Recent trends in modelling of turbulent combustion

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Abstract: Due to wide range of practical applications, modelling of turbulent combustion is one of the key areas in combustion research. This presentation will discuss the recent trend in turbulent combustion modelling – the appearance of universal, flexible models that combine features of existing categories. These approaches involve FDF (filtered density function) methods, generalised MMC (multiple mapping conditioning) and sparse-Lagrangian modelling. Jointly, these approaches allow for flexibility and the combination of useful properties of the original categories, most importantly generality and low computational cost. We discuss the general principles of universal modelling using MMC conditioning and sparse-Lagrangian simulations. As well we present some working examples. Special attention is paid to the application of MMC to premixed combustion.

Keywords: Combustion modelling, Turbulent flames, premixed and nonpremixed, MMC and sparse-Lagrangian methods

1. Introduction

Conventional models that are used for simulating turbulent combustion can be divided into the following categories [1]. 1) The models effectively based on the mixture fraction. Fast chemistry, flamelet, and CMC (conditional moment closure) models belong to this category. 2) The PDF (probability density function) methods which aim to reproduce the stochastic properties of reactive species. 3) The methods based on LES (large eddy simulation) or DNS (direct numerical simulation). Computational expense and generality of the models tends to increase significantly from the 1st category to the last, while DNS of complex flows with realistic kinetics are still out of reach for modern computers. While most of these categories were conventionally seen as being distinct and incompatible, research in recent years is marked by an emergence of universal and flexible approaches that combine useful features of the different categories. This presentation discusses and illustrates these new approaches.

2. Conditioning of mixing

The models that utilise the mixture fraction (Fast chemistry, flamelet, and CMC) are computationally efficient and involve accurate specification of mixing but have limited applications and lack generality to handle cases involving complex combustion phenomena (such as extinction and re-ignition). The PDF methods represent a more general albeit more computationally expensive approach, which can accurately treat complex kinetics but has difficulties in precise modelling of mixing. For a long time the mixture fraction and PDF methods were alternative (and to some extent competing) approaches for modelling turbulent combustion. With the introduction of MMC, this is no longer the case [2]. The MMC approach works to enforce conditional properties (such as conditional expectations modelled by CMC) on mixing while improving emulation of mixing and retaining the generality of the PDF methods.

In addition to the conventional dissipation time, the MMC models possess an additional parameter, called MMC localness. While the former parameter is selected to match large-scale properties of the simulated turbulent flow, the choice of the latter parameter reflects more refined properties of turbulent mixing determined by the scales belonging to the inertial interval of turbulence. Hence, MMC is explicitly aimed not only at simulation of the macroscopic effects of mixing (which is common for all mixing models) but also some of the microscopic effects of mixing. At this stage MMC is the only approach that is explicitly directed at modelling *micromixing*. Practically, the MMC localness parameter is selected to match the conditional variances, which are generated by small-scale fluctuations of the scalar dissipation.

MMC has evolved from its original version to a more flexible and simple to use generalized from. Its main feature is conditioning of mixing on MMC reference variables. Different types of reference variables have been explored in MMC modelling, including mixture fraction, scalar dissipation and shadow position.

3. Resolving large scales while modelling small scales

Large Eddy Simulations (LES) are known to improve simulation of turbulent flows in comparison with RANS-based models. At the same time, LES avoid the extensive computational expense which is associated with resolving down to the smallest turbulent scales in DNS. While the additional computational expense of LES, relative to RANS, is rewarded by well-simulated dynamic fields, LES simulations of chemical reactions often fall below expected quality. This happens due to neglecting subgrid fluctuations of reactive species, which are quite substantial (as long as LES is not over-refined to approach the full DNS regimes).

The response to the shortcomings of LES for reacting flows was to combine the LES and PDF methods into approach named FDF [3]. In this approach the large scales are resolved by LES while the subgrid distributions of species are not neglected but emulated. This can be done by Lagrangian particles or by multiple Eulerian fields (in the stochastic field method). The FDF approaches tend to produce very good results. The main factor that limits wide application of FDF methods is high computational cost due to the need of having many particles per each cell (or having many stochastic fields).

The computational cost of FDF methods can be substantially reduced: this is achieved in sparse-Lagrangian simulations. These simulations are not aimed at reproducing subgrid FDF of reactive scalars within each Eulerian cell (which represents the largest computational expense of conventional FDF simulations). This is replaced by the goal of having a representative stochastic value, which is distributed with the modelled FDF. These values are evaluated at Lagrangian particles, while having very few particles per cell or even having several cells per one particle can be sufficient for good simulations. In simple terms, the reactive scalars are simulated on a Lagrangian grid, while dynamic characteristics of turbulence are evaluated on the Eulerian grid. The variations of Lagrangian representations of the scalars emulate subgrid fluctuations.

4. Non-premixed flames

Practically, any substantial reduction in the number of particles is impossible to achieve without improving control of mixing. The sparse-Lagrangian methods work in conjunction with MMC modelling of mixing with conditioning on the mixture fraction. Simulations of Sandia flame D with as few as 10 thousand reactive particles have been demonstrating with a thousandfold reduction of computational cost as compared to conventional FDF simulations (which might deploy 20-50 million particles for a similar case).

Simulations of the whole series D, E and F have also been performed by sparse-Lagrangian MMC-LES simulations with only ~30 thousand particles [4]. Flame F is very close to extinction and is very difficult to reproduce correctly. The whole series have been simulated with exactly the same set of the model parameters.

4. Premixed flames

In the case of premixed flames, the PDF methods are known to work well for distributed regimes but, due to obvious reasons, have difficulties in reproducing flamelet regimes. The main problem is non-localness of simulated mixing that allows a direct mixing of the fresh and burned mixture (which is unphysical). MMC can be used as a remedy, localising mixing within the flame structure. The desired properties of the turbulent flames are to be enforced by conditioning of mixing, while the selection of different values for the MMC localness parameter allows for simulating distributed regimes, flamelet regimes or any regimes in between.

The selection of the MMC reference variable ξ that controls localization of mixing is illustrated in Figure 1. This variable can be qualitatively understood as the distance from the flame surface into the fresh mixture (this is conceptually similar to the level set approach). A constant density flow is assumed for simplicity. The area A of the surfaces of ξ=const increases as the flame is approached, while the flow of Lagrangian particles (each representing a certain mass) through these surfaces remains the same. Hence, the velocity of these particles in the reference space decreases from turbulent propagation speed u_t at a large distance from the flame to the laminar propagation speed u_0 at the flame. The details of the law associated with this decrease is very interesting, but it is still uncertain if this law is consistent with the relations of the inertial interval of turbulence. Fortunately, we do not need to emulate the whole distribution of the reference variables and are concerned only with the range near $\xi=\xi_f$ where the flame is located. Practically, the stochastic differential equation (sde) for simulation of the reference variables can be selected in different ways

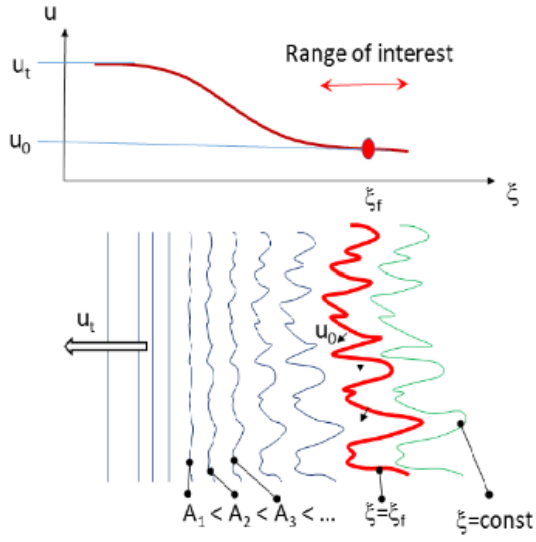

Fig. 1 Schematic of the choice of the MMC reference variable

In a summary, the flame is thin in the reference space ξ and propagates in this space with velocity close to the laminar propagation speed. The same flame is much wider in the physical space x and propagates in this space with the turbulent propagation speed. The structure of sample simulations with a simple one-step reaction mechanism is shown in Figure 2. The case under consideration corresponds to Re≈1000, Ka≈0.6 and the flame speed amplification $u_t/u_0 \approx 5$. The red dots represent particles at the flame, the blue dots represent the fresh mixture and the green dots represent the burned mixture. The flame is much thinner (~25 times) in the reference space than in the physical space. The top figure presents a snapshot of the x-ξ plane, while the bottom figures show scatter plots of the reaction progress variable C versus x and ξ correspondingly. The bottom figure is very close to the laminar flamelet solution, although some fluctuations with respect this solution are also apparent.

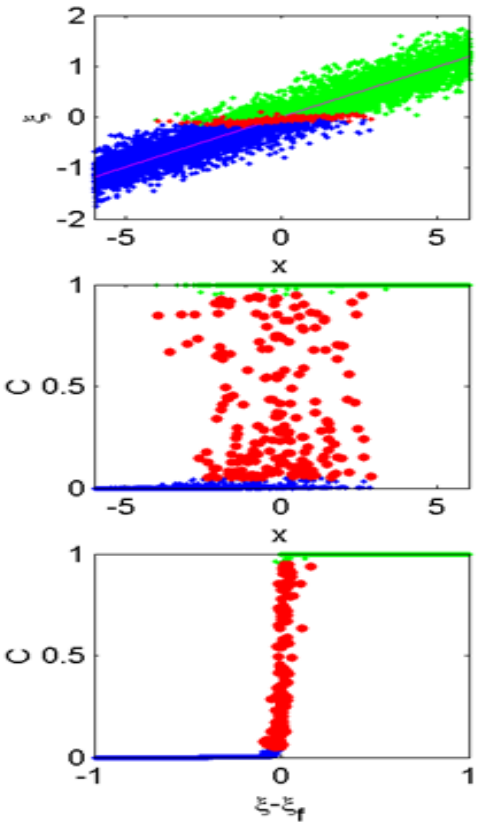

Fig. 2. Illustrative simulation of the flame propagation

5. Conclusions

Conceptual development of the last decade brought effective unification of the previously autonomous approaches to modelling of turbulent combustion. Most notable steps are incorporation of the PDF methods into LES framework and effective merges of the mixture-fraction based models with the PDF methods. These developments stimulate joint application of different turbulent models in a way that amplifies their strengths and negates their weaknesses.

6. Acknowledgement

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7 References

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