Deflagration-to-Detonation Transition in an Unconfined Space

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1 Introduction

This study is motivated by recent theoretical developments in premixed gas combustion revealing positive feedback between the advancing flame and the flame-driven pressure build-up, which results in the thermal runaway when the flame speed exceeds a critical level [1-4]. The present study is an application of this finding to the problem of deflagration-to-detonation transition (DDT) of a spherical flame expanding in an unconfined environment.

As has long been conjectured, in the unconfined system the expected transition might be caused by the flame acceleration induced by the Darrieus-Landau instability (wrinkling) [5-8]. Indeed, it has been shown recently [4], that for the wrinkled spherical flame the transition may be modeled even within the framework of a one-dimensional formulation by merely replacing the reaction rate term W by $\Sigma^2 W$, with Σ being the degree of folding [1] - the ratio of the total area of the wrinkled front to the area associated with its average radius R. For large radii $\Sigma \propto R^{d-2}$, where d is the wrinkled front fractal dimension [6-8]. Within Σ -based formulation the transition may be triggered at any initial temperature T_0 and pressure P_0 , as soon as R becomes large enough.

The present study is an extension of our recent exploration of the Σ -model (Sec. 4 of Ref. [4]), based on ignition-temperature kinetics and planar geometry, over (i) one-step Arrhenius kinetics and spherical geometry, and (ii) multistep hydrogen-oxygen kinetics and numerically more benign planar geometry.

2 Spherical geometry: one-step Arrhenius kinetics

For the spherical geometry the appropriately scaled set of governing equations reads:

continuity and state,

$$\frac{\partial \hat{\rho}}{\partial \hat{t}} + \frac{1}{\hat{r}^2} \frac{\partial \hat{\rho} \hat{r}^2 \hat{u}}{\partial \hat{r}} = 0, \quad \hat{P} = \hat{\rho} \hat{T}$$
(1)

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momentum,

$$\hat{\rho}\left(\frac{\partial\hat{u}}{\partial\hat{t}} + \hat{u}\frac{\partial\hat{u}}{\partial\hat{r}}\right) + \frac{1}{\gamma}\frac{\partial\hat{P}}{\partial\hat{r}} = -\frac{1}{\hat{r}^2}\frac{\partial\hat{r}^2\hat{\tau}_{rr}}{\partial\hat{r}} + \frac{\hat{\tau}_{\theta\theta} + \hat{\tau}_{\varphi\varphi}}{\hat{r}},\tag{2}$$

where

$$\hat{\tau}_{rr} = -\varepsilon Pr\left(2\frac{\partial\hat{u}}{\partial\hat{r}} - \frac{2}{3}\frac{1}{\hat{r}^2}\frac{\partial\hat{r}^2\hat{u}}{\partial\hat{r}}\right),\tag{3}$$

$$\hat{\tau}_{\theta\theta} = \hat{\tau}_{\varphi\varphi} = -\varepsilon Pr\left(2\frac{\hat{u}}{\hat{r}} - \frac{2}{3}\frac{1}{\hat{r}^2}\frac{\partial\hat{r}^2\hat{u}}{\partial\hat{r}}\right) \tag{4}$$

heat,

$$\frac{1}{\gamma}\hat{\rho}\left(\frac{\partial\hat{T}}{\partial\hat{t}} + \hat{u}\frac{\partial\hat{T}}{\partial\hat{r}}\right) + \left(1 - \frac{1}{\gamma}\right)\hat{P}\frac{1}{\hat{r}^2}\frac{\partial\hat{r}^2\hat{u}}{\partial\hat{r}} =$$
(5)

$$\varepsilon \frac{1}{\hat{r}^2} \frac{\partial}{\partial \hat{r}} \left(\hat{r}^2 \frac{\partial \hat{T}}{\partial \hat{r}} \right) - (\gamma - 1) \hat{\tau}_{rr} \frac{\hat{u}}{\hat{r}} - (\gamma - 1) \hat{u} \frac{\hat{\tau}_{\theta\theta} + \hat{\tau}_{\varphi\varphi}}{\hat{r}} + (1 - \sigma_p) \Sigma^2 \hat{W}$$

mass fraction,

$$\hat{\rho}\left(\frac{\partial\hat{C}}{\partial\hat{t}} + \hat{u}\frac{\partial\hat{C}}{\partial\hat{r}}\right) = \frac{\varepsilon}{Le}\frac{1}{\hat{r}^2}\frac{\partial}{\partial r}\left(\hat{r}^2\frac{\partial\hat{C}}{\partial\hat{r}}\right) - \Sigma^2\hat{W}$$
(6)

Here, $\hat{P} = P/P_0$ is the scaled pressure in units of the initial pressure, P_0 ; $\hat{C} = C/C_0$ is the scaled mass fraction of the deficient reactant in units of its initial value, C_0 ; $\hat{T} = T/T_p$ is the scaled temperature in units of $T_p = T_0 + QC_0/c_p$, the adiabatic temperature of burned gas (products) under constant pressure, P_0 ; T_0 is the initial temperature of unburned gas; Q is the heat release; $\sigma_p = T_0/T_p$; $\gamma = c_p/c_v$; c_p , c_v are specific heats; $\hat{\rho} = \rho/\rho_p$, where $\rho_p = P_0/(c_p - c_v)T_p$ is the density of combustion products in free-space isobaric deflagration; $\hat{u} = u/a_p$ is the scaled flow velocity; $a_p = \sqrt{\gamma(c_p - c_v)T_p}$ is the sonic velocity at $T = T_p$; $\hat{t} = t/t_p$, $\hat{r} = r/r_p$, $r_p = a_p t_p$, where the reference time is defined as $t_p = D_{th}^p/u_p^2$; D_{th}^p is the thermal diffusivity at $T = T_p$; u_p is the velocity of the free-space deflagration relative to the burned gas, regarded as prescribed; $\varepsilon = (u_p/a_p)^2 = (l_{th}/r_p)^2$ is the scaled thermal diffusivity; $l_{th} = D_{th}^p/u_p$ is the flame width; Pr and Le are the Prandtl and Lewis numbers, respectively; $\hat{W} = Wt_p/\rho_p C_0$ is the scaled reaction rate. For simplicity, molecular transport coefficients are assumed to be constant.

The reason for Σ^2 in Eqs. (5) (6) is explained as follows. According to the classical Zeldovich-Frank Kamenetskii analysis, for a low Mach number planar flame its propagation velocity is proportional to the square root of the reaction rate. On the other hand, the effective velocity of the wrinkled flame is proportional to its degree of folding, Σ [1]. Hence, the effective reaction rate of the wrinkled flame should be proportional to Σ^2 . Indeed, simulations of the Σ^2 - based models corroborate this assessment, at least for moderately high Σ -s (see Ref. [3] and Fig. 3(b) below).

The reaction rate W is modeled by the one-step Arrhenius kinetics, whose scaled version \hat{W} reads,

$$\hat{W} = Z\hat{\rho}^{n}\hat{C}\exp[N_{p}(1-\hat{T}^{-1})],\tag{7}$$

where $Z = \frac{1}{2}Le^{-1}N_p^2(1-\sigma_p)^2$ is the normalizing factor to ensure that at $N_p \gg 1$ and isobaric conditions $(\varepsilon \ll 1)$ the scaled planar deflagration speed relative to the burned gas approaches $\Sigma\sqrt{\varepsilon}$. Here $N_p = T_a/T_p$

is the scaled activation temperature.

According to the well known Gostintsev correlation [6], for large radii

$$R = At^{\frac{3}{2}}, \quad d = \frac{7}{3}$$
 (8)

and

$$\Sigma = \frac{3A^{\frac{2}{3}}R^{\frac{1}{3}}}{2u_p} = K\hat{R}^{\frac{1}{3}}, \text{ provided } \Sigma > 1$$
(9)

where

$$K = \frac{3A^{\frac{2}{3}}a_p^{\frac{1}{3}}(D_{th}^p)^{\frac{1}{3}}}{2u_p^{\frac{5}{3}}}$$
(10)

Equations (1)-(6) are considered over a semi-infinite interval $\hat{a} < \hat{r} < \infty$. Here \hat{a} is a small number to avoid dealing with the zero/zero limit at $\hat{r} \to 0$. The pertinent solution is required to meet the following initial and boundary conditions,

$$\hat{T}(\hat{r},0) = \sigma_p + (1-\sigma_p) \exp\left[(\hat{a}-\hat{r})/\hat{l}\right], \ \hat{C}(\hat{r},0) = 1, \ \hat{P}(\hat{r},0) = 1, \ \hat{\rho}(\hat{r},0) = 1/\hat{T}(\hat{r},0), \ \hat{u}(\hat{r},0) = 0$$
(11)

$$\partial \hat{T}(\hat{a},\hat{t})/\partial \hat{r} = 0, \quad \partial \hat{C}(\hat{a},\hat{t})/\partial \hat{r} = 0, \quad \hat{u}(\hat{a},\hat{t}) = 0, \tag{12}$$

$$\hat{T}(+\infty,\hat{t}) = \sigma_p, \quad \hat{C}(+\infty,\hat{t}) = 1, \quad \hat{P}(+\infty,\hat{t}) = 1, \quad \hat{\rho}(+\infty,\hat{t}) = 1/\sigma_p, \quad \hat{u}(+\infty,\hat{t}) = 0$$
(13)

The scaled flame radius \hat{R} is defined as,

$$\hat{R} = \left[3\int_{\hat{a}}^{\infty} (1-\hat{C})\hat{r}^2 d\hat{r} + \hat{a}^3\right]^{\frac{1}{3}}$$
(14)

In the chosen units the scaled velocity of Chapman-Jouguet detonation becomes,

$$\hat{D}_{CJ} = D_{CJ}/a_p = \frac{1}{2} \left(\sqrt{2(\gamma+1)(1-\sigma_p)} + \sqrt{2(\gamma+1)(1-\sigma_p) + \sigma_p} \right)$$
(15)

In numerical simulations the parameters employed are specified as follows,

$$Pr = 0.75, \ Le = 1, \ N_p = 4, \ n = 3, \ \gamma = 1.3, \ \varepsilon = 0.0025, \ \sigma_p = 0.125, \ K = 0.289, \ \hat{a} = 0.01, \ \hat{l} = 0.005.$$
(16)

In dimensional units this parameter set may correspond to,

$$T_{0} = 293 \text{K}, \ T_{p} = 2,344 \text{K}, \ T_{a} = N_{p}T_{p} = 9,376 \text{K}, \ P_{0} = 1 \text{atm}, \ a_{0} = 340 \text{m/s},$$
$$a_{p} = a_{0}/\sqrt{\sigma_{p}} = 962 \text{m/s}, \ D_{th}^{p} = D_{th}^{0}/\sigma_{p}^{1.75} = 1.9 \cdot 10^{-3} \text{m}^{2}/\text{s}, \ D_{th}^{0} = 5 \cdot 10^{-5} \text{m}^{2}/\text{s},$$
$$u_{0} = \sqrt{\varepsilon \sigma_{p}} a_{0} = 6 \text{m/s}, \ u_{p} = u_{0}/\sigma_{p} = 48 \text{m/s}, \ A = 1000 \text{m/s}^{\frac{3}{2}}.$$
 (17)

Parameters chosen in Eqs. (16) (17) are intended to represent a typical fast burning premixture rather than a specific, e.g. H_2/O_2 , system.

Note that relations (8) (9) are valid only for sufficiently large R where Σ exceeds unity. Otherwise Σ is set at unity. At the critical point where $\Sigma = 1$, according to Eqs. (9) (16) and Fig. 1, $\hat{R}_{cr} = K^{-3} = 41.429$

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Figure 1: Time records of the flame speed \hat{D} and degree of folding Σ . Unmarked line corresponds to the case of unwrinkled flame, $\Sigma = 1$. The hats on the labels have been omitted.

and $\hat{t}_{cr} = 700$.

Figure (1) depicts time records of Σ and $\hat{D} = d\hat{R}/d\hat{t}$. Here at the transition point $\Sigma_{DDT} = 2.86$, $\hat{t}_{DDT} = 5400$, $\hat{R}_{DDT} = 977$, or in dimensional units $R_{DDT} = 0.766$ m (see (17)).

Note that upon the transition the level of wrinkling is expected to drop dramatically, effectively reducing Σ to unity (see Fig. 13 of Ref. [3]). The post-transition raise of Σ on Fig.(1) should therefore be considered as the model's artefact. Figure (2) shows spatial profiles of state variables at several equidistant instants of time prior to the transition.



Figure 2: Profiles of scaled pressure (\hat{P}) , temperature (\hat{T}) , density $(\hat{\rho})$ and gas velocity (\hat{u}) at several consecutive equidistant instants of time adjacent to the transition point. The hats on the labels have been omitted.

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3 Planar geometry: hydrogen-oxygen system

To assess R_{DDT} for a realistic multistep chemistry, while avoiding the issue of an enormous disparity between the spatial scales involved aggravated by a large number of species and multicomponent transport, the discussion here is restricted to the numerically more benign case of a planar geometry. At the same time the parametric $\Sigma(R)$ dependency is assumed to be valid (see also Sec. 4 of Ref. [4]).

Figure (3) shows flame speed $D(\Sigma)$ dependency calculated for the stoichiometric hydrogen-oxygen mixture at $T_0 = 300$ K and $P_0 = 1$ atm. The chemical and transport models adopted follow those of Refs. [9-11]. In this case at $\Sigma = 1$ one ends up with $u_0 = 10.1$ m/s, $\sigma_p = 0.121$ and $u_p = u_0/\sigma_p = 83.5$ m/s. At the transition point $\Sigma_{DDT} = 8.2$.



Figure 3: Flame speed D(m/s) relative to unburned gas versus Σ for the planar geometry. Across the transition point D undergoes an abrupt increase from D = 78m/s to D = 2,800m/s. The right frame corresponds to the reduced area, 0 < D < 100m/s.

According to Gostintsev et al. [6], for $2H_2 + O_2$ mixture $A = 2,530 \text{m/s}^{\frac{3}{2}}$, and therefore $R_{DDT} = 14.9 \text{m}$ (see Eq. (9)). This outcome explains the difficulties with experimental reproduction of the effect in an open space.

4 Concluding remarks

- The above Σ -model presumably provides a qualitative reproduction of the classical experiment of Zeldovich & Rozlovskii [5] on DDT in a closed spherical vessel (15cm inner diameter) filled with the mixture of H₂(56.6%), O₂(41.4%), CS₂(2%) under elevated initial pressure (10atm). Here, prior to the transition occurring at $R_{DDT} = 2.5$ cm, the precursor shock does not reach the outer boundary, thereby imitating the situation in an unconfined environment.
- The Σ-model offers a simple mechanism which might be responsible for DDT in thermonuclear supernovae that attracts much attention nowadays [12].

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