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Self-similar accelerative propagation of expanding wrinkled flames and explosion triggering

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The formulation of Taylor on the self-similar propagation of an expanding spherical piston with constant velocity was extended to an instability-wrinkled deflagration front undergoing acceleration with $R_F \propto t^{\alpha}$, where R_F is the instantaneous flame radius, t the time, and α a constant exponent. The formulation describes radial compression waves pushed by the front, trajectories of gas particles, and the explosion condition in the gas upstream of the front. The instant and position of explosion are determined for a given reaction mechanism. For a step-function induction time, analytic formulas for the explosion time and position are derived, showing their dependence on the reaction and flow parameters including thermal expansion, specific heat ratio, and acceleration of the front.

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I. INTRODUCTION

Understanding of the structure and propagation of expanding spherical reaction fronts commands both fundamental interest and practical relevance. As examples, expanding spherical flames are employed to determine the laminar flame speeds of reactive mixtures [1–7], which in turn can be used to scrutinize their reaction mechanisms [8,9]. At the astrophysical scale, the onset of a supernova explosion is believed to be the consequence of an expanding nuclear reaction front [10,11]. From practical considerations, various combustion devices operate on the principle of spark ignition, while sparks are also frequently the source of accidental and intentional triggering of explosions.

The dynamics of expanding reaction fronts is richly endowed with combustion phenomena. To appreciate this statement, let us follow the events subsequent to the point deposition of a kernel of energy, leading to the formation of an embryonic flame. The critical issue at this early stage is whether a sustained propagation can be maintained. The front is smooth initially, as any tendency to develop flamefront cellular instability is suppressed by stretch induced by the expanding flame front, and the controlling physics here is stretch and mixture nonequidiffusion [1]. The front evolution depends on the Lewis number Le. In particular, it has been demonstrated [4,12] that sustained propagation is possible for Le > 1 mixtures, whereas for Le < 1 mixtures the flame needs to attain a minimum radius, through the initial energy deposited, before sustained propagation is possible.

As the flame grows in size and the stretch intensity reduces, diffusional-thermal cells would develop over the surface of Le < 1 flames. With further growth, the flame thickness relative to the global flame radius is reduced, leading to the onset of the Darrieus-Landau instability. This generates hydrodynamic cells over the flame surface regardless of the mixture Lewis numbers and will eventually dominate the surface morphology [13]. Furthermore, the continuous generation of new cells could lead to a concomitant increase in the total flame surface area per unit area of the globally spherical flame. This then implies a continuous increase in the reactant consumption rate for the global flame and correspondingly its propagation speed. That is, the flame self-accelerates [14–17]. This self-acceleration could lead to either or both of two possible outcomes: the wrinkled but nevertheless laminar flame could develop to detonation, constituting a deflagration to detonation transition (DDT) event [10], or the self-acceleration could further trigger the Rayleigh-Taylor, body-force, instability, which can also eventually lead to DDT. The DDT could take place either in free space or within a confinement; in the latter situation interaction with the acoustic dynamics of the confinement is expected to greatly facilitate the transition.

At present the dynamics and structure of the reaction wave in the first stage of propagation, when the flame surface is still smooth, have been studied quite extensively and are understood reasonably well, both theoretically and experimentally [4–6,12]. A theoretical analysis has also been performed on the transition to cellularity [13,18–20], with the predictions subsequently substantiated experimentally [21–23]. Studies on the subsequent development of the dynamics of the hydrodynamically wrinkled reaction front have been mostly concerned with the self-acceleration nature of the propagation, particularly on the possibility that the time exponent describing the temporal variation of the flame radius could attain a constant value. This would then imply that the acceleration is self-similar, having a fractal nature [14,15,21–25]. In particular, results from a recent experimental study [25] seem to support that this is indeed the case.

In view of the above considerations, we have initiated a systematic investigation on the structure and propagation of the hydrodynamically wrinkled flames leading to DDT. As a first step, we present herein a hydrodynamic formulation on the self-similar accelerative propagation of the wrinkled flame, describing the dynamic and scalar fields of the flame. We shall then employ this formulation to analyze the process of detonation triggering through heating of the gas ahead of the accelerating flamefront by the compression waves generated ahead of it. It is noted that while this mode of DDT is rather weak, and that the structure of the reaction front is not resolved at the

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present level of analysis, the study nevertheless demonstrates the potential utility of this formulation for further development.

II. SIMILARITY FORMULATION

We consider a deflagration front with the normal propagation speed S_L and the density expansion factor $\Theta = \rho_f/\rho_b$ propagating outwardly from an ignition point. Since we are interested in large scales, we shall neglect effects due to the initial flame stretch. Thus, at the early stage of burning, the front expands with a constant speed $dR_F/dt = \Theta S_L$ with respect to the ignition point. The front shape subsequently becomes corrugated due to flame instabilities, and the front accelerates. According to experimental and numerical studies [14,15,21–25], the evolution of the globally spherical front can be described by a power law

$$R_F(t) = R_0 + At^\alpha \approx At^\alpha, \tag{1}$$

where A, R_0, and α are some constants. In this expression R_0 does not coincide with the ignition "point" in that the self-similar mode of propagation starts at a later time [24]. Consequently, it may be treated either as a virtual origin for the fitting, or as a critical radius corresponding to the transition to the cellular flame structure. In any event, since DDT occurs at large r and t, at which the problem becomes scale invariant, R_0 may be omitted. Neglecting nonradial waves, the deflagration acts as an expanding spherical front pushing the cold medium outward. In the laboratory reference frame, the radial front velocity U_L and the average radial velocity of the flow immediately upstream of the front U_F $(r = R_F)$ are given by

$$U_L = dR_F/dt = \alpha At^{\alpha-1}, \tag{2}$$

$$U_F = \frac{\Theta - 1}{\Theta}U_L = \frac{\Theta - 1}{\Theta}\alpha At^{\alpha-1}. \tag{3}$$

The average front velocity with respect to the reactive mixture is $U_w = U_L/\Theta$.

The exponent α has been reported to fall in the range $\alpha = 1.25$–1.5 [14–17,20–25]. In particular, Gostintsev *et al.* [21,22] suggested $\alpha = 3/2$. In contrast, the well-controlled, recent experiments of Jomaas and Law [25], conducted in a quiescent environment, showed that α is about 4/3. Furthermore, it is basically independent of the chemical composition of the combustible mixture and as such the nature of cells, implying that the diffusional-thermal instability is suppressed by and subordinated to the Darrieus-Landau instability. As a result, the Lewis number and other chemical parameters do not affect the power-law dependence of Eq. (1).

Compressibility of the flow can be estimated by the ratio of the flow and sound speeds at the front, $M \approx u/c \approx U_F/c_F$. For typical hydrocarbon deflagrations, the Mach number M is low, $M \ll 1$, and as such we can use the isentropic approximation, which is valid for $O(M^3) \ll 1$. Consequently, the flame-generated compression wave is described by the spherically symmetric equations of continuity and motion

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial r}(\rho u) + 2\rho\frac{u}{r} = 0, \tag{4}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r} + \frac{1}{\rho}\frac{\partial P}{\partial r} = 0, \tag{5}$$

where $u(r,t) \equiv dr/dt$, $\rho(r,t)$, $P(r,t)$ are the velocity, density, and pressure of the cold gas. In the present work, the fresh medium is assumed to be a perfect gas obeying $P \propto \rho T$, with the sound speed $c = \sqrt{\gamma P/\rho}$, where γ is the specific heat ratio. We note that the present formulation can be readily extended to an arbitrary polytropic gas, $P \propto \rho^n$, with n being a free parameter for the problem. Following Taylor [26], who considered the similar problem of an expanding piston with a constant speed, for which the equations are scale invariant, we shall extend the formulation to one of an accelerating front, across which mass can pass through. For this purpose, we transform the space (r,t) to (η,τ), with $\eta \equiv r/\psi$ and $\tau \equiv (t/\varphi)^\alpha$, where φ and ψ are the characteristic time and length scales of the problem. Dimensional analysis then yields

$$\varphi = (c_0/A)^{\frac{1}{\alpha-1}}, \quad \psi = \left(c_0^\alpha/A\right)^{\frac{1}{\alpha-1}}, \quad \psi/\varphi = c_0, \quad \psi/A\varphi^\alpha = 1, \tag{6}$$

where c_0 is the initial upstream sound speed. Counterparts of the flow velocity and sound speed in the (η,τ) space are then given by

$$w(\eta,\tau) \equiv \frac{d\eta}{d\tau} = \frac{u(r,t)}{c_0\alpha}\tau^{\frac{1-\alpha}{\alpha}} = \frac{u(r,t)}{A\alpha}t^{1-\alpha} = \frac{u(r,t)}{U_L}, \tag{7}$$

$$s(\eta,\tau) = \frac{c(r,t)}{c_0\alpha}\tau^{\frac{1-\alpha}{\alpha}} = \frac{c(r,t)}{U_L}. \tag{8}$$

The deflagration therefore moves with a constant speed $w_L = 1$ in the (η,τ) space, with the front position and the flow velocity just ahead of it being $\eta_F = \tau$ and $w_F = (\Theta - 1)/\Theta$. Subsequently, Eqs. (4) and (5) become

$$\frac{1}{\rho}\left(\frac{\partial \rho}{\partial \tau} + w\frac{\partial \rho}{\partial \eta}\right) = -\frac{\partial w}{\partial \eta} - 2\frac{w}{\eta}, \tag{9}$$

$$\frac{\partial w}{\partial \tau} + w\frac{\partial w}{\partial \eta} + \frac{\alpha - 1}{\alpha}\frac{w}{\tau} = -\frac{1}{\alpha^2 c_0^2}\tau^{2\frac{1-\alpha}{\alpha}}\frac{1}{\rho}\frac{\partial P}{\partial \eta}. \tag{10}$$

We observe that the continuity equation is invariant with respect to the $(r,t) \to (\eta,\tau)$ transformation. Accounting for $P \propto \rho^\gamma$, $c^2 = dP/d\rho$, we have the following relations for an arbitrary variable χ [26]:

$$\frac{dc^2}{d\chi} = \frac{\gamma - 1}{\rho}\frac{dP}{d\chi}, \qquad \frac{1}{c^2}\frac{dc^2}{d\chi} = \frac{\gamma - 1}{\rho}\frac{d\rho}{d\chi}. \tag{11}$$

Equations (8) and (11) yield

$$\frac{1}{\rho}\frac{\partial P}{\partial \eta} = \frac{1}{\gamma - 1}\frac{\partial c^2}{\partial \eta} = \frac{\alpha^2 c_0^2}{\gamma - 1}\tau^{2\frac{\alpha-1}{\alpha}}\frac{\partial s^2}{\partial \eta}, \tag{12}$$

$$\frac{1}{\rho}\frac{\partial \rho}{\partial \eta} = \frac{1}{\gamma - 1}\frac{1}{c^2}\frac{\partial c^2}{\partial \eta} = \frac{1}{\gamma - 1}\frac{1}{s^2}\frac{\partial s^2}{\partial \eta}, \tag{13}$$

$$\frac{1}{\rho}\frac{\partial \rho}{\partial \tau} = \frac{1}{\gamma - 1}\frac{1}{c^2}\frac{\partial c^2}{\partial \tau} = \frac{1}{\gamma - 1}\left(\frac{1}{s^2}\frac{\partial s^2}{\partial \tau} + \frac{2}{\tau}\frac{\alpha - 1}{\alpha}\right). \tag{14}$$

With the result of Eqs. (12)–(14), Eqs. (9) and (10) take the form

$$\frac{1}{s^2}\left(\frac{\partial s^2}{\partial \tau} + w\frac{\partial s^2}{\partial \eta}\right) + \frac{2}{\tau}\frac{\alpha - 1}{\alpha} = -(\gamma - 1)\left(\frac{\partial w}{\partial \eta} + 2\frac{w}{\eta}\right), \tag{15}$$

$$\frac{\partial w}{\partial \tau} + w\frac{\partial w}{\partial \eta} + \frac{\alpha-1}{\alpha}\frac{w}{\tau} = -\frac{1}{\gamma-1}\frac{\partial s^2}{\partial \eta}. \tag{16}$$

We next introduce the scaled variable $\xi \equiv \eta/\tau = r/R_F = r/At^{\alpha}$. Then

$$\frac{\partial}{\partial \tau} = -\frac{\xi}{\tau}\frac{d}{d\xi}, \qquad \frac{\partial}{\partial \eta} = \frac{1}{\tau}\frac{d}{d\xi}, \tag{17}$$

and the set of partial differential equations (15)–(16) is transformed to the following set of ordinary differential equations:

$$\frac{dw}{d\xi} = -\left[2\frac{w}{\xi} + \frac{\alpha-1}{\alpha}\frac{2}{\gamma-1} + \frac{\alpha-1}{\alpha}\frac{w(\xi-w)}{s^2}\right] \times \left[1 - \frac{(\xi-w)^2}{s^2}\right]^{-1}, \tag{18}$$

$$\frac{ds^2}{d\xi} = (\gamma-1)\left[(\xi-w)\frac{dw}{d\xi} - \frac{\alpha-1}{\alpha}w\right]. \tag{19}$$

In the limit of $\alpha = 1$, the system (18)–(19) degenerates to the set of equations derived by Taylor [26]. Equations (18) and (19) constitute a scale-invariant problem describing the evolution of a deflagration-generated compression wave in the (η,τ) space. The variables w and s depend on each other and on the scale-invariant parameter ξ only. The front position is characterized by the locus $\xi_F = 1$. The matching relation for the problem is $w = w_F$ at $\xi = \xi_F$. Compressibility in the (η,τ) space is characterized by the Mach number at the front, $M = w_F/s_F$. We note that there is no "evolution" of the "compression wave" in the (η,τ) space, since there is no flame acceleration in terms of (η,τ). Therefore, both w_F and s_F are constants. In contrast, their counterparts in the (r,t) space are time dependent.

III. SOLUTION

It is nevertheless instructive to estimate the various terms in Eq. (18) and thereby explore analyticity through rational approximations. Because of the typically strong temperature dependence of the induction time, we are interested mainly in the unburned gas particles in the vicinity of the flame, where $w \approx (\Theta-1)/\Theta \sim 1$ and $\xi \approx 1$. While the magnitudes of w/ξ and $2(\alpha-1)/\alpha(\gamma-1)$ are $O(1)$, the other terms on the right-hand side of Eq. (18) are of the order of M^2/Θ or M^2/Θ^2 and hence can be omitted for $M \ll 1$ and typical values of $\Theta = 5$–10. Consequently, Eq. (18) is reduced to

$$\frac{dw}{d\xi} = -2\frac{w}{\xi} - \frac{\alpha-1}{\alpha}\frac{2}{\gamma-1}. \tag{20}$$

The last term in Eq. (20) is related to the unsteady effects in the velocity field of compression waves associated with an accelerating flame. Without this term, Eq. (20) would correspond to a constant density and quasisteady state approximation of the continuity equation. Equation (20) has the solution

$$w = \frac{B}{\xi^2} - D\xi, \tag{21}$$

where

$$D = \frac{\alpha-1}{3\alpha}\frac{2}{\gamma-1}, \qquad B = D + \frac{\Theta-1}{\Theta}. \tag{22}$$

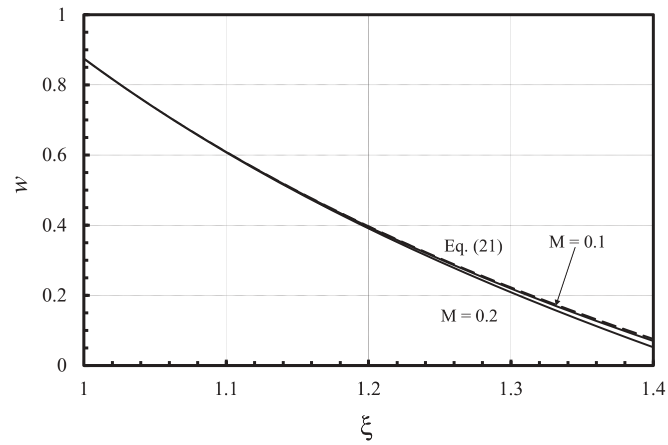

FIG. 1. Flow velocity in the (η,τ) space w versus the scale-invariant parameter ξ for $\Theta = 8$ and $\gamma = 7/5$: the numerical solution to Eqs. (18)–(19) for $M = 0.1$, 0.2 (solid), and the analytical approximation (21) (dashed).

The dashed plot in Fig. 1 shows formula (21). The set of equations (18) and (19) has also been solved numerically, with $w(\xi)$ shown as solid lines in Fig. 1, for $M = 0.1$, 0.2. It is seen that Eq. (21) agrees well with the numerical solution of Eq. (18) in the vicinity of the flame.

With the result of Eq. (21), Eq. (19) becomes

$$\frac{ds^2}{d\xi} = (\gamma-1)\left[\frac{2B^2}{\xi^5} - \left(D + \frac{3\alpha-1}{\alpha}\right)\frac{B}{\xi^2} - D\left(D+\frac{1}{\alpha}\right)\xi\right], \tag{23}$$

which can be integrated analytically as

$$s^2 = s_1^2 + (\gamma-1)\left[\left(D+\frac{3\alpha-1}{\alpha}\right)\frac{B}{\xi} - \frac{B^2}{2\xi^4} - \left(D+\frac{1}{\alpha}\right)\frac{D\xi^2}{2}\right], \tag{24}$$

with the integration constant s_1^2. The formulation (1)–(19) is self-consistent if $s = s_0$ at $w = 0$, with s_0 assuming the role of c_0. According to Eq. (21), $w = 0$ at $\xi = \xi_0$, with

$$\xi_0 = (B/D)^{1/3} = \left(1 + \frac{3\alpha}{\alpha-1}\frac{\gamma-1}{2}\frac{\Theta-1}{\Theta}\right)^{1/3}. \tag{25}$$

Substituting the relation $s(\xi_0) = s_0$ into Eq. (24), we find the value s_1,

$$s_1^2 = s_0^2 - \frac{6\alpha-3}{2\alpha}(\gamma-1)B^{2/3}D^{1/3}, \tag{26}$$

and Eq. (24) becomes

$$s^2 = s_0^2 + (\gamma-1)\left[\left(D+\frac{3\alpha-1}{\alpha}\right)\frac{B}{\xi} - \frac{B^2}{2\xi^4} - \left(D+\frac{1}{\alpha}\right)\frac{D\xi^2}{2} - \frac{6\alpha-3}{2\alpha}B^{2/3}D^{1/3}\right]. \tag{27}$$

Equation (25) provides the estimation for a spherical layer, where the present formulation is valid:

$$1 \leqslant \xi \leqslant \xi_0 \qquad \text{or} \qquad R_F(t) \leqslant r(t) \leqslant \xi_0 R_F(t). \tag{28}$$

For the standard set of parameters: $\Theta = 8$, $\gamma = 7/5$, and $\alpha = 4/3$, we have $\xi_0 \approx 1.46$.

We emphasize that Eqs. (20) and (21) were obtained by neglecting the terms of the order of M^2 in Eq. (18). However, the neglected terms increase with the distance from the flamefront. For this reason, Eqs. (20) and (21) do not work at large ξ, although the assumption $M^2 \ll 1$ is even better verified far upstream of the flame. Substituting the solution (21), (27) into Eq. (18), we find that the M^2 terms are meaningless within the domain (28) if $s_0 \gg 1$, and ξ_0 is of the order of unity. However, the value s_0 decreases with time; see Eq. (8). As soon as the reaction front acquires a near-sonic speed, $U_L \sim c_0$, i.e., $s_0 \sim 1$, the M^2 terms in Eq. (18) become important or even dominant, thereby making Eqs. (20) and (21) invalid. Consequently, the validity of the present formulation is determined by $1 \leqslant \xi \leqslant \xi_0$ and $s_0 \gg 1$.

In the (r,t) space, Eqs. (21) and (27) take the form

$$u(r,t) = \alpha\left(A^3 B \frac{t^{3\alpha-1}}{r^2} - D\frac{r}{t}\right), \tag{29}$$

$$\frac{T(r,t)}{T_0} = \frac{c^2(r,t)}{c_0^2} = 1 + (\gamma-1)\frac{\alpha^2}{c_0^2} \times\left[\left(D + \frac{3\alpha-1}{\alpha}\right)\frac{A^3 B t^{3\alpha-2}}{r} - \frac{A^6 B^2 t^{6\alpha-2}}{2r^4} - \left(D + \frac{1}{\alpha}\right)\frac{D r^2}{2t^2} - \frac{6\alpha-3}{2\alpha}A^2 B^{2/3} D^{1/3} t^{2\alpha-2}\right]. \tag{30}$$

In the scaled form, Eqs. (29) and (30) become

$$\frac{u}{c_0} = \alpha\left(B\frac{\tilde{t}^{3\alpha-1}}{\tilde{r}^2} - D\frac{\tilde{r}}{\tilde{t}}\right), \tag{31}$$

$$T/T_0 = 1 + (\gamma-1)\alpha^2 \times\left[\left(D + \frac{3\alpha-1}{\alpha}\right)\frac{B\tilde{t}^{3\alpha-2}}{\tilde{r}} - \frac{B^2\tilde{t}^{6\alpha-2}}{2\tilde{r}^4} - \left(D + \frac{1}{\alpha}\right)\frac{D\tilde{r}^2}{2\tilde{t}^2} - \frac{6\alpha-3}{2\alpha}B^{2/3}D^{1/3}\tilde{t}^{2\alpha-2}\right], \tag{32}$$

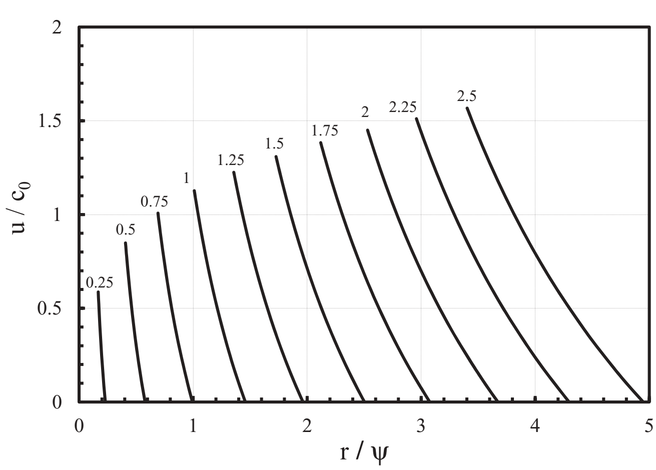

FIG. 2. Scaled radial flow velocity u/c_0 ahead of the deflagration front for $\Theta = 8, \gamma = 7/5$, and $\alpha = 4/3$ at the instants $t/\varphi = 0.25$–2.5 with the time intervals $\Delta t/\varphi = 0.25$.

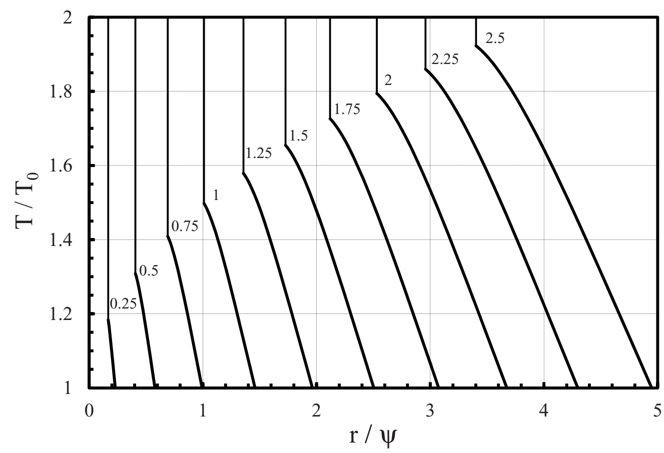

FIG. 3. Scaled temperature T/T_0 ahead of the deflagration front for $\Theta = 8, \gamma = 7/5$, and $\alpha = 4/3$ at the instants $t/\varphi = 0.25$–2.5 with the time intervals $\Delta t/\varphi = 0.25$.

where $\tilde{t} = t/\varphi$, $\tilde{r} = r/\psi$. We note again that Eqs. (31)–(32) work rigorously only in the vicinity of the reaction front. Within this limitation, the solution (31)–(32) completely satisfies the motion equation (5), and it obeys the continuity equation (4) with the accuracy of $O(d\ln\rho/dt)$. Such an accuracy is quite reasonable recognizing the weak logarithmic dependence and the relatively slow acceleration with $\alpha = 1.25$–1.5.

Equation (31) contains two independent thermal-chemical parameters, Θ and α, and there are three parameters in Eq. (32), Θ, α, and γ, related respectively to the chemical energy release, flame instabilities, and compression.

Figures 2 and 3 present Eqs. (31) and (32), respectively, for typical $\Theta = 8$, $\gamma = 7/5$, $\alpha = 4/3$. It is seen that the velocity and temperature of the unburned gas change noticeably during the time φ and at the length scale ψ. In particular, the flow velocity and temperature at the deflagration front behave as $U_F/c_0 \approx 1.17\,(t/\varphi)^{1/3} = 1.17\,(R_F/\psi)^{1/4}$ and $T_F/T - 1 \approx 0.42\,(t/\varphi)^{2/3} = 0.42\,(R_F/\psi)^{1/2}$.

IV. EXPLOSION TRIGGERING

We next consider the trajectories of the gas particles upstream of the flame. The trajectory equation for an arbitrary fresh gas parcel $\{r,t\}$ is

$$\frac{dr}{dt} \equiv u(r,t) = \alpha\left(A^3 B\,\frac{t^{3\alpha-1}}{r^2} - D\frac{r}{t}\right), \tag{33}$$

which describes the instant $t = t_c$ and position $r_c = r(t_c) = R_F(t_c)$ at which the element $\{r,t\}$ would be consumed by the reaction front. Obviously, t_c also determines the time interval $t_c - t$ left for an element before it is consumed by the front. Since the reaction front propagates faster than the front-generated flow, any fuel particle will be eventually consumed by the front if there is no deflagration-to-detonation transition (DDT). However, for certain conditions the reaction in a gas parcel may have attained the state of runaway and hence mostly completed before it is engulfed by the flame. Then the element may explode, hence initiating DDT. By assuming, realistically, that the temperature of a gas parcel increases only due to the reaction heat release, such an element would explode abruptly after an induction time t_i [13], which, while depending on the detailed reaction mechanism, is mainly a function of the temperature of the fresh mixture. The temperature dependence of the induction time is basically a "free functional" of the present formulation, in that in principle any complicated chemical kinetics can be accounted for. Since we are not concerned with detailed reaction mechanisms in this study, we just need t_i tabulated as $t_i = t_i(T)$, to specify the instant and position of DDT. Consequently, we have $t_i = t_i[T(r,t)] = t_i(r,t)$, since $T(r,t)$ is already determined by Eq. (30). The gas parcel $\{r,t\}$ explodes if the value $t_c - t$ at the position r at time t exceeds t_i at the same location and time. The condition for explosion is then given by [27]

$$t_i(t,r) + t - t_c(t,r) = 0. \tag{34}$$

Thus if Eq. (34) is satisfied at a certain instant t_0 at least at one position r_0, then the respective gas parcel $\{r_0,t_0\}$ would explode ahead of the flame. We are interested in the first instant at which such an explosion is possible, i.e., the smallest possible t satisfying Eq. (34) for any r. As soon as one parcel explodes, its neighbor would rapidly explode as well. This leads to rapid heat release and, eventually, to detonation triggering. As a result, the minimal solution to Eq. (34) determines the time instant and the position of DDT.

An analytic solution to Eq. (34) can be obtained by replacing the strong temperature dependence of the induction time by a step function: $t_i = 0$ if $T \geqslant T_i$ and $t_i \to \infty$ if $T < T_i$, where T_i is the ignition temperature at which the reaction runs away. Such an approximation is acceptable when the induction time is negligible as compared to the flame propagation time. If $t_i = 0$, then $t = t_c$ and $r = r_c = R_F(t_c)$, i.e., the explosion occurs immediately at the deflagration front as soon as the temperature just ahead of the flame reaches T_i. According to Eqs. (1) and (32), the instant and position of the explosion are

$$t_{\rm exp}/\varphi = \Omega^{\frac{1}{2(\alpha-1)}}, \qquad R_{\rm exp}/\psi = \Omega^{\frac{\alpha}{2(\alpha-1)}}, \tag{35}$$

where

$$\Omega = \frac{1}{(\gamma-1)\alpha^2}\left[B\left(D+\frac{3\alpha-1}{\alpha}\right) - \frac{B^2}{2} - \frac{D}{2}\left(D+\frac{1}{\alpha}\right) - \frac{6\alpha-3}{2\alpha}B^{2/3}D^{1/3}\right]^{-1}\left(\frac{T_i}{T_0}-1\right). \tag{36}$$

Figure 4 shows the instant and position of explosion, Eq. (35), versus the ignition temperature for the same parameters as in Figs. 2 and 3. In this event, Eq. (35) yields $t_{\rm exp}/\varphi = 3.74\,(T_i/T_0 - 1)^{3/2}$ and $R_{\rm exp}/\psi = 5.81\,(T_i/T_0 - 1)^2$, and we find the instant and radius of explosion as $t_{\rm exp} \approx (10 \sim 20)\varphi$, $R_{\rm exp} \approx (25 \sim 50)\psi$ for typical $T_i \approx (3 \sim 4)T_0$.

We next estimate the characteristic time and length scales of the problem. We observe that the flame dynamics is fully determined by the choice of φ and ψ, which in turn depend on c_0 and A; see Eq. (6). The sound speed at normal conditions is typically $c_0 \approx 3 \times 10^2$ m/s. The value of A, however, has not been extensively studied. Experimental measurements of Jomaas and Law [25] suggested that $A \approx 10^2$ m/s$^{4/3}$ for lean hydrogen-air flames at 8 atm with $\phi = 0.8$. Then the parameters in Eq. (6) are large: $\varphi \approx 30$ s and $\psi \approx 8$ km.

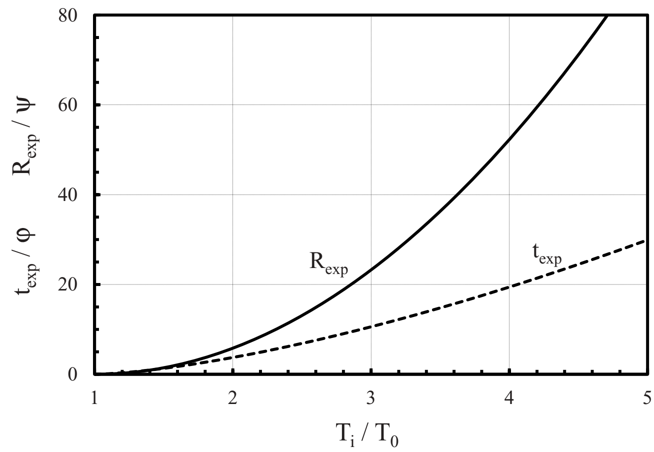

FIG. 4. Scaled instant and position of explosion, $t_{\rm exp}/\varphi$ and $R_{\rm exp}/\psi$, versus the scaled ignition temperature T_i/T_0 for $\Theta = 8$, $\gamma = 7/5$, and $\alpha = 4/3$.

The value A can also be estimated analytically as follows. Since the total burning rate is given by Eqs. (1)–(3) as

$$U_w = \frac{1}{\Theta}\frac{dR_F}{dt} = \frac{\alpha}{\Theta}A^{1/\alpha}R_F^{\frac{\alpha-1}{\alpha}}, \tag{37}$$

while the self-similar flame dynamics on large scales yields the dependence versus the Darrieus-Landau cutoff λ in the form [14]

$$U_w/S_L \approx \left(\frac{2\pi R_F}{\lambda}\right)^{\frac{\alpha-1}{\alpha}}, \tag{38}$$

we find

$$A \approx \left(\frac{2\pi}{\lambda}\right)^{\alpha-1}\left(\frac{\Theta S_L}{\alpha}\right)^{\alpha}, \quad \varphi \approx \frac{\lambda}{2\pi}c_0^{\frac{1}{\alpha-1}}\left(\frac{\alpha}{\Theta S_L}\right)^{\frac{\alpha}{\alpha-1}}, \quad \psi \approx \frac{\lambda}{2\pi}\left(\frac{\alpha c_0}{\Theta S_L}\right)^{\frac{\alpha}{\alpha-1}}. \tag{39}$$

For standard hydrocarbon combustion, the values in Eq. (38) are also large: $\varphi \approx (10^0 \sim 10^1)$ s, $\psi = (10^2 \sim 10^3)$ m.

These results yield the following insights into the phenomena of DDT. First, assuming that the formulation is appropriate to describe the mechanism of explosion triggering as postulated, then the large time and length scales would imply that unconfined DDT in terrestrial situations due to this mechanism is unlikely. Consequently the occurrence of terrestrial detonation in primarily spherical configuration is likely either through direct initiation or facilitated by interactions with acoustics from confinements or rigid boundaries in the event of DDT. On the other hand, these large dimensions are relevant for astrophysical phenomena such as the supernovae explosion, recognizing nevertheless the significantly different prevailing physics such as the equation of state and the huge gravitational force associated with these stars favoring the rapid development of the Rayleigh-Taylor instability.

Alternatively, it is reasonable to suggest that the formulation presented herein is just the first step in describing the present phenomenon, at the hydrodynamic level, and that an analysis of the diffusive-reactive inner structure of the front, and having it coupled to the hydrodynamics, may significantly revise the quantitative results. An impressive example of such an effect is the factor of 10^8–10^9 difference in the energy needed for the direct initiation of a spherical detonation wave [28], as compared to the estimate by Zel'dovich *et al.* [29], when the inner structure of the detonation wave including its curvature is considered.

V. CONCLUDING REMARKS

In this study we have presented a formulation describing the self-similar accelerative outward propagation of a wrinkled, globally spherical deflagration front. In particular, we have analyzed the dynamic and scalar fields associated with the flame propagation, including the flame-generated compression waves, the time evolution of the radial flow velocity and the sound speed ahead of the front, and the trajectories of the gas particles pushed by the flame. As a result, the burning time of each particle and, finally, the instant of explosion triggering can be determined. It is shown that unconfined DDT in terrestrial situations due to this mechanism is unlikely, since acceleration of the deflagration front due to flame instabilities is typically too weak. Additional implications of the results are discussed, and the potential for further development of the formulation is suggested.

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[1] C. K. Law, *Combustion Physics* (Cambridge University Press, New York, 2006).
[2] S. G. Davis and C. K. Law, Proc. Combust. Inst. **27**, 521 (1998).
[3] K. Kumar, J. E. Freeh, C. J. Sung, and Y. Huang, J. Propul. Power **23**, 428 (2007).
[4] M. P. Burke, Z. Chen, Y. Ju, and F. L. Dryer, Combust. Flame **156**, 771 (2009).
[5] A. P. Kelley, G. Jomaas, and C. K. Law, Combust. Flame **156**, 1006 (2009).
[6] A. P. Kelley and C. K. Law, Combust. Flame **156**, 1844 (2009).
[7] C. Ji, E. Dames, Y. L. Wang, H. Wang, and F. N. Egolfopoulos, Combust. Flame **157**, 227 (2010).
[8] C. K. Law, C. J. Sung, H. Wang, and T. F. Lu, AIAA J. **41**, 1629 (2003).
[9] T. F. Lu and C. K. Law, Prog. Energy Combust. Sci. **35**, 192 (2009).
[10] E. S. Oran, Proc. Combust. Inst. **30**, 1823 (2005).
[11] V. Bychkov, M. V. Popov, A. Oparin, L. Stenflo, and V. M. Chechetkin, Astron. Rep. **50**, 298 (2006).
[12] Z. Chen and Y. Ju, Combust. Theory Modelling **11**, 427 (2007).
[13] Ya. B. Zeldovich, G. I. Barenblatt, V. B. Librovich, and G. M. Makhviladze, *Mathematical Theory of Combustion and Explosion* (Consultants Bureau, New York, 1985).
[14] V. V. Bychkov and M. A. Liberman, Phys. Rev. Lett. **76**, 2814 (1996).
[15] D. Bradley, C. G. W. Sheppard, R. Woolley, D. A. Greenhalgh, and R. D. Lockett, Combust. Flame **122**, 195 (2000).
[16] D. Bradley, T. M. Cresswell, and J. S. Puttock, Combust. Flame **124**, 551 (2001).
[17] G. I. Sivashinsky, Proc. Combust. Inst. **29**, 1737 (2002).
[18] A. G. Istratov and V. B. Librovich, Doklady Akademii Nauk SSSR **168**, 43 (1966).
[19] A. G. Istratov and V. B. Librovich, Acta Astronaut. **14**, 453 (1969).
[20] J. K. Bechtold and M. Matalon, Combust. Flame **67**, 77 (1987).
[21] Y. Gostintsev, A. Istratov, and Y. Shulenin, Combust. Expl. Shock Waves **24**, 563 (1988).
[22] Y. Gostintsev, A. Istratov, N. Kidin, and V. Fortov, High Temperature, **37**, 282 (1999).
[23] G. Jomaas, C. K. Law, and J. K. Bechtold, J. Fluid Mech. **583**, 1 (2007).
[24] K. L. Pan and R. Fursenko, Phys. Fluids **20**, 094107 (2008).
[25] G. Jomaas and C. K. Law, Proc. of the 47th AIAA Aerospace Sciences Meeting and Exhibit, paper 1185 (2009).
[26] G. I. Taylor, Proc. R. Soc. London A **186**, 273 (1946).
[27] V. Bychkov and V. Akkerman, Phys. Rev. E **73**, 066305 (2006).
[28] L. He and P. Clavin, J. Fluid Mech. **277**, 227 (1994).
[29] Y. B. Zel'dovich, S. M. Kogarko, and N. N. Semenov, Sov. Phys. Tech. Phys. **1**, 1689 (1956).