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 \(\Sigma\) 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 \(\Sigma\)-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 \(\Sigma\)-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:

\[
\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial \rho r^2 \dot{u}}{\partial r} = 0, \quad \dot{P} = \dot{\rho} \dot{T}
\] (1)
The reaction rate \( W \) is modeled by the one-step Arrhenius kinetics, whose scaled version \( \hat{W} \) reads,

\[
\hat{W} = Z \rho^\epsilon \hat{C} \exp[\hat{N}_p(1 - \hat{T}^{-1})],
\]

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 \( (\epsilon \ll 1) \) the scaled planar deflagration speed relative to the burned gas approaches \( \Sigma \sqrt{\epsilon} \). Here \( N_p = T_a/T_p \).
In dimensional units this parameter set may correspond to,

\[ R = At^3, \quad d = \frac{7}{4} \]

and

\[ \Sigma = \frac{3A^2 R^2}{2u_p} = K \hat{R}^\frac{1}{4}, \text{ provided } \Sigma > 1 \]

where

\[ K = \frac{3A^2 a^2 \hat{\rho} (D_{th})^\frac{1}{2}}{2u_p^\frac{3}{2}} \]

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,

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

\[
\partial \hat{T}(\hat{a}, \hat{t}) / \partial \hat{r} = 0, \quad \partial \hat{C}(\hat{a}, \hat{t}) / \partial \hat{r} = 0, \quad \hat{u}(\hat{a}, \hat{t}) = 0,
\]

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

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

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

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

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

In numerical simulations the parameters employed are specified as follows,

\[ Pr = 0.75, \quad Le = 1, \quad N_p = 4, \quad n = 3, \quad \gamma = 1.3, \quad \varepsilon = 0.0025, \quad \sigma_p = 0.125, \quad K = 0.289, \quad \hat{a} = 0.01, \quad \hat{l} = 0.005. \]

In dimensional units this parameter set may correspond to,

\[ T_0 = 293K, \quad T_p = 2,344K, \quad T_a = N_p T_p = 9,376K, \quad P_0 = 1\text{atm}, \quad a_0 = 340m/s, \]

\[ a_p = a_0/\sqrt{\sigma_p} = 962m/s, \quad D^0_{th} = D^0_{th}/a_p^{1.75} = 1.9 \cdot 10^{-3}m^2/s, \quad D^0_{th} = 5 \cdot 10^{-5}m^2/s, \]

\[ u_0 = \sqrt{\sigma_p a_0} = 6m/s, \quad u_p = u_0/\sigma_p = 48m/s, \quad A = 1000m/s^2 \]

Parameters chosen in Eqs. (16) (17) are intended to represent a typical fast burning premixture rather than a specific, e.g. \( \text{H}_2/\text{O}_2 \), system.

Note that relations (8) (9) are valid only for sufficiently large \( R \) where \( \Sigma \) exceeds unity. Otherwise \( \Sigma \) is set at unity. At the critical point where \( \Sigma = 1 \), according to Eqs. (9) (16) and Fig. 1, \( \hat{R}_{cr} = K^{-3} = 41.429 \)
Figure 1: Time records of the flame speed $\hat{D}$ and degree of folding $\Sigma$. 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 $\Sigma$ 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 $\Sigma$ to unity (see Fig. 13 of Ref. [3]). The post-transition raise of $\Sigma$ 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.
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 $\Sigma_{DDT} = 8.2$.

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

4 Concluding remarks

- The above $\Sigma$ -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 $H_2(56.6\%), O_2(41.4\%), CS_2(2\%)$ 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 $\Sigma$-model offers a simple mechanism which might be responsible for DDT in thermonuclear supernovae that attracts much attention nowadays [12].

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References


