Combustion and Flame 157 (2010) 1467–1483

Contents lists available at ScienceDirect

Combustion and Flame

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

Investigation of an inhomogeneous turbulent mixing model for conditional moment closure applied to autoignition

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ARTICLE INFO

Article history:
Received 15 September 2009
Received in revised form 13 November 2009
Accepted 2 May 2010
Available online 1 June 2010

Keywords:
Scalar dissipation rate
Conditional moment closure
Autoignition
Mixing
Turbulence
Combustion

ABSTRACT

The present paper examines the case of autoignition of high pressure methane jets in a shock tube over a range of pre-heated air temperatures in engine-relevant conditions. The two objectives of the present paper are: (i) to examine the effect of the inhomogeneous mixing model on the autoignition predictions relative to the results obtained using homogeneous mixing models and (ii) to see if the magnitude of the change can explain the discrepancy between the predictions of ignition delay previously obtained with homogeneous mixing models and the experimental data. The governing equation of the scalar dissipation rate is solved for transient conditions and two different formulations of the same model are tested and compared: one using the linear model for the conditional velocity and one including the gradient diffusion model. The predicted ignition kernel location and time delay over a range of pre-combustion air temperatures are compared with results obtained using two homogeneous turbulent mixing models and available experimental data. The profiles of conditional velocity and the conditional scalar dissipation rate are examined. Issues related to the conditional velocity model are discussed. It is found that the differences in the predictions are due to the mixing model only. The inhomogeneous model using the gradient conditional velocity model produces much larger ignition delays compared to the other models, whereas the inhomogeneous form including the linear model does not produce any significant differences. The effect of the turbulent inhomogeneous model is larger at high air temperatures and decreases with decreasing air temperatures. In comparison with the measured ignition delays, the inhomogeneous-Gradient model brings a small improvement at high air temperatures over the results from the turbulent homogeneous models. At low air temperatures, other parameters need to be investigated in order to bring the predicted ignition delays and locations within the experimental data scatter.

1. Introduction

The accurate representation of the complex interactions between chemistry and turbulence is crucial for the development of new combustion devices, such as industrial furnaces, automotive engines and gas turbines. Computational models must be capable of incorporating finite-rate kinetics and predicting transient phenomena, such as ignition/extinction and autoignition in compression-ignition engines. In the context of autoignition, different turbulent combustion modelling approaches have been proposed including diverse levels of complexity, for example flamelet-based models [1], Conditional Moment Closure (CMC) [2] and probability density function (pdf) methods [3]. Over the past few years Direct Numerical Simulations (DNS) have also been increasingly used to provide further insight on existing models or physical phenomena that are not always reproducible through experimental data [4]. CMC methods solve additional transport equations for the conditional averages of scalars, such as species mass fraction and enthalpy, conditioned on the mixture fraction, in non-premixed turbulent combustion. The advantage of this approach is that the fluctuations about the conditional averages are much smaller than the fluctuations about the unconditional averages. Consequently, the conditional fluctuations can often be neglected leading to first order CMC, and detailed chemical kinetics can be included at low computational cost. First order CMC was successfully applied in several autoignition problems, including methane and methane-based blends [5–7], heptane [8], and spray [9,10]. Doubly-conditioning methods have been investigated for simplified cases of ignition [11]. De Paola et al. [12] applied a complete second order closure model to model autoignition and concluded that first order closure was sufficient when there was a rapid decay of the conditional scalar dissipation rate below its critical value. Three-dimensional CMC calculations of diesel engine simulations using Reynolds Averaged Navier–Stokes equations (RANS) [13] and forced ignition in Large Eddy Simulations (LES) [14] have been recently reported.

The scalar dissipation rate is a key quantity in turbulent combustion modelling, in particular for flamelet, CMC and pdf

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doi:10.1016/j.combustflame.2010.05.001

approaches [15]. The scalar dissipation rate, χ, represents the rate of mixing at the molecular level and is proportional to the mean square gradient of the scalar, Z, such as $\chi \equiv 2D\nabla Z \cdot \nabla Z$, where D is the molecular diffusivity of Z. Within the CMC framework, its conditional average at a particular value, η, of mixture fraction, ξ is of special interest with $\langle \chi|\eta \rangle = \langle D\nabla\xi \cdot \nabla\xi | \xi = \eta \rangle$. The angular brackets denote a conditional average over an ensemble of realizations of the flow, subject to the condition to the right of the vertical bar. Accurate modelling of the conditional scalar dissipation rate is crucial, as it appears in both the conditional species transport and temperature equations. However, evaluation of $\langle \chi|\eta \rangle$ is not straightforward. Further, CMC requires solution of the transport equations for the conditional averages to be consistent with that of the pdf transport equation [2]. When a presumed shape pdf is included, this condition can only be satisfied through the modelling of the conditional scalar dissipation rate derived from the pdf transport equation. Consequently, in cases of inhomogeneous turbulence, homogeneous mixing models do not provide closure for the conditional scalar dissipation rate that preserves consistency with the inhomogeneous pdf transport equation. Two of the most commonly used models in CMC are the presumed β-pdf model of Girimaji [16] and Amplitude Mapping Closure (AMC) [17]. Both models are derived assuming homogeneous turbulence. For validity, AMC requires some unmixed fluid to be present, setting a significant constraint in later stages of mixing. Girimaji's model may not be valid in shear layers. Klimenko and Bilger [2] showed how the conditional scalar dissipation rate could be evaluated in self-similar flows while Kronenburg et al. [18] developed a method for locally self-similar flows such as turbulent jet diffusion flames. Recently, Multiple Mapping Conditioning (MMC) methods have been developed using the concept of mapping closure [19]. In the simplest formulation, the mixture fraction can be selected as the only major species and MMC becomes equivalent to singly conditioned CMC. The advantage of MMC is that homogeneous turbulence is not assumed in the mapping process and as result, may be considered to be a generalisation of AMC for inhomogeneous cases. Further, the conditional scalar dissipation rate is in closed form [20]. However, modelling is still required for the conditional velocity. Previous CMC simulations for autoignition [5–13] only considered scalar dissipation rate models based on homogeneous turbulence, AMC being the most commonly used. El Sayed and Devaud [6] and El Sayed et al. [7] implemented first order CMC for the autoignition of high pressure methane jets in a shock tube using Girimaji's and AMC expressions. Both models gave similar results. The trend of predicted ignition delays were in reasonable agreement with experimental data, but an overprediction at low air temperatures and an underprediction at high air temperatures were noted. Detailed and optimised chemical kinetics were included and were unlikely to be the source of the discrepancies. The scalar dissipation rate was found to be a dominant term in the CMC equations, while the convective terms were smaller at most times. Thus, an improvement on the mixing model could directly affect the autoignition results. Three studies reported using CMC including an inhomogeneous formulation of the conditional scalar dissipation rate. Cleary and Kent [21] and Rogerson et al. [22] used the inhomogeneous model of Devaud et al. [23] with the gradient diffusion model for the conditional velocity in CMC for hood fire simulations and bagasse fired boiler, respectively. Sreedhara et al. [24] integrated the cross-stream averaged pdf transport equation to avoid numerical problems in low probability regions and ran CMC for piloted jet and bluff-body flames. In [21,24], the impact of the inhomogeneous mixing model was found to be small for the prediction of species concentrations and temperature. Rogerson et al. [22] did not include any further comparison on the effect of the mixing model.

The present paper re-examines the case of autoignition of high pressure methane jets in a shock tube over a range of pre-heated air temperatures in engine-relevant conditions. The two objectives of the present paper are: (i) to examine the effect of the inhomogeneous mixing model on the autoignition predictions relative to the results obtained using homogeneous mixing models and (ii) to see if the magnitude of the change can explain the discrepancy between the predictions of ignition delay previously obtained with homogeneous mixing models and the experimental data. The model proposed by Devaud et al. [23], derived through the integration of the pdf transport equation in mixture fraction space, will be implemented. In the present work, an inhomogeneous mixing model is expected to have a much larger effect on the prediction of ignition delay. At the early stages of jet development, the turbulent flowfield is far from being homogeneous. In contrast to the three previous studies [21,22,24], the governing equation of the scalar dissipation rate will be solved for transient conditions. To the authors' best knowledge, the inhomogeneous model has never been implemented for time-dependent or autoignition problems. Further, two different formulations of the same model will be tested and compared: one using the linear model for the conditional velocity and the second expression including the gradient diffusion model for the conditional velocity. The predicted ignition kernel location and time delay over a range of pre-combustion air temperatures will be compared with the results obtained using AMC and Girimaji's model and the experimental results of Wu [25]. The influence of the inhomogeneous mixing model will be assessed, as well as the impact of the conditional velocity model in the expression of the conditional scalar dissipation rate. Implementation of higher order or doubly-conditioning methods are beyond the scope of this paper. These may still be needed but further investigation is also required to examine (large) demand of computational resources and closure of many new terms. Thus, it is important to fully investigate the impact of the existing models in first order CMC before developing more complex CMC methods.

2. Inhomogeneous model

Devaud et al. [23] proposed a model for the Conditional Scalar Dissipation Rate (CSDR) without assuming homogeneous turbulence. Thus, this new method is applicable to a much wider range of flows compared to previous homogeneous-turbulence-based expressions and enforces consistency between the CSDR and the pdf transport equation. The model was presented in two formulations. The first formulation was the result of direct integration of the pdf transport equation in mixture fraction space, yielding an equation that was suitable for finite-volume discretization with no prior assumption regarding the form of the pdf required. The second formulation took a two-parameter presumed form of the pdf, in which the parameters were functions of mixture fraction and the variance. The results were compared with those of DNS for turbulent mixing in a channel flow and showed very good agreement [23]. In the present study, it is found that the first formulation of $\langle \chi|\eta \rangle$ is better suited to implementation in the commercial finite-volume CFD code, CFX [26], due to a smaller number of intermediate calculations. The derivation is briefly summarised below.

It is convenient to use density-weighted, or Favre, averages in turbulent combustion due to the large density fluctuations that occur in reacting flows. The Favre-averaged pdf, $\widetilde{P}(\eta)$, is related to the conventional pdf, $P(\eta)$, by

$$\rho_\eta P(\eta) = \langle \rho \rangle \widetilde{P}(\eta), \tag{1}$$

where $\langle \rho \rangle$ is the Reynolds mean density, $\rho_\eta = \langle \rho|\eta \rangle$ the conditional density and η a sample variable in mixture fraction space. The transport equation for $\widetilde{P}(\eta)$, is given by