On metastable deflagration in porous media combustion

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Abstract

A regime of low velocity deflagration in hydraulically-resisted flows as those occurring in porous beds is discussed. An asymptotic expression for the deflagration velocity is derived. The obtained dependency elucidates the mechanism controlling the gradual enhancement of the propagation velocity prior to the abrupt transition from slow to fast combustion. This enhancement is caused by the drag-induced diffusion of pressure ahead of the advancing front. The time of transition from the slow to fast propagation is estimated.

Keywords: *asymptotic analysis, combustion fronts, deflagration-to-detonation transition*

1 Introduction

As is well known there are basically two mechanisms controlling propagation of combustion waves in gaseous mixtures: molecular transport and adiabatic compression. Normally adiabatic compression is provided by the shock and the resulting combustion wave propagates at a supersonic speed. This coupling however is not inevitable. In hydrodynamically resisted flows, such as develop in porous beds, the burning velocity may fall significantly below its thermodynamic Chapman-Jouguet value, and under certain conditions may well become subsonic and therefore shockless. This fast combustion regime is called subsonic detonation [15].

Perhaps the physically simplest and yet experimentally quite feasible system for studying subsonic detonation is combustion in inert porous medium [12]. In this case, on the one hand, the distortions introduced by the porous matrix may be ignored while, on the other hand, the resistance of the matrix to the gas flow is often so strong that one may neglect the inertial effects and take Darcy's law as the momentum equation. In this high drag limit the shocks are ruled out and the pressure non-uniformities are equalized not by the acoustic waves but rather through the diffusion of pressure associated with low Reynolds number creeping flows.

To single out the impact of momentum loss the effective features of the reactive gas-porous medium system will be assumed to be controlled exclusively by its gaseous phase subjected to the resistance of the porous matrix. As an additional simplification the so-called small-heat-release

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(SHR) approximation will be employed where variations of temperature, pressure, density and gas velocity are regarded as small and, hence, the nonlinear effects are ignored everywhere but in the reaction rate term, generally highly sensitive even to minor temperature changes. In the non-dimensional formulation the resulting model reads [2],

$$\gamma\Theta_t - (\gamma-1)\Pi_t = \varepsilon\gamma\Theta_{xx} + \Psi f(\Theta), \tag{1}$$

$$\Psi_t = \varepsilon Le^{-1}\Psi_{xx} - \Psi f(\Theta), \tag{2}$$

$$\Pi_t = \Pi_{xx} + \Theta_t. \tag{3}$$

Here Π,Θ and Ψ are the appropriately scaled pressure, temperature and concentration of deficient reactant; $\gamma > 1$ is the specific heat ratio; ε is the thermal diffusivity/pressure diffusivity ratio and $\Psi f(\Theta)$ is the scaled reaction rate.

Eqs.(1), (2) represent the partially linearized conservation equations for energy and concentration of the deficient reactant, while Eq.(3) is a linearized continuity equation.

In the case of a homogeneous explosion, i.e when the spatial derivatives vanish, the system becomes,

$$\gamma\Theta_t - (\gamma-1)\Psi_t = \Psi f(\Theta), \tag{4}$$

$$\Psi_t = -\Psi f(\Theta), \tag{5}$$

$$\Pi_t = \Theta_t. \tag{6}$$

Equations (4)-(6) yield [5]

$$\Psi = 1 - \Theta. \tag{7}$$

For the sake of simplicity, following [5], we replace Eq.(2) by (7) for the general non-homogeneous case. The original formulation thus is substituted by a more tractable model involving only two equations

$$\gamma\Theta_t - (\gamma-1)\Pi_t = \varepsilon\gamma\Theta_{xx} + \Omega(\Theta), \tag{8}$$

$$\Pi_t = \Pi_{xx} + \Theta_t. \tag{9}$$

where $\Omega(\Theta) = (1-\Theta)f(\Theta)$. The model (8),(9) (according to the numerical simulations) preserves the main qualitative features of the original model (1)-(3), and will be studied hereafter.

For many realistic porous systems ε varies within the range $\varepsilon \sim 10^{-3} - 10^{-6}$ which makes it a natural small parameter.

When ε is small one may single out two distinct modes of combustion [15]: (i) fast wave driven by the diffusion of pressure and (ii) slow wave driven by the molecular transport. Moreover, numerical simulations reveal two possible regimes of propagation: depending on initial data the fast combustion wave (regime (i)) forms either immediately or after a long induction time as a result of an abrupt transition from slowly spreading deflagration driven by thermal diffusivity (see Fig. 1).

The first regime corresponds to the traveling wave solution of the system (8),(9). According to the numerical simulations [15] this solution is unique and, at least for some nonlinearities $\Omega(\Theta)$, is stable. Therefore this regime can be easily identified and, in principle, exists for an arbitrary long time interval. The second regime is slightly more involved. It was revealed numerically [2] that for some class of initial data the solution is close to the traveling wave solution of the Eq.(8) with $\Pi = 0$ in the following sense: the solution is close to the traveling wave, and its velocity is nearly constant. This behavior is typical for localized initial data and persists on a time interval of the order of $\varepsilon^{-1/2}$. This feature allows us to call the second regime metastable.

The first (fast) regime has been studied in a number of papers and is relatively well understood both mathematically [5][8],[9],[10] and physically [1],[3],[4]. There are however some new results concerning the second (slow) regime [3], [4] which are discussed in this study.

In order to evaluate the propagation velocity it is convenient to introduce the bulk burning rate defined as [6],

$$V(t) = \int_{-\infty}^{\infty} \Theta_t(x,t)dx = \int_{-\infty}^{\infty} \Pi_t(x,t)dx = \int_{-\infty}^{\infty} \Omega(\Theta(x,t))dx. \tag{10}$$

Note that when $(\Theta,\Pi)(x,t)$ is a traveling wave solution $(\Theta,\Pi)(x-ct)$, $V(t)=c$, but Eq.(10) is valid for general initial data.

For further considerations it is convenient to rewrite the system (8), (9) as

$$\Theta_t = \varepsilon\gamma\Theta_{xx} + \Omega(\Theta) + (\gamma-1)\Pi_{xx}, \tag{11}$$

$$\Pi_t = \Pi_{xx} + \Theta_t. \tag{12}$$

Initially the pressure field is assumed to be uniform $\Pi(x,0)=0$. The initial temperature $\Theta(x,0)$ is specified as a profile given by the traveling wave solution defined by,

$$\Theta_t = \varepsilon\gamma\Theta_{xx} + \Omega(\Theta), \quad \Theta(\infty,t)\to 0, \quad \Theta(-\infty,t)\to 1 \tag{13}$$

with

$$\Theta = \Theta_0(\xi), \quad \xi = \frac{x - c\sqrt{\lambda}t}{\sqrt{\lambda}}, \quad \lambda = \varepsilon\gamma, \tag{14}$$

where $c>0$ is the velocity of the deflagration wave. Substituting (14) into Eq.(13) yields,

$$-c\frac{d\Theta_0}{d\xi} = \frac{d^2\Theta_0}{d\xi^2} + \Omega(\Theta_0), \quad \Theta_0(\infty)\to 0, \quad \Theta_0(-\infty)\to 1 \tag{15}$$

Solving this eigenvalue problem we determine both a profile of the deflagration wave Θ_0 and its velocity c. In addition we require the following properties to be met:

i) The solution of Eq.(15) is unique;

ii) Propagation velocity $c \sim O(1)$;

iii) $\Omega(\Theta)$ is independent of ε;

iv) $\Omega(\Theta)$ is such that $\Theta(\eta) \sim exp(-c\xi)$ as $\xi\to\infty$

The above properties are held for the reaction rates normally employed in combustion.

A typical example of such a reaction rate is the Arrhenius kinetics [19],[18]:

$$\Omega(\Theta) = (1-\Theta)\exp(-\beta/\Theta) \tag{16}$$

where β is the scaled activation energy.

2 Asymptotic analysis

In this section we construct an approximate solution of the problem (11),(12) with initial conditions $\Pi(x,0)=0$ and (14).

The asymptotic approach we use here is described in [13]. Mathematical details and validation of the pertinent analysis can be found in [16].

It is clear that the pressure Π and its spatial derivatives are small for some relatively large time intervals, and the problem (11),(12) therefore can be treated asymptotically.

The idea of the asymptotic approach is rather simple. First we assume that pressure field Π is small and prescribed. Then Π_{xx} in Eq.(11) can be considered as a perturbation. Therefore the temperature field is independent of pressure in the first approximation. This fact in turn implies that the pressure Π in the first approximation can be obtained from Eq.(12) as a convolution of the heat kernel with the time derivative of the temperature, which again allows calculation of the first correction for the temperature field, and in particular the correction to the velocity of the front.

We seek the solution of Eq.(11) in the following form,

$$\Theta(x,t) = \Theta_0(\eta) + \sqrt{\lambda}\Theta_1(\eta, \sqrt{\lambda}t) + O(\lambda), \quad \eta = \frac{x - c\sqrt{\lambda}t - q(\lambda t)}{\sqrt{\lambda}}, \tag{17}$$

where $q(t)$ is a first correction to the position of the wave. The ansatz (17) is valid on the time interval $O(\lambda^{-1/2})$.

Substituting (17) into (11) and equating terms of successive powers of λ, one obtains

$$\Theta_1'' + c\Theta_1' + \Omega'(\Theta_0)\Theta_1 = -F, \quad F = \frac{dq}{d\tilde{t}}\Theta_0' + \frac{(\gamma-1)}{\sqrt{\lambda}}\Pi_{xx}, \tag{18}$$

where $\tilde{t} = \lambda t$ and $' = d/d\eta$.

This equation can be easily solved in terms of Θ_0. Indeed, presenting the correction as the product

$$\Theta_1(x,t) = z(\eta, \tilde{t})\Theta_0'(\eta) \tag{19}$$

and substituting (19) into (18) one obtains

$$z\left(\Theta_0'' + c\Theta_0' + \Omega(\Theta_0)\right)' + z''\Theta_0' + 2z'\Theta_0'' + cz'\Theta_0' = -F. \tag{20}$$

Multiplying right and left of (20) by $\Theta_0' \exp(c\eta)$ one obtains

$$\left(z'\Theta'^2 \exp(c\eta)\right)' = -F\Theta' \exp(c\eta). \tag{21}$$

Integration of Eq. (21) finally yields

$$\Theta_1(\eta, \sqrt{\lambda}t) = -\Theta_0'(\eta)\int_{-\infty}^{\eta} \frac{e^{-c\eta_1}d\eta_1}{\Theta_0'(\eta_1)^2}\int_{-\infty}^{\eta_1} F(\eta_2, t)\Theta_0'(\eta_2)e^{c\eta_2}d\eta_2. \tag{22}$$

It is clear (see property iv) that the function $e^{-c\eta_1}\Theta_0'(\eta_1)^{-2}$ in the outer integral (22) increases exponentially when $\eta_1 \to \infty$. Therefore this integral (as well as Θ_1) will be bounded only if the inner integral approaches zero for $\eta_1 \to \infty$. The solvability condition for this problem therefore can be written as,

$$\int_{-\infty}^{\infty} F(\eta, t)\Theta_0'(\eta)\exp(c\eta)d\eta = 0. \tag{23}$$

This condition determines $q(t)$. Using Eq.(18) the condition (23) can be rewritten as,

$$\frac{dq}{d\tilde{t}} = -\frac{(\gamma-1)}{\sqrt{\lambda}M}\int_{-\infty}^{\infty}\Pi_{xx}\Theta_0' \exp(c\eta)d\eta, \quad M = \int_{-\infty}^{\infty}{\Theta_0'}^2 \exp(c\eta)d\eta. \tag{24}$$

This expression can be simplified. Indeed Π_{xx} is a small and a slowly decaying function on the scale of η. On the other hand, $\Theta_0' \exp(c\eta)$ is close to a constant beyond some $\eta \sim O(1)$ i.e $x \sim O(\sqrt{\lambda})$, and rapidly decays for $\eta \le 0$. Thus the main contribution to the integral comes from the integration over the unburned gas region,

$$\int_{-\infty}^{\infty} \Pi_{xx}\Theta_0' \exp(c\eta)d\eta = \frac{-S}{\sqrt{\lambda}}\int_{c\sqrt{\lambda}t}^{\infty} \Pi_{xx}dx = \frac{S}{\sqrt{\lambda}}\Pi_x(c\sqrt{\lambda}t, t), \tag{25}$$

$$S = \int_{-\infty}^{\infty} \Omega(\Theta_0)\exp(c\eta)d\eta. \tag{26}$$

The last step is the calculation of the pressure distribution. Using the heat kernel Eq.(12) may be recast as follows,

$$\Pi(x,t) = \frac{1}{2\sqrt{\pi}}\int_0^t\int_{-\infty}^{\infty} \Theta_\tau(y,\tau)\exp\left(-\frac{(x-y)^2}{4(t-\tau)}\right)\frac{dyd\tau}{\sqrt{t-\tau}}. \tag{27}$$

Substituting the asymptotic solution for the temperature one obtains

$$\Pi(x,t) = \frac{-c}{2\sqrt{\pi}}\int_0^t\int_{-\infty}^{\infty} \Theta'\left(\frac{y-c\sqrt{\lambda}\tau}{\lambda}\right)\exp\left(-\frac{(x-y)^2}{4(t-\tau)}\right)\frac{dyd\tau}{\sqrt{t-\tau}} + O(\lambda). \tag{28}$$

Applying the Laplace formula we obtain

$$\Pi(x,t) = \frac{c\sqrt{\lambda}}{2\sqrt{\pi}}\int_0^t \exp\left(-\frac{(x-c\sqrt{\lambda}\tau)^2}{4(t-\tau)}\right)\frac{d\tau}{\sqrt{t-\tau}}. \tag{29}$$

Differentiation with respect to x yields

$$\Pi_x(x,t) = -\frac{c\sqrt{\lambda}}{4\sqrt{\pi}}\int_0^t \frac{(x-c\sqrt{\lambda}\tau)}{(t-\tau)}\exp\left(-\frac{(x-c\sqrt{\lambda}\tau)^2}{4(t-\tau)}\right)\frac{d\tau}{\sqrt{t-\tau}}. \tag{30}$$

Thus,

$$\Pi_x(c\sqrt{\lambda}t, t) = -\frac{c^2\lambda}{4\sqrt{\pi}}\int_0^t \exp\left(-c^2\lambda\frac{(t-\tau)}{4}\right)\frac{d\tau}{\sqrt{t-\tau}} = -\frac{c^2\lambda\sqrt{t}}{2\sqrt{\pi}}. \tag{31}$$

Substitution of (31) into (24),(25) yields

$$\frac{dq}{d\tilde{t}} = (\gamma-1)Nc^2\frac{\sqrt{t}}{2\sqrt{\pi}} \quad N = \int_{-\infty}^{\infty}\Omega(\Theta_0)\exp(c\eta)d\eta \Big/ \int_{-\infty}^{\infty}{\Theta_0'}^2\exp(c\eta)d\eta. \tag{32}$$

Scaling back to the original time scale one obtains

$$\frac{dq}{dt} = \lambda(\gamma-1)Nc^2\frac{\sqrt{t}}{2\sqrt{\pi}}, \tag{33}$$

and finally

$$V(t) = \sqrt{\varepsilon\gamma}c\left(1 + \frac{(\gamma-1)Nc}{2}\sqrt{\frac{\varepsilon\gamma t}{\pi}}\right). \tag{34}$$

This expression jointly with (17) implies that the slow deflagration persists on the time interval at least of the order of $\varepsilon^{-1/2}$. This estimate seems to be in line with the numerical observation reported in [4].

In order to check the accuracy of the relation (34) a number of numerical experiments with the system (11), (12) were performed. Figure 2 shows the value of the bulk burning rate obtained by direct numerical simulations of the system (11),(12) and the asymptotic relation (34). As is readily seen these two curves are indeed close on the time interval $\sim \varepsilon^{-1/2}$.

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Figure Captions

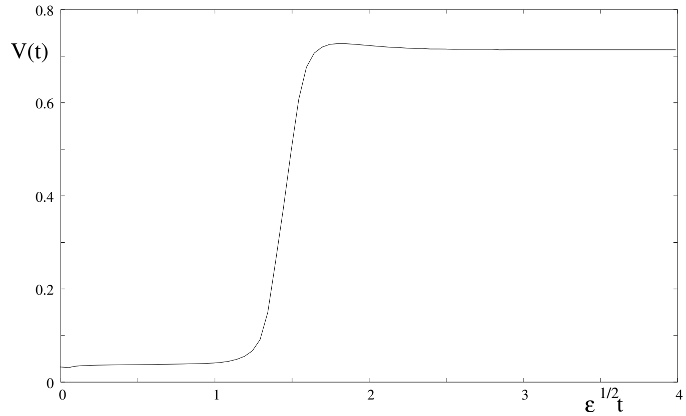

Figure 1. Transition from the slow to fast combustion ($\varepsilon = 10^{-3}$,$\gamma = 1.3$).

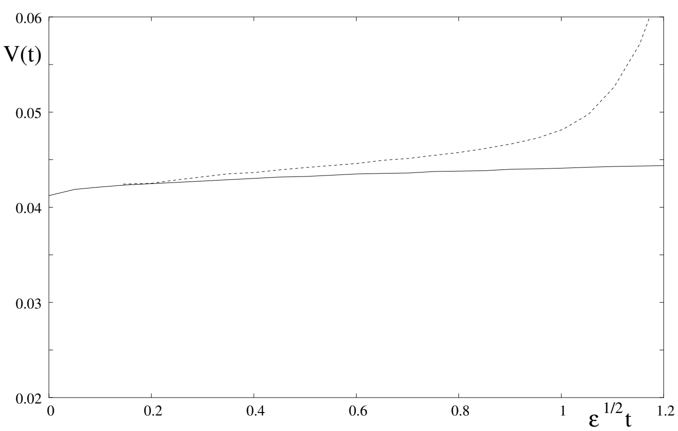

Figure 2. Asymptotic (solid line) and numerical (dashed line) values of the bulk burning rate versus scaled time ($\varepsilon = 10^{-3}$, $\gamma = 1.3$).