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Deflagration-to-detonation transition in an unconfined space

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ABSTRACT

Whereas deflagration-to-detonation transition in confined systems is a matter of common knowledge, feasibility of the transition in unconfined space is still a matter of controversy. With a freely expanding self-accelerating spherical flame as an example, it is shown that deflagration-to-detonation transition in unconfined gaseous systems is indeed possible provided the flame is large enough. The transition is caused by positive feedback between the accelerating flame and the flame-driven pressure buildup, which results in the thermal runaway when the flame speed reaches a critical level.

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 Section 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,

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

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,

$$\frac{1}{\gamma}\hat\rho\left(\frac{\partial \hat T}{\partial \hat t} + \hat u\frac{\partial \hat T}{\partial \hat r}\right) + \left(1 - \frac{1}{\gamma}\right)\hat P \frac{1}{\hat r^2}\frac{\partial \hat r^2 \hat u}{\partial \hat r}$$
$$= \varepsilon \frac{1}{\hat r^2}\frac{\partial}{\partial \hat r}\left(\hat r^2 \frac{\partial \hat T}{\partial \hat r}\right) - (\gamma - 1)\hat\tau_{rr}\frac{\hat u}{\hat r} - (\gamma - 1)\hat u \frac{\hat\tau_{\theta\theta} + \hat\tau_{\varphi\varphi}}{\hat r}$$
$$+ (1 - \sigma_p)\Sigma^2 \hat W \tag{5}$$

mass fraction,

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

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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 $t_p = D^p_{th}/u_p^2$; D^p_{th} 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; $l_{th} = D^p_{th}/u_p$ is the flame width; Pr and Le are the Prandtl and Lewis numbers, respectively; $\hat{W} = W t_p/\rho_p C_0$ is the scaled reaction rate. For simplicity, molecular transport coefficients are assumed to be constant.

The reason for Σ^2 in Eqs. (5) and (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 Figs. 1, 4, 6, 8 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 n is the reaction order, $Z = \frac{1}{2}Le^{-1}N_p^2(1 - \sigma_p)^2$ 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,

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

and

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

where

$$K = \frac{3A^{\frac{2}{3}}a_p^{\frac{1}{3}}(D^p_{th})^{\frac{1}{3}}}{2u_p^{\frac{5}{3}}} \tag{10}$$

Eqs. (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,

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

$$\hat{\rho}(\hat{r},0) = 1/\hat{T}(\hat{r},0), \ \hat{u}(\hat{r},0) = 0$$

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

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

$$\hat{u}(+\infty,\hat{t}) = 0$$

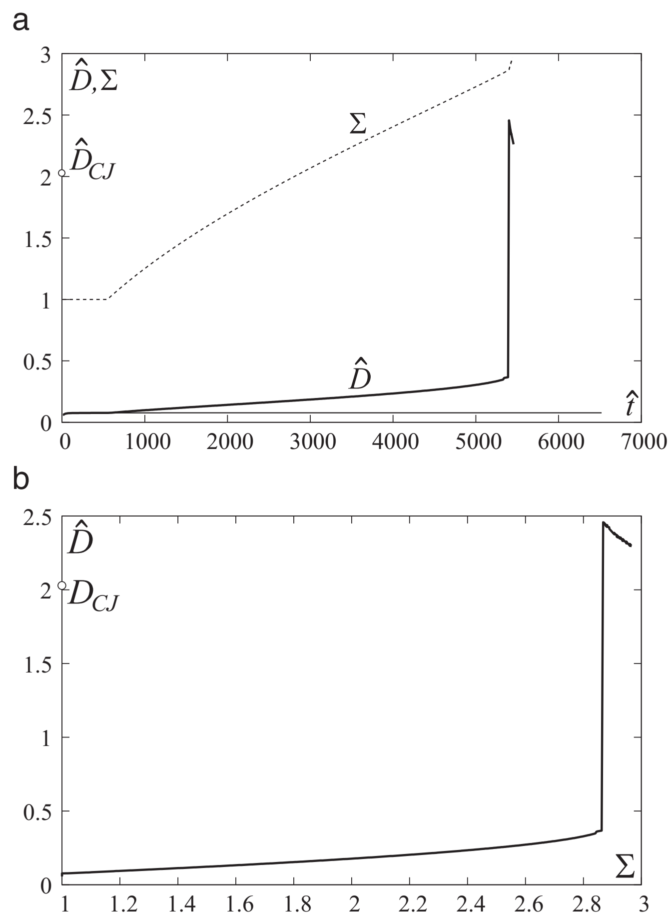

Fig. 1. Spherical flame. (a) Time records of the flame speed $\hat{D}$ and degree of folding Σ; spatial step $\hat{h} = 0.005$. Unmarked line corresponds to the case of unwrinkled flame, $\Sigma = 1$; (b) $\hat{D}(\Sigma)$-dependency.

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

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

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

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

The numerical method and its validation follow those of Ref. [9].

Parameters employed are specified as follows,

$$Pr = 0.75, \ Le = 1, \ N_p = 4, \ n = 3, \ \gamma = 1.3, \ \varepsilon = 0.0025, \ \sigma_p = 0.125, \tag{16}$$

$$K = 0.289, \ \hat{a} = 0.01, \ \hat{l} = 0.005.$$

In dimensional units this parameter set may correspond to,

$$T_0 = 293\,\mathrm{K}, \ T_p = 2,344\,\mathrm{K}, \ T_a = N_pT_p = 9376\,\mathrm{K}, \ P_0 = 1\,\mathrm{atm},$$

$$a_0 = 340\,\mathrm{m/s}, \ a_p = a_0/\sqrt{\sigma_p} = 962\,\mathrm{m/s}, \ D_{CJ} = a_p\hat{D}_{CJ} = 1.945\,\mathrm{m/s}, \tag{17}$$

$$\hat{D}_{CJ} = 2.022, \ D^p_{th} = D^0_{th}/\sigma_p^{1.75} = 1.9 \cdot 10^{-3}\,\mathrm{m^2/s}, \ D^0_{th} = 5 \cdot 10^{-5}\,\mathrm{m^2/s},$$

$$u_0 = \sqrt{\varepsilon\sigma_p}a_0 = 6\,\mathrm{m/s}, \ u_p = u_0/\sigma_p = 48\,\mathrm{m/s}, \ A = 1000\,\mathrm{m/s^{\frac{3}{2}}}.$$

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