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Analysis of the filtered non-premixed turbulent flame

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Results related to the filtered non-premixed turbulent flame statistics are presented. Considering non-premixed turbulent combustion modeling in the framework of large eddy simulations (LES), a turbulent flamelet equation is derived based on the filtered governing equations. Using a direct numerical simulation (DNS) data set, the statistical properties of two important parameters, the scalar dissipation and chemical source term, are analyzed in details. Numerical results show that for the scalar dissipation term, the probability density function (PDF) of the magnitude of the mixture fraction gradient changes is strongly dependent on the filter scale, whereas the PDF of the turbulent diffusivity is almost invariant. Theoretically from the scalar structure function a scaling law can be expected for the conditional mean of the difference between the filtered and nonfiltered scalars with respect to the filter scale, which is important for estimating the chemical source in the subgrid scale models.

1. Introduction

In reactive turbulence the interaction between the flame and flow is extremely complex. For problems with sufficiently high Reynolds numbers of practical interest, because of the large scale separation, both spatially and temporally, direction numerical simulations (DNS) are intractable. Thus models of the required relations need to be constructed. In non-premixed combustion simulation, the flamelet models originally developed by Williams [1] and Peters [2] play important roles. Physically if the flame scale is locally small compared with the turbulent dissipative scale, the flame structure remains to be laminar. Based on the flamelet equations, it is possible to largely reduce the dimensionality of the modeling parameters. The flamelet models have been widely applied [3–6] because of the clear physical meaning and high numerical efficiency. In recent years successful examples have been extended to various cases such as unsteady processes [7,8] and non-unity Lewis number effects [9]. The detailed budget analyses suggest that typically the flamelet assumption remains to be reasonable [10].

However, challenges in implementing the laminar flamelet models do exist. Especially in high Reynolds number turbulence the non-premixed flame structure is far away from being clearly defined, for instance unsteadyness and the strong influence from the premixed flame front associated with the triple flame [11,12]. When local extinction and re-ignition occur, premixed flame fronts are present to bring both premixed and nonpremixed features, which can violate the laminar non-premixed flamelet assumption. Moreover, in pre- and post-extinction flames the local mixing is strong; thus the local timescale may be important as well [12]. Turbulence can also lead to complex topological structures of the non-premixed flame front, for instance the flame patch and extinction hole, both of which are associated with the flame edge [13]. It can reasonably be expected that the flame edge influence will be enhanced with the increase of turbulence intensity. Although for the unsteady flamelet models the additional time scale can be modeled [8,14], physically extra modeling complexity need to be further investigated.

Large eddy simulations (LES) are especially appealing in turbulence simulation. With the appropriate subgrid scale models, the large-scale turbulent structures can feasibly be calculated by LES. However, subgrid scale modeling of the non-premixed flame also suffers from the aforementioned complexities. Efforts in this area have made some important progresses. In the thickened flame models [15,16] the flame is artificially stretched to fit the numerical resolution, but the overall flame speed remains invariant. Such a scenario can be reasonably interpreted in the framework of LES, because the filtering operation alters the detailed flame structures, for instance the reduced chemical kinetics and the temperature field; however, the overall flame speed must be invariant because the kernel of the filtered flame overlaps the nonfiltered flame zone. In other words the thickened flame models address the field quantities at the coarse grid level at the cost of distorting the fine scale structures. A different modeling idea is the filtered tabulated chemistry for LES (F-TACLES) [17], where the unclosed terms are

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determined directly from filtering the one-dimensional premixed laminar flame. For the flame normal structure the tabulated results are more efficient and robust than the thickened flame models, whereas the flame wrinkling effect need to be considered. The same strategy is also applied to study the non-premixed flame [18]. Specifically the unclosed terms in LES are estimated from a look-up table from filtering some representative non-premixed laminar flames, e.g. the counter flow flame, using as few as possible controlling variables, e.g. the filtered mixture fraction, the filtered progress variable and the filter size. But the same deficiency as in the premixed case appears, i.e. flame wrinkling is absent at the resolved scale level.

Here we aim to study the behavior of the non-premixed flames and the flamelet relation in the filtered field. Intuitively from the modeling viewpoint the filtered quantities can be of special interest to simplify the statistics at the subgrid scale because of the reduction of flame wrinkling, whose effect is among the main difficulties of flame modeling [18]. It is also worthy investigating if the complexities from flame turbulence interaction may be not or less relevant to model construction after filtering. In the present work from a priori analysis based on DNS, issues related to the numerical features of some involved parameters are addressed. This investigation aims to develop possible ideas for turbulent combustion modeling.

2. Analysis

The governing equation for the mixture fraction Z is

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot (\rho Z \vec{u}) = \nabla \cdot (D \rho \nabla Z) \tag{1}$$

and for the scalar Y_i, including temperature T and mass fraction of chemical species, is

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \vec{u}) = \nabla \cdot (D_i \rho \nabla Y_i) + \omega_i, \tag{2}$$

where $\vec{u}$ is the flow velocity, D and D_i are the molecular diffusivity of Z and Y_i, respectively. The non-premixed flamelet transform can be derived by mapping the spacial coordinates to the mixture fraction space [1,2]. The most favorable feature of this transform is to reduce the variable freedom to a low dimensional manifold.

In the context of LES, the dependent quantities are filtered at the resolved scale. The gradient transport model reads

$$\bar{\rho}(\widetilde{\vec{u}}\widetilde{Z} - \widetilde{\vec{u}Z}) = \bar{\rho} D_T \nabla \widetilde{Z} \tag{3}$$

$$\bar{\rho}(\widetilde{\vec{u}}\widetilde{Y}_i - \widetilde{\vec{u}Y_i}) = \bar{\rho} D_{T,i} \nabla \widetilde{Y}_i. \tag{4}$$

where D_T and $D_{T,i}$ are the subfilter diffusivity for Z and Y_i, respectively. Then the corresponding governing equations are

$$\frac{\partial \bar{\rho}\widetilde{Z}}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{Z}\widetilde{\vec{u}}) = \nabla \cdot [\bar{\rho}(D + D_T)\nabla \widetilde{Z}] = \nabla \cdot [\bar{\rho}\mathfrak{D}_T \nabla \widetilde{Z}], \tag{5}$$

for the filtered mix fraction equation $\widetilde{Z}$, and

$$\begin{aligned}\frac{\partial \bar{\rho}\widetilde{Y}_i}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{Y}_i\widetilde{\vec{u}}) &= \nabla \cdot [\bar{\rho}(D_i + D_{T,i})\nabla \widetilde{Y}_i] + \overline{\omega_i} \\ &= \nabla \cdot [\bar{\rho}\mathfrak{D}_{T,i} \nabla \widetilde{Y}_i] + \overline{\omega_i}\end{aligned} \tag{6}$$

for the filtered species concentration $\widetilde{Y}_i$. Here $\bar{\cdot}$ and $\tilde{\cdot}$ denote the filtered and density-weighted filtered quantities, respectively. In addition, to improve the numerical robustness D_T and $D_{T,i}$ can be determined by orientational average as $D_T = (\widetilde{\vec{u}}\widetilde{Z} - \widetilde{\vec{u}Z}) \cdot \nabla\widetilde{Z}/|\nabla\widetilde{Z}|^2$ and $D_{T,i} = (\widetilde{\vec{u}}\widetilde{Y}_i - \widetilde{\vec{u}Y_i}) \cdot \nabla\widetilde{Y}_i/|\nabla\widetilde{Y}_i|^2$, respectively.

To derive the turbulent flamelet transform relation, we introduce a Lagrangian coordinate system mapped to the mixture fraction Z space as

$$(x_1, x_2, x_3, t) \mapsto (Z, Z_2, Z_3, \tau), \tag{7}$$

where $\tau = t$ and Z_2 and Z_3 are two auxiliary coordinates, which are locally tangential to the $\widetilde{Z}$ isosurface and dependent on both x_i and t. To simplify the following mathematic expression, Z_2 and Z_3 are chosen as the curvilinear coordinates on the Z isosurfaces and orthogonal to each other. Following the analysis of freely propagating flame [19], a meaningful choice of the coordinate system is in the tangential direction it moves with the local tangential flow everywhere. More detailed discussion can refer to Refs. [19,20]. Thus the gradient operator ∇ can be expressed as

$$\nabla = \vec{n}\frac{\partial \widetilde{Z}}{\partial \vec{n}}\frac{\partial}{\partial \widetilde{Z}} + \frac{\vec{t_2}}{h_2}\frac{\partial}{\partial Z_2} + \frac{\vec{t_3}}{h_3}\frac{\partial}{\partial Z_3} = \vec{n}\frac{\partial \widetilde{Z}}{\partial \vec{n}}\frac{\partial}{\partial \widetilde{Z}} + \nabla_\perp, \tag{8}$$

where $\vec{n}$ is the unit normal to the $\widetilde{Z}$ isosurface, $\vec{t_2}$ and $\vec{t_3}$ are the unit directional vector for the Z_2 and Z_3 coordinates, and $h_{2,3}$ are their corresponding Lamé coefficients, and $\nabla_\perp$ denotes the gradient operator in the surface spanned by Z_2 and Z_3.

Following the chain law $\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t}\frac{\partial}{\partial Z} + \frac{\partial Z_2}{\partial t}\frac{\partial}{\partial Z_2} + \frac{\partial Z_3}{\partial t}\frac{\partial}{\partial Z_3}$, together with Eq. (5) and Eq. (6), the coordinate transform yields

$$\begin{aligned}&\bar{\rho}\frac{\partial \widetilde{Y}_i}{\partial \tau} + \bar{\rho}\left(\widetilde{\vec{u}} \cdot \nabla_\perp \widetilde{Y}_i + \frac{\partial \widetilde{Y}_i}{\partial Z_2}\frac{\partial Z_2}{\partial t} + \frac{\partial \widetilde{Y}_i}{\partial Z_3}\frac{\partial Z_3}{\partial t}\right) \\ &\quad = \frac{1}{2Le_T}\bar{\rho}\chi\frac{\partial^2 \widetilde{Y}_i}{\partial \widetilde{Z}^2} + \frac{\partial \widetilde{Y}_i}{\partial \widetilde{Z}}\nabla \cdot \left[\bar{\rho}(\mathfrak{D}_{T,i} - \mathfrak{D}_T)\vec{n}\frac{\partial \widetilde{Z}}{\partial n}\right] \\ &\quad + \nabla \cdot (\bar{\rho}\mathfrak{D}_{T,i}\nabla_\perp \widetilde{Y}_i) + \overline{\omega_i},\end{aligned} \tag{9}$$

where the turbulent scalar dissipation χ is defined as

$$\chi = 2D_T(\frac{\partial \widetilde{Z}}{\partial n})^2 \tag{10}$$

and the turbulent Lewis number $Le_T = D_T/\mathfrak{D}_{T,i}$.

Eq. (9) is the turbulent flamelet transform with respect to the resolved fields in LES, which generalizes such transform for the turbulent flame by Peters [2]. The present form is preferred because of its conciseness and the clear meaning of different terms. For the laminar cases such a transform indicates a strong correlation between the dependent field quantities and the scalar mixture fraction Z. Although formally similar to the laminar case, physically Eq. (9) is different in the following aspects. First, for the filtered flame the derivatives along the $\widetilde{Z}$ normal and along the flame tangential may behave differently compared with the laminar flamelet case, because the flame structure has been artificially changed by the filtering operation. The Lagrangian relation along the $\widetilde{Z}_2$ and $\widetilde{Z}_3$ directions, i.e. the second term on l.h.s., is involved. Such geometrical term can locally be influential. Second, the chemical reaction term is filtered and can not be interpreted using the filtered quantities $\widetilde{T}$ and $\widetilde{Y}_i$ because of the strong nonlinearity. Third, numerically the turbulent diffusivity coefficients $\mathfrak{D}_T$ and $\mathfrak{D}_{T,i}$ are flow dependent, but not the fluid parameters. Because the turbulent dissipation χ is defined via $\mathfrak{D}_T$ and thus the statistics of χ become more complex. For instance the possible negative diffusivity $\mathfrak{D}_T$, and thus possible negative χ from Eq. (10), will have impact on the numerical behavior of the flamelet transform Eq. (9).

Among all the new features χ and the filtered chemical source term $\overline{\omega_i}$ are of special importance. From the modeling viewpoint, the difference between reactive turbulence and nonreactive turbulence lies on the strong nonlinear reaction (and the relevant contribution) part. In principle the gradient components along the flame tangential share the nonreactive turbulence properties and modeling of them can follow the existing methods, for instance the dynamic subgrid model. In the following we focus on the properties of χ and $\overline{\omega_i}$, based on an a priori analysis of a DNS dataset.