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Detonation initiation in pipes with a single obstacle for mixtures of hydrogen and oxygen-enriched air

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ABSTRACT

This work presents an experimental and numerical study of a pulsed detonation combustion chamber. It consists of a pipe obstructed by one convergent–divergent nozzle, filled with a stoichiometric mixture of hydrogen and oxygen-enriched air. The proposed geometry is analysed with regard to its influence on the outset of detonation and its suitability for pulse detonation engines (PDEs). The study reveals the essential aspects for detonation initiation. The results of one of the configurations indicate a deterministic and reliable deflagration-to-detonation transition (DDT) with a short run-up distance, crucial for technical applications. The simulation reproduces the measurements in great detail and the origin of detonation is unequivocally identified.

1. Introduction

The motivation behind this work is the improvement of the efficiency of gas turbines via isochoric combustion. A better fuel consumption is achieved by the use of detonations as a more efficient means of combusting fuel-oxidizer mixtures and releasing its chemical energy content [1]. The detonation is initiated either directly or through the deflagration-to-detonation transition (DDT) [2]. The former requires an elevated amount of energy or rate deposition to successfully initiate a detonation [1]; hence, the latter provides an attractive alternative technique in combustion engines. The cornerstone of DDT-based engines is the ability to bring about a detonation transition in a reactive mixture using a deflagration ignited from a low-energy source. Therefore, a reproducible and reliable DDT from low-energy initiation sources is imperative for pulse detonation engines (PDEs).

The detonation front is a system consisting of a propagating shock wave followed by an induction zone and an exothermic reaction zone where the chemical energy is released as heat [3,4]. In other words, a coupling between the gas dynamics in the shock and chemical energy release must be obtained, since in a detonation the reaction is constantly induced by shock compression and its propagation is driven by thermal expansion due to the reaction. This leads to the central questions in the framework of any DDT investigation: (1) What are the conditions necessary for the transition? and (2) Which are the mechanims governing the transition?

One possible scenario indicates the increase of flame surface, mixing rate, and/or the change in the thermodynamic state of the reactants as essential mechanisms for flame acceleration. Lee [2] noted that the critical flame velocity preceding DDT reaches values close to the speed of sound in the products, which also matches closely the order of half of the theoretical Chapman–Jouguet detonation velocity $\frac{1}{2}V_{CJ}$ and the maximum possible deflagration velocity for a given mixture [4,5].

With regard to the second question, the early experimental investigations conducted in obstructed channels by Shchelkin and Troshin [6] propose turbulence as the first explanation for the acceleration and transition. The use of turbulence-generators considerably reduces the run-up distance. Therefore, rough walls and obstacles have been extensively used and turbulent flames have been associated with DDT processes. Turbulence and other type of instabilities contribute to the preconditioning, since the DDT is reluctant to occur in unconfined, freely propagating flames [7]. However, the attempt to explain DDT only by turbulence lacks a convincing coupling mechanism. A high mixing rate could generate local isochoric combustion and a blast wave emerging from the burned mass element, but it does not clarify the temporal and spatial coherence between the pressure waves and chemical reaction. An accepted regime transition theory is based on the spatial gradient of the chemical induction time τ_c and was introduced by Zeldovich et al. [8]. The ignition at the location of minimun τ_c and the propagation by further spontaneous ignitions through

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adjacent locations with slightly larger τ_c result in a reaction wave [9,10]. If the wave velocity lies between the speed of sound of the unperturbed medium and the V_{CJ} velocity, the reaction wave and the pressure waves induced by the expansion of the products couple and evolve into a self-sustained detonation [9,10]. An extensive study of this mechanism and its resulting regimes is presented by Liberman et al. in [10] and Kapila et al. in [11], for complex kinetics and for a one-step model, respectively.

The experimental examinations of Frolov et al. [12,13] focus on the practical use of detonation in combustion chambers. By using a shock wave-focusing nozzle, the detonation transition for hydrocarbon–air mixtures in relative short pipes was achieved. Without the use of the nozzle, unpractically long lengths are necessary for low reactive mixtures under normal conditions. This type of transition can be described as shock-to-detonation transition. These series of experiments [12,13] pointed out that the shock-to-detonation transition is a threshold phenomenon, which relies on mixture and combustion chamber geometry.

This paper presents the collaborative experimental and numerical study of DDT in a recently described configuration in which the flow is obstructed by a single obstacle [14]. The obstacle form consists of a convergent–divergent axisymmetric nozzle similar to Frolov et al.'s work [12,13] but equiped with a pre-combustion chamber instead of a shock tube device on the left hand side. The main objective is to analyse the effects this configuration has on the onset of detonation and identify the decisive aspects for DDT. To this end, different scenarios have been investigated. The problem is confronted by a joined experimental and numerical approach, thereby, enhancing the understanding of the processes involved. The findings of Gray et al. [14] are taken as a starting point. Important missing details inherent to the one-dimensional restrictions of Gray et al. [14] are completed by the current work. The results for one of the experimental cases deliver a deterministic and reliable behavior of DDT, which paves the way for its use in combustion systems.

The paper is organized as follows: Section 2 describes the features of the geometry under investigation and outlines the experimental facility and measurement devices. A description of the numerical model can also be found in Section 2. In Section 3, the experimental and numerical results are presented. The analysis and discussion of the results is included in Section 4. Section 5 summarizes the conclusions. Finally, the appendix contains the numerical model validation results.

2. Methods

2.1. Experimental setup

The experiments were conducted on a test stand with a shock-focusing geometry. This geometry is described in detail in [14] and consists of a hemispherical wave reflector at the inlet. The detonation chamber itself has an inner diameter of 40.3 mm. A spark plug is installed at the center of the wave reflector. The injection of fresh gases occurs over a circumferential slot at the boundary of the wave reflector. A shock-focusing nozzle is installed at 214.7 mm downstream of the center of the wave reflector with a blockage ratio of 75%, a converging half-angle of 45°, and a diverging half-angle of 4°. Twelve piezoelectric pressure sensors (PCB112A05) are installed at various locations before and after the nozzle, in order to capture the pressure evolution in the detonation chamber at a sampling frequency of 1 MHz. Figure 1 depicts a schematic of this configuration.

The test stand is designed to allow for various injection velocities as well as allowing for the ignition of a quiescent mixture. For the quiescent case (*CaseA*), the test stand is closed with ball valves and evacuated to below the desired air concentration. Then, oxygen and hydrogen are added using the method of partial pressures. The mixture used in these experiments is a stoichiometric mixture of hydrogen and air enriched to 40% oxygen by volume ($4H_2 + 2O_2 + 3N_2$). The amount of oxygen enrichment is based on matching the detonation cell width to that of a stoichiometric hydrogen-air mixture at the operating conditions in a micro gas turbine, namely, 3 bar and 400 K [14]. After filling, the mixture is circulated by means of another pump connected via a circulation line to the upstream and downstream sides of the test stand for five minutes. After circulation, the ball valves are opened and the mixture is ignited. The injection mass flows for the non-quiescent configuration (*CaseB*) were 20 kg/h air, 7 kg/h oxygen, and 1.47 kg/h hydrogen for the experiments presented in this paper. With these values, the bulk velocity in the combustor results in 8.7 m/s. Furthermore, a 100 mm long section just in front of the shock-focussing nozzle could be replaced by an acrylic glass tube, enabling high-speed observations of the flame. These were obtained with a Photron FASTCAM SA-Z.

2.2. Numerical methods

In the numerical part of this study, the compressible reactive Navier–Stokes equations are solved. These describe the mass, momentum, and energy conservation of the flow. The N species mass fractions of the reaction are modelled by N additional transport equations included in the set of differential equations, with $k = 1, \ldots, N$. Source terms must be incorporated into the N transport equations as well as the energy equation in order to take the changes during the reaction into account. These source terms are the mass reaction rate for the kth species $\dot{\omega}_k$ and the heat release due to combustion $\dot{\omega}_T$.

$$\sqrt{\rho}\frac{\partial\sqrt{\rho}}{\partial t} + \frac{1}{2}\frac{\partial \rho u_i}{\partial x_i} = 0 \tag{1}$$

$$\sqrt{\rho}\frac{\partial\sqrt{\rho}u_i}{\partial t} + \frac{1}{2}\left(\frac{\partial \rho u_j u_i}{\partial x_j} + \rho u_j \frac{\partial u_i}{\partial x_j}\right) + \frac{\partial p}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

$$\begin{aligned}&\frac{1}{\gamma-1}\frac{\partial p}{\partial t} + \frac{\gamma}{\gamma-1}\frac{\partial u_i p}{\partial x_i} - u_i\frac{\partial p}{\partial x_i}\\ &= \frac{\partial u_i \tau_{ij}}{\partial x_j} - u_j\frac{\partial \tau_{ji}}{\partial x_i} + \frac{\partial \Phi_i}{\partial x_i} + \dot{\omega}_T\end{aligned} \tag{3}$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_i Y_k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right) + \dot{\omega}_k \tag{4}$$

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \delta_{ij}\left(\mu_d - \frac{2}{3}\mu\right)\frac{\partial u_r}{\partial x_r} \tag{5}$$

$$\Phi_i = -\lambda\frac{\partial T}{\partial x_i} \tag{6}$$

Eqs. (1)–(3) are presented in the skew-symmetric form [15]. The advantage is the correct treatment of the kinetic energy. Although the equations are not in divergence form, the full scheme is conservative [15]. The perfect conservation property of mass, momentum, and total energy (chemical included) in high-order finite difference methods only applies when implicit time integrations are used and the numerical derivatives employ central stencils avoiding numerical dissipation [15,16]. Dissipation is introduced by the physical friction terms of the equations as well as by both an explicit filter of 6th order proposed in [17] and by an adaptive high-order shock-capturing filter [18]. The non-standard choice of the computational variables as $[\sqrt{\rho},\ \sqrt{\rho}u_i,\ p,\ \rho Y_k]^T$ responds to the simplification of