Pressure Diffusivity and Low-Velocity Detonation

Peter V. Gordon[a] and Gregory I. Sivashinsky[b]*
[a]Department of Mathematics, University of Chicago,
Chicago, IL 60637, USA
[b]School of Mathematical Sciences, Tel Aviv University,
Tel Aviv 69978, Israel

Abstract

The mechanism controlling occurrence of the low-velocity denotation in obstacle-laden systems is discussed. A quasi-one-dimensional model where the impact of obstacles is accounted for through a drag-force term is explored. It is shown that the hydraulic resistance gives rise to a powerful agency (diffusion of pressure) capable of driving the combustion wave both at fast subsonic as well as supersonic velocities. The latter mode is identified with the so-called choking regime often observed in obstacle-affected detonations.

Keywords: *quasi-detonation, choking regime, low-velocity detonation.*

1 Introduction

It has long been known that the flow impediments have a profound effect on gaseous detonation markedly reducing its propagation velocity compared to its thermodynamic, Chapman-Jouguet (CJ) value [1, 2]. Moreover, the obstacle-affected detonation may exhibit fascinating jumpwise transitions from a high-velocity sub-CJ *quasi-detonation* to a low-velocity detonation in a *choking regime* [3–9]. Whereas both detonation modes are supersonic relative to the fresh mixture, the choking regime is subsonic relative to the burned gas. As has been recently realized, this peculiarity of confined detonation may be successfully described in the framework of a quasi-one-dimensional ZND-Fanno formulation where the impact of obstacles is modeled by a drag-force term [10, 11]. Apart from the well-known sub-CJ quasi-detonation, the ZND-Fanno formulation yields both the low-velocity yet supersonic choking regime and the shockless subsonic regime driven by the drag-induced diffusion of pressure and occasionally observed in porous bed combustion [12] (Fig.1). The multiplicity of detonation regimes may thus be interpreted as a product of the interplay between two mechanisms controlling adiabatic compression: shocks and diffusion of pressure. For quasi-detonation (low

*Corresponding author.
E-mail address: grishas@post.tau.ac.il (G. Sivashinsky)

hydraulic resistance) the process is dominated by the first mechanism, while for the subsonic regime (strong hydraulic resistance) by the second. Yet, the relative impact of the above mechanisms on the intermediate choking regime remains unclarified. The objective of this note is to demonstrate that the choking detonation is physically quite similar to its subsonic counterpart, and may be sustained exclusively by the drag-induced diffusion of pressure. The shock accompanying the choking regime appears not as a driving agency, as occurs in conventional detonation, but rather as the forced outcome of supersonic propagation ensured by an extremely high level of the developing pressure diffusivity.

The ZND-Fanno formulation for reactive flows in obstructed channels, understandably, cannot describe all complexity of the process such as the choking regime, and is believed to capture the physics involved only in some average sense. There might be essential features and important mechanisms playing a role in experiments which are not accounted for in the model.

2 Formulation

In the frame of reference attached to the advancing detonation the set of equations describing its aero-thermo-chemical structure reads,

$$d[\rho(u-D)]/dx = 0 \quad \text{(continuity)} \tag{1}$$

$$d[\rho(u-D)u + p]/dx = f \quad \text{(momentum)} \tag{2}$$

$$d[\rho(u-D)(c_vT + \frac{1}{2}u^2) + pu]/dx = Q\omega \quad \text{(energy)} \tag{3}$$

$$d[\rho(u-D)C]/dx = -\omega \quad \text{(concentration)} \tag{4}$$

$$p = (c_p - c_v)\rho T \quad \text{(state)}\ . \tag{5}$$

Here, D, u, are the detonation and gas flow velocities in the laboratory frame of reference. T, C, p, ρ are the temperature, deficient reactant concentration, pressure and density, respectively. ω is the reaction rate defined by a one-step first-order Arrhenius kinetics,

$$\omega = A\rho C\exp(-E/RT)\ , \tag{6}$$

where A is the pre-exponential factor. The drag-force f is specified as [13, 14],

$$f = -2c_f\rho|u|u/d\ , \tag{7}$$

where d is the hydraulic diameter and c_f is the resistance factor. Other notations are conventional.

In the case of a porous bed saturated by an explosive mixture Eq.(7) is nothing but a high-Reynolds number version of the Forchheimer equation with $c_f = 0.58$ [15]. For spherical packings $d = 2\varphi d_p/3(1-\varphi)$, where φ is the porosity and d_p is the particle diameter [16]. To reduce the number of parameters involved the effects due to molecular transport and heat losses are discarded [10, 11]. The detonation is assumed to propagate throughout an initially quiescent homogeneous premixture whose temperature, pressure, density, and deficient reactant concentration are regarded as prescribed. Hence the upstream boundary conditions are,

$$T(+\infty) = T_0,\ C(+\infty) = C_0,\ \rho(+\infty) = \rho_0\ ,$$
$$p(+\infty) = p_0 = (c_p - c_v)\rho_0 T_0\ ,\ u(+\infty) = 0\ . \tag{8}$$

The integration of the continuity equation (1) then yields,

$$\rho(u - D) = -\rho_0 D\ . \tag{9}$$

Far behind the combustion wave, due to the flow deceleration and the reactant consumption,

$$u(-\infty) = 0\ ,\ \rho(-\infty) = \rho_0\ , C(-\infty) = 0\ , \tag{10}$$

and the global integration of the enthalpy equation, Eq. (3) +Q(Eq.4),

$$d[\rho(u - D)(c_v T + \frac{1}{2}u^2 + QC) + pu]/dx = 0 \tag{11}$$

yields

$$T(-\infty) = T_0 + QC_0/c_v = T_b\ ,$$
$$p(-\infty) = (c_p - c_v)\rho_0 T_b = p_b\ . \tag{12}$$

Thus, due to the boundary condition (Eq.10) and the absence of heat losses, the final temperature and pressure of the burned gas appear to be identical to those reached in the constant volume adiabatic explosion.

3 Low-Velocity Propagation

As opposed to the ideal CJ-detonation, in hydraulically resisted flows the propagation velocity is strongly affected by the processes occurring within the reaction zone. When calculating the velocity, in order to circumvent the familiar cold-boundary difficulty, it is often helpful to introduce a fictitious ignition (truncation) temperature T_{ign}, so that

$$\omega = 0 \ \text{ at } T < T_{ign}\ . \tag{13}$$

For the high-activation-energy limit adopted in the current study T_{ign} does not affect the final expression for D. In the following D is assumed to be comparable with the sonic velocity of unburned gas, a_0. Simultaneously a_0 is assumed to be much lower than a_b, the sonic velocity of the burned gas. The second condition is actually the requirement of strong heat release, $T_0 \ll T_b$, which is readily met in many practical systems. If within the reactive layer $p \sim p_b$ and $T \sim T_b$, then, since $u \sim D$, the inertial effects will be small i.e.,

$$\rho u(u - D) \ll p,\ \ \frac{1}{2}u^2 \ll c_v T\ . \tag{14}$$

As a result, the momentum and energy equations (2)(3) may be simplified to,

$$dp/dx = f \tag{15}$$

$$d[\rho(u - D)c_v T + pu]/dx = Q\omega \tag{16}$$

The integration of the enthalpy equation, Eq.(16) + Q Eq.(4), and utilization of Eqs.(1)(5) yields,

$$p = \rho_0(c_p T - c_v T_b + QC) \ . \tag{17}$$

At $T < T_{ign}$, due to the absence of molecular diffusion, the concentration remains at its initial level, $C = C_0$. Hence, at the ignition point,

$$p_{ign} = \rho_0(c_p T_{ign} - c_v T_0) \ . \tag{18}$$

Since $p_{ign} < p_b$, the last relation readily implies that

$$T_{ign} < T_0 + (1 - \gamma^{-1})(T_b - T_0) = T_+ \ . \tag{19}$$

T_+ is the temperature at the 'entrance' to the reaction zone and plays a pivotal role in controlling the reaction time scale, $A^{-1}\exp(E/RT_+)$ [17, 18]. The ignition temperature may therefore be written as

$$T_{ign} = T_0 + \alpha(T_+ - T_0) \text{ with } \alpha < 1 \tag{20}$$

If at $T_0 \ll T_b$ the parameter α is regarded as a finite number, T will be comparable with T_b within the whole reactive layer, in compliance with the conditions (14).

One thus ends up with a self-consistent reduced model based on the equations (1)(4)(5)(14)(16) and boundary conditions,

$$\begin{aligned} &T(0) = T_{ign}, \ p(0) = \rho_0(c_v T_{ign} - c_v T_0) \ , \\ &C(0) = C_0, \ T(-\infty) = T_b, \ p(-\infty) = p_b \ , \\ &C(-\infty) = 0 \ . \end{aligned} \tag{21}$$

Here the ignition point is set at $x = 0$. The emerging eigenvalue problem for the velocity D is formally identical to that for a strongly subsonic propagation ($D \ll a_0$) recently explored by the authors [18]. The asymptotic solution evaluated in [18] may therefore be safely extended over the current situation where $D \sim a_0$. Adapted for the drag-force specified by Eq.(7) the propagation velocity is thus given by the relation [18],

$$\frac{2c_f(1-\sigma)(1-\gamma^{-1})}{Aa_b^2 d} D^3 = \exp\left(-\frac{E}{RT_+}\right) \ . \tag{22}$$

With the appropriate choice of parameters the propagation velocity may be either supersonic or subsonic. For example, at $A = 10^{10}s^{-1}$, $E/R = 10,000°K$, $T_0 = 295°K$, $a_0 = 350m/s$, $\sigma = T_0/T_b = 0.15$, $\gamma = 1.3$, $\varphi = 0.4$, Eqs.(19)(22) yield: $T_+ = 681°K$ and $D = 253m/s$ (subsonic) at $d_p = 0.1cm$ and $D = 432m/s$ (supersonic) at $d_p = 0.5cm$.

The presence or absence of the shock in the upstream flow does not affect the picture in the reactive layer. Both subsonic and supersonic modes are sustained by the same mechanism:

the drag-induced diffusion of pressure.[1] To substantiate this assertion one may consider the pertinent evolution equation for the pressure. The latter is readily obtained from the continuity equation combined with the equation for momentum (15) and state (5),

$$\frac{\partial}{\partial t}\left(\frac{p}{a^2}\right) = \frac{\partial}{\partial x}\left(\frac{\mathcal{D}_{bar}}{a^2}\frac{\partial p}{\partial x}\right) . \tag{23}$$

Here a^2 is the local sonic velocity and

$$\mathcal{D}_{bar} = a^2 d/2\gamma c_f |u| \tag{24}$$

may be thus regarded as the local pressure diffusivity.[2]

At the entrance to the reaction zone,

$$\mathcal{D}_{bar} = a^2(T_+)d/2\gamma c_f u(T_+) \tag{25}$$

where

$$u(T_+) = D(1 - a^2(T_+)/a_b^2) . \tag{26}$$

In terms of $\mathcal{D}_{bar}(T_+)$ Eq.(22) may be recast as

$$D^2 = \frac{A\mathcal{D}_{bar}(T_+)}{1 - \gamma^{-1}(\sigma + (1-\sigma)(1-\gamma^{-1}))}\exp\left(-\frac{E}{RT_+}\right) , \tag{27}$$

which is quite similar structurally to the equation for deflagrative combustion driven by the thermal diffusivity [19, 20]. For the sonic propagation $D = a_0$, and, for example, at $a_0 = 350m/s$, $\sigma = 0.15$, $\varphi = 0.4$, $\gamma = 1.3$, $d_p = 0.5cm$. Eq.(25) yields

$$\mathcal{D}_{bar}(T_+) = 1.8 \cdot 10^4 cm^2/s \tag{28}$$

The developing pressure diffusivity may thus be as high as 10^4 times typical thermal diffusivity at the same pressure and temperature, which explains its ability to support supersonic propagation effectively without input from the upstream shock.

4 Concluding Remarks

The asymptotic relation (22) pertains to the part of the $D(d_p^{-1})$-curve below its lower turning point (Fig. 1). The rest of the curve including its upper turning point and the CJ-detonation may be evaluated utilizing Zeldovich's classical analysis [14]. For the drag-force specified by Eq. (7) one obtains [21],

$$\left(\frac{D_{CJ} - D}{D_{CJ}}\right)\exp\left[\frac{2E}{RT_{CJ,N}}\left(\frac{D - D_{CJ}}{D_{CJ}}\right)\right] \sim \frac{c_f D_{CJ}^3}{a_0^2 A d}\exp\left(\frac{E}{RT_{CJ,N}}\right) , \tag{29}$$

where $T_{CJ,N}$ is the post-shock (Neumann) temperature.

The low-velocity detonations are normally observed in obstacle-laden systems where the Reynolds analogy is strongly violated and the process may therefore be considered as effectively adiabatic. Yet, the low-velocity detonation may presumably be obtained also in smooth-walled tubes provided the impact of heat losses is somehow reduced.[3] According to Zeldovich and Kompaneets [22] such a situation may arise in transient turbulent flows where the temperature field settles down much slower than the flow field. This might possibly explain the occurrence of long-lived ‘strange waves’ discussed in Khoklov et al. [23] and Oran et al. [24]. There is indeed a strong similarity between these waves and the choking regime both in the levels of propagation velocity (about half of the CJ-velocity) and the post-shock pressure, comparable to that of a constant volume explosion.

Notes

1. The identity of the driving mechanisms is also reflected in the smoothness of the $D(d_p^{-1})$-curve in its passage through the sonic point $D = a_0$ (Fig. 1).

2. For the linear (Darcy) drag-law, $f = -\rho\nu u/K$, and constant temperature, $T = T_0$, Eq.(23) converts into the classical filtration equation, $p_t = \mathcal{D}_{bar}\ p_{xx}$, with $\mathcal{D}_{bar} = Ka_0^2/\gamma\nu$. Here K, ν are the porous bed permeability and kinematic viscosity, respectively [16].

3. As demonstrated by Manzhalei [25, 26], the low-velocity detonation may develop in smooth-walled glass capillaries. Quite in line with the theoretical findings based on the adiabatic approximation [10], there is a wide gap between the reaction zone and the leading shock.

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Figure Captions

Figure 1

Detonation velocity D versus reciprocal of the porous bed particle diameter d_p; adiabatic limit. D_{CJ}, a_0, a_b correspond to the Chapman-Jouguet detonation and sound velocities in the unburned and burned gas, respectively. Upper (lower) circles mark the border between quasi-detonation and choking (choking and subsonic) regimes.

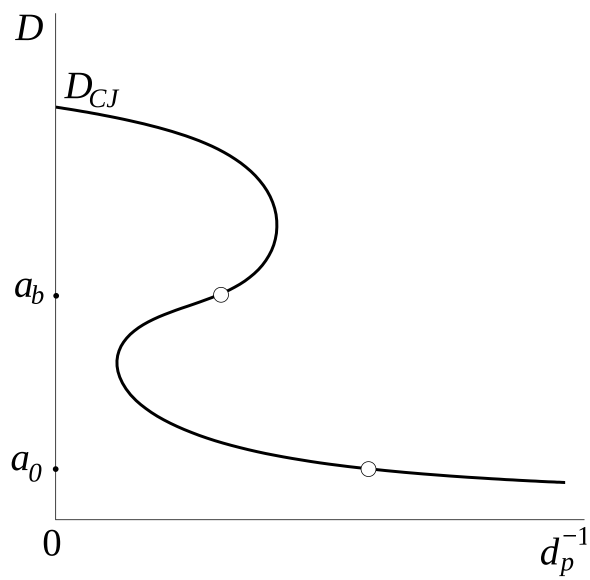

Figure 1