A MODIFIED PRESUMED PDF APPROACH TO MODELING PREMIXED TURBULENT FLAMES

A.N. Lipatnikov*, S. Nishiki, and T. Hasegawa*****
e-mail: lipatn@chalmers.se
*Department of Applied Mechanics, Chalmers University of Technology, 412 96, Gothenburg, Sweden
** Department of Mechanical Engineering, Kagoshima University, Kagoshima 890-0065, Japan
*** EcoTopia Science Institute, Nagoya University, Nagoya 464-8603, Japan

Abstract
Over past years, the use of a presumed Probability Density Function (PDF) $P(c)$ for combustion progress variable c has been becoming more and more popular approach to averaging reaction rates in premixed and partially premixed turbulent flames. In the present work, the ability of various presumed PDFs to predict the mean mass rate of product creation is quantitatively tested against data from 3D Direct Numerical Simulations (DNS) of premixed turbulent combustion in the flamelet regime. Commonly used presumed PDFs are shown to fail in predicting the mean rate, with the so-averaged rates being strongly sensitive to the shape of a presumed PDF. These limitations of the approach are attributed to a low probability of finding thin reaction zones in a typical premixed turbulent flame. In order for a presumed PDF to be able to predict this low probability and the mean rates of formation of various species in a turbulent flame, a modified approach is proposed to be used. The modification consists of determining a presumed $P(c)$ based on the mean reaction rate, rather than the second Favre moment (variance) of the c-field. Although the modified approach is not self-sufficient and requires a model for evaluating a single mean rate, such a complication could be justified by better predictive capabilities of the modified approach, indicated by the DNS data.

Introduction

When simulating combustion of a turbulent gas mixture, characterized by large magnitude of temperature fluctuations, the key challenge consists of averaging [or filtering if Large Eddy Simulation (LES) is concerned] reaction rates that depend strongly non-linearly on the temperature. The vast majority of models that address this challenge (i) characterize the state of reacting gas with a single scalar c called combustion progress variable ($c = 0$ and 1 in unburned mixture and combustion products, respectively) and (ii) aim at closing a single mean mass rate of product creation $\overline{W}_c$ in the following balance equation

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{c}\right) + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{c}\right) = -\frac{\partial}{\partial x_j}\overline{\rho u_j'' c''} + \overline{W}_c. \quad (1)$$

Here, t is the time, x_j and u_j are spatial coordinates and components of the flow velocity vector, respectively, ρ is the gas density, $\tilde{q} = \overline{\rho q}/\bar{\rho}$ and $q'' = q - \tilde{q}$ designate Favre-averaged and fluctuating quantities, respectively, with the Reynolds averages being denoted by overbars, e.g. $\bar{\rho}$, and summation convention applies to the repeated index j.

Moreover, such models commonly invoke the BML paradigm of thin flamelets [1], developed in seminal papers by Bray, Moss, and Libby [2-4]. Within the framework of this paradigm, (i) fresh reactants and equilibrium combustion products are assumed to be separated by thin, inherently laminar, self-propagating layers (often called flamelets)

that are wrinkled and stretched by turbulent eddies and (ii) the probability γ of finding intermediate (between unburned and burned) states of the mixture is assumed to be much less than unity. Accordingly, the probability of finding combustion products is approximately equal to the Reynolds-averaged combustion progress variable $\bar{c}$ and the Reynolds-averaged density $\bar{\rho}$ is evaluated as follows [4]

$$\bar{\rho} = \rho_u(1 - \bar{c}) + \rho_b\bar{c}, \tag{2}$$

$$\rho_b\bar{c} = \bar{\rho}\tilde{c}, \tag{3}$$

where subscripts u and b designate unburned and burned mixture, respectively.

While significant progress both in RANS and LES research into premixed turbulent combustion was already made by invoking the above paradigm, as reviewed elsewhere [1, 5, 6], certain important problems have not yet been resolved. For instance, in order to simulate emissions from an internal combustion engine, not only the rate W_c, but also rates of pollutant formation should be averaged invoking a chemical mechanism of burning. Moreover, in sufficiently intense turbulence, the paradigm of thin flamelets does not work properly [1, 5, 6] and, in particular, Eq. (3) is oversimplified.[1]

Among methods developed to address the above challenges, the presumed Probability Density Function (PDF) approach has been becoming a popular tool over past years. The approach consists of specifying a shape of a Favre PDF $\tilde{P}(c) = \rho(c)P(c)/\bar{\rho}$ for the combustion progress variable. Such a presumed PDF commonly invokes a few unknown parameters, which can be determined using the first $\tilde{c}$, second $\overline{\rho c''^2}/\bar{\rho}$, and eventually higher moments $\overline{\rho c''^n}/\bar{\rho}$, which are evaluated by solving proper balance equations closed by using the above $\tilde{P}(c)$. Such an approach is widely used for averaging reaction rates in premixed [7-13] and partially premixed [14-21] turbulent flames.

The goals of this work are to quantitatively test the presumed PDF approach using data obtained in Direct Numerical Simulations (DNS) [22, 23] and to propose a modification of the approach aimed at resolving certain inherent issues discussed in the following.

It is worth stressing that the well-known BML PDF, i.e. the sum of two Dirac delta functions associated with $c = 0$ and 1 [2-4], does not allow us to average $W_c(c)$, because $W_c(c = 0) = W_c(c = 1) = 0$. Accordingly, the following discussion is solely restricted to PDFs presumed in the range of $0 < c < 1$, while PDFs that do not address the intermediate range of $0 < c < 1$ are beyond the scope of the present paper.

DNS Data

Because the DNS were discussed in details elsewhere [22, 23], we restrict ourselves to a brief summary of them. The computational domain was a rectangular 8x4x4 mm and was resolved using a uniform rectangular mesh of 512x128x128 points. Three statistically planar 1D premixed flames characterized by three different density ratios ρ_u/ρ_b (see Table 1) were simulated by solving unsteady 3D continuity, Navier-Stokes, and energy equations, as well as a balance equation for the mass fraction of the deficient reactant and the ideal gas state equation. Combustion chemistry was reduced to a single global irreversible Arrhenius reaction of the first order, the Lewis number was equal to unity, and the dependence of the molecular transfer coefficients on the temperature was taken into account. The specific heat capacities were constant. The bulk viscosity, the pressure gradient diffusion,

[1]The latter remark does not concern Eq. (2). Indeed, if (i) the combustion progress variable is associated with the normalized temperature $(T - T_u)/(T_b - T_u)$ and (ii) ρT =const, then, Eq. (2) results straightforwardly from applying the definition of a Favre-averaged quantity $\tilde{q} = \overline{\rho q}/\bar{\rho}$ to $q = 1/\rho$.

Table 1: Flame characteristics

	Case H	Case M	Case L
ρ_u/ρ_b	7.53	5.0	2.5
S_L, m/s	0.600	0.523	0.416
δ_L, mm	0.217	0.191	0.158
S_t, m/s	1.146	0.9925	0.7862

the Soret and the Dufour effects were neglected. The characteristics of the counterpart laminar flames are reported in Table 1, where S_L and $\delta_L = (T_b - T_u)/\max|dT/dx|$ are the laminar flame speed and thickness, respectively.

Homogeneous isotropic turbulence (the rms velocity $u' = 0.526$ m/s, integral length scale $L = 3.45$ mm, Taylor microscale $\lambda = 2.05$ mm, Kolmogorov scale $\eta = 0.141$ mm, and Reynolds number $Re_t = u'L/\nu_u = 95.5$, where $\nu_u = 0.19$ cm^2/s is the kinematic viscosity of the unburned gas) was generated at the inlet boundary, entered the computational domain with a mean velocity U, and decayed along the direction x of the mean flow.

At an initial instant $t = 0$, a planar laminar flame was embedded into statistically the same turbulence assigned for the velocity field in the entire computational domain. Subsequently, the inflow velocity was increased twice, i.e. $U(t = 0) = S_L < U(t = t_1) < U(t = t_2) = S_t$, in order to keep the developing flame in the computational domain. At $t > t_2$, further increase in the inlet velocity was not required and the flame did not cross the inlet and outlet x-borders of the computational domain. The obtained turbulent flame speeds S_t are reported in Table 1.

Results discussed in the next section were obtained for $t > t_2$, with the instants t_2 being different in the three simulated cases. Averaging was performed both across the transverse yz-plane and over time interval $t_2 < t < t_3$, where t_3 corresponded to the end of the simulations, with the difference in t_2 and t_3 being of the order of $1.5L/u'$. The combustion progress variable was equal to the normalized temperature $(T-T_u)/(T_b-T_u)$. In the following, quantities [$\bar{\rho}$, $\tilde{c}$, $\overline{\rho c''^2}/\bar{\rho}$, $\overline{W}_c$, and $\tilde{P}(c)$, etc.] that are obtained by straightforwardly processing the DNS database will be called "true", contrary to "model" quantities evaluated invoking a presumed PDF.

As discussed elsewhere [22, 23], the three flames addressed in the DNS are characterized by a low probability γ and are associated with the flamelet regime [1-6] of premixed turbulent combustion.

Presumed PDFs to Be Tested

In the present work, the mean density

$$\bar{\rho} = \frac{\int_0^1 P(\xi)d\xi}{\int_0^1 \tilde{P}(\xi)/\rho(\xi)d\xi} = \frac{1}{\int_0^1 \tilde{P}(\xi)/\rho(\xi)d\xi} \tag{4}$$

and the mean rate of product creation

$$\overline{W}_c = \int_0^1 W_c(\xi)P(\xi)d\xi = \bar{\rho}\int_0^1 \frac{W_c(\xi)\tilde{P}(\xi)}{\rho(\xi)}d\xi \tag{5}$$

were evaluated invoking three presumed PDFs $\tilde{P}(c)$, i.e. (i) a beta-function (BF) PDF

$$\tilde{P}(c) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}c^{a-1}(1-c)^{b-1} \tag{6}$$

used in Refs. [7-11,13-15,21], (ii) a laminar flamelet[2] (LF) PDF

$$\tilde{P}(c) = A\delta(c) + Bf(c) + C\delta(1-c) \tag{7}$$

addressed in Refs. [9, 10, 12, 13] and (iii) a Dirac-delta-function (DDF) PDF

$$\tilde{P}(c) = \alpha\delta(c_1 - c) + (1-\alpha)\delta(c_2 - c) \tag{8}$$

to which joint PDFs $\tilde{P}(c, f)$ invoked to simulate partially premixed turbulent combustion in Refs. [16-20] are reduced if the mixture fraction f is constant.

In Eq. (6), a ratio of gamma functions $\Gamma(z) \equiv \int_0^\infty \eta^{z-1}\mathrm{e}^{-\eta}d\eta$ is used in order to satisfy the normalizing constraint of

$$\int_0^1 \tilde{P}(\xi)d\xi = 1. \tag{9}$$

Accordingly, the BF PDF involves two parameters a and b, which can be determined using the following constraints

$$\tilde{c} = \int_0^1 \xi\tilde{P}(\xi)d\xi, \tag{10}$$

$$\frac{\overline{\rho c^2}}{\bar{\rho}} = \tilde{c}^2 + \frac{\overline{\rho c''^2}}{\bar{\rho}} = \int_0^1 \xi^2\tilde{P}(\xi)d\xi \tag{11}$$

if the first and second Favre moments of the c-field are known. As shown elsewhere [7],

$$a = \tilde{c}(g^{-1} - 1), \qquad b = (1-\tilde{c})(g^{-1} - 1), \tag{12}$$

where

$$g \equiv \frac{\overline{\rho c''^2}}{\bar{\rho}\tilde{c}(1-\tilde{c})} \tag{13}$$

is a segregation factor.

In Eq. (7), $\delta(c)$ is Dirac delta function, $f(c)$ is equal to $1/\nabla c$ computed for the counterpart laminar flame, and the parameters A, B, and C are evaluated using Eqs. (9)-(11). As shown elsewhere [10],

$$B = \frac{\tilde{c} - \overline{\rho c^2}/\bar{\rho}}{I_1 - I_2}, \quad C = \frac{I_1\overline{\rho c^2}/\bar{\rho} - I_2\tilde{c}}{I_1 - I_2}, \quad A = 1 - I_0 B - C, \tag{14}$$

where the integrals

$$I_k = \int_0^1 \frac{\xi^k}{\nabla\xi}d\xi \tag{15}$$

are computed using the dependence of ∇c on c obtained from the laminar flame.

The DDF PDF satisfies the normalizing constraint given by Eq. (9) and involves three unknown parameters, α, c_1, and c_2, with $0 \le c_1 \le c_2 \le 1$. Therefore, two Eqs. (10) and (11) are not sufficient in order to evaluate the three parameters and one more constraint should be used, e.g.

$$\frac{\overline{\rho c^3}}{\bar{\rho}} = \tilde{c}^3 + 3\tilde{c}\frac{\overline{\rho c''^2}}{\bar{\rho}} + \frac{\overline{\rho c''^3}}{\bar{\rho}} = \int_0^1 \xi^3\tilde{P}(\xi)d\xi. \tag{16}$$

[2]Jin et al. [10] introduced also modified flamelet PDFs, but they did not improve results as compared with Eq. (7) under conditions of the present DNS.

Substitution of Eq. (8) into Eqs. (10), (11), and (16) yields

$$\tilde{c} = \alpha c_1 + (1-\alpha) c_2, \tag{17}$$

$$\tilde{c}^2 + \frac{\overline{\rho c''^2}}{\bar{\rho}} = \frac{\overline{\rho c^2}}{\bar{\rho}} = \alpha c_1^2 + (1-\alpha) c_2^2, \tag{18}$$

and

$$\tilde{c}^3 + 3\tilde{c}\frac{\overline{\rho c''^2}}{\bar{\rho}} + \frac{\overline{\rho c''^3}}{\bar{\rho}} = \frac{\overline{\rho c^3}}{\bar{\rho}} = \alpha c_1^3 + (1-\alpha) c_2^3. \tag{19}$$

The use of the DDF PDF substantially simplifies Eqs. (4) and (5), which read

$$\bar{\rho} = \alpha \rho(c_1) + (1-\alpha)\rho(c_2), \tag{20}$$

and

$$\overline{W}_c = \alpha W_c(c_1) + (1-\alpha) W_c(c_2), \tag{21}$$

respectively.

In the present work, the first $\tilde{c}$ and second $\overline{\rho c''^2}/\bar{\rho}$ Favre moments required to determine the parameters of the three aforementioned PDFs were evaluated by processing the DNS data. In order to get a better insight into the sensitivity of $\bar{\rho}$ and $\overline{W}_c$ to the shape of a presumed $\tilde{P}(c)$, we did not use the DNS data in order to compute the third moment in Eq. (19), but calculated this moment invoking the BF PDF. Thus, the two (BF and DDF) presumed PDFs were characterized by the same first, the same second, and the same third moments, with the first and second moments being taken from the DNS data.

Moreover, a simpler model proposed by Ribert et al. [16] was also invoked to determine the three parameters of the DDF presumed PDF, i.e.

$$c_1 = \tilde{c}(1 - g^{1/2}), \quad c_2 = \tilde{c} + (1-\tilde{c}) g^{1/2}, \quad \alpha = 1 - \tilde{c}. \tag{22}$$

In the following, the presumed PDF given by Eqs. (8) and (22) will be called the R-DDF PDF, by referring to the paper by Ribert et al. [16].

Results and Discussion

Figure 1 shows that, in all three cases H, M, and L, the mean densities (see left column) calculated invoking any of the considered presumed PDFs agree very well with the mean densities obtained straightforwardly from the DNS data (cf. broken curves 2-5 with solid curves 1) and with $\bar{\rho}$ yielded by the BML model (symbols). Thus, the presumed PDF approach allows us to average such a weakly non-linear dependence as $\rho = \rho_u/(1+\tau c)$. Here, $\tau = \rho_u/\rho_b - 1$ is the heat-release factor.

However, in the studied cases, the presumed PDFs yield substantially overestimated mean rate $\overline{W}_c$, cf. broken curves 2-5 with solid curves 1 in right column, with the DDF PDF performing worst (see curves 3 and 4, which are very close to one another). Moreover, comparison of curves 2 and 3 indicates that $\overline{W}_c$ is very sensitive to the shape of $\tilde{P}(c)$ even if not only the first and the second but also the third moments are the same for the BF and DDF PDFs.[3] Therefore, the presumed PDF approach fails in averaging such a strongly non-linear function as $W_c(c)$.

[3] A similar conclusion was recently drawn by Huang and Lipatnikov [24] using another method of research.

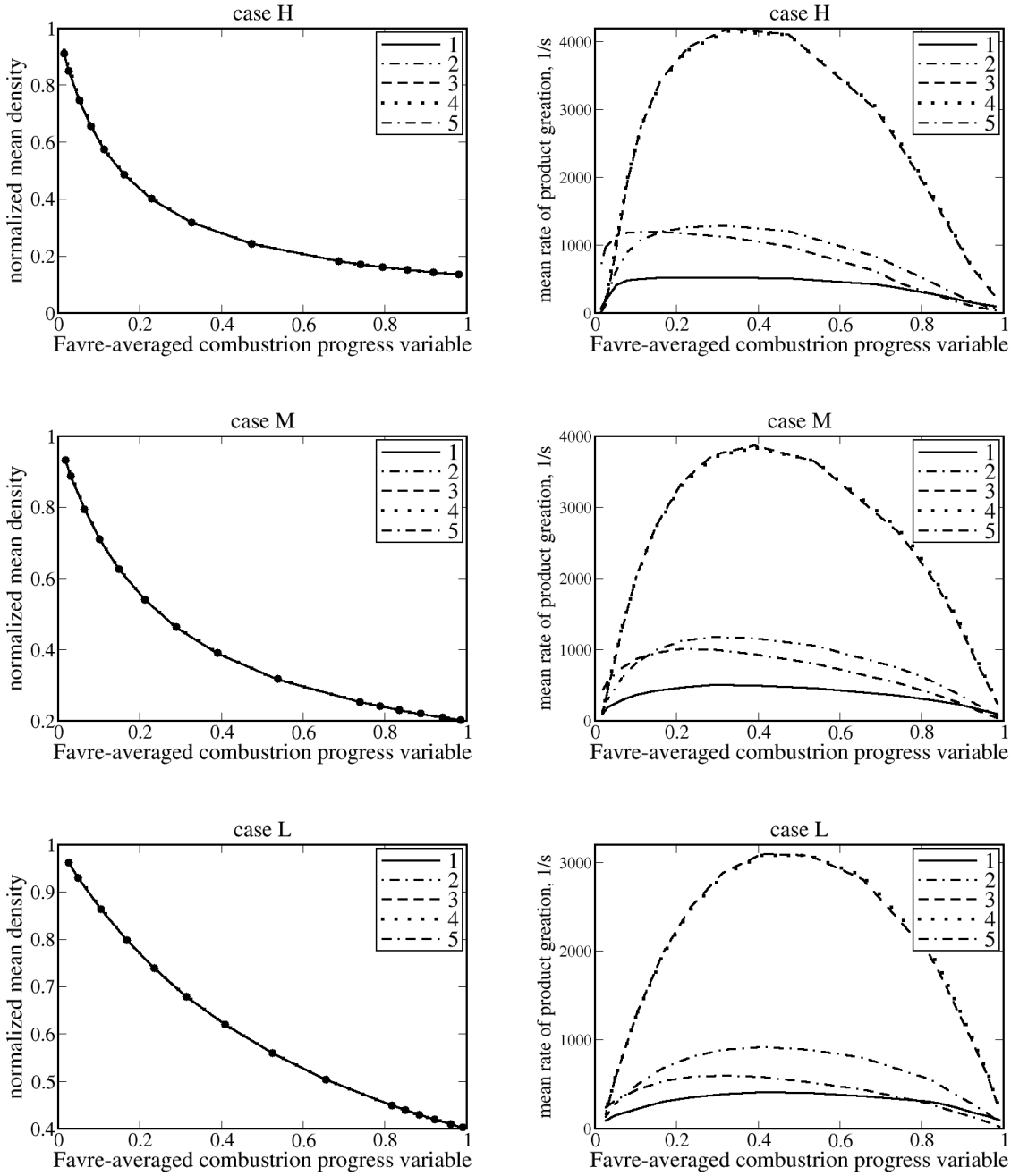

Figure 1: Normalized mean density $\bar{\rho}/\rho_u$ (left column) and mass rate $\overline{W}_c/\rho_u$ of product creation (right column) computed using different mass-weighted PDFs $\widetilde{P}(c)$ in cases H (top row), M (middle row), and L (down row). 1 - DNS data; 2 - BF PDF given by Eqs. (6) and (12); 3 - DDF PDF given by Eqs. (8), (17)-(19); 4 - R-DDF PDF given by Eqs. (8) and (22); 5 - LF PDF given by Eqs. (7) and (14). Circles show the normalized mean density $(1+\tau\tilde{c})^{-1}$ evaluated using the BML approach [2].

To better understand limitations of the presumed PDF approach, let us first consider the asymptotic case of infinitely thin flamelets, i.e. the segregation factor $g \to 1$. In this case, the first and second Favre moments are directly related with one another, i.e., $\overline{\rho c''^2} \to \bar{\rho}\tilde{c}(1-\tilde{c})$. Consequently, two Eqs. (10) and (11) are not independent, the number of independent equations is less than the number of unknown parameters, and a typical

presumed PDF approach is flawed in this asymptotic case.

In many premixed turbulent flames and, in particular, in three flames H, M, and L, addressed by the present DNS, flamelet thickness is finite, but small as compared to the mean flame brush thickness. Accordingly, the probability of finding intermediate states of the burning mixture is also finite, but low, i.e. $0 < \gamma \ll 1$. In this case, (i) the segregation factor is less than, but close to unity, i.e. $0 < 1 - g \ll 1$, and (ii) Eqs. (10) and (11) are two independent equations. However, a typical presumed PDF approach appears to be flawed in this case also.

Indeed, if W_c is notable in a finite range $c_{w,1} < c < c_{w,2}$ and the probability γ_w of finding such values of c is much less than unity, then, the influence of eventual variations in γ_w on $\tilde{c}$ and $\overline{\rho c''^2}/\bar{\rho}$ is negligible. Therefore, significantly different probabilities γ_w could be calculated either (i) by slightly varying $\tilde{c}$ and/or $\overline{\rho c''^2}/\bar{\rho}$ and retaining the shape of the presumed PDF or (ii) by slightly changing the shape of $\tilde{P}(c)$ and keeping both $\tilde{c}$ and $\overline{\rho c''^2}/\bar{\rho}$ constant. As a result, significantly different $\overline{W}_c$ can be computed invoking different presumed PDFs, cf. curves 2 and 3 in the right column in Fig. 1 or see Ref. [24]. Moreover, all so-averaged rates (curves 2-5) differ significantly from the true $\overline{W}_c$ (curves 1), because the presumed and the true PDFs characterized by the same $\tilde{c}$ and by the same $\overline{\rho c''^2}/\bar{\rho}$ yield significantly different probabilities γ_w. Due to $\gamma_w \ll 1$, this probability is very sensitive to variations in the PDF shape, with all other things being equal. Even the LF PDF (curves 5) aimed at modeling the flamelet regime of premixed turbulent combustion significantly overpredicts the true $\overline{W}_c$ (curves 1), because, due to flame-turbulence interaction, the true $f(c)$ in Eq. (7) differs substantially from $f(c) = 1/\nabla c$ obtained from the counterpart unperturbed 1D laminar flame.

Furthermore, in practical applications, the problem is even more severe, because the true values of $\tilde{c}$ and $\overline{\rho c''^2}/\bar{\rho}$ are not known, contrary to the above test, for which the true values are provided by the DNS data. In RANS or LES studies, these two moments are commonly computed by solving proper balance equations which involve unclosed terms such as turbulent scalar fluxes or scalar dissipation rate. Accordingly, even a small error in computing $\tilde{c}$ and $\overline{\rho c''^2}/\bar{\rho}$ (e.g. due to limitations of invoked closure relations) can result in substantial errors in calculating the low probability γ_w and, hence, in evaluating $\overline{W}_c$. For instance, parameters a and b in Eq. (12) are very sensitive to variations in g if $0 < 1 - g \ll 1$. Small parameters (like γ_w or a and b) cannot be determined accurately by subtracting one finite quantity from another finite quantity if the two quantities are calculated even with small errors, which are inevitable, not only for numerical reasons, but also and mainly due to limitations of physical models invoked to close the relevant balance equations.

The sensitivity stressed above is also shown in Fig. 2, which indicates that 15%-errors in evaluation of $\tilde{c}$ (see curve 1 in Fig. 2a or circles and triangles in Fig. 2b) or $\overline{\rho c''^2}/\bar{\rho}$ (see curve 2 in Fig. 2a or squares and diamonds in Fig. 2b) can change the probability B in Eq. (7) and the mean rate $\overline{W}_c$ by a factor of two, e.g. see solid curve 1 for error-factor $q = 0.85$ (i.e. $\tilde{c}$ is underestimated by 15%) in Fig. 2a or cf. dashed curve 3 and filled diamond at $\tilde{c} \approx 0.3$ in Fig. 2b. This limitation of the approach offers wide opportunities for tuning and can hide its poor predictive capabilities. For instance, filled square at $\tilde{c} \approx 0.3$ in Fig. 2b indicates that 15%-understimation of the true $\overline{\rho c''^2}/\bar{\rho}$ allow the BF PDF to yield the correct $\overline{W}_c$, whereas the same BF PDF based on the true second moment (dotted-dashed curve 2) overestimates the true mean rate (curve 1) by a factor of 2.5.

The above physical reasoning and straightforward test of the presumed PDF approach against DNS data indicate that the approach cannot be considered to be a predictive tool

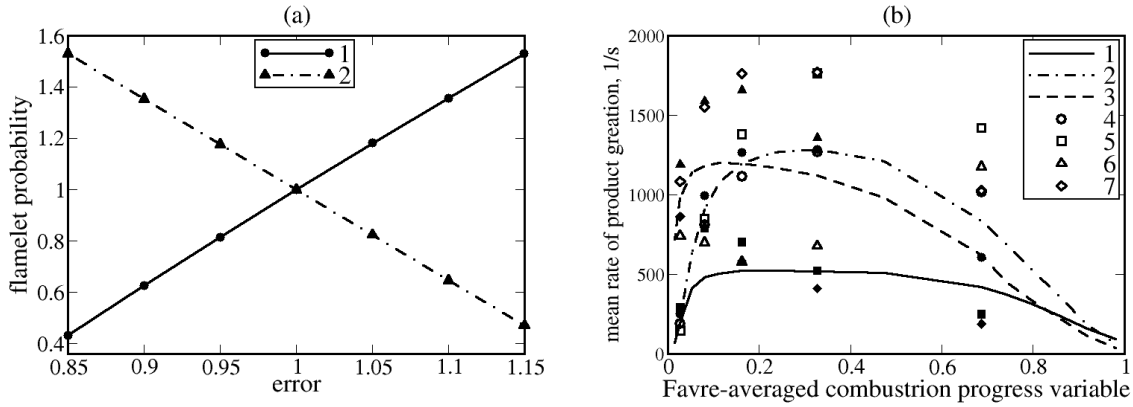

Figure 2: Sensitivity of the presumed PDF approach to variations in $\tilde{c}$ and $\overline{\rho c''^2}/\bar{\rho}$ in case H. (a) Probability B of finding flamelets on the surface $\bar{c} = 0.5$, calculated invoking the LF PDF given by Eqs. (7) and (14). Curves 1 and 2 show the normalized probability obtained by multiplying $\tilde{c}$ and $\overline{\rho c''^2}/\bar{\rho}$, respectively, with an error-factor q. The probability $B(q = 1)$ evaluated based on the true moments obtained from the DNS data is used to normalize $B(q)$. (b) Normalized mean mass rate $\overline{W}_c/\rho_u$ of product creation computed using (1) DNS data, (2) BF PDF given by Eqs. (6) and (12), and (3) LF PDF given by Eqs. (7) and (14). Symbols have been obtained by multiplying either $\tilde{c}$ (circles and triangles) or $\overline{\rho c''^2}/\bar{\rho}$ (squares and diamonds) with an an error factor $q = 0.85$ (open symbols) or $q = 1.15$ (filled symbols). Circles and squares - BF PDF, triangles and diamonds - LF PDF.

at least for the flamelet regime of premixed combustion characterized by a low probability γ. To the contrary, the approach is often assumed to perform well in intense turbulence associated with a noticeable γ and a substantial difference between the segregation factor g and unity. However, it is worth stressing that the basic limitations of the approach, highlighted in the above discussion, are associated with a low probability γ_w of finding a noticeable rate W_c, rather than with a low probability γ of finding $\varepsilon < c < 1 - \varepsilon$. Recent experimental [25-29] and DNS [30-33] studies have shown that, even in very intense turbulence, reaction zones characterized by noticeable rates of key combustion reactions that control heat release are thin and inherently laminar. These results imply that $\gamma_w \ll 1$ even if γ is not small. Accordingly, the predictive capabilities of the presumed PDF approach can be put into question even in intense turbulence.

Finally, it is worth stressing an inconsistency between a common practice of utilizing the presumed PDF approach and its basic features. On the one hand, the approach is claimed to be of particular interest for averaging rates W_k of production (consumption) of various species Y_k if complex combustion chemistry should be addressed (e.g. in order to simulate emissions). However, the knowledge of $\tilde{P}(c)$ will allow us to evaluate the mean rates $\overline{W}_k = \int_0^1 W_k(c)\tilde{P}(c)dc$ only if the instantaneous rates W_k are solely controlled by the combustion progress variable. Accordingly, when applying the presumed PDF approach to modeling a premixed turbulent flame, dependencies $W_k(c)$ are commonly obtained based on numerical simulations of the counterpart laminar premixed flames. In other words, the flamelet paradigm is invoked in order to average W_k by considering these rates to be functions of a single scalar variable c. However, on the other hand, the presumed PDF approach is basically flawed in the flamelet regime of premixed turbulent combustion, as argued above. This basic inconsistency has to be borne in mind.

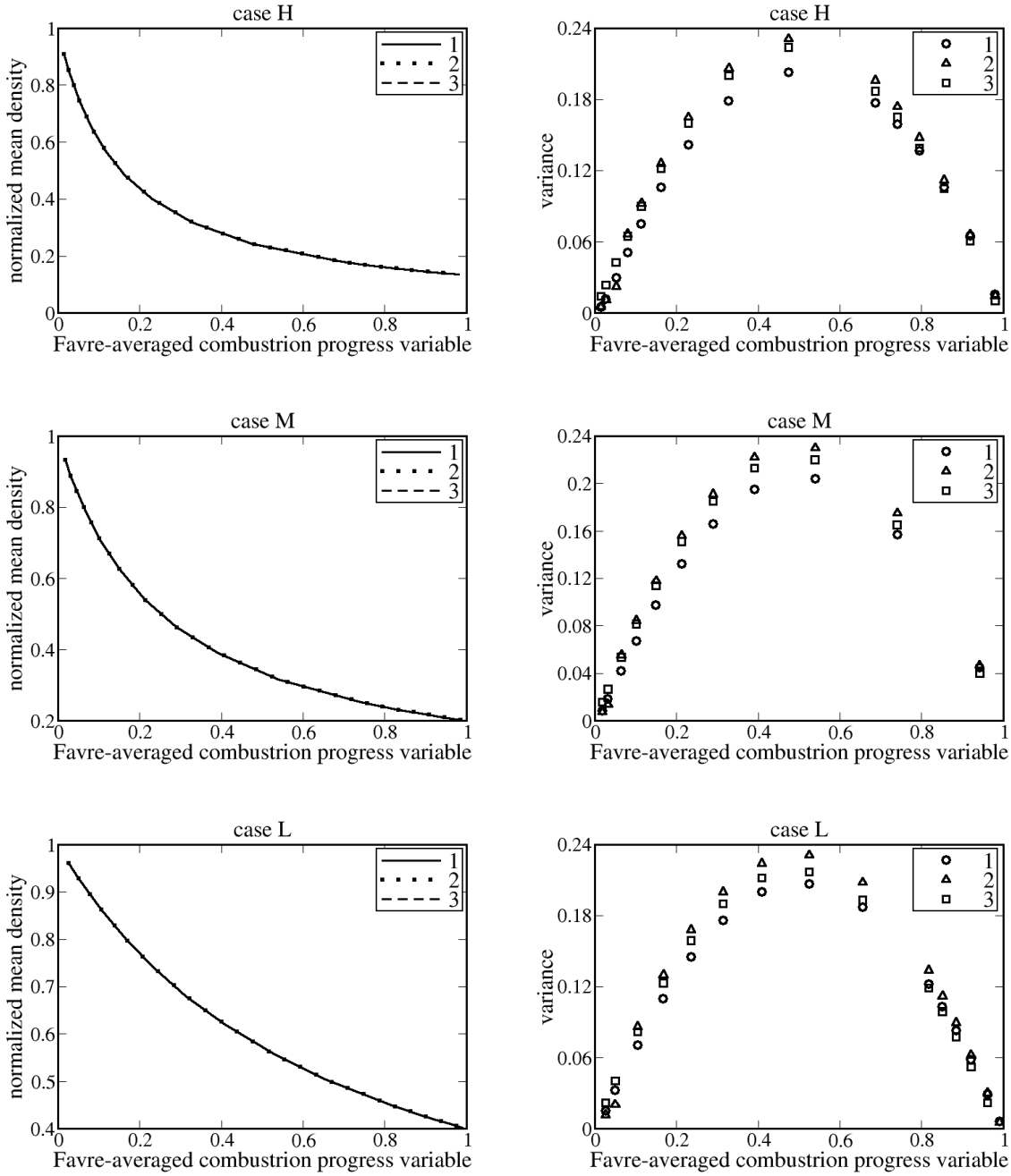

Figure 3: Normalized mean density $\bar{\rho}/\rho_u$ (left column) and the Favre variance $\overline{\rho c''^2}/\bar{\rho}$ (right column) computed using modified mass-weighted PDFs $\tilde{P}(c)$ in cases H (top row), M (middle row), and L (down row). 1 - DNS data; 2 - BF PDF given by Eqs. (5), (6), and (10); 3 - LF PDF given by Eqs. (5), (7) and (10).

Modified Presumed PDF Approach

A very simple way of resolving the above issues consists of substituting a common presumed PDF $\tilde{P}(c, \tilde{c}, \overline{\rho c''^2}/\bar{\rho})$ with a modified $\tilde{P}(c, \tilde{c}, \overline{W}_c)$. In other words, while parameters of presumed $\tilde{P}(c)$ are commonly determined using the two constraints given by Eqs. (10) and (11), we propose to retain Eq. (10), but to substitute Eq. (11) with Eq. (5). Due to such a modification, the presumed PDF will be tailored to predict the low probability γ_w, which plays the crucial role in evaluating the mean rates $\overline{W}_k$ for many species.

One penalty could consist of reducing capabilities for predicting the mean density and the Favre variance. However, Fig. 3 indicates that, under conditions of the present DNS, the modified PDF approach (i) predicts the mean density (left column) equally well as the common PDF approach and (ii) yields Favre variance (right column), which is sufficiently close to its true value (cf. curves 2 or 3 with curve 1) and is weakly sensitive to the PDF shape (cf. curves 2 and 3). Therefore, the modified PDF approach has yielded (i) the true values of $\tilde{c}$ and $\overline{W}_c$, because Eqs. (5) and (10) are invoked to determine the parameters of $\tilde{P}(c, \tilde{c}, \overline{W}_c)$, and (ii) values of $\overline{\rho c''^2}/\bar{\rho}$ approximately equal to the true values. To the contrary, the common PDF approach (i) has yielded the true values of $\tilde{c}$ and $\overline{\rho c''^2}/\bar{\rho}$, because Eqs. (10) and (11) are invoked to determine the parameters of $\tilde{P}(c, \tilde{c}, \overline{\rho c''^2}/\bar{\rho})$, but (ii) has significantly overestimated $\overline{W}_c$, which is, moreover, sensitive to the PDF shape. This comparison favors the modified PDF $\tilde{P}(c, \tilde{c}, \overline{W}_c)$ under the studied conditions.

It is worth also stressing that the modified PDF approach does not seem to face a basic problem if applied to modeling premixed turbulent combustion in the flamelet regime. Accordingly, the approach can be combined with manifolds $W_k(c)$ computed for the counterpart laminar flames. As far as premixed combustion in intense turbulence is concerned, further study is required in order to compare the common and modified approaches. Nevertheless, even in the intense turbulence, the ability to yield the correct values of $\overline{W}_c$ and γ_w appears to be of much more importance than the ability to yield the correct value of $\overline{\rho c''^2}/\bar{\rho}$.

Another penalty consists of the inability of the modified PDF $\tilde{P}(c, \tilde{c}, \overline{W}_c)$ to predict the mean rate $\overline{W}_c$, because this rate is used to determine the PDF. Accordingly, while the common approach yields the mean burning rate and the mean rates $\overline{W}_k$ within the framework of a single model, the modified approach is not self-sufficient and requires a model for evaluating $\overline{W}_c$. Subsequently, the modified approach can yield the mean rates $\overline{W}_k$. Nevertheless, such a complication appears to be fully justified bearing in mind poor predictive capabilities of the common approach at least in the flamelet regime of premixed turbulent combustion (see right column in Fig. 1). As far as a closure relation for $\overline{W}_c$ is concerned, a couple of models are available [5, 6] and some of them have been validated quantitatively by different groups against a wide set of representative experimental data obtained from substantially different flames under substantially different, but well-defined and simple conditions, as reviewed elsewhere [6, 34]. These models have been validated much better than models that invoke a presumed $\tilde{P}(c)$.

Conclusions

Commonly used presumed PDFs $\tilde{P}(c, \tilde{c}, \overline{\rho c''^2}/\bar{\rho})$ have failed in predicting the mean mass rate of product creation under conditions of the DNS addressed in the present paper.

In order to resolve the problem, a standard presumed PDF $\tilde{P}(c, \tilde{c}, \overline{\rho c''^2}/\bar{\rho})$ is proposed to be substituted with a modified presumed PDF $\tilde{P}(c, \tilde{c}, \overline{W}_c)$, i.e. parameters of the latter PDF are evaluated using the mean mass rate of product creation, rather than the variance.

Such modified PDFs have been shown to predict the variance $\overline{\rho c''^2}/\bar{\rho}$ reasonably well under conditions of the DNS analyzed in the present paper.

Future studies should address the usefulness of the modified presumed PDF $\tilde{P}(c, \tilde{c}, \overline{W}_c)$ for simulating emissions from highly turbulent premixed flames.

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