Advances in Turbulence X
Proceedings of the Tenth European Turbulence Conference
H. I. Andersson & P.-Å. Krogstad (Eds.)

Advances in PDF Methods for Turbulent Reactive Flows

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1 Introduction

Recent progress in PDF methods for turbulent reactive flows is reviewed, focusing on the work at Cornell on non-premixed turbulent combustion. Following an overview of PDF methods, recent calculations of two flames are described in Section 2, and then the important issue of modelling turbulent mixing is discussed in Section 3.

Modelling approaches to turbulent reactive flows [1][2] can be broadly categorized according to two attributes: first, how the flow and turbulence are represented; and, second, how the turbulence-chemistry interactions are modelled. The principal approaches to the flow and turbulence are [3]: Reynolds-averaged Navier-Stokes (RANS) turbulence modelling; large-eddy simulation (LES); and direct numerical simulation (DNS). At present, RANS is the dominant approach used in applications, whereas LES is the focus of much research [4][5]. While DNS is a powerful research tool [6], its range of applicability is severely limited (by computer power), much more so for reactive flows than for inert flows.

It is important to appreciate that the turbulence-chemistry interactions require modelling both in RANS and in LES [7]. The large-scale turbulent motions play the dominant role in the transport of momentum, heat and species, and consequently these are well-represented in LES by the resolved fields. But in reactive flows, especially combustion, the essential processes of molecular mixing and reaction occur on the smallest (sub-grid) scales, and therefore require statistical modelling in LES, as in RANS.

This paper is concerned with PDF methods [8][9][2], i.e., approaches for modelling turbulence-chemistry interactions through the solution of a transport equation for the joint probability density function (PDF) of the fluid composition (and other variables). The primary advantages of PDF methods are: that they are generally applicable (as opposed to being confined to homogeneously-premixed or two-stream non-premixed problems); the turbulent fluctuations of the fluid variables considered are completely represented through their joint PDF; and that arbitrarily complex and non-linear chemical reactions can be treated without approximation.

The two most widely used PDF methods in the RANS setting are the *composition PDF method*, and the *velocity-frequency-composition* method. In the

former, a RANS turbulence model (e.g., k-ε or Reynolds stress) is used, and the turbulent transport term in the PDF equation is modelled as gradient diffusion. In contrast, a complete closure is provided by the modelled transport equation for the joint PDF of velocity, composition and turbulence frequency [10]: separate mean momentum and turbulence-model equations are not required; and turbulent convective transport is in closed form, so that the gradient diffusion approximation is avoided.

In the LES setting, the filtered density function (FDF) [7] represents the distribution of compositions (on all scales), and conceptually it represents the PDF conditional on the resolved flow field [2]. The combined LES/FDF approach has been developed in recent years based on the composition FDF [11], and also on the velocity-composition FDF [12].

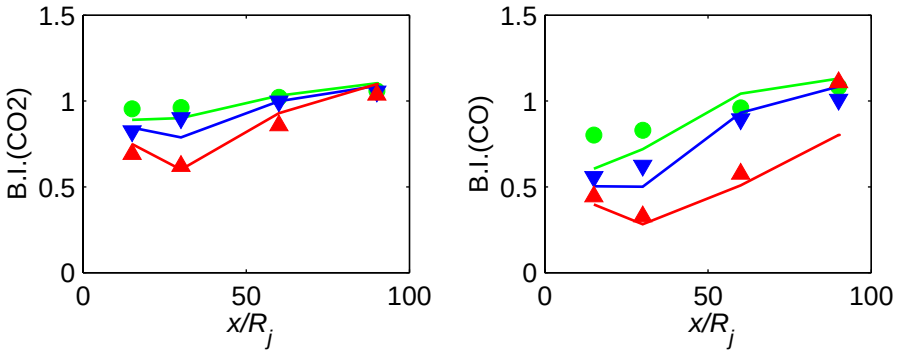
In the next section, recent PDF calculations of two non-premixed turbulent flames are reviewed in order to illustrate the ability of the method to represent accurately finite-rate turbulence-chemistry interactions. Then, in Section 3 we discuss the status of the modelling of molecular mixing, which is the principal modelling issue in PDF methods.

2 PDF Calculations of Turbulent Flames

In nonpremixed turbulent flames, whether or not finite-rate chemical effects are significant depends on the Damköhler number, Da, i.e., the ratio of characteristic mixing and reaction timescales. At high Da, simple models based on equilibrium chemistry or steady laminar flamelets can be successful (e.g., [13]). But as Da decreases, departures from equilibrium and flamelet behavior becomes pronounced, local extinction and eventually global extinction [14] occur. Several recent experiments have investigated such phenomena over a range of Da, achieved either by varying the jet velocities [14][15] or by varying the temperature and hence the reaction timescale. It is a good test and challenge for models to reproduce the observed behavior over the range of Da.

2.1 Piloted Jet Flames

The Barlow & Frank [14] flames have, deservedly, received much attention. The value of these experiments lies in: the design of the burner; the quality of the diagnostics; and, the range of conditions covered. By varying the jet and pilot flame velocities a series of six flames (designated A, B, $\ldots$, F) of decreasing Da are produced. Flame D is turbulent with little local extinction; flame F exhibits significant local extinction and is quite close to global extinction; whereas flame E is in between. There have been many calculations of flame D using several different approaches, but relatively few calculations of the more challenging flames E and F[16]. Velocity-composition-frequency joint PDF calculations of the Barlow & Frank flames are described by Lindstedt et al.[17], Xu & Pope [18] and by Tang, Xu & Pope [19]. In the latter works, the methane and NO chemistry



(a) (b)

Figure 1: Burning index based on (a) CO_2 and (b) CO against axial distance in flames D, E and F. Comparison of PDF calculations (lines) and experimental data (symbols).

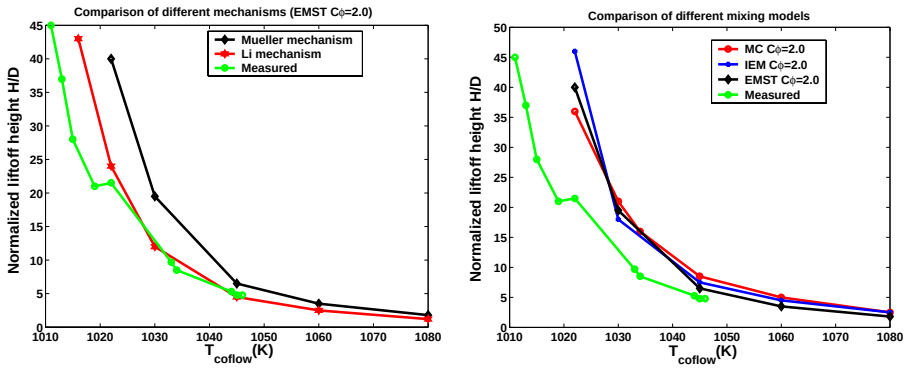
is described by a 19-species augmented reduced mechanism [20], and the mixing by the EMST mixing model [21].

Detailed comparisons between the calculations and experimental data (including conditional means and PDFs) are given in [18][19]. Here we present results just of the "burning index" BI which is an overall measure of finite-rate effects. The burning index can be based on different species and is locally defined: a value of 1 corresponds to complete combustion, and a value of 0 to complete extinction. Figure 1 shows the burning index based on CO_2 and CO as a function of axial distance for the three flames D, E and F. As may be seen, in general, the calculations represent accurately the minimum BI observed at 30 jet radii (due to local extinction) followed by the downstream recovery (due to reignition). Furthermore, the increase in local extinction between flames D, E and F is calculated accurately.

2.2 Lifted Jet Flame in a Vitiated Co-Flow

Cabra et al. [22] have studied experimentally the new configuration of a lifted flame formed by a H_2/N_2 jet issuing into a vitiated co-flow (at around 1045K). It is hypothesized that the stabilization mechanism for this flame is substantially different from that of lifted flames in cold co-flows. Specifically, mixing between the fuel and vitiated co-flow near the jet exit leads to a hot, lean mixtures which subsequently autoignite, thus anchoring the flame.

In further experiments using this burner at the University of Sydney the temperature of the vitiated co-flow has been varied over a narrow range (1010K-1045K) which results in lift-off heights between 45 jet diameters to 5 jet diameters



(a) (b)

Figure 2: Lift-off height versus co-flow temperature for the hydrogen jet flame in a vitiated co-flow (a) comparison of the Li and Mueller chemical mechanisms (b) comparison of MC, IEM and EMST mixing models.

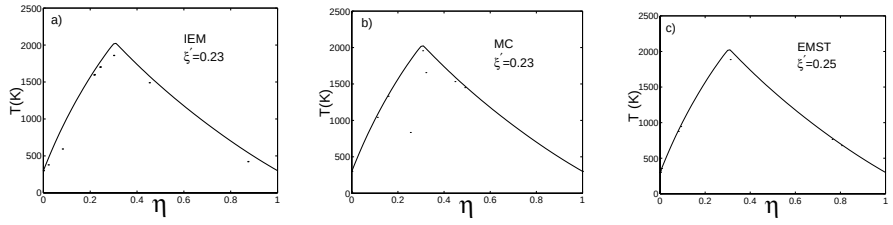
(as the temperature is increased).

There have been several PDF calculations of these flames [22][23][24][25]. From the latter work, we show in Fig. 2(a) the calculated lift-off height using two chemical mechanisms for hydrogen combustion: the Mueller mechanism [26]; and the Li mechanism [27] in which a few rates and enthalpies of formation are updated. It appears that the calculations with the Li mechanism are in excellent agreement with the experimental data. It is important to appreciate, however, that the experimental uncertainties in the temperature of the vitiated co-flow combined with the marked sensitivity of the lift-off height to this quantity results in experimental error bars that are larger than the differences between the calculations. What can be concluded is that both PDF calculations reproduce the experimental lift-off heights (within the error bars) and that they exhibit a sensitivity to the details of the chemical mechanism.

Figure 2(b) shows the calculated lift-off heights using the Mueller mechanism and the three most widely used mixing models, namely: the interaction by exchange with the mean (IEM) model [28][29]; the modified Curl (MC) model [30][31]; and the Euclidean minimum spanning tree (EMST) model [21]. As may be seen, for this flow, there is no great sensitivity to the choice of mixing model. This issue is discussed further in Section 3.

3 Modelling of Turbulent Mixing

In turbulence research on inert flows, there have been numerous studies of scalar mixing in which the primary focus is on the mean, variance and derivative statistics of a single inert scalar (e.g., temperature excess). The issues of mixing



(a) (b) (c)

Figure 3: Scatter plots of temperature versus mixture fraction in a PaSR using different mixing models (a) IEM (b) MC (c) EMST.

in turbulent combustion are significantly more involved. Typically, there are of order 20 compositions; the effect of molecular mixing on the shape of the PDF is important (not just the decay rate of the variances and covariances); fluctuations in mixing rates are significant in effecting local extinction; and (especially in premixed combustion) reaction and mixing can be strongly coupled.

The three most commonly used mixing models, IEM, MC and EMST, have known theoretical deficiencies, but at the same time, in some circumstances, they can yield quantitatively accurate results. A current objective of research in this area is to delineate the range of applicability of these different models.

The calculations of the lifted flame described above illustrate a case in which all three mixing models yield similar results. In contrast Ren & Pope [32] studied a partially stirred reactor (PaSR) in which radically different behavior is observed. As an example, Fig. 3 shows scatter plots of temperature versus mixture fraction given by the three models for a case of hydrogen combustion. In addition to the chemistry, the reactor is characterized by the residence time $\tau_{\rm res}$ and the turbulent mixing time $\tau_{\rm mix}$. For small values of $\tau_{\rm mix}/\tau_{\rm res}$ (e.g., $\tau_{\rm mix}\tau_{\rm res} < 1/20$) the PaSR approximates a PSR and the three mixing models yield essentially the same results. But for larger values of $\tau_{\rm mix}/\tau_{\rm res}$ the scalar variances become significant and, as observed in Fig. 3, the shapes of the joint PDFs predicted by the models can be quite different.

For the same PaSR test case, Fig. 4 shows the conditional mean temperature (at stoichiometric) as a function of the residence time for fixed $\tau_{\rm mix}/\tau_{\rm res} = 0.35$. As in a PSR, blow-out occurs at a critical value of $\tau_{\rm res}$, as indicated by the asterisks in Fig. 4. As may be seen, the three models have significantly different critical residence times with EMST being most resilient, and IEM being least. Similar conclusions were drawn by Subramaniam & Pope [33] in a significantly different test case.

An interesting development in the context of turbulent mixing is the development of the multiple mapping conditioning (MMC) approach [34]. This can be considered to be a marriage between the conditional moment closure [35] and the amplitude mapping closure [36][37]. For a turbulent reactive flow involving

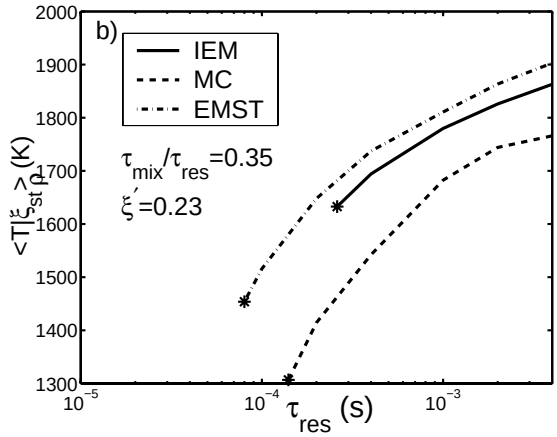


Figure 4: Mean temperature conditional on stoichiometric against residence time for a PaSR using different mixing models.

n_s species, it is hypothesized that (in the composition space) all compositions lie on a manifold of dimension $n_r < n_s$. (This hypothesis is also explored by Pope [38].) The manifold is parameterized by n_r reference variables to which the mapping closure is applied.

As a basic test of the mapping closure aspects of MMC, an analytic solution is obtained for the joint PDF of two scalars evolving in isotropic turbulence from a symmetric triple-delta-function initial condition. The shapes adopted during the evolution of the joint PDF are in excellent agreement with those obtained from DNS by Juneja & Pope [39].

Mixing models should remain an active area of research for some time, since they are a crucial element in PDF methods in both RANS and LES approaches, and current models have several well-appreciated shortcomings. There are also questions to be answered about the performance of the existing models. In the theory of non-premixed turbulent combustion, extinction and ignition events are associated with large and small values, respectively, of the scalar dissipation. How is it that these phenomena can be accurately calculated using existing mixture models which do not explicitly represent the distribution of scalar dissipation?

Acknowledgment

This work is supported by the Air Force Office of Scientific Research under Grant No. F-49620-00-1-0171, and by Department of Energy, grant number DE-FG02-90ER14128.

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