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A posteriori large-eddy simulations of a turbulent premixed flame in the thin reaction zones regime

Obulesu Chatakonda[1], Edward Knudsen[2], Evatt R. Hawkes[1,3], Mohsen Talei[3] and Heinz Pitsch[4]

[1]School of Photovoltaic and Renewable Energy
The University of New South Wales, Sydney, 2052 Australia
[2]Department of Mechanical Engineering, Stanford University, California, 94305, USA
[3]School of Mechanical and Manufacturing Engineering,
The University of New South Wales, Sydney, 2052 Australia
[4]Institute of Combustion Technology, Tempergraben 64, 52056, Aachen, Germany

Abstract

Large-eddy simulations (LES) have been successfully applied to premixed turbulent flames in the flamelet regime. However, in the context of LES, comparatively little effort has focused on modelling of premixed flames in regimes of combustion in which the small scale eddies can penetrate the flame, the most important of which is the so-called thin-reaction zones (TRZ) regime. In this work, *a posteriori* LES of a turbulent premixed, methane-air slot-jet are performed using strained and unstrained premixed flamelet solutions. The turbulent flame speed is calculated using the Hawkes model [13] in both static and dynamic coefficients versions. The LES results are compared with direct numerical simulation (DNS) data, demonstrating that the strained flamelet solution with the Hawkes model performs well in simulating turbulence perturbations of sub-grid premixed flame structures in the TRZ regime.

Introduction

Conventional gas-turbine combustors operate on diffusion flames where fuel burns near stoichiometric conditions, causing a high flame temperature and also an unacceptable level of emissions such as NO_x. Efforts to reduce the NO_x emissions have led to the development of lean premixed combustors. In these combustors, fuel is burned at a lower maximum temperature, thereby reducing NO_x formation. However, the flame speed decreases for leaner mixtures and therefore, these combustors operate at a high pressure and turbulence intensity, in order to burn the fuel faster [1]. At high turbulence intensity, when the Kolmogorov scale η is smaller than the thermal flame thickness δ_L but larger than the reaction layer thickness, smaller eddies penetrate into the preheat zone of the flame, thereby enhancing the flame-turbulence interactions. This regime of combustion is referred as the thin-reaction zones (TRZ) regime and is present in many modern practical combustors [2].

In recent years, large-eddy simulation (LES) has emerged as a useful tool for studying both fundamental and practical combustion problems. LES has proved to be successful in simulating premixed turbulent combustion, where flames are not perturbed by small scale eddies, *i.e.* where $\eta > \delta_L$, in the regime known as corrugated flamelet (CF) regime. However, comparatively fewer assessments have been performed for the TRZ regime.

Modelling of the chemical source term is a central modelling challenge in simulating premixed turbulent combustion. In LES, the small length scales are filtered out. Consequently, the reaction takes place mostly at sub-grid scales and therefore needs to be modelled accurately. A number of models have been proposed to tackle this problem, such as the level-set method (G-equation) [3, 4], the artificially thickened flame approach [5, 6, 7] and the flame surface density (FSD) concept [8, 9].

In addition to sub-grid modelling problems in LES, numerical resolution of the filtered flame is another challenge in premixed combustion simulations in which the filtered flame thickness is of the same order of the filter size. The lack of resolution causes error in computing scalar field gradients in the vicinity of the filtered flame front. The level-set approach addresses this issue to some extent. In this approach, the flame front is identified at a particular value of the level-set field $G = G_0$ and the flame structure is entirely prescribed based on the distance from the iso-surface of $G = G_0$. This assumption works when the flame is unperturbed by turbulent eddies, however, in the TRZ regime, the preheat zone of the flame is thickened by small eddies and may be partly resolved on the grid if the sub-grid Damköhler number is less than unity [10]. In order to address this issue, a method was proposed by Moureau *et al.* [11] and Knudsen *et al.* [12] that combines the level-set method with the progress variable equation. To close the level-set transport equation, a model for the turbulent flame speed is required. There are several models, such as Charlette *et al.* [5] and Colin *et al.* [7] which are mainly used in the CF regime. However, only a few models, such as Hawkes *et al.* [13] and Pitsch [10] have been proposed to account for flame-wrinkling due to unresolved turbulent scales in both CF and TRZ regimes.

In the present work, LES of a slot Bunsen burner are performed using two different grids in the TRZ regime. Chemistry is modelled using presumed PDFs with strained and unstrained flamelet solutions. The Hawkes model in both static and dynamic coefficients

Table 1: Simulation cases.

Flamelet	Mesh	Flame speed model	Case
Strained	9.3×10^6	Static	A
Strained	9.3×10^6	Dynamic	B
Unstrained	9.3×10^6	Static	C
Unstrained	9.3×10^6	Dynamic	D
Strained	1.2×10^6	Static	E
Strained	1.2×10^6	Dynamic	F
Unstrained	1.2×10^6	Static	G
Unstrained	1.2×10^6	Dynamic	H

versions is used to calculate the turbulent flame speed required for closing the level-set transport equation. The LES results are compared with the DNS of the same configuration performed by Sankaran *et al.* [1] at several streamwise locations. Model predictions are compared for different grids, strained and unstrained flamelet solutions and static and dynamic versions of the turbulent flame speed model. All cases studied in this paper are listed in Table 1.

Flow configuration and simulation parameters

The configuration is a slot Bunsen burner described in ref. [1] as case C. The domain is rectangular with the dimensions of $24\times21.6\times5.4mm^3$ in the streamwise, transverse and spanwise directions, respectively. The central slot width h is $1.8mm$. The velocity of the central jet U_0 is $100m/s$, and the Reynolds number based on this velocity is 2100. The central jet is surrounded by a co-flow stream of $25m/s$. A preheated mixture of methane and air at $800K$ is injected into the central slot in presence of a co-flow of burned products at the adiabatic flame temperature. The mixture fractions of the both streams are identical and have an equivalence ratio of 0.7. The operating pressure is $1atm$. At these conditions, the laminar burning velocity S_L and laminar flame thickness δ_L are $1.8m/s$ and $0.3mm$, respectively. The inflow turbulence intensity is about 33% of the bulk velocity. The resulting Karlovitz and Damköhler numbers for the above conditions based on the inlet values are 225 and 0.4, respectively, indicating that the flame is near the upper boundary of the TRZ regime.

Numerical methods

The LES were performed using NGA, a parallel, semi-implicit and finite-difference code developed for low Mach number flows [14]. The pressure was set by solving an elliptic equation that enforces conservation of mass. Closure of the sub-grid scale (SGS) stress tensor was achieved with the dynamic Smagorinsky eddy viscosity model. Following ref. [15], the combustion process was parameterised using a reaction progress variable $\tilde{C}$ and the mass fraction of the hydrogen radical, $\tilde{Y}_H$, for which transport equations were solved. Here, Y_H facilitates an additional parameter space to include strain effects in the tabulation of strained flamelet solutions. A detailed rationale for choosing H species in particular is described in ref. [15]. The subfilter fluxes in the transport equations of $\tilde{C}$ and Y_H were modelled using the turbulent diffusivity computed from a dynamic Smagorinsky-type model [15].

For the spatial discretisation of velocities and scalar gradients, a second and third order accurate scheme was used, respectively. The time integration was performed using a second order implicit Crank-Nikolson method and an iterative predictor and corrector updating scheme was utilised.

Grid and boundary conditions

Two different grids were used. The first grid consisted of 9.3×10^6 cells with filter width ratios of $\Delta/\eta = 4$ and $\Delta/\delta_L = 0.25$, where Δ is the LES filter size, which is the same as the grid size. The second mesh consisted of 1.2×10^6 cells, and had filter width ratios of $\Delta/\eta = 8$ and $\Delta/\delta_L = 0.5$. A fine grid was used at the central jet whereas the grid was stretched in the co-flow region.

An inlet velocity was specified at the inflow boundary. The velocity and gas composition at the inflow were smoothly transitioned between the central jet and co-flow according to the function specified in ref. [1]. Periodic boundary conditions were used in the spanwise direction, whereas a non-reflecting outflow boundary condition was used at the jet exit and in the transverse direction. Inflow turbulence was obtained using velocity information from a single realisation of a homogeneous isotropic turbulence (HIT) field. This was superimposed to the bulk velocity profile at the inlet.

Reaction rate closure

Coupled progress variable $\tilde{C}$ and level-set equations are solved to calculate the filtered progress-variable and hydrogen mass fraction reaction rate. A detailed description of this method is given in refs. [11, 12]. The key advantage of this approach is that the level-set model tracks the flame position irrespective of the grid resolution, whereas the progress variable equation describes the flame structure and flame-turbulence interactions. Thereby, coupling these two equations overcomes some of the modelling challenges in the TRZ regime. The solution algorithm is briefly described here. Firstly, the level-set (G) equation is solved to obtain the flame position. The turbulent flame speed in the level-set equation is modelled using the Hawkes model with both static and dynamic model coefficients. In the dynamic version, an approximate Germano identity was used to obtain the model coefficients. Using the G field, a progress variable field C_G is constructed with the equation provided in ref. [12]. This progress variable field is then used to access the reaction rate closure from the flamelet solutions with a presumed PDF of progress variable and Y_H. In the final step, the progress variable transport equation is solved using the computed reaction source term to obtain the progress variable field. This progress variable and Y_H values are used to calculate the density, species mass fractions, laminar flame speed, and laminar flame thickness from the solution of strained and unstrained flamelets. Chemistry tabulation for both unstained and strained flamelets are obtained using FlameMaster [17] program with 17 species methane-air mechanism, also employed in the DNS [1].

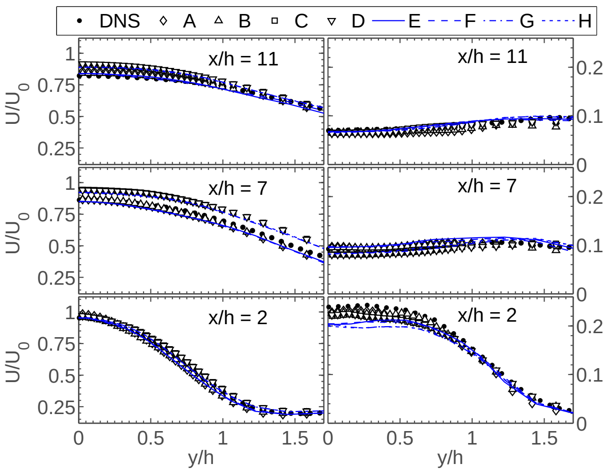

Figure 1: Time averaged streamwise velocity component U and fluctuating velocity U_{rms}.

Results

Profile of mean and rms velocities

Time averaged streamwise velocity U and velocity fluctuations U_{rms} for all cases listed in Table 1 are plotted in Figure 1. All the values are normalised with the inlet bulk velocity U_0. As can be seen, the mean streamwise velocities match well with DNS for both grids when the strained flamelet solution is used, whereas using the unstrained flamelet solution leads to over prediction of mean velocity at downstream location $x/h = 7$. Also, it can be observed that the results of the fine and coarse grids are similar. These results show that the streamwise velocity is less sensitive to the grid resolution but more sensitive to the strain effects in the flamelet. Figure 1 also shows that the rms velocity fluctuations are in good agreement with the DNS for both flamelet solutions. As can be seen, at $x/h = 2$, coarse grid simulations under predict the rms velocity more than the fine grid. Both dynamic and static versions of the turbulent flame speed model show almost the same results.

Profiles of progress variable and temperature

The instantaneous iso-surfaces of the progress variable $\tilde{c} = 0.065$ are shown in Figure 2 for the DNS, cases B and D. It is evident from this figure that the strained flamelet solution resembles the DNS data. However, the flame height is underpredicted when unstrained flamelet solution is used.

Time averaged progress variable C and temperature $\tilde{T}$ are shown in Figure 3 at several streamwise locations. As can be seen, the strained flamelet solution clearly shows a good agreement with the DNS at all streamwise locations and also for both grids, whereas using the unstrained

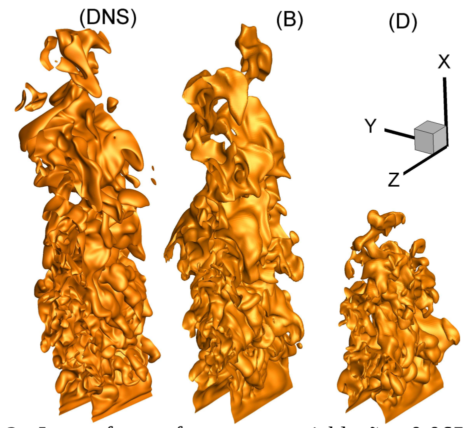

Figure 2: Iso-surfaces of progress variable $\tilde{c} = 0.065$ for the DNS [1], cases B and D.

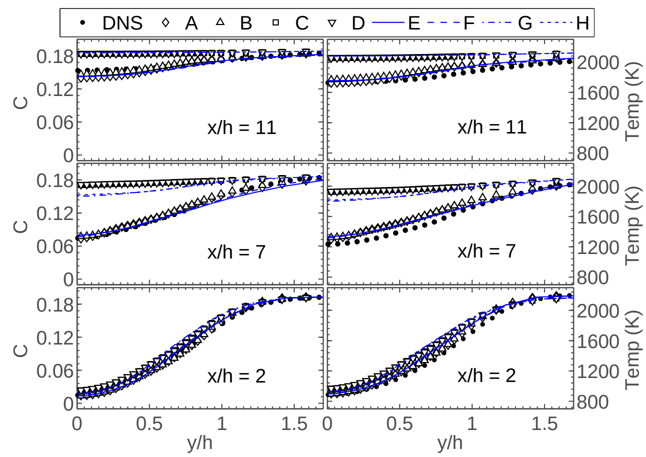

Figure 3: Time averaged progress variable C and temperature T.

flamelet solution leads to over prediction of the progress variable and temperature at downstream locations. Figure 3 also shows that the temperature profiles are similar to the progress variable profiles.

Profile of minor species

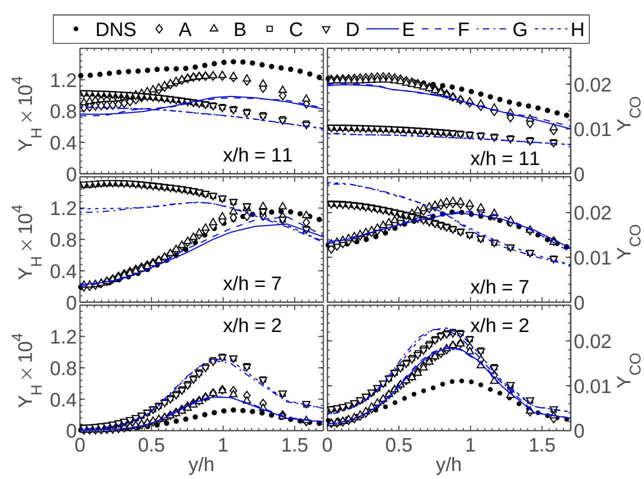

Figure 4: Time averaged H (Y_H) and CO (Y_{CO}) mass fractions.

Figure 4 shows the profiles of Y_H and Y_{CO} for all cases. As can be seen, both Y_H and Y_{CO} profiles have similar trends to the DNS when the strained flamelet solution is used. However, the agreement between DNS and the strained flamelet solution is only good at $x/h = 7$. Also, it can be observed that the unstrained flamelet solution is not able to even predict the DNS trends. This may be due to the significant overprediction of the progress variable downstream of the flame as shown in Figure 3.

The effect of grid resolution is predominant at downstream locations. Looking at Y_H profiles in Figure 4 shows improved results compared with the DNS at x/h =7 and 11, whereas, near the nozzle, the grid does not have much effect. Also, dynamic and static versions of the turbulent flame speed model lead to very similar results.

Conclusions

LES of a premixed slot Bunsen flame were used to study the performance of the Hawkes turbulent flame speed model using both strained and unstrained flamelets to tabulate chemical states, laminar flame thickness and laminar flame speed for two different grids. The turbulent flame speed model was implemented in both static and dynamic coefficients versions. All simulation results were compared with DNS of the same configuration at several streamwise locations.

It was shown that the Hawkes flame speed model in conjunction with the strained flamelet tabulation is able to simulate turbulent perturbations of flame structures and matches well with the DNS. Both static and dynamic model showed very similar performance in predicting the turbulent flame speed. Progress variable and temperature results revealed that the strain effects on the flamelets are very significant. Also, comparison of the flame height for different cases showed that the strained flamelet solution predicts the correct flame propagation. The effect of grid was only observed when comparing minor species such that the fine grid improved the species mass fraction predictions.

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