge function $\Theta(\epsilon)$ such that

$$\Theta = 1 \quad \text{if } \tilde{c} \geqslant \epsilon, \tag{5a}$$

$$\Theta = 0 \quad \text{if } \tilde{c} < \epsilon, \tag{5b}$$

where $\epsilon \ll 1$ is a small parameter. They showed that this deviation introduces a shift in the velocity of the front given by

$$v \approx v^*_{\mathrm{KPP}} - \pi^2/|\ln \epsilon|^2, \tag{6}$$

where $v^*_{\mathrm{KPP}} = 2$ is the KPP wave speed for the $\tilde{\omega}(\tilde{c}) = \tilde{c}(1-\tilde{c})$ profile used.

Two key conclusions fall out of this expression: First, the basic KPP wave speed scaling still holds, *even though* the $\tilde{\omega}(\tilde{c})$ function does not satisfy Eq. (3). Second, the wave speed has a correction which is very strong even for very small ϵ, being in the form of a logarithm. Furthermore, while this result was developed for a Heaviside leading edge function, it turns out to

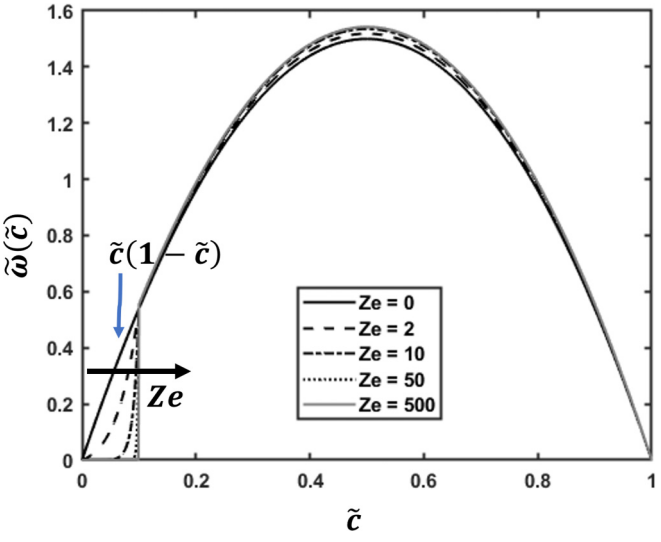

FIG. 2. Reaction rate function, $\tilde{\omega}(\tilde{c})$, showing leading edge correction for increasing values of Ze for $\epsilon = 0.1$.

be independent of the functional nature of $\Theta(\epsilon)$ to this order, as shown by Dumortier *et al.* [29] and Benguria *et al.* [30].

Consider next the effects of slight endothermicity of the leading edge of the flamelet, conceivable under certain conditions where the fuel decomposes into intermediates. The simplest of these source functions have been studied in the literature in the context of response of a biological neuron when excited by an external stimulus [31,32] and are termed Fitzhugh-Nagumo source terms given by $\tilde{\omega}(\tilde{c}) = \tilde{c}(1-\tilde{c})(\tilde{c}-\gamma)$, where the parameter $\gamma \in (0, 1/2)$ determines the inflection point. There are fundamental differences in the nature of the traveling wave solutions to reaction diffusion equations with Fitzhugh-Nagumo source terms and the KPP source terms satisfying Eq. (3). The KPP source term results in a velocity spectrum with a lower bound [see Eq. (4)] above which uniformly traveling wave solutions exist. On the other hand, the Fitzhugh-Nagumo model results in a unique traveling wave solution with the velocity uniquely given by [33]

$$v_0 = \frac{1}{\sqrt{2}} - \gamma\sqrt{2}. \tag{7}$$

Note that this correction reduces the wave speed, but in a manner that is linearly dependent upon γ, as opposed to the quadratic and logarithmic correction to the leading-edge function in Eq. (6). Fitzhugh-Nagumo source functions, with leading edge correction functions of the form used in Eq. (5), have also been studied [34,35]. This deviation was shown to introduce a shift in the velocity of the front given by [34]

$$v \approx v_0 + K(\gamma)\epsilon^{1+2\gamma}, \tag{8}$$

where $K(\gamma) = \frac{\Gamma(4)}{\Gamma(1+2\gamma)\,\Gamma(3-2\gamma)}\,\frac{\sqrt{2}\gamma}{(1+2\gamma)^{2\gamma}}$ is a positive constant. Note that as $\epsilon \to 0$, the above equation limits to the solution given by Eq. (7). However, as $\gamma \to 0$, this does not limit to Eq. (6) since the two source functions are different; i.e., $\tilde{\omega} = \tilde{c}(1-\tilde{c})$ and $\tilde{\omega} = \tilde{c}(1-\tilde{c})(\tilde{c}-\gamma)$, respectively.

Given how strong these finite flame thickness corrections can be to the KPP wave speed, the objective of this study was to study the nature of this correction for leading edge functions, $\Theta(\epsilon)$, representative of those encountered in high activation energy flames. While the leading order result in Eq. (6) is independent of the functional form of $\Theta(\epsilon)$, the general form of the higher order correction terms is not addressed in the literature, or its dependencies upon key combustion parameters, such as activation energy. Addressing these corrections is the focus of this paper.

II. PROBLEM FORMULATION AND METHODOLOGY

A. Problem formulation

Consider the balance equation for a Favre averaged progress variable $\tilde{c}$ for a one-dimensional (1D) statistically stationary flame given by Eq. (1). Figure 1 shows the schematic of such a flame with the corresponding boundary conditions, given by

$$\tilde{\omega}(\tilde{c} \to 0) = \tilde{\omega}(\tilde{c} \to 1) = 0. \tag{9}$$

Following the asymptotic analysis of Williams [36], Buckmaster [37], and the simplified source function analyzed by Clavin *et al.* [38], we consider source functions of the form

$$\tilde{\omega}(\tilde{c}) = A(\mathrm{Ze}, \epsilon)\begin{cases}\tilde{c}(1-\tilde{c})e^{-\mathrm{Ze}(1-\tilde{c}/\epsilon)} & \tilde{c} < \epsilon \\ \tilde{c}(1-\tilde{c}) & \tilde{c} \geqslant \epsilon\end{cases}, \tag{10}$$

where $A(\mathrm{Ze}, \epsilon)$ is a normalizing factor such that $\int_0^1 \tilde{\omega}(\tilde{c})\, d\tilde{c} = 1$, Ze is the Zeldovich number defined as $\mathrm{Ze} = E_A/R(T_B - T_U)$, E_A is the activation energy, R is the gas constant, and T_U and T_B are the unburnt and burnt gas temperatures. Note that the above source function satisfies Eq. (3a), i.e., $\tilde{\omega} \geqslant 0$. Endothermicity effects at the brush leading edge, suggested to be a much weaker effect from the analysis presented in the previous section, will be briefly discussed in Sec. III.

Figure 2 shows the variation of the resulting source function [Eq. (10)] with increasing values of Ze for $\epsilon = 0.1$. Notice that as $\mathrm{Ze} \to \infty$ the leading edge function limits to the Heaviside step function discussed in the context of Eq. (5), analyzed by Brunet and Derrida [28].

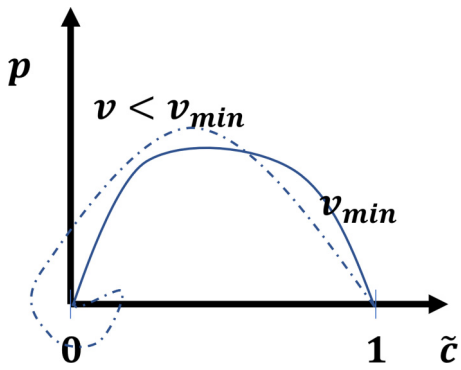

FIG. 3. Illustration of solution trajectory to Eq. (11) in phase space ($\tilde{c}$, p) for two different values of wave speed.

B. Computational methodology

Denoting $p = -d\tilde{c}/d\zeta$, Eq. (1) becomes

$$dp/d\tilde{c} = [vp - \tilde{\omega}(\tilde{c})]/p, \tag{11}$$

and the boundary conditions are given by

$$p(\tilde{c} = 0) = p(\tilde{c} = 1) = 0. \tag{12}$$

Note that the singular points of Eq. (11) are ($\tilde{c} = 0$, $p = 0$) and ($\tilde{c} = 1$, $p = 0$). Thus, in phase space ($\tilde{c}$, p), the solution to Eq. (11) is a heteroclinic trajectory joining the two singular points. The numerical solution for the equation is obtained using a shooting method in phase space [39,40]. Figure 3 shows an illustration of such solution trajectories for two different values of wave speed. There exists a minimum value of wave speed above which the solution is restricted to the physically meaningful region of $0 \leqslant \tilde{c} \leqslant 1$ [2,16]. This computed minimum wave speed is discussed further in the next sections.

III. RESULTS AND DISCUSSION

A. Numerical solution: KPP case

Figure 4 plots the dependence of the wave speed upon dimensionless flame thickness ϵ for several values of Ze. Also plotted in the figure is the asymptotic result, Eq. (6). Starting

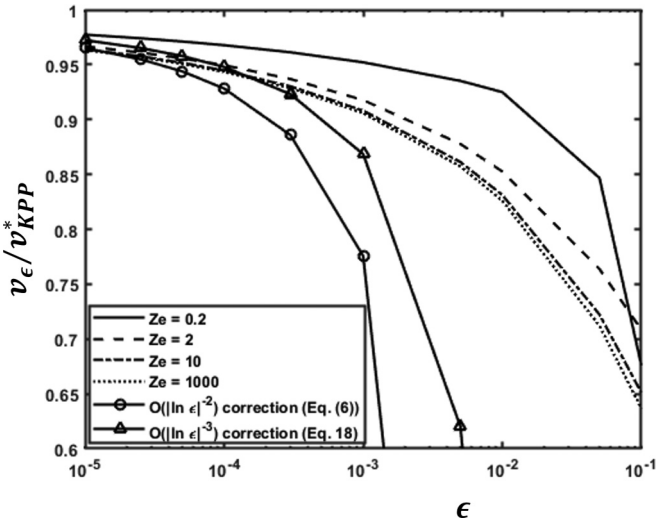

FIG. 4. Numerically computed minimum wave speed (normalized by KPP wave speed) dependence upon ϵ, as well as the $O(|\ln\epsilon|^{-2})$ correction from Eq. (6).

with the large Ze limit, notice that there is a significant correction introduced from the KPP result even for small values of ϵ ($\sim 10^{-3}$). Insights into this large sensitivity to small but nonzero flame thickness is provided by Eq. (6), which shows that the correction is of $O(1/|\ln\epsilon|^2)$.

Figure 5 plots these same results as a function of Ze for different values of ϵ. Several observations are evident. The wave speed decreases with increasing values of Ze for any value of ϵ. This intuitively makes sense, because, as shown in Fig. 2, an increase in Ze pulls the wave profile farther and farther from its baseline. The rate of decrease, however, increases with increasing ϵ. Further, as $\mathrm{Ze}\to\infty$, the value of wave speed saturates and the saturated wave speed decreases with increasing ϵ. We will address these limiting values further in the next section.

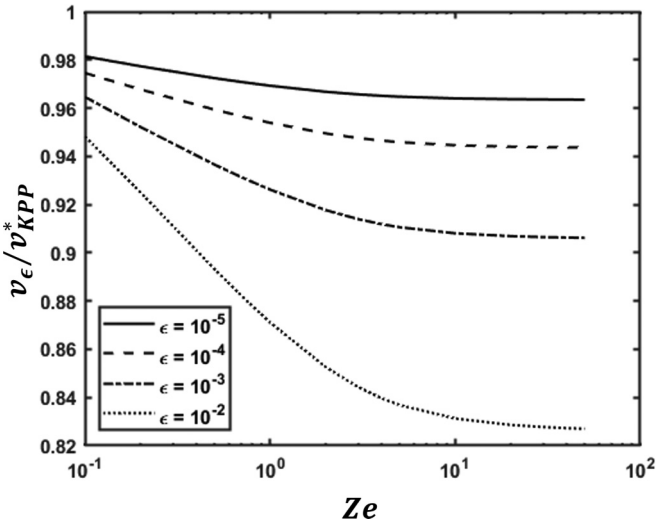

FIG. 5. Variation of wave speed (normalized by KPP wave speed) with parameter Ze for different values of ϵ.

B. Asymptotic result for Ze $\gg$ 1 cases

This section derives higher order corrections to the KPP wave speed, generalizing the result from Benguria *et al.* [41]. In the $\mathrm{Ze}\to\infty$ limit, the leading-edge function hence is given by

$$\tilde{\omega}(\tilde{c}) = \begin{cases} 0 & \text{if } \tilde{c} < \epsilon \\ \tilde{c}(1-\tilde{c}) & \text{if } \tilde{c} \geqslant \epsilon \end{cases}. \tag{13}$$

Following Benguria *et al.* [41], we can develop the following expression for the wave speed from a variational principle to arrive at

$$v^2 \geqslant \sup_{\phi(s)} \left(\frac{\frac{F(1)}{s_0} + \int_0^{s_0} \frac{F[\phi(s)]}{s^2} ds}{\int_0^{s_0} \left(\frac{d\phi}{ds}\right)^2 ds} \right), \tag{14}$$

where $F(\phi) = \int_0^\phi \tilde{\omega}(q)dq$, s_0 is an arbitrary parameter, and the supremum is taken over all the positive increasing functions $\phi(s)$ such that $\phi(0) = 0$ and $\phi(s_0) = 1$ and for which all the integrals in the above variational principle are finite [41].

The maximizing function $\hat{\phi}(s)$ is given by the solution of the Euler-Lagrange equation [41],

$$\frac{d^2\hat{\phi}}{ds^2} + \lambda \frac{\tilde{\omega}(\hat{\phi})}{s^2} = 0. \tag{15}$$

such that $\hat{\phi}(0) = 0$, $\hat{\phi}(s_0) = 1$, and $\hat{\phi}'(s_0) = 0$. Note that the variational principle computes a lower bound with any "trial function" chosen as $\phi(s)$.

For the considered leading function, the analytical solution to Eq. (15) is not tractable, so we use a linear approximation for the source function [$\tilde{\omega}(\tilde{c} \ll 1) \sim \tilde{c}$] to understand the functional form of the higher order corrections. The resulting trial function for the variational principle is given by

$$\frac{d^2\hat{\phi}}{ds^2} = 0 \quad 0 \leqslant \hat{\phi} < \epsilon, \tag{16a}$$

$$\frac{d^2\hat{\phi}}{ds^2} + \lambda \frac{\hat{\phi}}{s^2} = 0 \quad \epsilon \leqslant \hat{\phi} \leqslant 1. \tag{16b}$$

The solution to the above Ordinary Differential Equation which maximizes the variational principle is given by [41]

$$\hat{\phi}(s) = \begin{cases} s & 0 \leqslant \hat{\phi} < \epsilon \\ \alpha\sqrt{s}\cos\left[\frac{1}{2}\cot(\phi_*)\ln\left(\frac{s}{\epsilon}\right) - \phi_*\right] & \epsilon < \hat{\phi} \leqslant s_0 \end{cases}, \tag{17}$$

where $= \sqrt{\epsilon}\sec\phi_*$, $s_0 = \frac{1}{\epsilon}$, and ϕ_* is the first positive solution of the equation $\phi_* \tan\phi_* = \frac{1}{2}|\ln\epsilon|$.

Substituting the trial function [Eq. (17)] into the variational principle [Eq. (14)], we obtain

$$v_\epsilon/v^*_{\mathrm{KPP}} \geqslant 1 - \frac{\pi^2}{|\ln\epsilon|^2} + \frac{7\pi^2}{4}\frac{1}{|\ln\epsilon|^3} + O(|\ln\epsilon|^{-4}). \tag{18}$$

This higher order correction can also be used as a function to fit the finite Ze results from the computations in order to render the results as functions of Ze only; i.e., we determine the dependence of the coefficients $C_1(\mathrm{Ze})$ and $C_2(\mathrm{Ze})$ upon Ze in the expression from the computations:

$$v_\epsilon = v^*_{\mathrm{KPP}}\{1 - \pi^2[1/2|\ln\epsilon|^2 + C_1(\mathrm{Ze})/|\ln\epsilon|^3 + C_2(\mathrm{Ze})/|\ln\epsilon|^4]\}. \tag{19}$$

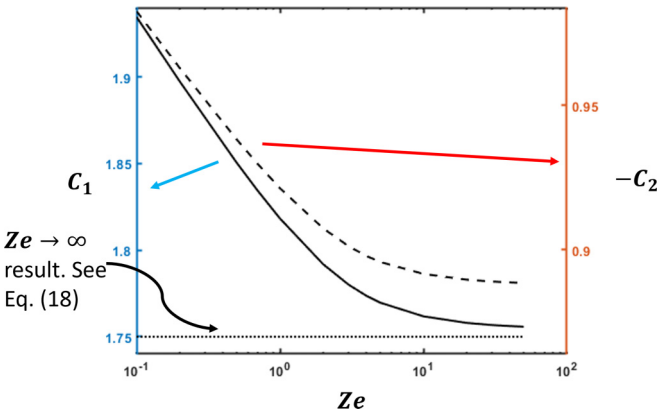

FIG. 6. Coefficients C_1 and C_2 vs Ze as defined in Eq. (19) obtained using least squares curve fit numerically. Overlaid in dotted line is the value of C_1 obtained from variational principle for Heaviside cutoff function explained in Sec. III B.

These values of C_1 and C_2 results are plotted in Fig. 6 as functions of Ze. For reference, the limiting value of $C_1 = 7/4$ in the Ze $\to \infty$ from Eq. (18) is also shown. The figure shows that C_1 and C_2 are both functions of Ze, but that the dependence is rather weak, varying by about 25% and 15% over the entire Ze range for C_1 and C_2. In other words, the dominant factor influencing the correction of the KPP flame speed is flame thickness, with the details of the reaction rate profile as parametrized by Ze, exhibiting a nonzero, but weaker effect. This also indicates that similar results should be observed for a range of related leading-edge functions. The figure also shows both the C_1 and C_2 values saturating for large Ze, with the C_1 value converging to the dashed line [Eq. (18)].

Consider next the effects of weak endothermicity at the flame brush leading edge. We analyzed corrections to the leading-edge function of the Fitzhugh-Nagumo form. Although the wave speed was a function of the parameter γ, the effect was negligible for $\gamma \ll 1$ and so not plotted here. This result was expected due to the linear nature of the correction of the wave speed, presented in Sec. I.

IV. CONCLUSIONS

This study has considered the effects of a laminar flame-type source function introduced to the Favre averaged progress variable equation to account for the deviation in the reaction rate from a concave shape. This deviation is attributed to the Arrhenius kinetics coupled with the finite flamelet thickness. Without this deviation, the flame speed can be computed from KPP theory and depends only on the leading edge of the flame (pulled fronts). With the deviation however, there is a significant correction introduced to the KPP pulled front wave speed. This correction is of the form $|\ln \epsilon|^{-n}$ and is computed numerically. In the limit of high Zeldovich number, the Arrhenius term is shown to behave as a Heaviside step function and the corresponding coefficient of the $O(|\ln \epsilon|^{-3})$ is shown to be predicted by variational principle [41].

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