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Prediction of local extinction and re-ignition effects in non-premixed turbulent combustion using a flamelet/progress variable approach

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Abstract

The flamelet/progress variable approach (FPVA) has been proposed by Pierce and Moin as a model for turbulent non-premixed combustion in large-eddy simulation. The filtered chemical source term in this model appears in unclosed form, and is modeled by a presumed probability density function (PDF) for the joint PDF of the mixture fraction Z and a flamelet parameter λ. While the marginal PDF of Z can be reasonably approximated by a beta distribution, a model for the conditional PDF of the flamelet parameter needs to be developed. Further, the ability of FPVA to predict extinction and re-ignition has also not been assessed. In this paper, we address these aspects of the model using the DNS database of Sripakagorn et al. It is first shown that the steady flamelet assumption in the context of FPVA leads to good predictions even for high levels of local extinction. Three different models for the conditional PDF of the flamelet parameter are tested in an a priori sense. Results obtained using a delta function to model the conditional PDF of λ lead to an overprediction of the mean temperature, even with only moderate extinction levels. It is shown that if the conditional PDF of λ is modeled by a beta distribution conditioned on Z, then FPVA can predict extinction and re-ignition effects, and good agreement between the model and DNS data for the mean temperature is observed.

Keywords: Non-premixed combustion; Turbulent flame; Modeling

1. Introduction

The accurate description of extinction and re-ignition effects in non-premixed turbulent combustion is of importance for the prediction of flame stabilization [1]. The transported probability density function (PDF) method [2] has been successfully used in numerical simulation of flames with moderate to strong extinction events [3]. Although the results compare well with experimental data for flames with different levels of extinction, the accuracy has been shown to depend on the mixing model, specifically on the time scale ratios employed. Transported PDF methods also become computationally expensive, especially when used in large-eddy simulation (LES) and when the number of chemical species is large. Other commonly used combustion models are the flamelet model [1,4,5] and the conditional moment closure model [6] for non-premixed turbulent combustion. These methods are computationally less expensive even if complex chemical mechanisms are considered. The latter two models are commonly combined with a presumed PDF model to describe

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the mean values of the density and reactive scalars. Because of the simplifying assumptions made in the derivation of the flamelet equations, the steady state flamelet model and also the unsteady flamelet model, for example, as applied by Pitsch et al. [7], fail in situations where local extinction and re-ignition are important. In another recent study, the unsteady flamelet model has been shown to predict extinction quite accurately, but cannot account for re-ignition [8,9].

Many attempts have been made to extend the applicability of flamelet models to combustion with local extinction and re-ignition. Mauss et al. [10] have solved the unsteady flamelet equations for a methane jet diffusion flame near extinction to predict CO-formation. Pitsch and co-workers [11,12] have developed a stochastic, interacting flamelet model, which extends the unsteady flamelet model to account for re-ignition effects due to the interaction of different flamelets. In an a priori study, it has been shown that this model is in reasonable agreement with DNS data, but the implementation of the model into a CFD-solver is non-trivial.

Pierce and Moin [13,14] have recently proposed a model based on the steady flamelet approach and applied this model in LES of turbulent combustion in a confined combustor. In this flamelet/progress variable approach (FPVA), a flamelet parameter based on a reactive scalar is used rather than the scalar dissipation rate. This allows, in principle, to predict extinction and re-ignition effects. In using a combined reactive scalar/mixture fraction approach with a presumed PDF, this model is similar to that of Janicka and Kollmann [15], where transport equations for mixture fraction and a reactive scalar are solved, and the unclosed chemical source term is obtained by using the presumed joint PDF of both scalars. Similar ideas have also been used by Bruel et al. [16] in the modeling of auto-ignition processes using the flamelet approach with a presumed-shape PDF for the mixture fraction and progress variable. However, important differences to the FPVA are the choice of the scalar state relationship, the flamelet parameter, and the presumed PDF.

The objective of the present paper is to assess and improve the flamelet/progress variable approach. We will first present the FPVA model with an emphasis on revealing the assumptions made in the model. We will then assess the performance of the FPVA against results obtained from direct numerical simulations (DNS) of decaying isotropic turbulence with a one-step reversible chemical reaction at different levels of local extinction and re-ignition [8,9]. In addition to investigating each of the FPVA assumptions individually with respect to their ability to predict extinction and re-ignition effects, we also propose and test improvements of the model in the following sections.

2. Flamelet/progress variable approach

The flamelet model [5,4] considers a turbulent diffusion flame as an ensemble of laminar flamelets. This model introduces the mixture fraction Z as a conserved scalar. The species mass fractions and temperature are related to the mixture fraction by the solution of the flamelet equations. A parameter appearing in this model is the dissipation rate of the conserved scalar defined as

$$\chi = 2D_Z(\nabla Z)^2, \tag{1}$$

where D_Z is the molecular diffusivity of the mixture fraction. The steady flamelet equations are given by

$$-\rho\frac{\chi}{2}\frac{\partial^2\boldsymbol{\phi}}{\partial Z^2} = \boldsymbol{\omega}, \tag{2}$$

where the scalar dissipation rate appears as an external parameter. In Eq. (2), ρ is the density, $\boldsymbol{\phi}$ is the vector of the species mass fractions and temperature, and $\boldsymbol{\omega}$ denotes their respective source terms. Assuming a unique functional dependence of the scalar dissipation rate on the mixture fraction, the state relation given by Eq. (2) can be written in the form

$$\boldsymbol{\phi} = \boldsymbol{\phi}(Z, \chi_{\mathrm{st}}), \tag{3}$$

where χ_{st} is the scalar dissipation rate at $Z = Z_{\mathrm{st}}$. The solution of the flamelet equations can be represented by the so-called S-shaped curve, whose upper and lower branches describe the stable burning and non-burning solutions, respectively, and the middle solution branch is unstable. The turning point between the upper and middle branches corresponds to $\chi = \chi_{\mathrm{q}}$. Since multiple solutions exist for certain values of the dissipation rate, a unique parameterization of the flamelet solutions in terms of the scalar dissipation rate cannot represent the entire solution space. Typically, in applications of the flamelet model, only the burning branch of the S-shaped curve is considered. Even if the lower branch of the non-burning solutions is also considered for $\chi > \chi_{\mathrm{q}}$, it is obvious that there exists a discontinuity in the solution at $\chi = \chi_{\mathrm{q}}$, and intermediate states of the reactive scalar between fully burning and fully extinguished cannot be described. This implies that any physical state between the fully burning and extinguished state in the steady state flamelet model will be projected onto the burning or the non-burning solution, depending on the value of the stoichiometric scalar dissipation rate. Hence, the flamelet model parameterized with the scalar dissipation rate does a vertical projection onto the S-shaped curve.

The flamelet/progress variable approach introduces a new flamelet parameter λ, which is based on a reactive scalar and uniquely identifies each single flame state along the S-shaped curve,

including the unstable branch. Flamelets experiencing a transition from the burning to the extinguished flame state or those which are likely to re-ignite are then projected horizontally onto the S-shaped curve. The flamelet parameter λ is defined through a reactive scalar C, which has been introduced by Pierce and Moin [14,17] to be a linear combination of major reaction products. In the present paper, for convenience, we choose C to be the reduced temperature. Different choices can be made for the flamelet parameter λ, as long as it uniquely describes all states along the S-shaped curve. Here, we will define λ to be the temperature at stoichiometric mixture fraction of a given steady flamelet. It will be seen later that this definition will have advantages in the model for the joint PDF. We can then express the solutions of Eq. (2) in terms of λ as

$$\boldsymbol{\phi} = \boldsymbol{\phi}(Z, \lambda). \tag{4}$$

Note that this is different from Eq. (3) as it includes all solutions of the steady state flamelet equations. For any given combination of Z and C, λ can be determined by inverting Eq. (4), which assumes that an unique inversion exists. However, this is not the case at the boundaries of the mixture fraction space, where C for all flamelets goes to a single value. It is interesting to note that if a turbulent reactive flow can be described by Eq. (4), meaning that all flame states correspond to solutions of the steady flamelet equations, then Z and λ are independent. This is an important property, since it simplifies the modeling of the joint PDF of Z and λ and can also be used as a criterion for testing the validity of Eq. (4).

Without further assumptions, the mean values of the scalars $\boldsymbol{\phi}$ can be determined from

$$\widetilde{\boldsymbol{\phi}}(t, \mathbf{x}) = \int_{\lambda^-}^{\lambda^+} \int_0^1 \boldsymbol{\phi}(Z, \lambda) \widetilde{P}(Z, \lambda; t, \mathbf{x}) \, \mathrm{d}Z \, \mathrm{d}\lambda, \tag{5}$$

where $\widetilde{P}(Z, \lambda; t, \mathbf{x})$ is the Favre joint PDF of Z and λ. The integration limits λ^+ and λ^- correspond to the solution of Eq. (2) for $\chi_{\mathrm{st}} \to 0$ and $\chi_{\mathrm{st}} \to \infty$, respectively. In turbulent combustion, the PDF of any scalar is a function of space and time. In the following, for simplicity of notation, we will not write the implicit dependence on $\mathbf{x}$ and t. Using Bayes' theorem, the joint PDF can be written in terms of a conditional PDF, $\widetilde{P}(\lambda|Z)$, and a marginal PDF, $\widetilde{P}(Z)$, as

$$\widetilde{P}(Z, \lambda) = \widetilde{P}(\lambda|Z) \widetilde{P}(Z). \tag{6}$$

It is possible to solve a PDF-transport equation for $\widetilde{P}(Z, \lambda)$ and then integrate Eq. (5) to obtain $\widetilde{\boldsymbol{\phi}}$. The FPVA, as proposed by Pierce and Moin [13,14], is based on a presumed PDF method. It has been shown by several authors that the PDF of a passive scalar can reasonably be approximated by a beta distribution [18–20]. However, it is well known that PDFs of reacting scalars usually cannot be simply represented by presumed distributions. Pierce and Moin [13,14] have used a beta distribution for the marginal PDF of the mixture fraction. Similar to Janicka and Kollmann [15], they assumed λ and Z to be independent and choose a delta function for the PDF of λ.

To summarize, essentially four different assumptions have been employed in the FPVA. First, it is assumed that $\boldsymbol{\phi}$ is only a function of Z and λ, and that this function is given by the solution of the steady state flamelet equations. In the following, we will call this the steady flamelet assumption. Second, to model the joint PDF, Z and λ are assumed to be independent. Note that, as described earlier, this is already a direct consequence of the steady flamelet assumption, but here it is of interest to address these assumptions individually. Finally, assumptions three and four are the presumed forms for the marginal PDFs of Z and λ, respectively, where the marginal PDF of the mixture fraction is modeled by a beta distribution. To model the joint PDF, the FPVA assumes that λ and Z are independent with the marginal PDF of the flamelet parameter described by a delta function.

3. Numerical experiment

In this paper, a priori testing of the FPVA and the underlying modeling assumptions will be presented using data from the DNS experiment performed by Sripakagorn et al. [8,9]. A one-step, reversible chemical reaction of the form $\mathrm{F} + \mathrm{O} \rightleftharpoons 2\mathrm{P}$ evolves in decaying isotropic turbulence, where F, O, and P represent fuel, oxidizer, and products, respectively. In this numerical simulation, a chemical reaction without heat release has been studied. It is well known that heat release effects the flow field significantly. However, it has been found that results from incompressible DNS can capture important dynamic features, such as extinction and peak temperature [21,22]. The non-dimensional chemical source term is a function of Z and the reduced temperature θ only, and is given by

$$\begin{aligned}\omega_\theta = {} & 2A \exp\left\{-\frac{\beta}{\alpha}\right\} \exp\left\{-\frac{\beta(1-\theta)}{1-\alpha(1-\theta)}\right\} \\ & \times \left[Z_{\mathrm{st}}(1-Z_{\mathrm{st}})\left(\frac{Z}{Z_{\mathrm{st}}}-\theta\right)\left(\frac{1-Z}{1-Z_{\mathrm{st}}}-\theta\right) - \frac{1}{K}\theta^2\right].\end{aligned} \tag{7}$$

Here, A is the frequency factor, $\alpha = (T_{\mathrm{st,c}} - T_{\mathrm{st,u}})/T_{\mathrm{st,c}}$ is the heat release parameter, $\beta = \alpha T_{\mathrm{a}}/T_{\mathrm{st,c}}$ is the Zeldovich number, T_{a} is the activation temperature, and K is the equilibrium constant of the global reaction. $T_{\mathrm{st,c}}$ and $T_{\mathrm{st,u}}$ are the temperatures for complete adiabatic conversion and the

unburned temperature evaluated at $Z_{st} = 0.5$, respectively. All parameters used in this study can be found in [8,9]. For a one-step global reaction, the mass fractions of the chemical species are linearly related to the temperature, so that in addition to the mixture fraction equation only an equation for the temperature needs to be solved. For the comparison with DNS data, we chose the reduced temperature $\theta = (T - T_{st,u})/(T_{st,c} - T_{st,u})$ as the reaction progress variable, i.e., $C = \theta$. The shape of the beta distribution for a scalar ϕ is determined by its mean $\widetilde{\phi}$ and variance $\widetilde{\phi''^2}$, and can be written as $\widetilde{P}(\phi) = \beta(\phi; \widetilde{\phi}, \widetilde{\phi''^2})$. This requires the solution of transport equations for $\widetilde{\phi}$ and $\widetilde{\phi''^2}$. In this idealized problem, the turbulent flow field is incompressible, and hence, the flow is decoupled from the chemical reaction process. The equations for the first two moments of Z and C then simplify to:

$$\frac{\partial \widetilde{Z}}{\partial t} = 0, \tag{8}$$

$$\frac{\partial \widetilde{Z''^2}}{\partial t} = -2D_Z(\widetilde{\nabla Z''})^2, \tag{9}$$

$$\frac{\partial \widetilde{C}}{\partial t} = \widetilde{\omega}_C, \tag{10}$$

$$\frac{\partial \widetilde{C''^2}}{\partial t} = -2D_C(\widetilde{\nabla C''})^2 + 2\widetilde{C''\omega''_C}, \tag{11}$$

where $\widetilde{\omega}_C$ is the filtered or averaged chemical source term.

Here, we will consider two cases with different values for the frequency factor A in Eq. (7), and hence varying degrees of local extinction and re-ignition. A measure of local extinction and re-ignition is the burning index [23], presented here to compare the two different cases for $A = 80{,}000$ (a moderate extinction case) and $A = 30{,}000$ (a case with strong extinction). The burning index is based on the reduced temperature and is defined as

$$BI_\theta = \frac{\widetilde{\theta|Z_{st}}}{\theta(Z_{st}, \widetilde{\chi}_{st})}, \tag{12}$$

where $\theta(Z_{st}, \widetilde{\chi}_{st})$ is the flame temperature conditioned on stoichiometric mixture as given by the burning branch of the steady flamelet equations with $\widetilde{\chi}_{st}$ taken from the DNS. The temperature of the burning flamelet at χ_q is used for $\widetilde{\chi}_{st} > \chi_q$. Values of BI_θ near unity indicate fully burning states and values near zero characterize complete extinction. The burning index BI_θ and $\widetilde{\lambda}$, also directly evaluated from the DNS, are shown in Fig. 1 as functions of time. Time has been normalized by the eddy turnover time t_{eddy} [8,9]. It is interesting to note that the flamelet parameter

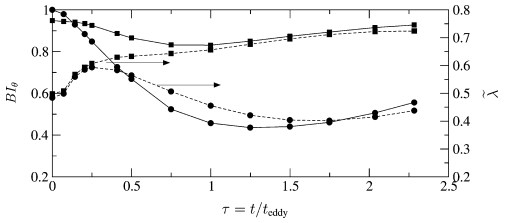

Fig. 1. The evolution of the burning index BI_θ (solid lines) and the mean value of the flamelet parameter $\widetilde{\lambda}$ (dashed lines) extracted from the DNS for $A = 80{,}000$ (squares) and $A = 30{,}000$ (circles).

introduced in the model shows the same behavior as BI_θ after a transitional time $\tau \sim 0.5$. Note also that from the definition of λ, $\widetilde{\lambda|Z_{st}}$ is equal to $\widetilde{\theta|Z_{st}} = BI_\theta\theta(Z_{st}, \widetilde{\chi}_{st})$.

4. Results and discussion

In this section, we will test the assumptions of the FPVA model against the DNS data, and modeling needs will be identified. This ultimately leads to an improved model for a presumed shape of the conditional PDF for the flamelet/progress variable approach, which will be tested using the DNS data.

4.1. Steady flamelet assumption

For a comparison with DNS data, Eq. (10) is integrated numerically. To individually test the steady flamelet assumption as defined in the previous section, the mean chemical source term $\widetilde{\omega}_C$ is evaluated from Eq. (5) by using the joint PDF $\widetilde{P}(Z, \lambda)$ taken from the DNS data.

Figure 2 compares the evolution of the progress variable, or the reduced temperature for the present case, obtained by invoking the steady flamelet assumption against data from the DNS. Graph A in Fig. 2 shows the result for the case with moderate extinction. The prediction of $\widetilde{C}$ is in very good agreement for $\tau < 1.5$ and deviates only marginally

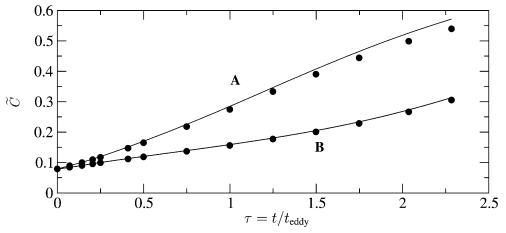

Fig. 2. The evolution of the progress variable invoking the steady flamelet assumption (solid lines) compared with DNS data (circles); (A) $A = 80{,}000$ (moderate extinction) and (B) $A = 30{,}000$ (strong extinction).

from the DNS results at later times. The evolution of the mean progress variable for the case with strong extinction is shown by curve B in Fig. 2. The results obtained from the steady flamelet assumption are again in good agreement with the DNS results. Then it can be concluded that the steady flamelet assumption is a valid model for the present problem, as long as the exact shape of $\widetilde{P}(Z,\lambda)$ is known. This means that the scalars can be represented by Eq. (4) and that the steady state solution of the flamelet equations, including the solution for the unstable branch of the S-shaped curve, are sufficient for the level of accuracy shown in Fig. 2. Furthermore, transitional effects such as partial burning and re-igniting flamelets can be well described by flame states corresponding to the unstable middle branch. However, we will see below that the flamelet parameter is not entirely independent from the mixture fraction away from Z_{st}, which indicates that in these regions the steady flamelet assumption is not completely satisfied.

4.2. Single flamelet closure

Pierce and Moin [13] applied the FPVA to LES, where they assumed that $\widetilde{P}(\lambda|Z)$ is independent of Z. Then, they presumed the marginal PDF $\widetilde{P}(\lambda)$ to be a delta distribution

$$\widetilde{P}(\lambda) = \delta(\lambda - \lambda^*), \tag{13}$$

where $\lambda^* = \lambda(\widetilde{Z}, \widetilde{Z''^2}, \widetilde{C})$ describes a single representative flamelet. In the following, this model is referred to as single flamelet closure. By assuming that the mixture fraction follows a beta distribution characterized by $\widetilde{Z}$ and $\widetilde{Z''^2}$, the flame state in each LES cell can be determined with the value of $\widetilde{C}$ obtained from the solution of a transport equation. Hence, a flamelet library can be precomputed which returns λ^* as a function of $\widetilde{Z}, \widetilde{Z''^2}$ and $\widetilde{C}$. Using the flamelet library, Eq. (10) is integrated numerically with the mean chemical source term evaluated by

$$\widetilde{\omega_C}(\widetilde{Z}, \widetilde{Z''^2}, \widetilde{C}) = \int_0^1 \omega_C(Z,\lambda^*)\beta(Z;\widetilde{Z}, \widetilde{Z''^2})\,\mathrm{d}Z. \tag{14}$$

The mean and variance of the mixture fraction are computed from the DNS by volume averaging. The DNS data are used to initialize the equation for $\widetilde{C}$. Numerical results for the two different cases are shown in Fig. 3, where the evolution of $\widetilde{C}$ is shown and the flamelet parameter λ^* is compared with $\widetilde{C|Z_{st}}$ from the DNS data. For the case with moderate extinction (Fig. 3A), the mean value of the progress variable (solid line) is overpredicted after $\tau \sim 0.5$, which corresponds approximately to the time when extinction in the DNS becomes important [8,9]. Note that a small overprediction of the mean temperature can correspond to a large error of the local temperature in the reaction zone.

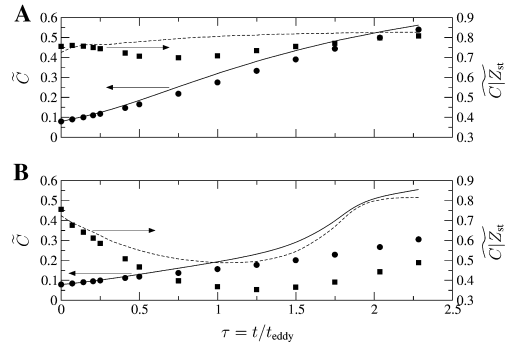

Fig. 3. The evolution of the progress variable invoking single flamelet closure (solid lines) compared with DNS data (circles) and comparison of the mean progress variable conditioned on Z_{st} (dashed lines) with DNS data (squares); (A) $A = 80{,}000$ (moderate extinction) and (B) $A = 30{,}000$ (strong extinction).

This can be seen by comparing the conditional mean temperature at stoichiometric conditions from the DNS data (squares) with the predictions from the FPVA (dashed line) in Fig. 3. The results obtained for the case with strong extinction, shown in Fig. 3B, deviate considerably from the DNS data. With the single flamelet closure, the FPVA under-predicts the local rate of extinction and overpredicts re-ignition, resulting in higher mean temperatures. The reason for this can be found by comparing the conditional PDF of λ at $Z = Z_{st}$ from the DNS with the presumed PDF, shown in Fig. 4. The bimodal shape of $\widetilde{P}(\lambda|Z_{st})$ confirms that a computational cell contains an ensemble of extinguished and burning flame states. However, the single flamelet model uses a delta function at λ^*, which is between the peaks of $\widetilde{P}(\lambda|Z_{st})$. Due to the non-linearity of the chemical source term, this will lead to a larger value of the mean chemical source term $\widetilde{\omega}_C$, and consequently to the higher mean temperatures observed in Fig. 3.

To predict extinction and re-ignition, the broad distribution of the conditional PDF must be taken into account. An improved model for $\widetilde{P}(\lambda|Z)$ will be proposed in the following section.

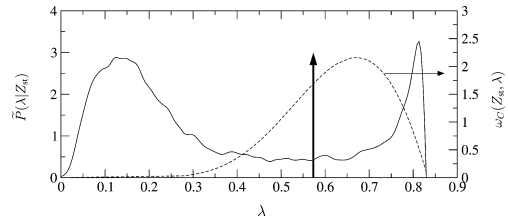

Fig. 4. Comparison of the conditional PDF $\widetilde{P}(\lambda|Z_{st})$ from the DNS for $A = 30{,}000$ at $\tau = 1.5$ (solid line) with the single flamelet closure. The vertical arrow indicates the delta function, $\delta(\lambda - \lambda^*)$, and the dashed line shows the chemical source term $\omega_C(Z_{st},\lambda)$.

4.3. Modified closure

The bimodal nature of $\widetilde{P}(\lambda|Z)$, as illustrated in Fig. 4, indicates that higher moment information for the λ-distribution is required for the present case. That is, the assumption of a delta distribution for the PDF of λ fails, because it can only describe the first moment. Cha and Pitsch [24] have introduced a beta function for the conditional PDF of a reactive scalar in the context of higher order conditional moment closure modeling. They found that this function cannot accurately describe the shape of the PDF in general. However, enforcing the second conditional moment within the higher order conditional moment strategy can lead to good results which are relatively insensitive to the conditional variances. Ultimately, to derive a working model for LES, we want to presume a beta function for the marginal PDF of the flamelet parameter λ. If the steady flamelet assumption is valid, then λ and Z are independent, and $\widetilde{P}(\lambda|Z) = \widetilde{P}(\lambda)$. Hence, we will start here by assuming a beta distribution as a presumed PDF for the flamelet parameter conditioned on Z as

$$\widetilde{P}(\lambda|Z) = \beta(\lambda; \widetilde{\lambda|Z}, \widetilde{\lambda''^2|Z}). \tag{15}$$

This model requires, in addition to the equation for $\widetilde{\lambda|Z}$, the solution of a transport equation for the flamelet parameter variance conditioned on Z. Here, we extract the conditional mean and variance of λ in addition to $\widetilde{Z}$ and $\widetilde{Z''^2}$ directly from the DNS, and use these values to solve Eq. (10) with the chemical source term evaluated according to Eq. (5) and the conditional PDF given by Eq. (15). Figure 5 compares the reduced temperature obtained from this model (solid lines) with the DNS results (circles) and with the model discussed earlier, where only the flamelet assumption is invoked. From this figure it can be seen that Eq. (15) provides a good model for the conditional PDF, even in the presence of strong local extinction and re-ignition events (also shown by Fig. 5B).

The dashed-dotted lines in Fig. 5 show results with the additional assumption that λ and Z are independent, i.e., with

$$\widetilde{P}(Z,\lambda) = \beta(\lambda; \widetilde{\lambda}, \widetilde{\lambda''^2})\beta(Z; \widetilde{Z}, \widetilde{Z''^2}), \tag{16}$$

where a beta PDF now describes the unconditional PDF of λ. The result is a strong overprediction of the mean temperature especially for the case with moderate extinction. Eq. (16) is used to model $\widetilde{\omega}_C$ by taking the moments for λ and Z from the DNS to integrate Eq. (10) in time. The initial distribution of the mixture fraction follows a beta function with two peaks at $Z \to 0$ and $Z \to 1$, respectively. The determination of a flamelet parameter is not unique at these two points. We assign to these states values for λ corresponding to the state for $\chi \to \infty$, which introduces an error in the determination of the moments for λ. However, it was found that the error associated with these multi-valued points is relatively small. To understand the deviation between the DNS data and the FPVA model with Eq. (16) in Fig. 5, the conditional PDFs of λ from the DNS at two different times are shown in Fig. 6. The conditional PDFs are symmetric around $Z_{st} = 0.5$, so that only one half of $\widetilde{P}(\lambda|Z)$ is shown. Figure 6A shows the results

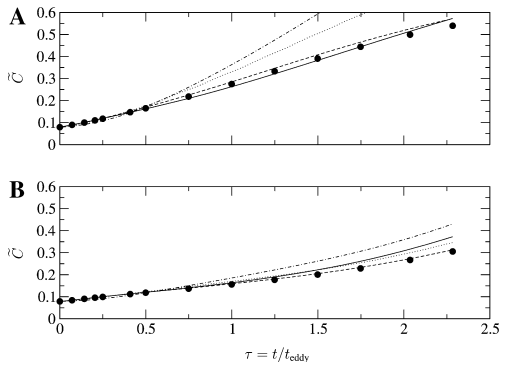

Fig. 5. The evolution of the mean progress variable computed with FPVA. The joint PDF of Z and λ is evaluated from Eq. (15) (solid lines), Eq. (16) (dashed-dotted lines), and the joint PDF taken from the DNS data (dashed lines). Also shown is the mean progress variable from the DNS results (circles). The dotted lines represent the results from LES with a filter size of 4^3 DNS cells; (A) $A = 80{,}000$ (moderate extinction) and (B) $A = 30{,}000$ (strong extinction).

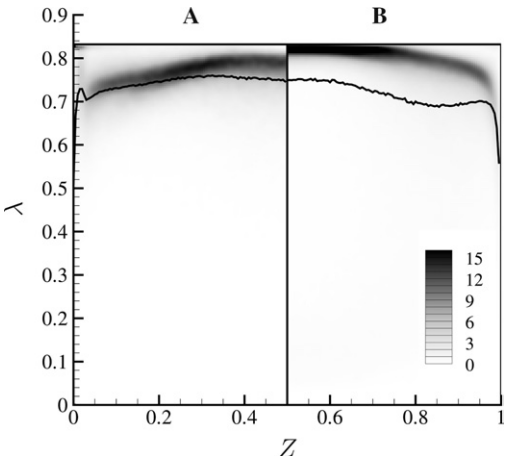

Fig. 6. Iso-contours of the conditional PDF, $\widetilde{P}(\lambda|Z)$ extracted from the DNS for $A = 80{,}000$ (moderate extinction) at two different times: (A) $\widetilde{P}(\lambda|Z)$ at $\tau = 0.2$, where extinction effects are dominant; (B) $\widetilde{P}(\lambda|Z)$ for $\tau = 1.5$, where re-ignition effects are of importance. The conditional PDFs are symmetric around $Z_{st} = 0.5$, so that only one half of $\widetilde{P}(\lambda|Z)$ is shown. Solid lines show the conditional mean value of the flamelet parameter, $\widetilde{\lambda|Z}$.

for $\tau = 0.2$, where flame quenching and subsequent extinction are dominant. Figure 6B shows the results for $\tau = 1.5$, where flamelets re-ignite due to the reduced scalar dissipation rates. Around $Z_{st} = 0.5$, the assumption that λ and Z are independent is seen to be reasonable, which in turn shows that the steady flamelet assumption is valid in this region. However, for values of the mixture fraction $Z < 0.2$ and $Z > 0.8$ this is not the case. This can be understood by considering unsteady transport phenomena of a flamelet during extinction and re-ignition. The chemistry in a diffusion flame takes place in a thin layer around Z_{st}. During extinction and re-ignition, the stoichiometric temperature changes due to an imbalance between chemistry and diffusive transport. The time to reach a quasi-steady state throughout the flamelet is given by a diffusive time scale, which can be approximated as $t_d \sim Z_{st}^2/\chi$. The functional form of the scalar dissipation rate dependence on the mixture fraction can be described, for instance, from a counterflow or mixing layer configuration [1,5]. Important here is only that the dissipation rate tends to zero when the mixture fraction approaches its minimum and maximum possible value. It follows then from t_d that the diffusion time tends to infinity, which prohibits the chemical species from reaching a steady state solution in these regions. The characteristic time scale for extinction is related to t_d and hence, the structure of a flamelet during the extinction process is, at high and low values of Z, different from that of a corresponding steady flamelet. Although such regions are generally not very important, for the present DNS the evaluation of the mean chemical source term is strongly effected by these discrepancies, since especially for early times very lean and very rich regions occur with high probability. The reason for the strong impact of areas of very high and low mixture fraction is that the present study has been performed using the data of the entire DNS-domain, and hence corresponds to a Reynolds-averaged (RANS) approach.

An improvement could be expected for LES where a significant part of the kinetic energy and scalar variance is resolved. In LES, the sub-filter variance $\widetilde{Z''^2}$ in a computational cell is typically small, leading to a relatively narrow PDF $\widetilde{P}_{cell}(Z)$. Because of the weak dependence of λ on Z, it can be argued that λ and Z are then locally independent, and the FPVA with the presumed sub-filter PDF described by Eq. (16) would lead to better results than those obtained by the RANS approach. This has been confirmed by performing large-eddy simulations, in which the LES-filter size has been varied. Figure 5 shows as an example the results from a simulation with a filter size of 4^3 DNS cells. Especially for the case with stronger extinction, the results are significantly improved compared with the RANS results using the unconditional PDF. With increasing resolution, the numerical results approach the solution obtained with the conditional PDF model.

The application of the extended FPVA requires, in addition to $\widetilde{Z}$, $\widetilde{Z''^2}$, and $\widetilde{C}$, a model for the variance of the progress variable. Here, we solve a transport equation for this quantity given by Eq. (11). This equation contains two unclosed terms, the dissipation rate of the reactive scalar, and the covariance of the progress variable and the chemical source term. In the present RANS-type study, we model the covariance appearing in Eq. (11) using Eq. (15) and the beta distribution for the mixture fraction.

The comparison between the modeled covariance and the results obtained from the DNS are shown in Fig. 7. In addition, the evolution of the covariance conditioned on Z_{st} is shown. The overall agreement with the DNS data is quite good, particularly for the case with strong extinction. For the case with moderate extinction, the covariance is slightly under-predicted between $\tau = 0.25$ and 1.0. For both cases, the covariance is overpredicted at later times.

The second unclosed term in Eq. (11) is the dissipation rate of the progress variable. This quantity can be obtained from the ratio of the time scales of the reactive and non-reactive scalars $\gamma = \tau_C/\tau_Z$ where the time scales are defined as $\tau_Z = \widetilde{Z''^2}/\widetilde{\chi}$ and $\tau_C = \widetilde{C''^2}/\widetilde{\chi}_C$ and appropriate models for $\widetilde{Z''^2}$, $\widetilde{C''^2}$, and $\widetilde{\chi}$. A model for γ has been provided by Cha and Trouillet [27,28]. Results obtained with this time scale model have been shown to be in good agreement with DNS data for homogeneous isotropic turbulence [26] and for a turbulent non-premixed jet [27]. Employing the model by Cha and Trouillet [27,28] and the closure for the covariance, the

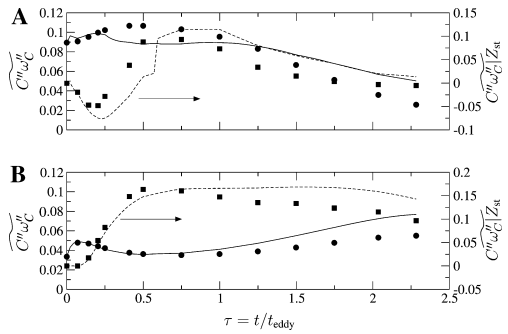

Fig. 7. The evolution of the covariance appearing in Eq. (11) obtained with FPVA and conditional beta distribution (solid lines) compared with DNS results (circles). Also shown is the covariance, conditioned on Z_{st} from the model (dashed lines) and the DNS data (squares); (A) $A = 80{,}000$ (moderate extinction) and (B) $A = 30{,}000$ (strong extinction).

FPVA model is closed and can be applied to LES of turbulent non-premixed combustion.

5. Conclusions

The flamelet/progress variable approach of Pierce and Moin [14,13] has been studied using a DNS database for non-premixed turbulent combustion in isotropic turbulence. The key modeling assumptions in FPVA are investigated with a particular emphasis on assessing the ability to describe extinction and re-ignition. Using the joint PDF of Z and λ from the DNS, it is shown that the steady flamelet assumption in the context of FPVA predicts extinction and re-ignition effects accurately. However, the further assumption of a delta distribution for the marginal PDF of the flamelet parameter leads to an overprediction of the temperature. A presumed beta distribution for the conditional PDF of the progress variable is shown to considerably improve the results. Applying the beta distribution as a model for the marginal PDF provides less accurate results because of the correlation between λ and Z for $Z \neq Z_{st}$, which is caused by the unsteadiness in these regions. This is assumed to be of minor importance for an LES closure, but also suggests that an unsteady flamelet model would further improve the results.

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