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Large Eddy Simulations of forced ignition of a non-premixed bluff-body methane flame with Conditional Moment Closure

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ABSTRACT

Large Eddy Simulations (LES) of forced ignition of a bluff-body stabilised non-premixed methane flame using the Conditional Moment Closure (CMC) turbulent combustion model have been performed. The aim is to investigate the feasibility of the use of CMC/LES for ignition problems and to examine which, if any, of the characteristics already observed in related experiments could be predicted. A three-dimensional formulation of the CMC equation was used with simple and detailed chemical mechanisms and sparks with different parameters (location, size) were used. It was found that the correct pattern of flame expansion and overall flame appearance were predicted with reasonable accuracy with both mechanisms, but the detailed mechanism resulted in expansion rates closer to the experiment. Moreover, the distribution of OH was predicted qualitatively accurately, with patches of high and low concentration in the recirculation zone during the ignition transient, consistent with experimental data. The location of the spark relative to the recirculation zone was found to determine the pattern of the flame propagation and the total time for the flame stabilisation. The size was also an important parameter, since it was found that the flame extinguishes when the spark is very small, in agreement with expectations from experiment. The stabilisation mechanism of the flame was dominated by the convection and sub-grid scale diffusion of hot combustion products from the recirculation zone to the cold gases that enter the burner, as revealed by analysis of the CMC equation.

1. Introduction

Ignition of non-premixed turbulent flames is important from a fundamental point of view, but also for practical applications, such as aviation and industrial gas turbines. In the former, high altitude re-light is of special interest, since the conditions (low pressure and temperature) may hinder the atomisation of the liquid fuel spray and hence the evaporation of the droplets, which may lead to unsuccessful ignition events. It is, therefore, important to understand better the processes that take place during the different phases of ignition and flame expansion. There are three stages involved in the ignition of a gas turbine flame [1,2]: (i) deposition of energy, (ii) evaporation of liquid fuel and (iii) flame expansion and stabilisation. This study focuses only on the last part. A gaseous flow is considered and it is assumed that hot gases have been created in a region of the flow and the way the flame expands is investigated.

The approach of Large Eddy Simulations (LES) has been used in this work. In LES, the larger, energy-containing scales are directly resolved, whereas the smaller scales are modelled [3]. LES of reacting flows using different combustion models have attracted much interest lately. Pitsch and Steiner have performed LES of Sandia flame D using a Lagrangian-type flamelet model [4]. Sandia flames D and E have been studied by Ihme and Pitsch using a flamelet/progress variable model [5]. Raman and Pitsch investigated a bluff-body stabilised burner (Sydney burner) using a recursive filter-refinement procedure [6], while a steady state laminar flamelet approach was used by Kempf et al. to study the same burner [7]. Very few LES studies of ignition are available. Jones and Navarro-Martinez [8,9] and Domingo et al. [10] have studied auto-ignition problems using a sub-grid scale probability density function model and tabulated chemistry, respectively. For spark ignition, LES of an ignition sequence in a gas turbine engine has been performed by Boileau et al. [11], with the igniters modelled as hot jets and the evaporation of the liquid fuel was included in the simulations. It was shown that the flame jumped from sector to sector driven by a mean flow in the azimuthal direction, caused by the imbalance between the production of the burnt gases in the flame and their outflux through the combustion outlet [11]. LES of ignition in a rocket-like configuration [12] has shown that the flame initially expands like a premixed spherical flame and later changes direction to propagate towards the nozzle. Finally, LES of spark ignition of a turbulent methane jet has also been performed re-

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cently [13]. The upstream propagation of the jet flame was captured with great accuracy and the lift-off height predictions were very close to experimental findings. All these simulations demonstrate that complex unsteady phenomena, such as extinction, auto-ignition and flame propagation can be captured by LES, combined with an intelligent combustion model.

In the present work, Conditional Moment Closure is used as a combustion model in LES. The CMC [14] is based on the fact that the fluctuations of the reacting scalars conditioned on the mixture fraction ξ are much smaller than the fluctuations of the unconditional reacting scalars. This means that closure may be provided for the chemical source term in terms of the conditional averages, either in terms of the first conditional moments (first order closure) or of higher moments. In a LES context, equations are solved for the conditionally filtered reacting scalars and their unconditional values can be calculated by integration over mixture fraction space. By nature, the CMC approach includes unsteady effects, which makes it an ideal candidate for the study of transient problems, such as ignition. The explicit presence of the scalar dissipation rate (see Section 2.2) enables it to capture the effects of small scale mixing [2]. The fact that convection and turbulent diffusion terms appear in the CMC equation (see Section 2.2 and Eq. (11)) suggests that the physical processes involved in the flame propagation phase are also included.

The CMC model has been used in the past in a RANS context in studies of many different turbulent combustion problems. These include attached [15,16] and lifted jet flames [17–19], where good agreement with the experimental results for the lift-off height was achieved and the correct flame stabilisation mechanism was reproduced. First order closure has been used in two-dimensional studies of spray auto-ignition [20,21], but also in three-dimensional simulations of diesel engines [22]. The results were overall good, despite the fact that the conditional fluctuations were neglected. This may be attributed to the relatively low scalar dissipation rate, compared to the extinction value, reducing the effect of the fluctuations [2]. Recirculating flames have been investigated with first-order CMC [23], where reasonable agreement with experimental measurements was achieved, with some discrepancies in the concentration of OH, which was attributed to the over-prediction of the scalar dissipation from the CFD solver and discrepancies for CO and H_2, the sources of which are unclear. Simulations of a counterflow flame [24] showed good agreement with the experimental measurements. Finally, reasonable agreement with experimental data was observed in a soot formation problem [25], where some of the discrepancies were attributed to the soot model.

The CMC equation was recently formulated for LES [26] and has been used to study a turbulent methane/air jet flame (Sandia D) [26], a bluff-body flame [27] and a lifted flame, sustained by auto-ignition [28]. In these papers, the nature of the flames allowed for variation of the conditional averages to be considered only in one (1D-CMC) [27] or two directions (2D-CMC) [28] or three directions but with the grid being very coarse on the plane vertical to the axis [26] ($64 \times 4 \times 4$ CMC cells). Using a coarser CMC grid than the RANS or LES grid is an essential feature of the practical implementation of CMC and reduces the computational cost. To further assume homegeneity in one or two physical space directions is justified if the nature of the studied flame allows it; essentially if the conditional averages are not strong functions of space. However, in forced ignition problems, the conditional averages show very large spatial variations (there are fully burnt and fully unburnt regions) and all three directions are of equal importance to the expansion of the flame. The application of CMC in LES in such problems can help reveal its strengths and shortcomings.

Recently, a number of spark ignition experiments of turbulent non-premixed flames have been performed at the University of Cambridge with laboratory scale burners to investigate closely the fundamentals of the process. Many different phenomena have been observed in these experiments. The various stages of flame expansion have been identified (kernel growth and flame expansion) and a probabilistic nature has been observed. The fact that there are fluctuations of the mixture fraction means that in a position where, on average, flammable mixture is found, instantaneously it is possible to have a mixture which is not flammable (either on the lean or the rich side). If energy is deposited at that instant, it is possible that the ignition event will be unsuccessful. Additionally, due to the unsteady nature of the turbulent strain that may quench the kernel and the possibility that the flame may not be able to propagate against the flow, the probability of a successful ignition event is not equal to the probability of finding flammable mixture (flammability factor). Moreover, three modes of failed ignition events have been identified [2]: (i) failure to initiate a kernel, (ii) creation of kernel, which is, however, convected away and (iii) flame growth in a substantial part of the combustor, but inability to obtain overall flame stabilisation. These topics are discussed in detail in Refs. [2,29] for gaseous flows and Ref. [30] for spray combustion.

In this paper, LES of ignition events of a bluff-body stabilised turbulent non-premixed methane flame, using the CMC model, are presented. In particular the experiment of Ref. [29] is simulated. The fuel is injected radially through a slit before the exit of the bluff-body (more details about the configuration are presented in Section 2.5.1), creating a reasonably well-mixed recirculation zone that presents an opportunity to additionally examine how good the CMC predictions will be in a flow with well-mixed regions. There is availability of qualitative and quantitative experimental measurements for the validation of the inert flow and the ignition simulations. Preliminary LES of this experiment with tabulated chemistry have also appeared [31], where is was shown that the time-history of the velocity and the mixture fraction can have an impact on the success or failure of a spark. That work further highlighted the value of LES for ignition problems. The purpose of this paper is to examine whether the CMC is appropriate for problems of forced ignition and flame expansion in non-premixed configurations. Furthermore, this paper aims to investigate how accurately the different phenomena observed in the experimental studies can be reproduced and how the location and size of the spark affects the way the flame expands. Chemical mechanisms of different complexity are presented to investigate which, if any, of the characteristics of flame expansion can be reproduced using a simple (and hence less computationally expensive) chemical mechanism.

In the next section, the LES and the CMC methods are described, presenting the equations that are solved and the models that are being used. The numerical set-up and the presentation of the investigated burner is also included. The results are presented and discussed in Section 3 and finally the conclusions are drawn in Section 4.

2. Modelling

2.1. Large Eddy Simulations

In LES, the larger scales are directly resolved, while the smaller scales are modelled. The Favre-filtered continuity and momentum equations are [32,33]:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_i} = -\frac{\partial \bar{p}}{\partial x_j} + \frac{\partial \tilde{\tau}_{ij}}{\partial x_i} - \frac{\partial\left(\bar{\rho}\tau^r_{ij}\right)}{\partial x_i} \tag{2}$$

where $\bar{\rho}$ is the resolved density, $\tilde{u}_i$ is the resolved velocity in the i direction, $\tilde{\tau}_{ij} = \overline{\mu}\left[2\widetilde{S}_{ij} - \frac{2}{3}\delta_{ij}\frac{\partial \tilde{u}_k}{\partial x_k}\right]$ is the resolved stress tensor and