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Engine hot spots: Modes of auto-ignition and reaction propagation

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ABSTRACT

Many direct numerical simulations of spherical hot spot auto-ignitions, with different fuels, have identified different auto-ignitive regimes. These range from benign auto-ignition, with pressure waves of small amplitude, to super-knock with the generation of damaging over-pressures. Results of such simulations are generalised diagrammatically, by plotting boundary values of ξ, the ratio of acoustic to auto-ignition velocity, against ε. This latter parameter is the residence time of the developing acoustic wave in the hot spot of radius r_o, namely r_o/a, normalised by the excitation time for the chemical heat release, τ_e. This ratio controls the energy transfer into the developing acoustic front. A third relevant parameter involves the product of the activation temperature, E/R, for the auto-ignition delay time, τ_i, normalised by the mixture temperature. T, the ratio, τ_i/τ_e, and the dimensionless hot spot temperature gradient, $(\partial \ln T/\partial \tilde{r})$, where $\tilde{r}$ is a dimensionless radius. These parameters define the boundaries of regimes of thermal explosion, subsonic auto-ignition, developing detonations, and non-auto-ignitive deflagrations, in plots of ξ against ε.The regime of developing detonation forms a peninsula and contours, throughout the field. The product parameter $(E/RT)(\tau_i/\tau_e)/\partial \ln T/\partial \tilde{r}$ expresses the influences of hot spot temperature gradient and fuel characteristics, and a unique value of it might serve as a boundary between auto-ignitive and deflagrative regimes. Other combustion regimes can also be identified, including a mixed regime of both auto-ignitive and "normal" deflagrative burning. The paper explores the performances of a number of different engines in the regimes of controlled auto-ignition, normal combustion, combustion with mild knock and, ultimately, super-knock. The possible origins of hot spots are discussed and it is shown that the dissipation of turbulent energy alone is unlikely to lead directly to sufficiently energetic hot pots. The knocking characterisation of fuels also is discussed.

1. Introduction

Reactive hot spots can arise for a number of reasons: partial mixing with hot gas or burned products, heat transfer from hot surfaces, and turbulent energy dissipation in flowing reactants. Their size may be of the order of millimetres. Following Zel'dovich [1], a gradient of reactivity can give rise to an auto-ignition velocity, u_a. At one extreme this can lead to a detonation, at another, to a benign, controlled auto-ignitive propagation. The rate of change of the heat release rate at the hot spot determines the associated amplitude of the generated pressure pulse and, if u_a is high enough, to be close to the acoustic speed, a, this pulse can be coupled with the heat release in a detonation wave.

Earlier findings [2,3] from direct numerical simulations, DNS, of hot spot auto-ignitions in 0.5 H_2/0.5 CO/air mixtures showed a peninsula could be constructed, within which detonations could develop. The boundaries were defined by the dimensionless groups, a/u_a, and$r_o/a\tau_e$, in which r_o is the radius of a spherical hot spot and τ_e is the excitation time. This is the time during which most of the heat release occurs at the end of the auto-ignition delay time, τ_i [4].

This approach has been employed in studies of engine knock and super-knock in gasoline engines [5–10]. The phenomena leading to super-knock are a rather complex sequence of events comprising the primary formation of hot spots that pre-ignite and initiate premature flame propagation, with earlier increases in pressure and temperature in the unburned mixture. A secondary, more reactive, hot spot may then be generated in the reactants and lead to a developing detonation, following the theory developed in [2,3]. While the salient features of the latter appear to be understood, the mechanisms causing the primary hot spots are still the subject of debate. The earlier the initial pre-ignition, the more severe is the secondary auto-ignition. The cyclical nature of "super-knock" is discussed in Section 5. The paper focuses on the secondary hot spots and the parameter range within which a detonation can develop. The original simulations have been extended to other fuels and focus on the secondary hot spots, by relating the detonation peninsula also to the auto-ignitive activation energy

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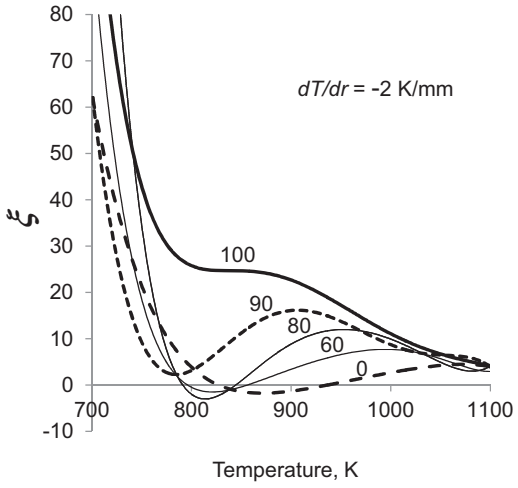

Fig. 1. Computed values of ξ for five different octane numbers of primary reference fuels at 4 MPa and $\partial T/\partial r = -2$ K/mm.

of the mixture and hot spot temperature gradient. This extended understanding is able to characterise engine auto-ignition over a wide range of conditions from benign auto-ignition, through mild knock, to super-knock and offers a fundamental approach to assessing the anti-knock characteristics of fuels.

2. Auto-ignition in the strong ignition regime

The auto-ignition delay time at a given pressure is expressed by:

$$\tau_i = C\exp(E/RT), \tag{1}$$

and

$$\partial\tau_i/\partial T = \tau_i\left(E/RT^2\right). \tag{2}$$

The localised auto-ignitive activation temperature, E/R, is expressed by:

$$\partial \ln \tau_i/\partial(1/T) = E/R. \tag{3}$$

Assuming that the reactivity gradients arise solely from changes in temperature with the radius, r, the auto-ignition propagation velocity is

$$u_a = \partial r/\partial\tau_i = (\partial r/\partial T)(\partial T/\partial\tau_i). \tag{4}$$

Detonations are associated with the auto-ignitive front propagating at close to the acoustic velocity, a, and it is convenient to introduce the dimensionless ratio, ξ:

$$\xi = a/u_a = (\partial T/\partial r)(\partial\tau_i/\partial T)a. \tag{5}$$

The way in which ξ decreases with increasing temperature is shown for the Primary Reference Fuels, *i*-octane/*n*-heptane, in Fig. 1, for five different Octane Numbers, and an assumed value of $(\partial T/\partial r)$ of -2 K/mm. The data on τ_i are from [11], and the values of a are from [12]. Between about 700 and 800 K there is a sharp decrease in $(\partial\tau_i/\partial T)$ with T and, consequently, also in ξ. This is countered in the regime of negative temperature coefficient, but is subsequently resumed at about 1000 K, as ξ approaches unity. In the absence of a negative temperature coefficient, the same temperature gradient that can ignite a detonation at a high temperature, quenches it at a lower temperature, as noted in [13].

A critical value of the temperature gradient, signified by suffix c, occurs when $\xi = 1.0$, and from Eq. (5),

$$(\partial T/\partial r)_c = (\partial T/a\partial\tau_i) \tag{6}$$

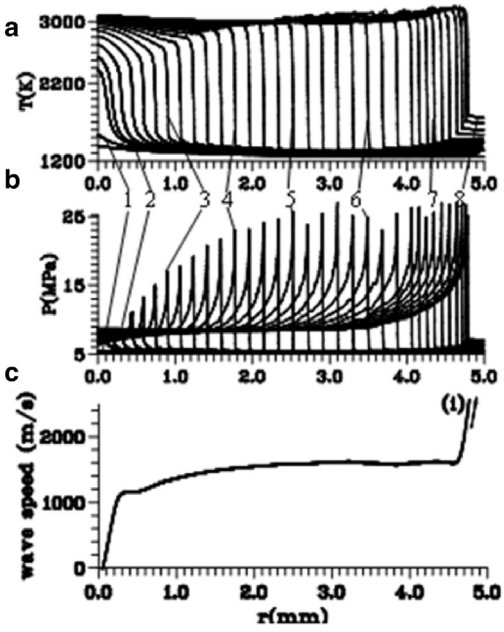

Fig. 2. History of a hot spot, $r_o = 3$ mm, with $\xi = 1$, stoichiometric 0.5 H_2/0.5 CO/air, $T_o = 1200$ K and $P_o = 5.066$ MPa, $\tau_i = 39.16\,\mu$s. Time sequence (μs) 1—35.81, 2—36.16, 36.64, 4—37.43, 5—37.72, 6—38.32, 7—38.86, 8—39.13. (a) Temperature, (b) pressure and (c) combustion wave speed.

From Eqs. (5) and (6),

$$\xi = (\partial T/\partial r)(\partial T/\partial r)_c^{-1} \tag{7}$$

For a given mixture and its conditions, ξ is proportional to $\partial T/\partial r$.

From Eqs. (2) and (5),

$$\xi = -\tau_i\left(E/RT^2\right)(\partial T/\partial r)a. \tag{8}$$

Both Voevodsky and Soloukhin [14], and Meyer and Oppenheim [15], employing H_2/O_2 mixtures, used Eq. (2) to define the boundary between strong and weak auto-ignitions. Strong ignition was defined as a stable detonation, with near-instantaneous and uniform auto-ignition, and a low value of $(\partial\tau_i/\partial T)$. Meyer and Oppenheim suggested a threshold value of $\partial\tau_i/\partial T$ for this regime of $-2\,\mu$s/K.

Figure 2 shows results from the DNS studies of [2,3], for a detonation developing rapidly from a hot spot of radius 3 mm, in a stoichiometric mixture of 0.5 H_2/0.5 CO/air, with $\xi = 1.0$ at 1200 K, $\tau_i = 39.16\,\mu$s, and $a = 731$ m/s. The Chapman–Jouguet wave speed is soon attained within the hot spot. The temperature gradient across the hot spot was -2.426 K/mm, and the value of $(\partial\tau_i/\partial T)$ was $-0.564\,\mu$s/K, smaller than the value of Meyer and Oppenheim. A hot spot developing into a thermal explosion was also investigated in [2,3] with $\varphi = 0.75$ and at 1000 K. This showed a value of $(\partial\tau_i/\partial T)$ of $-32\,\mu$s/K. Similar plots of hot spot histories for other conditions appear in [2,3].

3. Excitation time and the detonation peninsula

This features the other relevant dimensionless group formulated in [2,3]. The nature of an auto-ignition also depends upon the rate at which the heat is released at the end of the delay time [4,13]. The time for the acoustic wave to move through the hot spot of radius r_o, divided by the excitation time, τ_e, is defined by ε:

$$\varepsilon = r_o/a\tau_e. \tag{9}$$

It is a measure of the energy transferred into the acoustic front: the acoustic wave transit time through the hot spot, divided by the time for the heat release.