Available online at www.sciencedirect.com
ScienceDirect
Proceedings of the Combustion Institute 32 (2009) 1445–1453
Proceedings of the Combustion Institute
www.elsevier.com/locate/proci

Direct Numerical Simulation analysis of the Flame Surface Density transport equation in the context of Large Eddy Simulation

Nilanjan Chakraborty [a,*], R.S. Cant [b]

[a] Engineering Department, University of Liverpool, Brownlow Hill, Liverpool, Merseyside L69 3GH, UK
[b] Cambridge University, Engineering Department, Trumpington Street, Cambridge CB2 1PZ, UK

Abstract

Turbulent reaction rate closure modelling using the concept of Flame Surface Density (FSD) is now well-established in the context of Reynolds Averaged Navier Stokes (RANS) simulations. In the present study, three-dimensional DNS data is explicitly filtered in order to evaluate different terms of the FSD transport equation in the context of Large Eddy Simulation (LES). Existing sub-models for these unclosed terms are assessed with respect to the filtered DNS data, resulting in a recommended modelled form for each term. Previously assessed modelling of the propagation and curvature terms is combined with new model formulations for the turbulent transport and strain rate terms to produce a complete modelled FSD transport equation for use in LES. Displacement speed is shown to play a pivotal role in the modelling of several terms and its curvature dependence is explicitly accounted for in order to ensure that the FSD model will be valid in both the corrugated flamelets and the thin reaction zones regimes.

Keywords: Flame Surface Density (FSD); Large Eddy Simulation (LES); Direct Numerical Simulation (DNS); Displacement speed; LES combustion modelling

1. Introduction

Large Eddy Simulation (LES) has become an important tool for the analysis of turbulent combustion especially in problems involving significant large-scale unsteadiness, e.g. in thermo-acoustic instability in gas turbine combustors. Modelling of turbulent premixed flame propagation using the concept of Flame Surface Density (FSD) is well established in the context of Reynolds Averaged Navier Stokes (RANS) simulation. By contrast, extension of the FSD concept for LES combustion modelling is relatively recent [1–6]. Other LES combustion models [7–12], including those based on artificially thickened flames and the sub-grid scale wrinkling factor, are closely related to models for the sub-grid FSD.

Modelling the FSD transport equation is expected to have advantages over simpler algebraic FSD models in cases where the level of sub-grid wrinkling is high and the flame propagation is highly unsteady [13]. Moreover, straining and curvature effects can be represented directly in the FSD transport equation by using a suitable model for the displacement speed of the flame. At

* Corresponding author. Fax: +44 1517944848.
E-mail addresses: n.chakraborty@liverpool.ac.uk (N. Chakraborty), rsc10@eng.cam.ac.uk (R.S. Cant),

1540-7489/$ - see front matter © 2009 The Combustion Institute. Published by Elsevier Inc. All rights reserved.
doi:10.1016/j.proci.2008.06.028

present, most FSD modelling does not account for the strain rate and curvature dependence of displacement speed and is valid only for the corrugated flamelets regime [14]. In the thin reaction zones regime the curvature contribution to displacement speed becomes a leading order effect [14], and hence cannot be ignored.

In LES, the level-set approach has proved successful in addressing flame propagation behaviour in the thin reaction zones regime [15], while Sankaran and Menon [16] have recently proposed a development of the Linear Eddy Model (LEM) for LES in the same context. By contrast, FSD based models have yet to be extended properly to the thin reaction zones regime. Some FSD and wrinkling factor models [2,3,8–10] do include straining and curvature effects through the use of an efficiency function, although the applicability of this approach within the thin reaction zones regime is not yet clear. Recent work has provided a detailed examination of the curvature and propagation terms of the FSD transport equation [17], and has indicated the importance of the displacement speed in closing these terms.

In this paper, FSD transport equation modelling is extended to the thin reaction zones regime based on *a priori* DNS analysis. Three-dimensional DNS with single-step Arrhenius chemistry has been carried out for freely propagating statistically planar turbulent premixed flames. The DNS data is explicitly filtered for LES using a Gaussian filter. The modelling assumptions for the FSD transport equation are assessed by comparing the LES-modelled terms with filtered DNS data.

The rest of the paper is organised as follows. The mathematical background is presented in Section 2, followed by a brief description of the numerical implementation in Section 3. The results are presented and discussed in Section 4, and the main conclusions are summarised in the final section of the paper.

2. Mathematical background

Combustion DNS in 3D with detailed chemistry has become feasible only recently and remains immensely computationally expensive. For the present investigation, three-dimensional DNS with a single step irreversible Arrhenius reaction mechanism is used. A reaction progress variable c is defined in terms of product mass fraction Y_P as $c = (Y_P - Y_{P0})/(Y_{P\infty} - Y_{P0})$, which increases monotonically from zero in fresh gas (subscript 0) to unity in fully burned products (subscript ∞). The LES filtered transport equation for reaction progress variable is given by:

$$\partial(\bar{\rho}\tilde{c})/\partial t + \partial(\bar{\rho}\tilde{u}_j\tilde{c})/\partial x_j = \overline{\dot{w} + \nabla\cdot(\rho D\nabla c)} - \partial(\bar{\rho}\widetilde{u_j c} - \bar{\rho}\tilde{u}_j\tilde{c})/\partial x_j \qquad (1)$$

where $u_j, \rho, \dot{w}$ and D denote the jth component of velocity, density, reaction rate and mass diffusivity, respectively, while $\overline{Q}$ and $\tilde{Q} = \overline{\rho Q}/\bar{\rho}$ stand, respectively, for LES filtered and Favre filtered values of a general quantity Q. The term $\bar{\rho}(\widetilde{u_j c} - \tilde{u}_j\tilde{c})$ in Eq. (1) denotes the sub-grid flux of reaction progress variable. The combined reaction rate and molecular diffusion rate is given by:

$$\overline{\dot{w}} + \overline{\nabla\cdot(\rho D\nabla c)} = \overline{(\rho S_d)}_s\Sigma_{\text{gen}} \qquad (2)$$

where $\overline{(Q)}_s$ denotes the surface average of a general quantity Q as given by $\overline{(Q)}_s = \overline{Q\,|\,\nabla c\,|}/\overline{|\,\nabla c\,|}$ and $\Sigma_{\text{gen}} = \overline{|\,\nabla c\,|}$ is the generalised FSD as suggested by Boger et al. [1]. Here, S_d is the displacement speed, defined as $S_d = (\dot{w} + \nabla\cdot(\rho D\nabla c))/(\rho\,|\,\nabla c\,|)|_{c=c^*}$, which is the speed with which a given isosurface of $c = c^*$ moves normal to itself with respect to an initially coincident material surface. The transport equation for the generalised FSD is expressed as [18]:

$$\frac{\partial\Sigma_{\text{gen}}}{\partial t} + \frac{\partial(\tilde{u}_j\Sigma_{\text{gen}})}{\partial x_j} = -\frac{\partial}{\partial x_i}[\overline{(u_i)}_s - \tilde{u}_i]\Sigma_{\text{gen}} + \overline{\left((\delta_{ij} - N_iN_j)\frac{\partial u_i}{\partial x_j}\right)_s}\Sigma_{\text{gen}} - \frac{\partial}{\partial x_i}[\overline{(S_dN_i)}_s\Sigma_{\text{gen}}] + \overline{\left(S_d\frac{\partial N_i}{\partial x_i}\right)_s}\Sigma_{\text{gen}} \qquad (3)$$

The terms on the right-hand side of Eq. (3) represent the effects of (1) sub-grid transport, (2) strain rate, (3) propagation and (4) curvature. All of these terms are unclosed and hence require modelling.

3. Numerical implementation

A series of DNS runs has been carried out for freely propagating statistically planar turbulent premixed flames in a cubical domain. The boundaries normal to the mean direction of flame propagation were specified as acoustically non-reflecting using the NSCBC formulation [19], while the transverse boundaries were specified as periodic. The combustion DNS code SENGA [17] was used, in which spatial differentiation is carried out using 10th-order central differences for interior points, decreasing to 4th-order one-sided differences close to non-periodic boundaries. Time advancement is carried out using a third order low storage Runge–Kutta scheme. The velocity field was initialised with homogeneous isotropic turbulence generated in Fourier space using a Batchelor–Townsend energy spectrum, while the flame was initialised using a steady one-dimensional laminar flame solution. The laminar flame thickness is defined as $\delta_L = 1/\text{Max}(|\nabla c|)$ and about 10 grid points are kept within δ_L in order to resolve the flame structure. The domain length ($l_0 \approx 10\delta_L$) and unstrained laminar flame