Large Eddy Simulation of premixed flames with multi-step global reaction mechanisms

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Abstract. Large Eddy Simulation is a powerful tool to simulate the unsteady lean premixed flames and to predict combustion instabilities. However the resolution of an LES grid is typically larger than the thickness of practical flames. In artificially thickened flame concept the mixing in the flame region is enhanced by explicitly increasing heat and mass diffusivity while decreasing the average reaction rates. The resulted flame is resolvable and propagates with the correct speed but the flame response to small turbulent structures is decreased which should be compensated. A novel flame thickening technique is applied here to implement a multi-step global reaction mechanism in an LES solver. This method exploits the intrinsic numerical diffusion of the upwind biased discretization schemes to implicitly enhance mixing in the flame region hence thickening the flame to sizes resolvable on an LES grid. Unlike the previous thickening method this technique does not increase the diffusion in the plane tangent to the flame front hence reduces the loss of the flame surface. Simulation of a lean premixed low swirl methane-air flame reveals that this new method tends to keep some of those small flame structures which are smeared out by the previous flame thickening methods.

1. Introduction

The increasing demand for decreased emissions levels of the gas turbines has led to the development of the lean premixed combustion concept in which the fuel and oxidizer are perfectly mixed prior to ignition. The lean premixed flames can operate at lower temperatures therefore produce less pollutants. The desire to operate the gas turbines at the lowest emissions level possible results in a flame which operates very close to the lean blow off limit condition. The intrinsic dynamic behavior and the tendency of the lean premixed flames to become unstable necessitate the study of the stability mechanisms and operational limitations of this kind of flames. In Large Eddy Simulation the large scales of the flow which depend on the overall geometry are simulated and only the smallest scales which behave more universally are modeled. Therefore, Large Eddy Simulation is a promising tool to simulate the unsteady lean premixed flames and to predict their stability limits.

Economical requirements limit Large Eddy Simulation of reacting flows to simplified chemistry where the detailed chemical reaction chains are replaced by multi-step global or elementary mechanisms, hence reducing the number of transport equations in CFD codes. These models are ideal to be incorporated into CFD codes as they provide the reaction rates through simple mathematical expressions. However, these mechanisms are originally derived to predict
selected features of the detailed chemistry, e.g. CO concentration, temperature, laminar flame speed, etc., therefore the reaction rates given by these mechanisms should be corrected for the CFD problem at hand. In particular grid resolution and turbulence-chemistry effects should be considered.

The flame front thickness is usually less than the LES resolution for practical applications and it is not possible to resolve the flame on the LES grid which can lead to numerical problems. There are several techniques proposed to overcome this difficulty. Artificially thickened flame concept (Colin et al., 2000) suggests the simulation of a flame which is thicker than the real flame but has the same flame speed. Flame front tracking technique (Peters, 2000), G-equation approach, treats the flame as a propagating surface represented by isosurfaces of an scalar $G$ while flame surface density approach is based on using a filter larger than the computational grid size.

In this work a novel flame thickening technique is proposed and is implemented in an in-house LES solver to correct the reaction rates given by a three step global mechanism for methane-air flames. This technique is then compared to the previous thickening techniques in simulating a lean premixed low swirl methane-air flame and their ability in resolving the flame dynamics and structures are compared.

2. LES solver

The LES solver used in this work is an in-house code which has been successfully applied to a range of different problem areas, including gas turbine combustors, afterburners, ramjet combustors, jet noise predictions, pulsed detonation, etc. The LES solver applies the Smagorinsky sub-grid scale model to solve the Favre-averaged Navier-Stokes equations including species transport equations. Preconditioning is used to efficiently solve low velocity flows. A cell-centered finite-volume scheme with explicit three-stage Runge-Kutta time stepping is used to integrate the equations in time. The convective flux is approximated with a third order accurate characteristic upwind scheme with low diffusion whereas a locally centered compact second order scheme approximates the diffusive flux. A Total Variation Diminishing (TVD) limiter (Laney, 1998) is used to suppress the non-linear instabilities.

A three step global mechanism from the literature (Meredith & Black, 2006) is used to simulate methane-air flames.

\[ 2\text{CH}_4 + 3\text{O}_2 \rightarrow 2\text{CO} + 4\text{H}_2\text{O} \]
\[ 2\text{CO} + \text{O}_2 \rightarrow 2\text{CO}_2 \]
\[ 2\text{CO}_2 \rightarrow 2\text{CO} + \text{O}_2 \]

where the reaction rates are given by an Arrhenius expression:

\[ r_i = A_i T^{\beta_i} e^{-\frac{E_{ai}}{RT}} \prod_{j=1}^{N_j} [X_j]^{a_{ij}} \]

This reduced mechanism has been originally optimized to give correct CO concentration and temperature and not to predict the correct laminar flame speed. Therefore the laminar flame speed of this mechanism was first evaluated using the 1D version of the numerical solver on a resolved grid of 0.01mm in size. The laminar flame speed of methane-air mixture at equivalence ratio of 0.62 was found to be 12.34cm/s which is very close to the laminar flame speed of 12.4cm/s calculated from the detailed chemistry using the commercial code CHEMKIN.
3. Artificially thickened flame

According to the theories of laminar premixed flame the flame speed and thickness can be expressed as (Glassman, 1996):

\[
s_0^l \propto \sqrt{D \overline{W}}, \quad \delta_0^l \propto D \overline{s_0^l}
\]

(2)

where \( D \) is the molecular diffusivity, \( \overline{W} \) is the mean reaction rate, \( \delta_0^l \) is the flame thickness and \( s_0^l \) is the laminar flame speed. The basic idea of the flame thickening concept is to thicken the flame by a factor \( F \) so that it is resolvable on an LES grid while keeping the laminar flame speed of \( S_L \) unchanged. This can be done by increasing the molecular diffusivity \( D \) and thermal diffusivity \( \alpha \) by the factor \( F \) and decreasing the mean reaction rate \( \overline{W} \) by the same factor (Colin et al., 2000). This means that the species mass fraction transport equation

\[
\frac{\partial \rho Y^{(i)}}{\partial t} + \frac{\partial \rho u Y^{(i)}}{\partial x} = \frac{\partial}{\partial x} \left( \rho D \frac{\partial Y^{(i)}}{\partial x} \right) + \dot{\omega}
\]

is simply replaced by

\[
\frac{\partial \rho Y^{(i)}}{\partial t} + \frac{\partial \rho u Y^{(i)}}{\partial x} = \frac{\partial}{\partial x} \left( \rho F D \frac{\partial Y^{(i)}}{\partial x} \right) + \frac{\dot{\omega}}{F}
\]

(4)

and the thermal diffusivity in energy equation is also multiplied by \( F \).

Though the thickened flame allows the propagation of the flame on a coarse grid it unfortunately reduces the flame response to the smaller turbulent structures and the flow field wrinkling of the flame (Colin et al., 2000). Colin et al. (2000) and Charlette et al. (2002) have derived the wrinkling correction factor \( E \) to compensate for the loss of flame surface due to reduced flame wrinkling. The final species mass fraction transport equation reads

\[
\frac{\partial \rho Y^{(i)}}{\partial t} + \frac{\partial \rho u Y^{(i)}}{\partial x} = \frac{\partial}{\partial x} \left( \rho E F D \frac{\partial Y^{(i)}}{\partial x} \right) + \frac{E \dot{\omega}}{F}
\]

(5)

There is yet another drawback with this approach as the increased thermal and molecular mass diffusivity can severely affect the mixing process in the whole domain. Increasing the diffusivity of these properties only in the flame front region is enough for the purpose of flame thickening. Therefore, dynamic flame thickening techniques are proposed to track the flame front and increase the diffusion only in the flame region. The suggested thickening factors in the literature, (Strakey & Eggenspieler, 2010) for instance, have the following form:

\[
F = 1 + (F_{max} - 1) \tanh(\beta \frac{RR}{RR_{max}})
\]

(6)

where \( RR \) is the local reaction rate and \( RR_{max} \) is the maximum reaction rate evaluated from simulating the resolved flame. This function ensures a thickening of the flame while keeping the diffusivity intact elsewhere, hence not over-predicting the mixing in the whole flow field.

4. Upwind thickened flame

Numerical diffusion associated with numerical schemes has the potential to locally increase the diffusion and can be exploited to thicken the flame. Non-diffusive schemes such as central differencing are usually not stable and lead to oscillations and this additive numerical viscosity is needed to overcome numerical problems. The numerical diffusion appears as a result of upwinding the variables in the discretization of the convection term in transport equations and depending on the numerical scheme may appear as any even order derivative term resulted from
the truncation error of Taylor series used to approximate the variables in discretization schemes. Specifically if this error appears as a second derivative it behaves exactly as a physical diffusion and can be quantified as an excess viscosity in the flow. For instance, the first order upwind scheme in 1D gives an additional viscosity of $\frac{1}{2} u \Delta x$ on a uniform grid of $\Delta x$ in size.

The convective scheme used in the current solver is a very low diffusion scheme which is incapable of thickening the flame to levels needed to resolve it on the LES grid, however a non-linear stability mechanism based on total variation diminishing technique (Laney, 1998) is also implemented that can change the level of upwinding in case of occurrence of low range large gradient changes of flow variables therefore increasing the local diffusion. Across the flame and particularly in the head and tail of the flame these changes are large and the TVD technique gives high levels of upwinding that can act the same way as the increased diffusivity in the above mentioned flame thickening method. The TVD limiter can be designed so that it gives different levels of upwinding (additive diffusivity) in different gradient scenarios. It is important that only the density (which represents the energy diffusion) and the fuel mass fractions are upwinded so that the momentum equation is not affected.

This technique was first used to simulate a one dimensional flame and showed similar behavior to the flame thickening method. However, there are two disadvantages with this technique. First, the numerical diffusion can only happen in existence of a velocity therefore it may not be able to provide enough thickening of the flame in a very low velocity problem. Second, analytical expressions for numerical viscosity exist for only few numerical schemes under very simplified conditions and the value of added numerical diffusivity should be approximated in this technique. The numerical diffusion depends on the numerical scheme, grid spacing, velocity, shape of the grid cell, the direction of velocity vector, etc. However, all these factors are universal and do not depend on the problem at hand. Therefore, once the numerical diffusion of a scheme is quantified as a function of these factors it can be used in all other applications.

Increasing the diffusivity only in the direction normal to the flame front is enough to thicken the flame while the flame thickening method increases the diffusivity equally in all directions therefore increases the mixing in all directions. This increased mixing in the directions other than normal to the flame front can significantly smear out the small wrinkles of the flame and necessitates complicated wrinkling correction factors. The upwind thickening technique on the other hand is directional due to two reasons. First, the numerical diffusion is anisotropic and depends on the velocity vector and the cell alignment relative to the velocity vector and the flame front. Second and more important, the TVD limiter may give different upwinding levels in different directions at the same computational cell depending on the local conditions hence giving an anisotropic diffusivity that can resolve the smaller wrinkles and may simplify the wrinkling correction factors. It is worth to mention that these wrinkling correction factors depend on quantities which are not universal and depend on overall geometry of the problem at hand.

As the first step to quantify the numerical diffusion of the numerical scheme used in the LES solver the numerical diffusion of the TVD limiter was assumed to behave as a second derivative and to give a numerical viscosity of the form:

$$\nu_{num} = \alpha u \Delta x$$

where $\alpha$ is a constant. The value of $\alpha = 0.25$ was then chosen which gives the correct flame speed for a 1D premixed methane-air flame at equivalence ratio of 0.62 traveling in a free stream of $u = 2m/s$ in velocity. Figure 1 shows the variation of the laminar propagation speed of the above flame with free stream velocity simulated with both upwind thickening technique and the dynamically flame thickening method with $\beta = 1$ and $F_{max} = 10$. The laminar flame speed shows less dependence on the free stream velocity for dynamically thickening of the flame compared to the upwind thickening technique. The laminar flame speed decreases as the free stream velocity
increases which indicates that equation 7 with $\alpha = 0.25$ over-predicts the numerical diffusion at higher free stream velocities.

As mentioned earlier, the numerical diffusion is anisotropic and the important value of the numerical viscosity at the flame front, the one that controls the flame propagation speed, is the one that enhances the diffusion in the direction normal to the flame front (flame propagation direction). This additional diffusivity is responsible for thickening the flame and the reaction rates should be compensated for it according to the basic flame thickening concepts. The numerical viscosity normal to the flame in 3D is approximated as:

$$
\nu_{num.} = \frac{1}{4} \left| T_x U \Delta x \right| + \left| T_y V \Delta y \right| + \left| T_z W \Delta z \right| + \left| \nabla T \right|
$$

where the temperature gradient vector is used to represent the direction normal to the flame. The reaction rates are first corrected to compensate for the added numerical diffusion in the same way as in thickened flame technique. The flame should travel with the laminar flame speed after this correction. Then the reaction rates are corrected to give a specified turbulent flame speed $S_T$ approximated by a classic Clavin-Williams form (Clavin & Williams, 1979).

$$
\dot{r}_{i,eff} = \dot{r}_i \left( \frac{S_T}{S_L} \right)^2 \frac{D_l}{D_{eff}}
$$

$$
D_{eff} = D_l + D_{sgs} + D_{num.}
$$

$$
S_T = S_L \sqrt{1 + \frac{k_{sgs}}{S^2_L}}
$$

where diffusivity $D$ is the viscosity divided by Schmidt number and Prandtl number in species transport equations and energy equation respectively.

The same turbulent flame speed correction is also applied in the dynamically thickened flame model instead of the original wrinkling correction factor in order to compare these two approaches in their ability in resolving the small flame wrinkles.
Figure 2. Schematics of the experimental test rig (a) showing the burner nozzle, perforated-plate/swirler-vane configuration and the co-flow region and the perforated-plate/swirler-vane configuration (b).

Figure 3. Flame front structure at a surface normal to the axial direction at 45mm downstream of the nozzle exit (a) visualized by temperature isolines of $700 - 1700 K$ and at the center-plane (b) visualized by temperature contours.

5. Test case: low swirl burner

The low swirl burner test rig simulated in this work is installed at Lund University, Sweden. Figure 2 shows the burner experimental test rig, in which a constant mass flow of lean premixed methane-air mixture at equivalence ratio of 0.62 is blown into the 50mm diameter burner nozzle. First, the flow passes through two perforated plates which aim at providing a uniform flow across the entire nozzle diameter. Then the flow passes through a perforated-plate/swirler-vane configuration, figure 2, which is located approximately one diameter upstream of the burner exit. This perforated plate and the eight swirler vanes encircling it, divide the flow into two regions: a near wall swirling flow and an axial core flow. The perforated plate also gives a
pre-specified range of turbulence scales to the core flow. The burner nozzle is surrounded by a wide 0.35m/s axial co-flow to prevent disturbances from the surroundings as shown in figure 2. This configuration results in a detached flame stabilized in less than one diameter downstream of the burner exit without any flame holders. This flame is characterized by extreme dynamics both in the core and the shear layer regions and has slight translational oscillations in the axial direction. This flame has a wide range of structures.

The flow-flame in the low swirl burner was simulated using the upwind thickening technique until it was fully developed. Figure 3 shows the flame structure at two different angles at this developed conditions. Then simulations with both upwind flame thickening and dynamically flame thickening with $F_{\text{max}} = 10$ were performed for a short time period to investigate their effects on the flame front structures. The aforementioned turbulent flame speed correlation was used for both cases. Figures 4 and 5 show the temperature isolines for several snapshots of the flow for both simulations.

Figure 4. Flame front structure at a distance of 45mm downstream of the burner exit visualized by the temperature isolines of $700 - 1700\,K$ for the flame simulated by dynamically thickened flame technique. Figures (a), (b), (c), and (d) correspond to times 60, 200, 300 and 600 microseconds respectively. The time is measured from the conditions shown in figure 3.
Figure 5. Flame front structure at a distance of 45mm downstream of the burner exit visualized by the temperature isolines of 700 – 1700K for the flame simulated by upwind thickened flame technique. Figures (a), (b), (c), and (d) correspond to times 60, 200, 300 and 600 micro-seconds respectively. The time is measured from the conditions shown in figure 3.

These figures show that the dynamically thickened flame model results in a more uniform temperature distribution inside the hot region as it is indicated by concentric isolines while the upwind thickening results in a more non-uniform distribution. This is due to increased diffusion resulted from flame thickening. At first glance it may appear that the dynamically flame thickening method provides more flame thickening as the density of isolines is higher at the flame front for upwind thickening. Figure 6 is a closer view on the flame structures at the last snapshot for both simulations and there are several locations on the flame front specified with numbers on it. Figure 7 shows the temperature profiles normal to the flame front at the positions shown in figure 6 which represent the local flame thickness at these locations. It shows that in two type of regions the flame thickness is about equal for both techniques: the regions where the flame front is flat and the regions where the flame is concave (where the flame front is retreated back into the hot body of the fluid or in other words where the cold gases have penetrated into the hot region) and flame is thicker only in the regions where the flame
Figure 6. A closer view on the flame front structures visualized by temperature isolines of 700–1700K. The locations at which the flame front thickness is evaluated are shown by numbers on the left figure. Figure (a) is from dynamically thickened flame technique simulations and figure (b) from upwind thickened method.

Figure 7. Thickness of the flame at several locations visualized by temperature profiles across the flame front. Figures (a), (b), (c), (d), (e) and (f) correspond to locations 1, 6, 2, 4, 3 and 5 respectively. The temperature, $\mathit{Y}$ axis are in Kelvin and the distance in the direction normal to the flame front, $X$ axis, is in millimeters.

front is convex (where the hot gasses have penetrated into the cold region). The reason for this phenomenon may be explained by the added diffusivity in the direction tangent to the flame. When the flame locally penetrates into the cold region the hot regions in the vicinity start to warm up the back part of the flame which will increase the flame thickness. This phenomenon will eventually either not let the wrinkles to form or will smear out the existing wrinkles and will result in loss of flame surface that should be compensated by a proper wrinkling correction factor. This loss of flame surface can be easily seen in the temperature isolines as the time goes on. The flame simulated with dynamically thickened flame will eventually extinguish as the wrinkling correction factor is not implemented to compensate for the loss of flame area.

6. Concluding remarks

The upwind flame thickening technique seems promising for simulating premixed flames. It needs less complicated wrinkling correction factors compared to previous thickening flame techniques as the range of resolved flame structures is larger compared to dynamically thickened flame
technique. However the numerical viscosity of the numerical techniques should be better approximated. It is also important to note that using this technique is only possible if the velocities involved are high enough for thickening the flame to levels resolvable on the LES grid.

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