Laminar Flamelets in Turbulent Combustion Modelling

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Summary

A brief review is presented of so-called laminar flamelet models of turbulent combustion processes, using premixed combustion as an example. Circumstances where this simple modelling strategy can fail are explored.

Introduction

Although it is widely accepted that combustion of hydrocarbon fuels contributes to global warming, and should be curtailed, the necessary alternative power sources are not yet widely available. We must therefore expect fuel to continue to be burned, particularly for road and air transport, for the foreseeable future. The combustion process is highly turbulent in almost all practical devices and circumstances are such that the rate of heat release is sensitive to the resulting turbulent mixing processes. Turbulence and combustion interact with each other in complex and incompletely understood ways so the design of combustion engines must make use of empirically based turbulent combustion models.

One class of model that can be used for this purpose is based on the assumption that a turbulent flame can be approximated by a laminar flame which is distorted and wrinkled by the flow but retains the internal structure of a laminar flame. This so-called *laminar flamelet* approximation which is widely used in both RANS (Libby & Williams, 1980; Peters, 2000) and LES (Nambully et al, 2014; Knudsen et al, 2013; Butz et al., 2015) calculations is the subject of the present brief review. The laminar flames of these models may be premixed or nonpremixed, steady or nonsteady, with or without heat transfer; here, for illustration, we confine our attention to steady premixed flames. We shall identify several different types of laminar flamelet model, and discuss their advantages and circumstances in which they may fail.

A laminar flamelet assumption may for example be used (Vervisch et al, 2011) simply to produce a table of species compositions and reaction rates in terms of a suitably chosen reaction progress variable; an assumed probability density function (PDF) for this variable then provides an estimate for mean properties. This should be relatively insensitive to disturbances of the preheat zone as long as the reaction zone remains unaffected. A second type of flamelet model estimates the mean reaction rate as

$$\overline{\omega}_c = \rho_R S_{L0} \Sigma$$

where ρ_R is the density of unburned reactants, S_{L0} is the laminar flame speed and Σ is the flame surface density.

A third type of model involves a laminar flamelet expression for the PDF, P(c;**x**), We have the following relationship (Bray 2011):

$$\Sigma(c;\mathbf{x}) \approx \Sigma(\mathbf{x}) = < |\nabla c| | c > P(c:\mathbf{x})$$

where the PDF is written

$$P(c;\mathbf{x}) = \alpha(\mathbf{x})\,\delta(c) + \beta\,(\mathbf{x})\,\delta(1-c) + \gamma\,(\mathbf{x})\, f_{lam}(c)$$

Here $\alpha(\mathbf{x})$ and $\beta\,(\mathbf{x})$ are the probabilities for reactants and products, respectively, $\gamma\,(\mathbf{x})$ is the reaction mode probability, and $f_{lam}(c)$ is the internal PDF for the reaction mode, where the subscript indicates that this is to be evaluated in the laminar flamelet approximation. This quantity is written (Bray, 2011)

$$f_{lam}(c) \approx 1/(\Delta\eta\sigma_{lam})$$

where $\Delta\eta$ represents the thickness of laminar flame included in the model and σ_{lam} is the gradient $dc/d\eta$ at a location η in the flame.

It has been shown (Bray, 2011) that this flamelet PDF leads to a simple and explicit mean reaction rate model

$$\overline{\omega}_c = \frac{e\tilde{c}(1-\tilde{c})}{(1+\tau\tilde{c})\delta *} \rho_R S_{L0}$$

where e is the deviation of $\overline{\rho c''^2}$ from its maximum possible value, ie

$$e = 1 - \frac{\overline{\rho c''^2}}{\bar{\rho}\tilde{c}(1-\tilde{c})}$$

and

$$\delta^* = \int_{\eta_{\min}}^{\eta_{\max}} \frac{c(1-c)}{(1+\tau c)} d\eta$$

This expression shows the mean reaction rate in the flamelet approximation to be proportional to e and to the laminar flame speed. If e is small then the flamelet probability $\gamma(x)$ will also be small. In the limit $\gamma \langle\langle\ 1$, where the mixture consists predominately of packets of unburned and fully burned mixture separated by thin reaction zones, the mean heat release rate is controlled mainly by small-scale mixing. The rate at which this occurs, characterised by the scalar dissipation rate, $\tilde{\chi}_c$, is then related to the mean reaction rate by (Libby & Bray, 1980)

$$\bar{\omega}_c = \frac{1}{(C_M - 1/2)} \bar{\rho} \tilde{\chi}_c$$

where

$$C_M = \overline{c\omega_c} / \bar{\omega}_c$$

can usually be treated as a constant; its value typically lies between 0.7 and 0.8 (Swaminathan & Bray, 2011) for lean hydrocarbon and hydrogen-air flames. This replaces the problem of modelling the mean reaction rate with the equally difficult challenge of predicting the mean scalar dissipation – but it does emphasise that burning is now mixing – controlled. Scalar dissipation rate closures for LES are proposed and assessed in (Butz et al., 2015; Ma et al., 2014; Langella et al., 2015; Langella & Swaminathan 2016).

The simple laminar flamelet assumptions outlined above can fail for a variety of reasons, including flame stretch, intense small-scale turbulence, and flame-flame interactions. Chen et al. (1996) report results of experiments showing departures from laminar flame structure in the preheat zone of a turbulent flame and this flame is shown to be predicted quite well using flamelets (Langella & Swaminathan 2016). Dunstan *et al* (2012) use data from DNS of three turbulent flame geometries, a planar propagating flame, a stagnation point flame, and a vee flame, to explore turbulent flame propagation and deviations from laminar flamelet burning. The magnitude of the composition gradient is generally greater than that of an unstretched laminar flame, indicating thinning of the flame by turbulent straining. However, this increase is found to be small near the hot side.

Dunstan *et al* (2012) use direct numerical simulations (DNS) of two side-by-side vee flames to study flame-flame interactions. They identify seven different types of interaction and their data suggests that the one they call *tunnel closure*, in which a tube of unburned gas surrounded by products is stretched by the flow until the sides of the tube touch each other, appears to be the most probable. The problem of incorporating flame interactions into models is briefly discussed.

Conclusions

We have reviewed evidence concerning the occurrence of laminar flame structures in premixed turbulent combustion and influences of flame stretch, intense turbulence, and flame-flame interactions have been explored. DNS data suggests that the preheat zone structure differs from that of an unstretched laminar flame much more strongly than does the high temperature side. Significant modelling advantages are apparent when laminar flame structures are assumed. However, we still cannot predict with certainty what errors will result from adopting a flamelet modelling strategy.

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