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FLUID AGE-BASED MODELLING FOR TURBULENT PREMIXED COMBUSTION IN FREE SHEAR FLOWS

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ABSTRACT

Age-based modelling is developed for the progress variable pdf in turbulent premixed combustion. The modelling is assessed using DNS data for a turbulent Bunsen flame. The age-based model reproduces the good performance of analogous flamelet-based modelling approaches, such as the filtered laminar flame approach, but provides additional benefits. The age-based approach provides a model for the shape of the filter kernel used to obtain the pdf from the laminar flame and a scaled-β function filter kernel is introduced for use in high-Reynolds number turbulent jet flames. In the present low-Reynolds number DNS, however, it is found that a Gaussian filter provides a better model. The results motivate application of the age-based model for the progress variable pdf in more general age-based modelling for partially-premixed turbulent combustion.

INTRODUCTION

Turbulent premixed combustion is characterised by thin reaction fronts that are wrinkled, thickened and potentially quenched by the underlying turbulent flow. Despite the complexity of the interactions between combustion chemistry and turbulence, the reaction-diffusion dynamics of combustion drive the thermo-chemical state onto a low-dimensional manifold (Pope, 2013). A classical model for the chemical manifold arising in a turbulent premixed combustion is a one-dimensional laminar premixed flame, resulting in a one-dimensional manifold that may be parametrised by a reaction progress variable, c, defined such that it varies monotonically from zero in the reactants to unity in the products. Given that direct numerical simulation (DNS) is computationally prohibitive for high-Reynolds number combustion systems, the filtered or ensemble-averaged quantities required for large eddy simulation (LES) or Reynolds-Averaged Navier-Stokes (RANS) simulation can be modelled by integrating properties of the chemical manifold over a modelled-probability density function (pdf) for the progress variable. For example, the Favre-averaged chemical source term $\dot{\omega}_c$ for progress variable is given by

$$\widetilde{\dot{\omega}}_{c\mathscr{F}} = \int_0^1 \mathscr{F}_{\dot{\omega}}(c)\tilde{p}_c(c;\mathbf{x},t)dc \qquad (1)$$

where $\mathscr{F}_{\dot{\omega}}$ returns the reaction rate on the manifold at c and subscript $\mathscr{F}$ indicates the property has been modelled using the flamelet manifold. Evolution of the density-weighted progress variable pdf $\tilde{p}(c)$ may be modelled directly with a transport equation (Pope, 1985) or a presumed-pdf shape may be parametrised as a function of progress variable moments.

Presumed-pdf models for progress variable can be classified broadly into algebraic (Bradley *et al.*, 1994), flamelet (Bray *et al.*, 2006; Jin *et al.*, 2008; Moureau *et al.*, 2011) and data-driven (Tsui *et al.*, 2016; de Frahan *et al.*, 2019) approaches. The β-pdf is an algebraic function of the mean and variance of progress variable that is employed widely in flamelet generated manifold modelling of premixed flames (Van Oijen & De Goey, 2000; Domingo *et al.*, 2005).The β-function generally provides an acceptable description of the mixing of simple non-reactive scalars. However the pdf shape of reaction progress variable is affected by the reaction-diffusion dynamics within the flame, with chemical reaction tending to thin out the probability density within the reaction zone. The β-function is independent of chemical kinetics and does not account for the effects of different fuels and combustion conditions on the pdf shape and this can lead to erroneous combustion predictions.

Flamelet-based models for the progress variable pdf shape have been developed in order to take account of the effects of reaction-diffusion dynamics for given combustion conditions. Bray *et al.* (2006) modelled the shape of the progress variable pdf based on the structure of a one-dimensional laminar flame, setting the magnitude of the pdf inversely proportional to the spatial gradient of progress variable in the laminar flame. Their original formulation was restricted to flames with very high variance. Jin *et al.* (2008) modified this approach by truncating the pdf shape in c-space in order to match the required progress variable variance. The truncated pdf model is equivalent to the sub-filter density function given by spatially-filtering the progress variable in the one-dimensional flame using a top-hat filter, as illustrated in Fig. 2, although Jin *et al.* (2008) do not explicitly state the correspondence with spatial filtering. The use of a top-hat filter by Jin et al. results in an unrealistic discontinuity at the extremes of the distribution. Moureau *et al.* (2011) proposed a filtered laminar flame model for the LES sub-filter progress variable pdf. Moureau *et al.* (2011) used a Gaussian filter, which avoids the discontinuities in the pdf shape given by a top-hat filter, and adjusted the laminar flame filter scale relative to the turbulent LES filter scale in order to obtain the desired level of sub-filter progress variable variance. Moureau *et al.* (2011) also provide modelling that can be used to relate the sub-filter progress variable variance to established modelling for sub-filter flame wrinkling in the context of LES. These flamelet approaches have be introduced by the respective authors using unstrained freely-propagating laminar flames. However the underlying methods can be applied equally using strained one-dimensional (e.g. counter-flow) laminar flames in order to account for the effect of strain on the profile of progress variable through the flame.

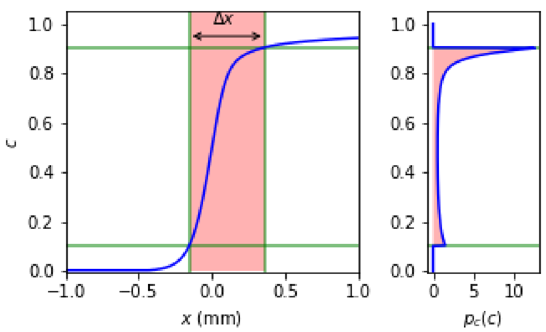


Figure 1: Spatial profile of progress variable in a laminar flame (left), a top-hat filter of width Δx (rectangular shading) and the corresponding pdf given by the model of Jin *et al.* (2008)(right).

Tsui *et al.* (2016) went further in order to account for effects of turbulent strain on the flame's internal structure. They used data from one-dimensional Linear Eddy Model turbulent premixed flame simulations for a given set of combustion conditions in order to obtain the pdf shape as a function of its mean and variance. For a given flame (fixed Lewis number, heat release parameter and Zel'dovich number), turbulent combustion is characterised by at least two further independent non-dimensional numbers (e.g. Reynolds and Karlovitz numbers). The results of Tsui et al. (Tsui *et al.*, 2016) suggest that the pdf shape is dependent on a single shape parameter, such as the variance, over a wide range of Reynolds and Karlovitz numbers.

The present study contributes to development of an age-based modelling framework for partially-premixed combustion (Richardson & Soriano, 2019) that uses information from multi-dimensional flamelet manifolds to describe the thermochemical state in turbulent flames, to model the scalar dissipation rates within that manifold, and to provide presumed-pdf shapes for the reference variables describing that manifold. Richardson & Soriano (2019) have shown that contours of fluid age within relevant reaction-diffusion manifolds can be used to model the statistical dependence of progress variable on mixture fraction in a wide variety of partially-premixed combustion applications, as illustrated in Fig. 2. The iso-age line in Fig. 2 is already a significant improvement over established models for the joint mixture fraction-progress variable pdf, even though it treats the conditional pdf of progress variable simply as a δ-function, which is clearly unsatisfactory in the limit of turbulent premixed combustion.

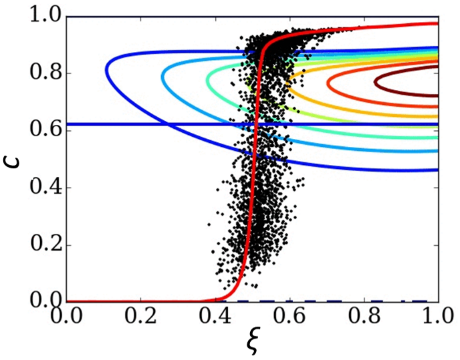


Figure 2: The one-point distribution of mixture fraction (ξ) and progress variable (c) in an equivalence ratio-stratified turbulent jet flame DNS (black points). Multi-coloured contours show the progress variable chemical source terms from a two-dimensional flamelet model for the problem. The joint distribution given by the conventional assumption of statistical dependence between ξ and c is represented by the blue horizontal line. The dependence of progress variable on mixture fraction predicted by an iso-line of fluid age in the two-dimensional flamelet is shown by the red 's'-shaped contour.(Richardson & Soriano, 2019)(right).

The focus in this study is application of the age-based approach to modelling of the progress variable pdf. In the perfectly-premixed context, the age-based pdf approach is analogous (although not equivalent) to Moureau *et al.*'s spatially-filtered laminar flame approach, and similarly good results are anticipated, but it provides a broader theoretical basis for extending flamelet-based presumed pdf models to more general inhomogeneous combustion systems. The article proceeds with an introduction to age-based modelling of the progress variable pdf, and analysis of its performance evaluated using DNS data for a premixed Bunsen flame.

DNS SIMULATION

The analysis considers data from DNS of a turbulent premixed Bunsen flame illustrated in Fig. 3. The simulation configuration has been studied previously by Richardson *et al.* (2010) however new simulations have been performed in order to incorporate transport equations for fluid age. A planar-jet of lean pre-heated methane-air mixture issues at 100 ms^{-1} from a H =1.8 mm wide slot into a

25 ms^{-1} co-flow of adiabatic combustion products. Synthetic homogeneous isotropic velocity fluctuations are imposed at the jet inflow. The flow is periodic in the spanwise direction. All other boundaries are open and modelled using partially-non-reflecting characteristic boundary conditions. The unburnt methane-air mixture has equivalence ratio of 0.7 at 800 K and 1 atm. The flame is simulated with the Sandia DNS code S3D (Chen *et al.*, 2009) employing a 13-species chemistry model (Sankaran *et al.*, 2007) and mixture-averaged molecular transport models. Further details of the numerical methods are given by Richardson *et al.* (2010). Data presented correspond to a statistically-converged steady state.

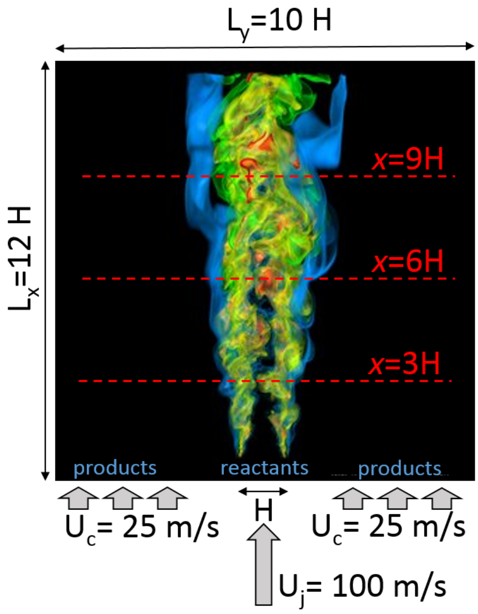


Figure 3: Illustration of the Bunsen flame configuration, including a volume rendering of the instantaneous heat release rate.

AGE-BASED MODELLING

The fluid age is defined as a spatially and temporally-varying continuum property of the fluid, equal to the mass-weighted average time that the atoms at each point have spent within a specified domain (Shin *et al.*, 2017). The fluid age a is governed by

$$\frac{\partial a}{\partial t} + \mathbf{u} \cdot \nabla a = \frac{1}{\rho} \nabla \cdot (\rho \mathscr{D} \nabla a) + 1 \tag{2}$$

assuming Fickian molecular transport with equal diffusivity $\mathscr{D}$ for all species (Ghirelli & Leckner, 2004). $\mathbf{u}$ is the velocity vector and ρ is the fluid density. The source term on the right hand side of Eq. 2 is equal to unity, representing the increase of age due to the passage of time.

In order to assess the fluid age-based modelling in the present DNS, which has two inlet streams (i.e. the jet and the coflow), the modelling is formulated in terms of the jet fluid age a_j. The jet fluid age is obtained from solution of transport equations in the DNS for the jet fluid mixture fraction ξ_j and the mass-weighted jet fluid age ϕ_j:

$$\frac{\partial \phi_j}{\partial t} + \mathbf{u} \cdot \nabla \phi_j = \frac{1}{\rho} \nabla \cdot \left(\rho \mathscr{D} \nabla \phi_j\right) + \xi_j \tag{3}$$

$$\frac{\partial \xi_j}{\partial t} + \mathbf{u} \cdot \nabla \xi_j = \frac{1}{\rho} \nabla \cdot \left(\rho \mathscr{D} \nabla \xi_j\right). \tag{4}$$

The jet fluid age is then recovered as $a_j = \phi_j/\xi_j$. In the simulations the mixture fraction and age are assigned the diffusivity of nitrogen since this makes up the majority of the mass in the fluid.

The fluid age is an attractive reference variable for modelling chemically-reactive systems since, in contrast with a reaction progress variable, its source term is uniform in space, meaning that the fluid age mixes like other conserved scalars for which algebraic and transport equation models for statistical moments and probability density function (pdf) shapes are well established (Shin *et al.*, 2017, 2019).

It is emphasised that the datum point for age is arbitrary and there is no unique *global* mapping between age and reaction progress in a propagating premixed flame. Instead, the present age-based modelling assumes a *local* statistical dependence between age and progress variable. The age-based closure for unconditional Favre-averaged reaction rate is given by

$$\widetilde{\dot{\omega}}_{c\mathscr{F}} = \int_{-\infty}^{\infty} \mathscr{F}_{\dot{\omega}}(a_{\mathscr{F}}) \tilde{p}_{a_{\mathscr{F}}}(a_{\mathscr{F}};\mathbf{x},t) da_{\mathscr{F}}, \tag{5}$$

which requires modelling for the functional dependence $\mathscr{F}_{\dot{\omega}}(a_{\mathscr{F}})$ of reaction rate on a local age parameter $a_{\mathscr{F}}$ and for its pdf $\tilde{p}_{a_{\mathscr{F}}}$. $a_{\mathscr{F}}$ is a fluid age parameter in the flamelet manifold rather than in the turbulent flow. In general the flamelet age $a_{\mathscr{F}}$ is not equal to the value of fluid age a in the actual turbulent flow, but it is assumed that the there is a linear mapping between the pdfs of the two variables at each point $(\mathbf{x},t)$ in the flow.

In this study, the flamelet manifold is given by a one-dimensional freely-propagating laminar flame calculation for the same reactant conditions as the DNS, including a transport equation for the fluid age. Setting flamelet age equal to zero at the inlet to the simulation domain, the flamelet age increases monotonically in the downstream direction through the flame. The flamelet solution can be recorded alternatively as a function of the spatial coordinate x, the mixture fraction c, or the flamelet age $a_{\mathscr{F}}$. The freely-propagating flame is solved numerically in physical space using S3D, however an equivalent solution can be obtained by transforming the governing equations into progress variable space (Lodier *et al.*, 2011; Richardson & Soriano, 2019).

The motivation for expressing the closure in terms of age (Eq. 5) rather than progress variable (Eq. 1) is that age is a passive scalar and may admit simpler presumed-pdf modelling. Three approaches for modelling $\tilde{p}_{a_{\mathscr{F}}}$ are considered: top-hat, Gaussian or scaled β-function distributions. The shape of the scaled β-function is modelled using jet fluid mixture fraction moments following Shin *et al.* (2019). Shin *et al.* showed that one-point statistics of jet fluid mixture fraction and age display strong negative correlation in a turbulent slot jet suggesting the following relationship between the mixture fraction and age pdfs,

$$\tilde{p}_{a_j}(a_j) = \tilde{p}_{\xi_j}\left(\tilde{\xi}_j + \frac{\xi_j''}{a_j''}(a_j - \tilde{a}_j)\right) \qquad (6)$$

where a_j'' and ξ_j'' are Favre root mean square values. The validity of this model for the Bunsen DNS case is investigated below. Given the assumption that the jet fluid age and flamelet age are linearly related, and modelling $\tilde{p}_\xi$ as a β-distribution, the scaled β-distribution for $a_\mathscr{F}$ is given by

$$\tilde{p}_{a_\mathscr{F}}(a_\mathscr{F}) = \beta\left(\tilde{\xi}_j + \frac{\xi_j''}{a_\mathscr{F}''}(a_\mathscr{F} - \tilde{a}_\mathscr{F}); \tilde{\xi}_j, \widetilde{\xi''^2}\right). \qquad (7)$$

Given that flamelet age moments $\widetilde{a_\mathscr{F}}$ and $\widetilde{a''^2_\mathscr{F}}$ are not available directly from the turbulent flow, the flamelet age moments required for each of the three presumed-pdf models for $a_\mathscr{F}$ are determined numerically in order to match the Favre-mean $\widetilde{c}_\mathscr{F}$ and Favre-variance $\widetilde{c''^2}_\mathscr{F}$ predicted using the flamelet manifold with the progress variable statistics $\tilde{c}$ and $\widetilde{c''^2}$ in the turbulent flow, with

$$\widetilde{c}_\mathscr{F} \equiv \int_{-\infty}^{\infty} \mathscr{F}_c(a_\mathscr{F})\tilde{p}_{a_\mathscr{F}}(a_\mathscr{F};\mathbf{x},t)da_\mathscr{F}; \qquad (8)$$

$$\widetilde{c''^2}_\mathscr{F} \equiv \int_{-\infty}^{\infty} (\mathscr{F}_c(a_\mathscr{F}))^2\,\tilde{p}_{a_\mathscr{F}}(a_\mathscr{F};\mathbf{x},t)da_\mathscr{F} - (\widetilde{c}_\mathscr{F})^2. \qquad (9)$$

The progress variable and mixture fraction statistics in the turbulent flow are evaluated in this study using the DNS data. In predictive LES or RANS they can be obtained from modelled transport equations or other sub-filter LES closures. Once the flamelet age pdf is determined, the mapping $\mathscr{F}_c(a_\mathscr{F})$ can be used to evaluate the corresponding progress variable pdf:

$$\tilde{p}_c = \tilde{p}_{a_\mathscr{F}}\left(\frac{\partial \mathscr{F}_c}{\partial a_\mathscr{F}}\right)^{-1} \qquad (10)$$

The process of determining the progress variable pdf from $\mathscr{F}_c(a_\mathscr{F})$ is illustrated in Fig. 4, taking the example of a Gaussian presumed-pdf for $\tilde{p}_{a_\mathscr{F}}$.

RESULTS
Presumed-pdf modelling for the jet fluid age

Eq. 6 provides a model for the relationship between the mixture fraction and age pdfs in a turbulent jet. Two instances of these pdfs from the DNS are presented in Fig. 5 in standardised form, where the standardised mixture fraction is $\hat{\xi}_j = (\xi - \tilde{\xi})/\xi''$ and and standardised jet fluid age is $\hat{a}_j = (a_j - \tilde{a}_j)/a_j''$. Eq. 6 implies that $\tilde{p}(-\hat{a}_j) = \tilde{p}(\hat{\xi}_j)$. The plot also shows the standard Gaussian distribution and a standardised-β distribution (based on the unstandardised mixture fraction moments). Close to the jet centre-plane, where the skewness of the mixture fraction distribution is low, the standardised pdfs of mixture fraction, age and the scaled β-function all lie close to the standard Gaussian distribution. At the periphery of the jet (e.g. at the $x = 6H, y = 1.5H$ location shown) the mixture fraction distribution is highly skewed. This skewed shape is described accurately by the β-function distribution. However the shape of the age distribution remains close to Gaussian, suggesting that a simple Gaussian model for the age-pdf is appropriate for the present case.

The observation that the jet fluid age distribution is Gaussian is at odds with the results of Shin *et al.* (2019). Possible reasons for the different character of the mixture fraction-age dependence in the near field of these two slot jet DNS studies include differences in Reynolds number

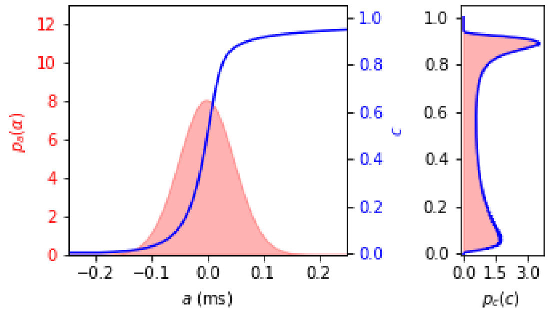
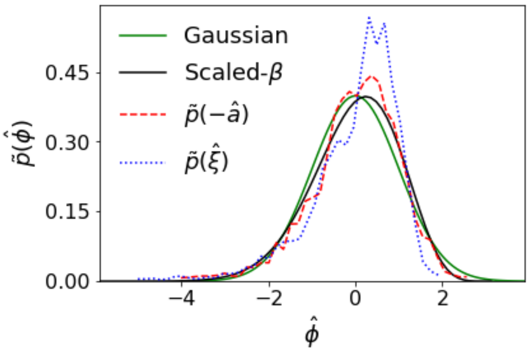
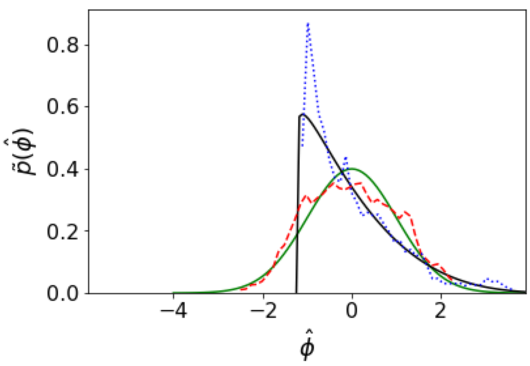


Figure 4: Age-space profile of progress variable $\mathscr{F}_c$ in a laminar flame (left), and the Gaussian model for the age-pdf (shaded) giving a corresponding progress variable pdf with $\tilde{c} = 0.5$ and $\widetilde{c''^2} = 0.1$ (right).



(a) y=0



(b) y=1.25H

Figure 5: Standardised distributions of jet fluid age and mixture fraction, the standardised Gaussian and the β-function pdf based on the mixture fraction mean and variance. Data for x=6H.

and the specification of turbulence at the inlet. Shin *et al.* (2019) simulated a flow with $\mathcal{O}300,000$ jet Reynolds number, which is two orders of magnitude greater than the present case, and with more realistic specification of shear-generated turbulence at the inlet. The higher-Reynolds number results of Shin *et al.* (2019) are likely more representative of practical combustion systems, for which Eq. 6 may still be valid. In the present low Reynolds number case with synthetic turbulence at inlet a Gaussian distribution for age is a simpler and better model and the scaled-beta distribution is not analysed further. A Top Hat profile for the age distribution is clearly unrealistic in all cases, however it is retained in the subsequent analysis in order to illustrate sensitivity of the progress variable modelling to the shape of the age distribution.

Age-based modelling for the progress variable distribution

The progress variable pdf is presented in Fig. 6 for six locations in the Bunsen flame, along with three models for the progress variable pdf: the β-pdf, based on the mean and variance of progress variable, and the age-based pdf assuming either a Top Hat or a Gaussian distribution for the flamelet age. The β-function distribution gives unrealistic predictions of the progress variable pdf shape, in agreement with previous analysis (Jin *et al.*, 2008). The age-based models give a substantial improvement in the pdf shape prediction, and this is attributed to basing the pdf-shape on the structure of the flamelet. The Top Hat age pdf gives discontinuities at the extrema of the presumed pdf. The Gaussian age-pdf leads to a desirable smoothing of those discontinuities. The flamelet manifold used in the present modelling is based on a freely-propagating one-dimensional flame. Given the high Karlovitz number of the turbulent flame, further refinement might be possible by basing the modelling on strained laminar flames or using the Linear Eddy Model approach given by Tsui *et al.* (2016).

Predictions of the Favre-average progress variable chemical source term at $x/H = 3,6$ and 9 are also presented in Fig. 6. Data for the 'Empirical-pdf' use the progress variable distribution in the DNS combined with the reaction source term function $\mathscr{F}_{\dot{\omega}}$ from the flamelet. The difference between the Empirical-pdf and the DNS results indicates the error in the chemistry model ($\mathscr{F}_{\dot{\omega}}(c)$) associated with the one-dimensional flamelet. It is observed that the difference between the DNS and Empirical-pdf results is substantially smaller than between the best and worst presumed-pdf models, emphasising that accurate modelling of the presumed pdf-shape is central to the overall accuracy of the flamelet approach. All of the presumed-pdf models are tested using the same flamelet chemistry model, so that perfect modelling of the pdf would recover the Empirical-pdf results.

The inaccuracy of the β-pdf shape results in very large errors in the predicted Favre-average reaction rates. The age-based pdf models provide a substantial improvement since they account for the effect of the flame's reaction-diffusion dynamics on the progress variable distribution. Results for the Gaussian age-based pdf are arguably an improvement over the Top Hat-based approach, although there are small regions where the Top Hat predictions are closer to the Empirical-pdf results. Again, considering the high Karlovitz number in the turbulent flame, further improvement in predictions might be possible by basing the age-based modelling on one-dimensional strained flames.

CONCLUSIONS

Age-based modelling for the progress variable pdf is formulated and assessed using DNS data for premixed turbulent combustion. The age-based approach reproduces the good performance of previous flamelet-based approaches for modelling the progress variable pdf: the predicted pdf shape is very close to the empirical pdf shape and, following integration with the laminar flame model for reaction rates, it provides a substantial improvement in reaction rate closure compared to the usual β-function pdf model. Basing the modelling on an age variable however offers a number of additional advantages compared to, for example, the filtered laminar flame approach. The age-based approach allows for more general modelling of the shape of the filter kernel used to generate the pdf from the flamelet manifold, and a scaled-β pdf approach is introduced in order to account for effects of turbulent shear on the age distribution. In the present low-Reynolds number flame however, a Gaussian model gives better predictions for the age distribution. Overall, it is demonstrated that the age-based approach provides accurate modelling for the progress variable pdf and provides a valid basis for further development of more general age-based modelling for partially-premixed turbulent combustion.

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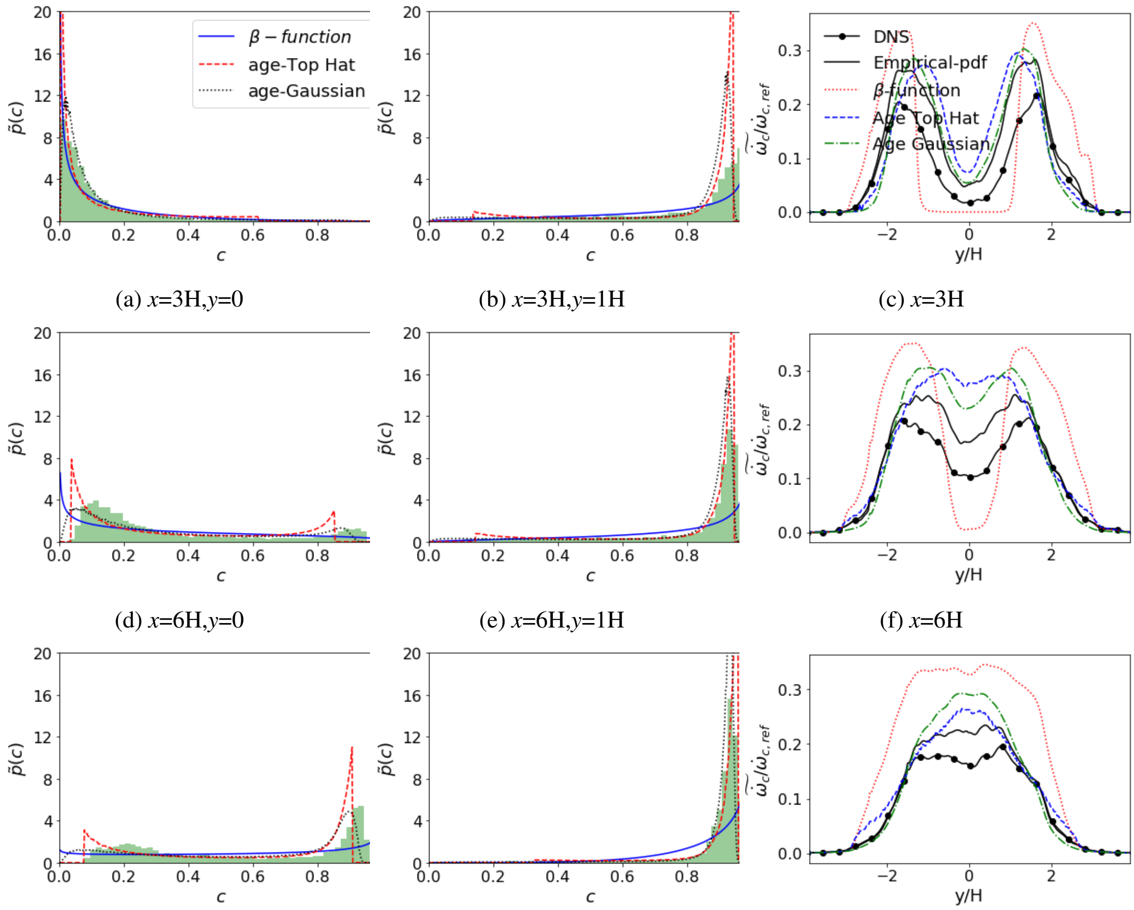

(a) x=3H,y=0 (b) x=3H,y=1H (c) x=3H

(d) x=6H,y=0 (e) x=6H,y=1H (f) x=6H

(g) x=9H,y=0 (h) x=9H,y=1H (i) x=9H

Figure 6: Standardised distributions of jet fluid age and mixture fraction, the standardised Gaussian and the β-function pdf based on the mixture fraction mean and variance. Data for x=3H.

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