Modeling Premixed Turbulent Combustion using a Level-set Flamelet Approach

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Abstract

Modeling of a lean premixed propane/air turbulent flame stabilized by a bluff body is presented. The laminar flamelet library approach, which has been successfully used for modeling of non-premixed turbulent flames, is applied to premixed combustion. In this approach the mean flame location and mean flame thickness are modeled by a level-set G-equation and the variance of G. Different empirical expressions modeling the turbulent flame speed and flame brush thickness are tested. The detailed species, temperature and density are calculated using a presumed probability density function together with a laminar flamelet library. A laminar flamelet library with species mass fractions, density and temperature as a function of a coordinate normal to the flame surface is calculated using a one dimensional laminar flame code and provided prior to this work. The sensitivity of the results to the model components is examined. Comparison of calculations and experimental data is presented.

Introduction

Modeling of turbulent premixed combustion is a challenging subject because of the uncertainties in the current understanding of mechanisms by which turbulence, chemical reactions and heat transfer interact. In principle, direct numerical simulation (DNS) of the Navier-Stokes equations and species transport equations is most desirable, since it keeps detailed information about turbulent flames. However, DNS is limited to low Reynolds number flows, therefore most of the possible methods for simulation of engineering turbulent flames are based on spatial-, ensemble or time averages of the governing transport equations, which leads to two types of unknowns to be modeled. One is the Reynolds stresses/turbulent transport fluxes, the other is the mean reaction rate. The former has been modeled by the 'gradientdiffusion' type model and shown a relative success in engineering applications, though there are controversies such as 'counter-gradient diffusion' found in premixed turbulent combustion. The latter, the mean reaction rate, has been less successful in arriving at an universally acceptable modeling. There are several approaches proposed in the literature [1]. A simple but popular model among industrial applications is the phenomenological approach, by which the mean reaction rate is directly modeled by the known properties such as the mean concentrations of species and the turbulent mixing time scale and assuming chemical reactions are infinitely fast. An example is the model based on the Eddy Dissipation Concept (EDC). There are also types of models based on solving a transport probability density function (PDF) equation; the presumed PDF based the reaction progress variable model (e.g. the Bray, Libby and Moss model) or the flame surface density models.

In this work we explore a different method, the level-set flamelet library approach. The reason is that most of the above mentioned models are aimed at solving the transport equations of wanted species and therefore are under the limitation of two factors. First is the inability or poor accuracy in modeling the detailed species mean reaction rates in turbulent combustion, and secondly, the computer CPU time and storage requirement for solving these transport equations. In the flamelet library approach, the transport equations of conserved scalars are solved and there is no need to model or solve any species transport equations. The flamelet library approach has been most successfully applied in calculation of turbulent non-premixed combustion [2] and partially premixed flames [3]. However it is less often used in premixed turbulent flames, due to the fact that there are no such conserved scalars in premixed flames as the mixture fraction in diffusion flames and partially premixed flames.

Mathematical Formulation

We will describe a flamelet library approach for premixed turbulent flames in the following. For laminar premixed flames, the propagation of the flame front (e.g. the inner layer location of a laminar flame) in a flow field can be described by a level-set G-equation. We define G = 0 to be the instantaneous position of the flame and let negative values of G represent unburnt and positive represent burnt gas. By applying time averaging to the G-equation one can find the mean flame location, e.g. $\overline{G} = 0$ [3]. In the flamelet library approach the turbulent flame is viewed as different laminar flamelets which randomly fluctuate around the mean flame position. The properties of the laminar flamelet are given as a function of a spatial coordinate, normal to the flame surface, in a flamelet library. Ensemble averages can then be employed to calculate the mean flame properties, such as

$$\begin{split} \widetilde{T}(x,y,z) &= \frac{1}{\overline{\rho}} \int_{-\infty}^{\infty} \wp(\xi,\kappa) \rho(d(x,y,z) - \xi,\kappa;T_u,p,\phi) T(d(x,y,z) - \xi,\kappa;T_u,p,\phi) d\xi d\kappa \\ \\ &\overline{\rho} = \int_{-\infty}^{\infty} \wp(\xi,\kappa) \rho(d(x,y,z) - \xi,\kappa;T_u,p,\phi) d\xi d\kappa \end{split}$$

where $T(\xi, \kappa; T_u, p, \phi)$ and $\rho(\xi, \kappa; T_u, p, \phi)$ denote the laminar flamelet library of temperature and density as functions of the flamelet coordinate ξ and flame stretch κ , under different preheat stream conditions, such as the equivalence ratio ϕ , temperature T_u and pressure p. \tilde{T} and $\bar{\rho}$ denote the Favre averaged temperature and time averaged density. The mean species mass fractions can be obtained in a similar way. In the laminar flame coordinate, $\xi = 0$ denotes the inner layer location; ξ is the distance to the inner layer location; $\xi >> 0$ denotes the post-flame zone and $\xi << 0$ denotes the preheat zone. d(x, y, z)is the mean distance in the flow field point (x, y, z) to the mean flame front ($\overline{G} = 0$). \overline{G} calculated by the level-set equation does not contain any information of the distance from a flow field to the flame front. In order to obtain d(x, y, z) a re-initialization step is employed, i.e. the equation $\partial \overline{G}/\partial t = 1 - |\nabla \overline{G}|$ is solved numerically until a steady state solution ($\partial \overline{G}/\partial t = 0$) is obtained. The re-initialization step does not change the location of mean flame position $\overline{G} = 0$; after the re-initialization \overline{G} represents the mean distance to the mean flame position, i.e. $d(x, y, z) = \overline{G}$. Finally, in order to model the presumed PDF, one needs the information of the flame thickness or the variance of G, $(\overline{G'}^2)$. A summary of the different submodels we have used in the flamelet library approach for premixed turbulent flames is given in Table 1. S_T is the turbulent flame speed, which is used for calculation of \overline{G} .

Models	Turbulent flame speed / thickness	Reference
S-1	$S_T = S_L + 0.46u' + 0.2 \left(S_L u'\right)^{1/2}$	[3]
S-2	$S_T = S_L + u'$	[4]
G-1	$\overline{G'}^2$ by transport equation	[5]
G-2	$\overline{G'^2} \approx (S_T k / 6\epsilon)^2$	$\operatorname{present}$
G-3	$\overline{G'^2} \approx 25 mm^2$	$estimated^1$

¹estimated from the experiments [6] at the x = 150mm plane.

Table 1: Turbulent flame speed and flame thickness models

Experimental Setup

The results from the calculations are compared to experimental data[6] from measurements performed in a rectangular channel with height (y) 120mm and width 240mm. The premixed combustion was stabilized in the channel by a triangular, 40mm by 40mm, 240mm long, prism-shaped flame holder with one corner pointing upstream. Measurements were carried out at three different (x) locations; 150mm, 350mm and 550mm downstream of the flame holder trailing edge. The velocity, temperature and some species are measured [6] by LDA, CARS and gas analysis equipments (a chemiluminescence analyzer for NO_x, two non-dispersive infrared instruments for CO and CO₂, a paramagnetic analyzer for O₂ and flame ionization detector for unburned hydrocarbons).

Results and Discussion

There are a few uncertainties needed to explore in the flamelet library approach. (1) In the mean G-equation, the unknown turbulent flame speed (S_T) requires further modeling. The turbulent flame speed is a sensitive parameter, which increases rapidly as the intensity of turbulence (u'/S_L) increases for low u'/S_L , the increase of S_T is much slower for moderately high u'/S_L , followed by flame quenching at high u'/S_L . There is no consistent theory to predict the whole range of S_T profile [7]. (2) How sensitive are the results to the different model parameters/submodels? We address these issues in the modeling of a turbulent lean premixed propane/air flame ($\phi = 0.6$), pressure p = 1 atm, preheated to $T_u = 600K$. First, the laminar flamelet library is calculated using a one dimensional laminar flame code employing detailed chemical reaction mechanism of propane combustion [8], involving 82 elementary steps and 30 species. The unstretched laminar flame speed is $S_L = 74.3 cm/s$. The flow field is modeled by the Favre averaged Navier-Stokes equations together with two-equation $k - \epsilon$ turbulence model. The value of u'/S_L is about 10 and the Karlovitz number defined in [7] is between 0.05 and 0.2 in the mean flame front, therefore the flame is in the flamelet regime [7]. Figure 1 shows the comparison of results



Figure 1: Comparison of computed mean species mole fractions and temperature with the experimental data, along perpendicular direction at $150 \ mm$ downstream of the flame holder. The submodels are described in Table 1

calculated using different flame speed and flame thickness models at 150mm downstream the flame holder. It is seen that a sensitive parameter in the level-set flamelet library approach is the turbulent flame speed S_T . The calculations are performed using the turbulent flame speed model of Damkohler and the model proposed in [3]. Several flame thickness models are tested.

As seen, at x = 150mm, the major species CO_2 and O_2 as well as the temperature are well predicted by the these models. In particular, the peak species mole fractions of CO_2 and O_2 and the peak of temperature in the central of the channel are well predicted by all the models, as compared to the experimental data. The minor species such as CO are more sensitive to the flame thickness model. A thinner flame has a higher peak value of CO and vice versa. The reason for this is that in the laminar flamelet of lean fuel combustion, CO is only seen in the flame zone. In the post flame zone, because of the excess of oxygen, the CO formed in the flame inner layer is quickly oxidized. In the limit of a thin laminar flamelet, the mean CO mass fraction found in a turbulent flame is proportional to $\wp(G(x, y, z), \kappa)Y_{CO}(0)$. Here $\wp(G(x, y, z), \kappa)$ is the PDF of flame occurring at the point (x, y, z). This value depends solely on the flame thickness and the flame location.

At x = 550mm (not displayed) the comparison between the result and the experiments shows similar results. A slight difference is found at the mean flame location. In the measurements the mean flame location is close to the channel walls. The major species and temperature away from the mean flame location is fairly well predicted. Again the predicted CO peak differs by more than 50% from the experiments.

The flamelet library approach generally simulated a better distribution of species and temperature field, compared to fast-reaction models such as the EDC model.

Summary

Modeling of premixed turbulent flames by the level set G equation and the flamelet library approach is presented. The Favre averaged Navier-Stokes equations together with the standard $k - \epsilon$ turbulence model are used to model the mean flow field. The models are calibrated with a lean premixed propane/air turbulent flame in a rectangular channel stabilized by a bluff body flame holder. The flamelet library approach generally simulated a better distribution of species and temperature field, compared to fastreaction models such as the EDC. In particular the maximal values of major species and temperature are not sensitive to the model parameters. The mean flame location is fairly sensitive to the modeling of the turbulent flame speed. The intermediate species are more sensitive to the turbulent flame thickness model. This information shows the need for better models for the turbulent flame speed and flame thickness in turbulent premixed flame modeling.

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