Combustion and Flame 183 (2017) 144–156

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

A compact shock-focusing geometry for detonation initiation: Experiments and adjoint-based variational data assimilation

J.A.T. Gray*, M. Lemke, J. Reiss, C.O. Paschereit, J. Sesterhenn, J.P. Moeck

Institut für Strömungsmechanik und Technische Akustik, Technische Universität Berlin, Müller-Breslau Str. 8, Berlin 10623, Germany

ARTICLE INFO

Article history:
Received 12 November 2016
Revised 17 December 2016
Accepted 9 March 2017
Available online 23 June 2017

Keywords:
Detonation
Shock focusing
DDT
Data assimilation
Adjoint equations

ABSTRACT

A shock-focusing geometry is proposed for a pulse detonation combustor, which exhibits a very short length for detonation initiation. This characteristic is imperative for the practical integration of such a combustor into a gas turbine. Experimental investigations are conducted in order to gain more understanding of the underlying processes and confirm the reliability of the geometry with respect to the success rate of the deflagration-to-detonation transition (DDT). The pressure evolution is measured at various locations in the detonation tube. Based on these data, a numerical simulation governed by the reactive, compressible Navier–Stokes equations is adapted by means of an adjoint-based data assimilation, where Arrhenius and diffusion parameters are adjusted. The resulting numerical model reproduces the experimental results very well and is used to obtain even more detailed information.

1. Introduction

Pulse detonation combustion has been a topic of intense research for several decades. The motivation is the increased efficiency of the Fickett–Jacobs cycle, which takes advantage of the near constant volume combustion of a detonation [1]. Thereby, it is important that as much of the combustion as possible takes place as a detonation wave and not as a turbulent flame. The advantage lies in the fact that the detonation wave exhibits a much higher pressure increase than the turbulent (deflagration) flame and, therefore, a significant increase in cycle efficiency. This leads to isochoric combustion also being referred to as pressure-gain combustion.

The generation of a detonation may be achieved by various means. The most straightforward of these is simply the direct initiation by introducing a large amount of energy (most frequently by means of a spark) in a short enough time and small enough space that a blast wave is generated, which continues as a self-sustaining detonation wave. This method, however, requires large amounts of energy and expensive high-voltage equipment and is, thus, not suited for gas turbine applications. For instance, the energy sufficient for the direct initiation of a hydrogen–air detonation at atmospheric conditions is nearly 10 kJ [2]. In contrast, the minimum ignition energy for a hydrogen–air deflagration is 0.02 mJ [3], nearly 9 orders of magnitude lower. The process of accelerating a deflagration to a detonation wave is known as the deflagration to detonation transition (DDT). Frequently used means of achieving DDT are based on creating a local explosion in the mixture by either shock–obstacle interaction [4] or by using shock focusing [5,6]. Ciccarelli et al. present a very comprehensive summary of alternatives to the direct initiation of a detonation, including the so-called SWACER (shock wave amplification by coherent energy release) mechanism in [7]. Much work has been done in recent years using obstacles in order to initiate DDT. Gamezo et al. [8] investigated the effect of obstacle spacing using numerical simulations. They found that small obstacle spacing increases initial flame acceleration, but hinders DDT, as Mach stems are not created. Paxson et al. [9] conducted an analysis on the effect of obstacles on the performance of pulse detonation combustors using a quasi-one-dimensional simulation verified by experiments. They determined that enhanced friction and heat transfer caused by the obstacles can result in a decrease in specific impulse of over 10%, though the majority of the loss results from heat transfer. Therefore, the number, size, and axial extent of obstacles should be kept as small as possible.

In the present work, a detonation combustion chamber is investigated which uses a single obstacle (nozzle) in order to focus the leading shock. Such leading shocks are typically ahead of accelerating fast deflagration flames [7,10]. By focusing this shock wave, a local explosion can be generated, which will transform

---

* Corresponding author.

E-mail addresses: joshua.gray@tu-berlin.de (J.A.T. Gray), mathias.lemke@tnt.tu-berlin.de (M. Lemke).

http://dx.doi.org/10.1016/j.combustflame.2017.03.014

into a self-sustaining detonation wave. The geometry of this combustion chamber results in very reliable DDT over a relatively short distance.

Due to the high temperatures and pressures as well as the relatively high speed at which the detonation process occurs, only limited information may be obtained from experiments by conventional means. In this study, flush-mounted pressure sensors and high-speed imagery, including shadowgraphy, are employed. In order to gain a deeper understanding of the DDT process a data assimilation technique is used for a more comprehensive analysis.

In general, the process of incorporating measurements (observations) into a mathematical model of the real system is known as data assimilation. It aims at finding a state among all possible states of a considered numerical model that matches the observations in an optimal sense. Applications are known from many fields (e.g., meteorology, climatology, oceanography, geoscience and control engineering). Usually, sparse measurements are used to predict the state of a considered system at spatiotemporal locations where no measurements are available. The behavior of the full system is estimated based on the physical understanding of the governing processes. Another application is parameter estimation for the creation of realistic models (e.g., [11]). The goal is to analyze a real system by means of a mathematical model. Thus, it enables advanced analysis of the detonation combustion chamber under consideration.

For data assimilation, two main approaches can be identified: stochastic filtering and variational methods. Both involve different techniques. As an extensive paper review exceeds the scope of this manuscript the reader is referred to [12,13]. In the present work, a variational approach is used [14–16]. More specifically, an adjoint-based variational parameter estimation strategy is designed and applied. Diffusion coefficients and Arrhenius-based chemistry parameters of the reactive Navier–Stokes equations are adapted until the numerical solution optimally matches the experimental observations. The resulting numerical simulation provides the full state in space and time and, thereby, quantities which are not able to be experimentally determined.

Variational data assimilation has been applied to incompressible [17] and compressible [18] flow configurations. Adjoint equations for reactive flows are mentioned in the context of uncertainty [19,20] and sensitivity analysis [21] as well as optimization tasks [22]. In the present work, data assimilation is used for the first time for the analysis of detonation initiation.

The paper is structured as follows: Section 2 describes the setup for the detonation test stand and the experimental procedures. In Section 3, the adjoint-based data assimilation framework is derived and discussed. The results of both the experimental investigations and the data assimilation procedure are presented in Section 4, including a comprehensive analysis of the processes occurring in the combustor.

2. Experimental considerations

2.1. Mixture scaling

The detonation sensitivity of gaseous mixtures is highly dependent on the reactivity of the gas. This can most readily be seen in experiments in confined tubes and channels. The dimensions of the tube or channel must meet or exceed a critical value, namely the size of the detonation cell, disregarding the limiting case of the so-called spinning detonation. As the reactivity of a mixture varies (due to changes in fuel, equivalence ratio, pressure, temperature, etc.), so does the detonation cell size and, therewith, the critical dimension of the confining detonation chamber. Ng et al. [23,24] developed an empirical model to estimate this cell size λ based on the induction length Δ_I and a non-dimensional stability parameter χ:

$$\lambda = f(\chi)\Delta_I. \tag{1}$$

The stability parameter is defined as

$$\chi = \varepsilon_I \Delta_I \frac{\dot{\sigma}_{\max}}{u_{\mathrm{CJ}}}, \tag{2}$$

where ε_I is the activation energy, u_{CJ} is the Chapman–Jouguet particle velocity, defined as the velocity of the gas behind the detonation wave in the shock-based frame of reference, and $\dot{\sigma}_{\max}$ is the maximum of the thermicity per definition of Kao and Shepherd [25].

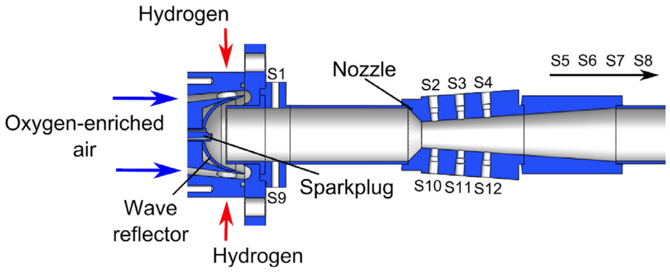

Fig. 1. Detonation initiation geometry used in experiments, with a wave reflector at the inlet, a focusing nozzle at a distance of 158 mm from the spark plug in the middle of the wave reflector, and pressure sensors S1–S12 installed at various positions. The distances of the pressure sensors from the spark plug are given in Table 1.

It has been shown in previous studies [26] that the benefits of pressure-gain combustion are dominant in regimes of lower pressure ratios (i.e., for operating conditions in micro gas turbines). A typical operating condition for such a machine would be initial conditions in the detonation chamber of 3 bar and 400 K. Using the described model from Ng et al., the corresponding cell size at these operating conditions for a hydrogen–air mixture is 2.9 mm. In order to decrease the cell size of the gaseous mixture at atmospheric conditions (1.013 bar and 293 K), the air may be enriched with oxygen. Increasing the oxygen concentration in the air to 40% by volume results in the same detonation cell size as that for the operating conditions of a typical micro gas turbine. Therefore, a stoichiometric mixture of air enriched to 40% oxygen and hydrogen was used for the following work.

2.2. Experimental setup

The experiments were conducted on a modular test stand, which allows for various types of obstacles to be installed in order to initiate DDT. For the purposes of this study, a nozzle was used with an upstream converging half-angle of 45° and a downstream diverging half-angle of 4°. The detonation tube has a diameter of 40.3 mm and the nozzle has a diameter of 20 mm at the throat, corresponding to a blockage ratio of 75%. The geometry of the combustion chamber is shown in Fig. 1. The premise behind using a nozzle as a DDT obstacle is the focusing of the leading shock wave. Work has been conducted on shock focusing at an endwall (e.g., [27] and [28]) with hemispherical, parabolic, or wedge-shaped forms. However, less research has been conducted on nozzles in which the incident shock and subsequent detonation travel in the same direction. Frolov et al. [6] used a parabolically shaped nozzle with a blockage ratio of 73%. An initial shock wave was produced in a propane–air mixture using a solid propellant gas generator (no flame) separated from the tube by a diaphragm. A focusing nozzle was placed in a tube with an inner diameter of 52 mm at a distance of 2000 mm from the diaphragm. This resulted in DDT at over 3500 mm from the diaphragm. In [29], Frolov et al. investigated a scaled version of the previous nozzle in