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Direct comparison of PDF and scalar dissipation rates between LEM simulations and experiments for turbulent, premixed methane air flames

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ABSTRACT

We present a direct comparison between the predicted and measured probability density functions (PDF) of the reaction progress variable and conditioned values of the scalar dissipation rates (SDR) in premixed turbulent flames. The predictions are based on simulations of premixed flames using the linear-eddy model (LEM), parameterised by a wide range of integral length scales and turbulent Reynolds numbers. The experimental results are highly spatially resolved temperature and species data from the Cambridge–Sandia swirl burner. The LEM simulations display remarkable accuracy in capturing the features observed experimentally. Further, the results reveal that the LEM calculated PDF and SDR for premixed flames remain relatively steady under a variety of turbulent conditions, including variations in the integral length and turbulent Reynolds number. In general, it appears to be practical to use representative pseudo-turbulent PDF and SDR models for a range of turbulence intensities and length scales.

1. Introduction

Several practical models for turbulent premixed combustion rely on an accurate representation of the probability density function (PDF) of a reaction progress variable, which is often parameterised by the mean and variance of that progress variable [1–6]. These presumed PDF approaches are often implemented in conjunction with tabulated chemical variables to achieve detailed chemistry calculations in turbulent combustion simulations. Such models have been developed for both the Reynolds-averaged Navier–Stokes (RANS) and large eddy simulation (LES) paradigms. Previous work has shown that the accuracy of these methods depends to a considerable extent on the accuracy of the function presumed for the PDF of the progress variable [1].

A number of different presumed PDF models have been previously investigated for premixed combustion. The often used β-PDF does recover the extreme properties expected of the true PDF, such as δ functions at the zero and unity extremes of reaction progress for maximal variance, and single δ functions at the mean for zero variance. However, it fails to reproduce the shape of the true PDF in more general cases [1]. The issue is related to the fact that the shape of the true PDF appears to be a function of how the chemical reaction rates vary as a function of the progress variable; hence, different chemical kinetics lead to different shapes of the PDF of progress variable. The form of the β-PDF – which is of course entirely independent of the chemical kinetics – can lead to significant inaccuracies. Most critically, there can be a biasing error, as the discrepancies tend to occur at the same values of the progress variable for any particular flame.

One of the primary concerns in the design of modern engines is the reduction of harmful pollutants; specifically, the current generation of numerical models must be able to predict both the thermodynamic properties of the reacting mixture and the formation of these minor species with sufficient accuracy to resolve the parts per million produced. A prominent example is the prediction of prompt flame NO_x via the Fenimore pathway [7]. The predicted NO_x values from this mechanism are strongly affected by the choice of the PDF model, as this pathway is sensitive to the predicted temperatures and flame profile in the reactive regions.

In an attempt to account for the effects of chemistry on the shape of the PDF, Bray *et al.* [8] proposed using a premixed laminar flame to model the functional dependence of the PDF on progress variable. The proposed probability dependence of the flame existing at any given state is inversely proportional to the magnitude of the gradient of the temperature. Their original formulation only provided coverage for flames with very high variance. Jin et al. [1]

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then proposed a modification to the Bray PDF that extends the original formulation to cover all possible mean and variance combinations. This is accomplished by truncating the PDF shape function as needed to match the mean and variance parameters. It was found to significantly improve the fit of the PDF to that extracted from Direct Numerical Simulation (DNS) results. A shortcoming of this method is that, at the point of truncation, the model PDF has a sharp drop to zero, whilst the true PDF tends to be more rounded.

To address this issue, a one-dimensional turbulent method was proposed to take the place of the typical laminar flame calculation to tabulate pseudo-turbulent PDF models for RANS and LES closures. The Linear-Eddy Model, an inexpensive one dimensional stochastic mixing model, has demonstrated the ability to capture important effects from the interaction between chemistry and turbulence on the PDF distributions sufficiently well [9–11]. This model provides us with a mechanism to investigate the general flame characteristics at very high turbulence intensities, much beyond the capability of current DNS strategies. In turn, it permits us to analyse the behaviour of the PDF constructed at these highly turbulent states.

While the LEM has been implemented to investigate the shape of the PDF distributions [9,10], such simulations were performed to analyse the PDF for specific flames. The current study is primarily interested in the tabulation of a PDF lookup table useful for subsequent RANS and LES flame computations (a pre-processing operation not unlike pre-calculating the β-function and storing that in a lookup table). At first, there was a suggestion that one ought to try to match the turbulence statistics in the LEM calculations to those that one expects to find in the later turbulent flame calculation. Indeed, a possibility is that one might need to add a dimension to the lookup table (something like the local turbulent Reynolds number) to account for variations in local turbulence properties in the turbulent flame calculation and their effect on the shape of the PDF. This is a large part of the motivation for the LEM work presented here: do the turbulence properties affect the shape of the PDF? If so, how? How important is it to match the LEM turbulence properties used in generating the PDF lookup table to those that will be found in the turbulent flow to be calculated later?

A related question can be asked about the local gradient of progress variable in a premixed turbulent flame which is closely related to the scalar dissipation rate (SDR). For premixed combustion, the SDR, χ_c, of a temperature-based reaction progress variable is,

$$\chi_c(T,\phi) = \alpha_c(T,\phi)\nabla c \cdot \nabla c, \tag{1}$$

where $\alpha_c(T,\phi)$ and ∇c are the thermal diffusivity at the local temperature and equivalence ratio and the gradient of the progress variable, respectively.

The SDR is an important quantity to both non-premixed and premixed combustion modelling [12,13]. It is an unclosed term that appears in the transport equation for the variance of progress variable, where χ_c directly measures the decay rate of fluctuations through turbulent micromixing [13]. Since the burn rate of many combustion processes depends on the contact area and local gradient between the reactants, it is reasonable for most combustion models to assume that the mean burning rate of the flames either explicitly or implicitly depends on the scalar dissipation rate. For example, Conditional Moment Closure (CMC) uses the scalar dissipation rate conditioned by the progress variable to calculate micromixing [13]; not surprisingly, modelling the conditional scalar dissipation term $\chi_c|c^*$ conditioned on the local and global progress of reaction emerges as one of the main difficulties in applying CMC to turbulent premixed flames [14].

The same LEM method can be used to generate a model for the conditional scalar dissipation, where one simply conditionally averages the scalar dissipation in the LEM temperature profiles that are used to construct the PDF model. The unconditional mean SDR can be obtained by convolving the conditional SDR with the model PDF. This allows for the construction of pseudo-turbulent PDF and SDR models that are perfectly consistent with one another. While it is possible to obtain PDF and SDR distributions for premixed combustion from DNS, the associated cost is generally prohibitive for flows with relevant turbulent conditions [1]. More importantly, studies typically tend to focus on the analysis of the PDFs and SDRs at specific points within the domain. This leads to the problem that although DNS and experiments can provide valuable insight to the behaviour of the PDF and SDR [15–17], they cannot provide usable input models for subsequent RANS and LES combustion calculations, which is the primary motivation behind the current work. The incorporation of turbulence characteristics in the PDF distributions could provide a solution to the deficiencies seen in a number of current PDF models, such as the *ad hoc*β-pdf or the laminar approaches. Having more accurate PDF and SDR models would be beneficial to a number of RANS and LES strategies as closures for turbulent premixed combustion typically rely on some variant of the PDF or SDR model for the reaction progress variable as the input [12,13].

Recent detailed measurements of species and temperature have been made by the Cambridge–Sandia swirl burner [16,18–20]. This swirl burner was designed specifically to explore the influence of stratification on the flame. However, the very detailed nature of the scalar and velocity measurements have made the data set attractive as a target for premixed flame model validation as well [21,22]. In particular, the comprehensive database allows conditioning on a number of different variables, including equivalence ratio (for the stratified flames), temperature (or progress of reaction) or any other suitable scalar.

In this paper we use the experimental dataset to obtain detailed PDFs of the progress of reaction. The temperature is used to characterise the extent of reaction, for direct comparison with the PDFs generated from LEM simulations for three different swirl (and turbulence) levels. We consider the measured and computed variances, as well as the detailed shape of the PDFs in the comparison. In addition, we are also able to directly evaluate the unconditional mean SDR values obtained from experiment and LEM simulations. In the following sections we discuss the numerical approach, followed by a summary of the experiments and the data treatment used.

2. Numerical conditions: premixed combustion

2.1. Linear-Eddy model

The Linear-Eddy Model has been demonstrated to replicate the flow statistics for simple turbulent conditions with acceptable accuracy [23–27]. Given the one-dimensional nature of the model, the computational costs remain relatively low for most practical cases. Here, the LEM is used in a pre-processing manner for the tabulation of discrete PDF and SDR models, which can be implemented in subsequent RANS and LES applications.

The LEM can be divided into two modules. The deterministic component consists of the usual one-dimensional gas dynamics evolution equations, whereas the stochastic component consists of random *eddy events*. The turbulence concept of LEM postulates a random process that rearranges fluid elements along a line in order simulate the chaotic vortices that appear in turbulent fields. These one-dimensional vortices, known as *triplet maps*, generate discontinuous fluid motions, which lead to a random walk of fluid elements. The eddy event frequency per unit length of the domain is governed by Kerstein [26],

$$\lambda_{LEM} = \frac{54}{5}\frac{\nu Re_t}{C_\lambda l_0^3}\frac{(l_0/l_k)^{5/3}-1}{1-(l_k/l_0)^{4/3}}, \tag{2}$$