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Effect of gaseous oxidizer composition on the detonability of isooctane–air sprays

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ABSTRACT

Experimental and numerical study of the detonation has been conducted in heterogeneous reactive two-phase media made of liquid isooctane sprays dispersed in gaseous oxidizing atmospheres. Influence of the oxidizer composition on conditions of detonation formation and propagation regimes, with particular attention on the existence of the so-called cellular structure, has been studied.

Experiments have been performed under standard initial conditions of temperature and pressure (293 K, 1 bar) in a 4-m long vertical, square cross-section (53×53 mm^2) detonation tube. The mean isooctane droplet size was of about 30 μm. When oxidizing mixture was made of air ($O_2 + \beta N_2$ with $\beta = 3.76$), three detonation regimes have been observed with increasing equivalence ratio: a spinning regime, a marginal one with half a cell structure, and a normal multi-headed detonation regime. At smaller dilution ratio ($\beta = 2$ and 1), only the multi-headed detonation regime was observed, with smaller cell size. When nitrogen is replaced by argon as inert diluent, the detonation structure is multi-headed; the cellular structure is more regular and the cell size is smaller than with nitrogen.

Numerical simulations have been performed with the EFAE code, with taking in consideration the chemical composition of the oxidizing phase and the effects of the two-phase mixture richness. Results of 2D and 3D numerical simulations, as a function of the equivalence ratio and the dilution, display propagation regimes and detonation cell sizes in reasonable agreement with the experimental results.

1. Introduction

Possibility to initiate a detonation in reactive two-phase system made of liquid fuel sprays dispersed in oxidizer or reactive gaseous environment is of great interest in relation with the safe use, storage and transportation of liquid fuels in the chemical and oil industry, and with aerospace propulsion. Indeed, a more recent interest arose from the works undertaken to take an advantage of the detonation combustion regime in the development of new propellers e.g., the Pulsed Detonation Engine (PDE) or the Rotative Detonation Engine (RDE).

Two-phase liquid spray–gaseous mixtures are foreseen to drive these detonation engines. In spite of the numerous works done during the last fifty years since the reference work by Dabora et al. [1], the conditions of existence of a detonation in such a two-phase system and its characteristics and structure are far to be known as well as in homogeneous gaseous mixtures. Initiation of a self-sustained detonation in liquid fuel–air sprays has not been really demonstrated. Most of detonation propagation regimes in liquid fuel sprays have been observed in oxygen or suroxygenated air gaseous environment [2,3].

Moreover, the evidences of existence of the detonation cellular structure were until our recent works [4,5,6], quasi-inexistent. The only existing experimental data are principally those of Papavassiliou et al. [7], Alekseev et al. [8], and Austin et al. [9]. One reason of this lack of reliable data is the difficulty to perform detonation experiments in two-phase liquid sprays with well-controlled characteristics and in reproducible conditions. Therefore, we have designed and built a specific experimental setup [4,5,6], allowing to study the initiation of a detonation in a square cross section (53×53 mm^2) and 4-m long tube, filled with liquid sprays of different composition and having a well-controlled granulometry (8 μm, 30 μm, 45 μm). Thus, we have shown that it was possible to initiate a detonation propagation regime in various hydrocarbon–air sprays. The critical conditions of existence of the detonation and the observed detonation regimes depend on the nature of the fuel and the granulometry of the sprays. However, the majority of the studies of detonation combustion regime for practical systems focused on low-molecular weight hydrocarbons (less than five carbon atoms, C_2–C_5) that are more detonable. Though, the fuels of practical interest (storable in

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Table 1
Position of pressure gauges along the tube.

Transducers	O–K1	K1–K2	K2–K3	K3–K4	K4–K5	K5–K6	K6–K7
Distance (cm)	135	50	24.1	50	23	13.5	17

liquid form) correspond to higher molecular weight hydrocarbons (six carbon atoms C_6 and more). It is those, which are particularly the subject of the present study. Thus, we have chosen to focus here on "isooctane" as liquid fuel and examine the effect of gaseous oxidizer composition.

Besides, several recent works [10,11] have focused both experimentally and theoretically especially on the effect of gaseous oxidizer composition on the pressure evolution during constant volume explosion. Large amplitude oscillations have been observed during the final stage of combustion, which poses dramatic safety issues in terms of high pressure waves. These strong shocks during fast deflagrations were attributed to a new physical phenomenon named "Combustion-induced Rapid Phase Transition (CRPT)". It was found that the addition of inert diluents, such as N_2, CO_2, He, Ar or even H_2O, can prevent the anomalous hazardous behavior of combustion in the studied reactive mixtures.

2. Experimental method

The experimental setup developed for the purpose of this study has been described elsewhere [4–6]. It mainly consists of a stainless steel vertical detonation tube of 4-m length and square cross-section (53×53 mm^2).

An important feature of this experimental installation is the liquid spray generation technique by means of an ultrasonic atomizer which produces a quasi-monodispersed spray, in well-controlled conditions. The mean droplet size is controlled beforehand by a Phase Doppler Interferometry system.

The atomizer is located at the bottom of the setup. The liquid droplets exit the spray generator at a quasi-zero velocity and are transported along the vertical detonation tube by the sustaining gaseous flow up to the open upper end. An optical device at the bottom of the tube detects the presence of the spray. Liquid and gaseous flowrates are monitored by flowmeters. The equivalence ratio of the mixture is determined by adjusting the flowrates of liquid and gases. When the tube is filled up with the mixtures, the flowrates are stopped and the tube is closed at the bottom and the top ends by two rotative electro-pneumatic valves.

Initiation is performed at the bottom of the tube by means of an auxiliary shock tube (booster) separated from the main one by a 0.2 mm Mylar membrane and filled with a stoichiometric ethylene–oxygen mixture (in most experiments the initial pressure of the mixture in the booster is 2 bar). After ignition, a detonation propagates in the booster and provokes the rupture of the membrane, thus generating a shock wave propagating towards the top of the tube in the two-phase reactive mixture. The progression of this shock along the tube is recorded by means of seven short rise time (1 μs) Kistler 603B piezoelectric pressure transducers. Table 1 shows spacings between the gauges in the tube.

These pressure gauges were connected to amplifiers "Kistler 5011", and output signals were recorded on an eight channels central unit "Graphtec Hard Disk Logger GL 1100". Signals delivered by these pressure gauges allow to determine the pressure at the shock front and the pressure evolution in the flow behind the front. These data are also used to estimate the average detonation velocity between neighboring gauges and its evolution along the tube.

Besides, a steel plate covered with soot, typically 420 mm long and 53 mm wide, is used to record the detonation cell pattern by the method of Mach tracks, at the top of the tube.

3. Experimental results

The experiments were carried out with 99.5% grade liquid isooctane (iso-C_8H_{18}) sprays having a mean diameter D_{10} of 30 μm.

First series of experiments have been performed in mixtures $C_8H_{18}/(O_2 + \beta N_2)$ with β varying from $\beta = 3.76$ corresponding to air case, down to $\beta = 2$ and $\beta = 1$ (where β is the molar ratio of N_2 to O_2). The equivalence ratio r was varied from 0.8 to 1.7.

In a second series of experiments, argon was used as the inert diluent of the gaseous phase, and two dilutions ($\beta = 2$ and $\beta = 3.76$), were tested.

All the experiments were performed under standard conditions of temperature and pressure (293 K, 1 bar).

3.1. Experiments in air ($\beta = 3.76$)

As demonstrated in previous works [4,5,6], the incident shock generated at the bottom of the tube initiates a detonation with a quasi-constant front velocity after about 2–3 m of propagation. The average values of the detonation velocity and detonation pressure measured in the upper part of the tube (mainly by means of gauges K6 and K7) as function of the equivalence ratio r are displayed in Figs. 1 and 2.

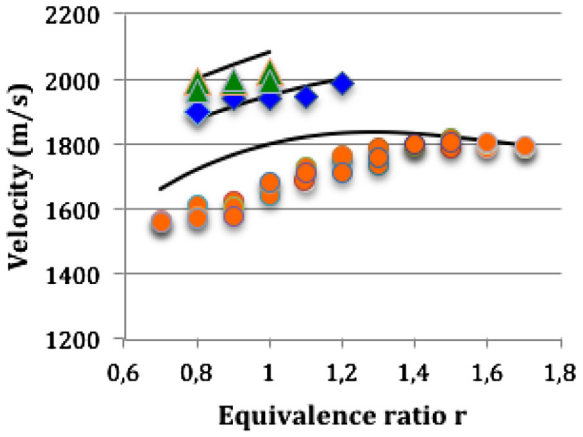

Fig. 1. Variation of the terminal detonation velocity of $C_8H_{18}/(O_2 + \beta N_2)$ mixtures as function of r, [(●): $\beta = 3.76$; (◆): $\beta = 2$ and (▲): $\beta = 1$], with corresponding ideal CJ parameters (—).

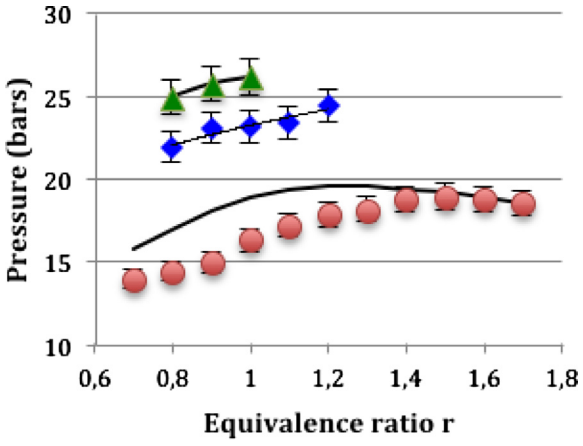

Fig. 2. Variation of the detonation pressure of $C_8H_{18}/(O_2 + \beta N_2)$ mixtures as function of r, [(●): $\beta = 3.76$; (◆): $\beta = 2$ and (▲): $\beta = 1$], with corresponding ideal CJ parameters (—).