EFFECTS OF HYDRAULIC RESISTANCE AND HEAT LOSSES ON DETONABILITY AND FLAMMABILITY LIMITS

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As is well known, in order to ensure detonative or deflagrative combustion in a confined or obstacle-laden system its effective (hydraulic) diameter should exceed a certain critical value, quenching diameter. Since the propagation mechanisms of detonations and deflagrations are of an essentially different nature, there is no reason to expect that their quenching diameters will coincide. Indeed, it has long been observed that the quenching diameters for detonations are generally larger that those of deflagrations, i.e. there are tubes wide enough to allow for deflagrations but not detonations [1, 2]. A simple model reproducing the effect in the context of subsonic porous bed combustion has recently been proposed [3]. In this system, due to the strong hydraulic resistance, the pressure-driven wave spreads at a fast yet subsonic velocity [4-8]. The disparity between the quenching diameters is explained in terms of the disparity between the associated reaction times, $\tau \sim \exp(E/RT)$. In the pressure-driven regime, τ is controlled by the relatively low temperature at the entrance to the reaction zone rather that its exit, as occurs in deflagrative combustion [5-8]. This makes the pressure-driven wave more vulnerable to heat losses. A similar effect is expected to take place also for conventional supersonic detonation where τ is controlled by the post-shock (Neumann) temperature which is normally lower than its deflagrational counterpart. The objective of the current study is a more systematic exploration of this question. The results obtained show that the post-shock and flame temperatures are not the only factors controlling the quenching diameters disparity. The latter is also affected by the change in the resistance law in the transition from deflagrative to detonative propagation, as well as by the magnitude of the pre-exponential factor in the Arrhenius kinetics. As a consequence a situation may arise where the quenching diameter of detonation exceeds that of deflagration. The latter picture is favored by the systems with relatively low activation energies and high pre-exponentials.

The problem is analyzed within the framework of a quasi-one-dimensional formulation for the reactive flow in a smooth-walled tube. The impact of walls is modeled through a drag-force and heat-loss terms added to the momentum and energy balance equations. In the frame of reference attached to the advancing wave the set of governing equations reads,

$$\frac{d}{dx}\big(\rho(u-D)\big)=0\,,\qquad P=\big(c_p-c_v\big)\rho T \quad \text{(continuity and state)} \tag{1}$$

$$\frac{d}{dx}\left(\rho(u-D)u+P-\frac{4}{3}\mu\frac{du}{dx}\right)=-f \quad \text{(momentum)} \tag{2}$$

$$\frac{d}{dx}\left(\rho(u-D)(c_vT+\frac{1}{2}u^2)+uP-Pr^{-1}\mu\frac{dT}{dx}-\frac{4}{3}\mu u\frac{du}{dx}\right)=QW-h \quad \text{(energy)} \tag{3}$$

$$\frac{d}{dx}\left(\rho(u-D)C-\big(Le\,Pr\big)^{-1}\mu\frac{dC}{dx}\right)=-W \quad \text{(concentration)} \tag{4}$$

Here D is the propagation velocity in the laboratory frame of reference, $\mu = \mu_0 (T/T_0)^{0.7}$ is the dynamic viscosity, where the subscript (0) pertains to the initial state of the mixture; $W = A\rho^2 C \exp(-E/RT)$ is the reaction rate, defined by a one-step non-stoichiometric bimolecular Arrhenius kinetics; A is the pre-exponential factor; $f = 2C_f \rho u|u|/d$, $h = 2\alpha C_f d^{-1} \rho |u| \left(c_p (T - T_0) + u^2/2\right)$ are the terms controlling the momentum and heat losses, respectively; d is the hydraulic diameter; α is the momentum-heat-loss similarity factor; C_f is the hydraulic resistance factor depending on the Reynolds number; $Re = \rho |u| d/\mu$. For smooth tubes considered in this study $\alpha = 1$ (Reynolds analogy). For deflagrative and detonative propagation $C_f = 16\,Re^{-1}$ and $C_f = 0.3164\,Re^{-1/4}$, respectively.

The wave is assumed to propagate through an initially quiescent homogeneous mixture where temperature, pressure, density and the deficient reactant concentration are regarded as prescribed. Hence the upstream boundary conditions are

$$T(+\infty) = T_0;\ C(+\infty) = C_0;\ P(+\infty) = P_0;\ \rho(+\infty) = \rho_0;\ u(+\infty) = 0 \tag{5}$$

Far behind the wave, because of the flow deceleration and the reactant consumption

$$C(-\infty) = 0;\ u(-\infty) = 0 \tag{6}$$

In detonative combustion the effects due to molecular transport normally may be ignored everywhere except for h, f terms depending on the Reynolds number.

The emerging eigen-value problem for the propagation velocity D is solved along the lines of the classical Zeldovich analysis of non-ideal detonations [9], and its recent extensions based on the activation energy asymptotics [10-13]. At high activation energies the bulk of the chemical heat release occurs in a thin reactive layer located at a certain distance behind the shock. One thus ends up with the so-called square-wave model allowing analytical treatment. The resulting expression for the quenching diameter reads,

$$d_{det}^{q} = F \left(\frac{a_0}{A\rho_0} \right)^{4/5} \left(\frac{\mu_0}{\rho_0 a_0} \right)^{1/5} \exp\left(\frac{4E}{5RT_{N,CJ}} \right) \tag{7}$$

Here $T_{N,CJ}$ is the post-shock (Neumann) temperature in the ideal CJ-detonation, a_0 is the sonic velocity at the initial temperature T_0. F is the nondimensional factor depending on specific-heat ratio $\gamma = c_p/c_v$ and $\sigma_N = T_0/T_{N,CJ}$.

In deflagrative propagation, since $D << a_0$, one may ignore dynamic compressibility as well as the inertial and viscous dissipation effects in the energy equation (3). The conventional high activation-energy analysis [14] then leads to the following expression for the quenching diameter,

$$d_{dfl}^{q} = G \left(\frac{\mu_0}{A\rho_0^2} \right)^{1/2} \left(\frac{E}{RT_0} \right)^{3/2} \exp\left(\frac{E}{2RT_P} \right) \tag{8}$$

Here $T_P = T_0 + QC_0/c_p$ is the adiabatic temperature of combustion products. G is the dimensionless factor depending on the Prandtl and Lewis number (Pr, Le) and $\sigma_P = T_0/T_P$. Eqs. (7), (8) readily imply that since $T_P > T_{N,CJ}$, d_{det}^{q} will exceed d_{dfl}^{q}, provided the

activation energy is high enough. The effect is enhanced by the transition from laminar to turbulent resistance law introducing the factors 4/5 and 1/2 in the exponentials of Eqs.(7), (8). If in the detonative combustion the developing flow would be laminar, 4/5 should be replaced by 1/2 preserving but weakening the effect. Yet, if the pre-exponential A is high enough then at relatively low activation energies the picture inverts yielding wider detonability limits. There is a range of tube diameters where the mixture a capable of supporting detonation but not deflagration.

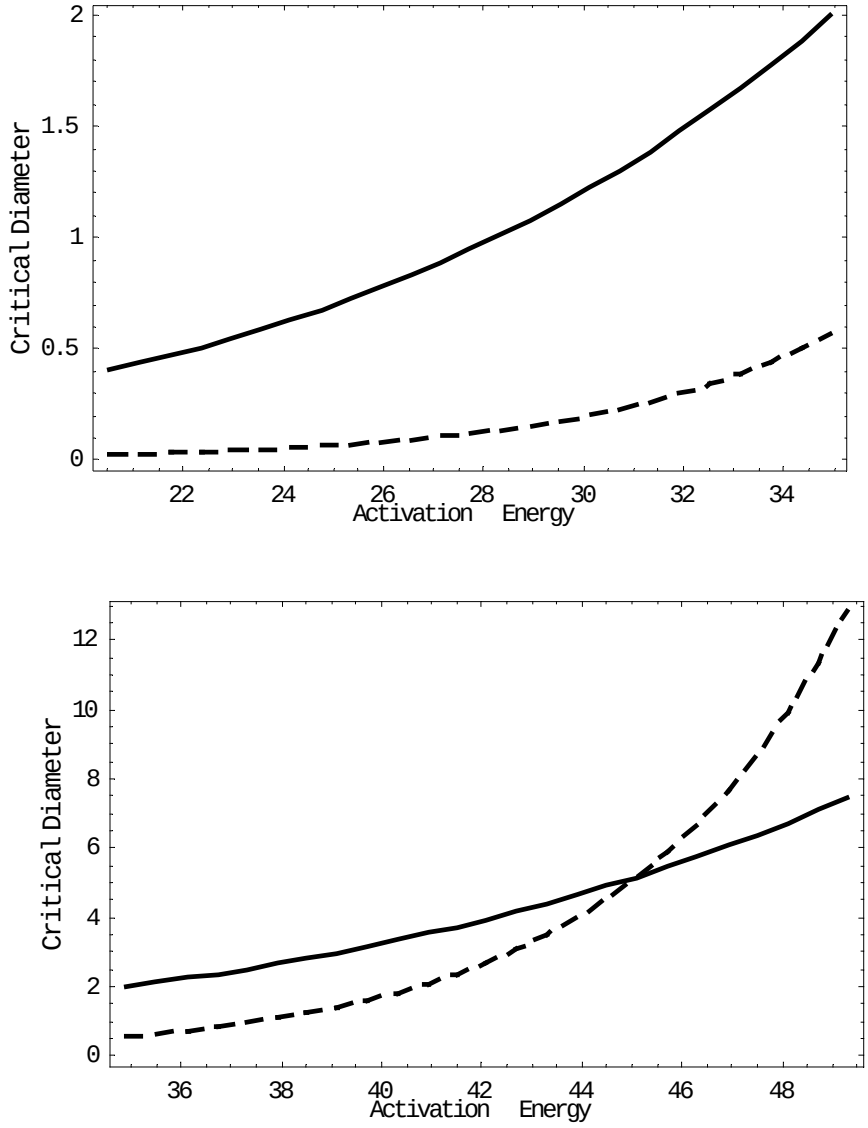

Figure 1. Quenching diameter d^q (mm) vs scaled activation energy E / RT_0. Solid and broken lines correspond to deflagrative and detonative regimes, respectively.

Figure 1 plots d^q_{dfl} and d^q_{det} dependencies on the scaled activation energy E / RT_0, calculated for a set of parameters suggested by the data on the ethylene-air mixture [15]:

$$T_0 = 293\,K, \quad P_0 = 10^5\ Pa, \quad \rho_0 = 1.58\,kg/m^3, \quad T_P = 2625\,K, \quad T_{N,CJ} = 1081\,K,$$
$$A = 3.2 \cdot 10^8\ m^3/(kg \cdot s), \quad \mu_0 = 7.73\,kg/(s \cdot m), \quad \gamma = 1.15, \quad Le = 1, \quad Pr = 1, \qquad (8)$$
$$F = 0.548, \quad G = 4.813.$$

The high-activation-energy limit and other assumptions underlying Eqs. (7), (8) make the above conclusions more of a qualitative guide than a quantitative prediction. It is therefore desirable to conduct direct numerical simulations of the original model (1)-(4) dealing with

the distributed reaction rate and accounting for the molecular transport and inertial effects both in deflagrative and detonative regimes.

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