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ScienceDirect

Combustion and Flame 154 (2008) 186–190

Combustion and Flame

www.elsevier.com/locate/combustflame

Autoignition due to hydraulic resistance and deflagration-to-detonation transition

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Received 13 August 2007; received in revised form 12 November 2007; accepted 22 November 2007

Available online 24 January 2008

Abstract

A further development of the friction-based concept of the deflagration-to-detonation transition is presented. Employing Zeldovich's quasi-one-dimensional formulation for combustion in hydraulically resisted flows, the autoignition of the unburned gas subjected to the friction-induced precompression and preheating is assessed. It is shown that autoignition, triggering the transition, is readily attainable for quite realistic parameters.

Keywords: Autoignition; Deflagration-to-detonation transition

1. Introduction

It has long been known that the deflagration-to-detonation transition (DDT) seldom occurs in unconfined systems but may be significantly facilitated in the presence of obstacles/confinement. In the traditional attempt to explain the phenomenon, the role of confinement is reduced exclusively to generation of hydrodynamic disturbances (turbulence). The latter promotes extension of the flame interface, resulting in flame acceleration and, hence, enhancement of the flame-supported compression waves, which allegedly leads to formation of hot spots, triggering localized explosions and transition to detonation [1–3].

Recently, in the course of studying obstacle-affected deflagrative combustion, it was realized that there is a complementary aspect of the flame–confinement interaction which somehow escaped proper attention and which seems to be of crucial importance. Apart from inducing hydrodynamic disturbances, confinement also exerts resistance to the gas flow, causing reduction of its momentum, which appears to be an agency perfectly capable of provoking the DDT event even if the flame folding and predetonational acceleration are effectively suppressed, as is the case in quasi-one-dimensional formulations [4]. The hydraulic resistance causes a gradual precompression and hence preheating of the unburned gas adjacent to the advancing deflagration, which leads (after an extended induction period) to localized autoignition, triggering an abrupt transition to detonation.

The nature of the results obtained—the explosive character of the transition, velocity and pressure overshoots, predetonational expansion and shrinking of the reaction zone, sublinear dependence of predetonation distance on the tube diameter (all these effects are well known experimentally)—gives serious grounds for the belief that a good deal of the actual DDT dynamics is captured quite adequately. One

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0010-2180/$ – see front matter
doi:10.1016/j.combustflame.2007.11.007

should acknowledge, however, that so far all tests of the new concept have been focused mainly on the general topology of the transition and, to facilitate numerical simulations, have dealt with parameter ranges ensuring a rather mild scale separation (wide reaction zones, small hydraulic diameters, fast flames) compared to those typical of real life systems [4,5]. In light of this constraint, the current study offers a quantitative assessment showing that the transition due to hydraulic resistance is indeed readily attainable for quite realistic parameters.

2. Analysis

Assume that ahead of the advancing flame the reactive gas is totally frozen chemically. Then there will obviously be no predetonational autoignition and the flame will assume a certain friction-affected mode of subsonic propagation driven by molecular transport. We shall call this mode chemically frozen preheat zone (CFPZ) frictional flame.

The impact of friction manifests itself in the formation of a precompressed and preheated layer adjacent to the flame front. This layer is generally wide compared to the diffusive width of the CFPZ flame (Fig. 1).

Note that due to precompression the velocity of the frictional flame may noticeably exceed the velocity of the open-space flame, other conditions being identical.

Imagine now that on the reactant side of the flame the pressure and temperature profiles fall precisely within the autoignition range pertinent to the given mixture. Such an outcome may naturally be interpreted as an assurance that under normal conditions, i.e., when the freezing constraint is removed, the unburned gas will explode, presumably triggering the transition. However, if the unburned gas is only

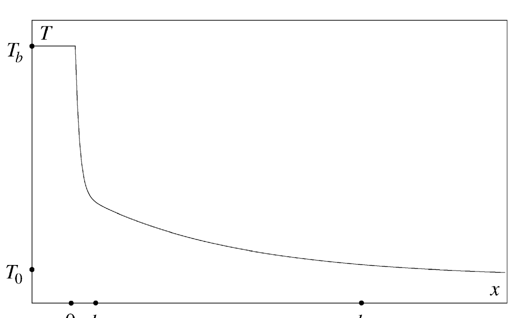

Fig. 1. Temperature profile of the CFPZ frictional flame. T_0, T_b are the initial and final temperatures. The reaction zone is located at $x = 0$. l_d, l_p mark the diffusive and precompressed layers.

slightly affected by the reaction, the CFPZ flame may serve as a good approximation to the actual friction-affected flame, not subjected to any restriction on distribution of the reaction. Such a situation is expected to emerge when the activation energy of the system is high enough.

In order to evaluate the pressure/temperature profiles of the CFPZ flame, Zeldovich's [6] quasi-one-dimensional formulation is adopted, where the presence of obstacles/walls is accounted for by means of the velocity-dependent drag-force term added to the momentum equation. The transport effects as well as heat losses are discarded, and the flame is treated as a hydrodynamic discontinuity moving at a prescribed velocity D relative to the laboratory frame. The diffusive width of the flame is therefore assumed to be small compared to the friction-induced length-scale (Fig. 1).

The current study deals with subsonic combustion only, $D < a_0$, a_0 being the sonic velocity in the fresh mixture. Moreover, we shall consider the limit $D \ll a_0$, readily held for premixed gas flames. In this situation the impact of inertial effects may be discarded, and in the frame of reference attached to the settled CFPZ flame, the set of equations describing its aero-thermo-chemical structure reads

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

$$\mathrm{d}p/\mathrm{d}x = f \quad \text{(momentum)}, \tag{2}$$

$$\mathrm{d}\big[\rho(u-D)(c_\mathrm{v}T + QC) + pu\big]/\mathrm{d}x = 0 \quad \text{(enthalpy)}, \tag{3}$$

$$\mathrm{d}\big[\rho(u-D)C\big]/\mathrm{d}x = -J\delta(x) \quad \text{(concentration)}, \tag{4}$$

$$p = (c_\mathrm{p} - c_\mathrm{v})\rho T \quad \text{(state)}. \tag{5}$$

Here u is the gas flow velocity in the laboratory frame of reference. T, C, p, ρ = temperature, deficient reactant concentration, pressure, and density, respectively. J = localized reaction rate intensity, determined by the flame velocity D (see Eq. (18) below). $c_\mathrm{p}, c_\mathrm{v}$ = specific heats, assumed to be constant. Q = heat release. f = drag force, specified as

$$f = -2C_\mathrm{f}\rho|u|u/d, \tag{6}$$

where d = hydraulic diameter and C_f = drag coefficient.

For porous beds $C_\mathrm{f} = 0.58$ [7]. For well-shaken spherical packings $d = 0.44d_\mathrm{p}$, d_p being the particle diameter.

For tubes C_f depends on the Reynolds number and the wall roughness. While involving more parameters, the tube case leads to the results qualitatively similar to those of porous beds, and for brevity's sake is not discussed here.