A Lagrangian Based Scalar PDF Method for Turbulent Combustion Models

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In this paper, a new "presumed" Probability Density Function (PDF) approach coupled with a Lagrangian tracking method is proposed for turbulent combustion modeling. The test and the investigation of the model are conducted by comparing the model results with DNS data for a premixed flame subjected in a decaying turbulent field. The newly constructed PDF, which incorporates the instantaneous chemical reaction term, demonstrates consistent improvement over conventional assumed PDF models. It has been found that the time evolution of the mean scalar, the variance and the mean reaction rate are strongly influenced by a parameter deduced by a Lagrangian equation which takes into account explicitly the local reaction rate. Tests have been performed for a moderate Damköhler number, and it is expected the model may cover a broader range of Damköhler number. The comparison with the DNS data demonstrates that the proposed model may be promising and affordable for implementation in a moment-equation solver.

Key Words : Turbulent Premixed Flame, Lagrangian Trajectory, Presumed PDF Method, Turbulent Combustion Modeling

1. Introduction

Various PDF (Probability Density Function) models encountered in combustion simulations have been for decades, potential candidates for modeling turbulent combustion (Toor, 1962; Pope and Anand, 1984). The main reason can be found in the inherent statistical approach, which enables to capture the fundamental aspect of turbulence-chemistry interaction residing in turbulent reactive flows. For example, the highly non-

linear mean reaction rate (one of the main critical variables) can be easily estimated from the PDF definition (Borghi, 1988a). Among existing PDF approaches, which are categorized by "presumed" PDF (Jones and Whitelaw, 1982; Girimaji, 1991a; Kim, 2002), and "calculated" PDF (Durand et al., 1996), the present study is focused on the former approach which usually demands the knowledge of the first and second moments of the concerned variable for estimating the PDF distribution. The latter approach requires a balance equation of PDF, and is better suitable for modeling the mixing term since the highly non-linear chemical reaction term appears in a closed term. The choice of PDF method ("presumed" or "calculated") depends on the range of validity when one considers the Damköhler number regime of Borghi's diagram (Borghi, 1985). The PDF in the limit of very fast reactions can be

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considered as a bimodal PDF shape which is encountered at a very high Damköhler number. For the limit of slow reactions, a Gaussian-like PDF shape is expected at a relatively low Damköhler number. The PDF approach can handle a wide range of Damköhler numbers since it can reproduce any PDF distribution shape depending on the values of the mean and the second order moment. If the limit of very fast reaction is well suited for the flamelet approach introduced earlier by Mao and Toor (1960), the PDF method may cover the whole range of flame structure from the wrinkled flame regime to the thickened flame regime. Furthermore, if the characteristics of the mean reaction rate are concerned, it is clear that the "presumed" PDF method that does not require numerical techniques such as Monte-Carlo method abundantly used in PDF balance equation (Pope, 1981) has advantages over the "calculated" PDF method, due to the simplicity. Nevertheless, the flamelet approach has its own advantages when multi-species reaction is considered ; this is because the PDF approach encounters a growing dimensionality problem, which requires the assumption of statistical independence between the species engaged. A number of "presumed" PDF methods are found in the literature, e.g. Rhodes (1972) with triangular form, by Borghi (1988a) with rectangular form and clipped Gaussian form proposed by Lockwood (1975). A PDF shape constructed from Lagrangian equations was also proposed by Gonzalez (1986). In all these PDF methods, geometrical information of assumed PDF is evaluated by solving the first and second order transport equations for the concerned reactive scalar. The proposed approach in this study is a blended model based on rectangular PDF form of Borghi (1988a) in which PDF height, width and peaks heights are estimated not only by the two scalar moments, but also by a Lagrangian tracking method using IEM (Interaction by Exchange with the Mean) equations. The modeling procedure starts from building the joint PDF of reactive and inert species at each point of the reactive medium with the assumption of high activation temperature for global reaction

in order to simplify the calculation of trajectories of fluid particles. The basic modeling concept had been introduced by Moon and coworkers (1992). In the following section, formulation of the newly proposed model will be described, followed by the results demonstrating the model prediction capability in a premixed homogeneous and isotropic turbulent reactive flow.

2. Formulation of the Lagrangian PDF Model

2.1 The basic equations

The idea of the Lagrangian PDF model is to combine the classical assumed PDF approach with a Lagrangian set of equations in which a parameter containing local chemistry information is added to the usual three parameters defining the PDF shape. Figure 1 shows several rectangular assumed PDF shapes of Borghi (1988a) which will be served as the datum PDF prior to the final form to be found with the aid of IEM equations. In this classical model, each three parameters defining the geometry of probability distribution of the reactive species are deduced from the first and second moment of reactive scalar. This is achieved by solving their transport equations
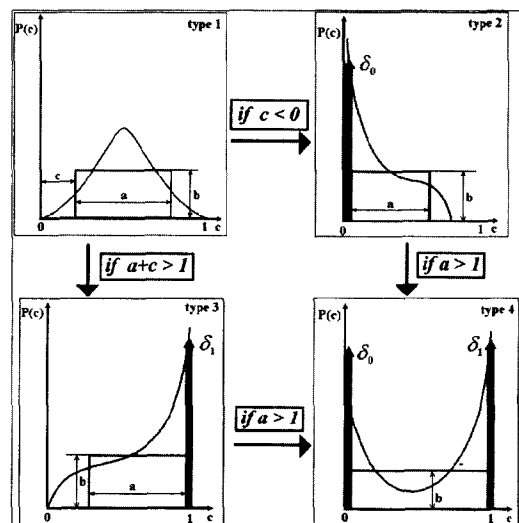

Fig. 1 Presumed shape of PDF by Borghi (1988a) : Each shape depends on three parameters which are function of $\bar{c}$ and $\overline{c'^2}$

simultaneously, and then, depending on the value of the mean and the variance, the calculated three parameters will correspond to one of the four shapes shown in Fig. 1. In the absence of turbulent convection $(\bar{u}=0)$ and with the assumption of negligible or low heat release $(\rho=cst)$, the transport equations of the two moments for the isotropic turbulent field are as follows:

$$\frac{d\bar{c}}{dt}=\bar{\omega} \qquad (1)$$

$$\frac{d\overline{c'^2}}{dt}=-\varepsilon_c+2\overline{c'\omega} \qquad (2)$$

where c is the reacting progress (or regress) variable representing the degree of reactant consumption by the chemistry. It is defined as $c=Y_F/Y_{FM}$, where Y_F is the fuel mass fraction and Y_{FM}, the maximum fuel mass fraction achievable in the mixture. $c=1$ corresponds to the fresh gas side whereas $c=0$ to the burnt gas side. $\bar{\omega}$ is the mean reaction rate to be evaluated by

$$\bar{\omega}=\int_{-\infty}^{+\infty}\dot{\omega}(c)\,P(c)\,dc \qquad (3)$$

ε_c is the dissipation rate of $\overline{c'^2}$. For the moment, we have assumed a direct proportionality between the turbulent characteristic time, τ_t and reactive scalar exchange time, τ_{ex} as in the classical approach. Modeling the dissipation rate yields:

$$\varepsilon_c\cong\frac{\overline{c'^2}}{\tau_{ex}}=C_d\frac{\overline{c'^2}}{\tau_t} \qquad (4)$$

where C_d is a trimming constant for comparisons. In the section 4.2, a more elaborated closure model for the dissipation rate is used for this study where a closure based on $k^{0.5}/U_L$ of Said et al.(1988b) is tested against the upper closure. $k^{0.5}/U_L$ is the ratio between turbulent and laminar characteristic speeds where k stands for turbulent kinetic energy whereas U_L stands for the laminar flame propagation speed. An additional parameter containing local chemistry information is deduced from the classical Lagrangian equation; here, we have borrowed the IEM model of Yamazaki et al.(1970) which represents the Lagrangian evolution of one fluid particle in a turbulent medium with

$$\begin{cases} \dfrac{dc}{dt}=\dfrac{\bar{c}-c}{\tau_{ex}}+\dot{\omega}(c) & (5) \\[2ex] \dfrac{d\phi}{dt}=\dfrac{\bar{\phi}-\phi}{\tau_{ex}} & (6) \end{cases}$$

Indeed, the first term of the RHS is the modeled term of $\dfrac{1}{\rho}\dfrac{\partial}{\partial x_i}\left(\rho D\dfrac{\partial Y_F}{\partial x_i}\right)$ which is just the diffusion term in the reactive species transport equation, with $1/\tau_{ex}$ being the mixing exchange frequency. ϕ is the fictive inert species that has been introduced in order to construct the Lagrangian trajectory.

2.2 The Lagrangian model

Figure 2 shows a trajectory calculated by the Lagrangian equations in the phase space $(c,\ \phi)$. Note that the trajectory contains local chemistry information (Eqs. (5) and (6)) which is not explicitly accessible with Eqs. (1) and (2), since these equations are based on Reynolds averaged equations. One can see that the real trajectory (solid line) can be approximated by the line AI, IS and SB (dashed line). The IS part can be viewed as a result of sudden combustion effect supported by our hypothesis of high activation temperature of the global reaction. The point M represents the spot of mean values of both reactive and inert species in the phase space. The point I resides on the line AM, and the location is determined when
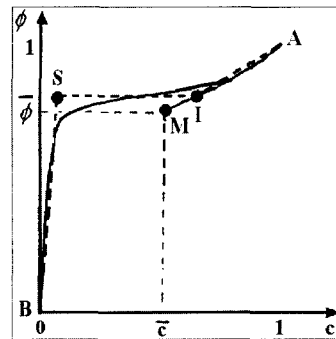

Fig. 2 The Lagrangian trajectory in the phase space of reactive and inert scalar (Solid line: real trajectory evaluated by IEM equation; Dashed line: modeled trajectory in the event of local ignition)

$$c_I - \bar{c} = \tau_{ex} |\dot{\omega}(c)| \qquad (7)$$

This assumption is arbitrary, and the above equation is an implicit relation that permits us to determine c_I as a function of τ_{ex}, $\bar{c}$ and local chemical reaction rate. During the whole study, we have supposed that the local chemical reaction rate, $\dot{\omega}(c)$ is uniquely dependent on c assuming that the medium is adiabatic and that the combustible and oxidizer are linearly related to c. The physical meaning of the parameter c_I can be clarified if we consider the solution graphically. Figure 3 shows the graphical solution of Eq. (7) where c_I is found by the intersection between $\dot{\omega}(c)$ and $\dfrac{c - \bar{c}}{\tau_{ex}}$ curves. It is obvious that there will be only one c_I such that $c_I > \bar{c}$. c_I becomes closer to $\bar{c}$ as $\bar{c}$ increases, due to Arrhenius-like reaction, and $\dot{\omega}(c)$ is elevated as the reaction becomes faster, and then, c_I will be closer to $c=1$. Thus c_I can be represented as an ignition starting point where the combustion event abruptly takes place prior to local mixing (represented by AI line). The point S is supposed to be at stationary state and at near zero so that the concentration at S, c_S, can be evaluated by the following equation :

$$0 = \frac{\bar{c} - c}{\tau_{ex}} + \dot{\omega}(c) \qquad (8)$$

Meanwhile, at the extreme case of very small values of τ_{ex} (the slope $1/\tau_{ex}$ being too high), the intersection between $\dot{\omega}(c)$ and $\dfrac{c - \bar{c}}{\tau_{ex}}$ would not let grab any point S near zero. There exists only $c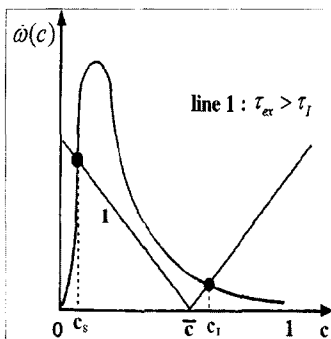_S$ close to $\bar{c}$. This corresponds to the case when either the local reaction is weak or the turbulence frequency is high, and that there exist a certain value of τ_{ex} as a function of $\bar{c}$ and chemistry for which there is no ignition. In other words, the ignition can hardly occur. Figure 4 demonstrates the Lagrangian trajectory in the case of non occurrence of ignition, and Figure 5 the graphical solution. We will therefore, define an ignition exchange time, τ_I as a limiting bound between ignition event with sudden reaction and weak reaction. This is represented in Fig. 5 by the line $\dfrac{c - \bar{c}}{\tau_I}$ which is adjacent to the curve $\dot{\omega}(c)$. All the above figures, Figs. 1 to 5, are schematic diagram used to help visualize how the Lagrangian PDF model is constructed.
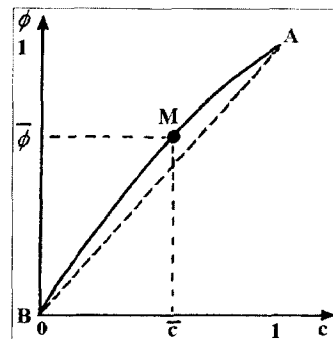

Fig. 4 The Lagrangian trajectory in the phase space of reactive and inert scalar in the event of negligible reaction

Fig. 3 Schematic plot of the graphical solution for the Eq. (7) in the event of local ignition
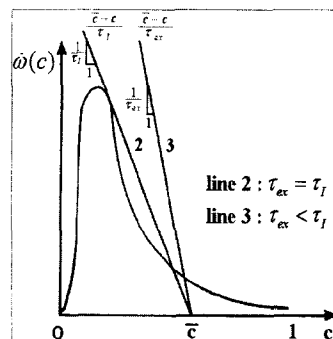

Fig. 5 Schematic plot of the graphical solution in the event of negligible reaction (Line 2 : Border between ignition event and negligible local reaction ; Line 3 : The case of negligible local reaction)

Fig. 7 Presumed shape of PDF by Lagrangian PDF
        model : Each shape depends on four para-
        meters (a, b, δ_0, δ_1: function of $\bar{c}$ and $\overline{c'^2}$;
        c_I : fourth parameter given by Lagrangian
        trajectory)

6. The Construction of PDF

For the case of $\tau_{ex} < \tau_I$, we have imposed the form of PDF defined in Fig. 1 since a Gaussian-like or clipped Gaussian form of PDF distribution is always possible for non reactive scalar. For the case of $\tau_{ex} > \tau_I$, the PDF is constructed at the expense of Lagrangian trajectory calculation. In Fig. 6 showing the link between inert scalar PDF with reactive scalar PDF, it can be found that for the domain $0 < c < c_I$, there are no presence of the probability distribution for the reactive species, c. This is because after triggering high rate of reaction at c_I location, the reaction rate is very high, resulting no probability of existence for $c < c_I$. For the nearby region of c_S, near $c=0$, a peak has formed in reactive PDF (which is not the case with the PDF of the inert scalar) since the slope of the trajectory is high in the region. Figure 6 clearly demonstrates this effect via the PDF shape of reactive scalar. It should be noted that the parameter c_I is just the additional parameter containing the local chemistry information besides three other parameters defining the shape of PDF cited earlier.

Figure 7 is a schematic representation of the newly constructed PDF shapes by the Lagrangian trajectory showing an empty space in PDF distribution between the peak at $c=0$ and the rectangular form. Trajectory found at each time step will serve for the evaluation of c_I at all time
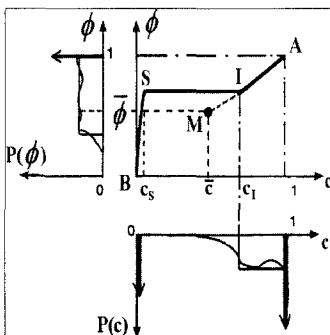

Fig. 6 Schematic of the link between inert scalar
        PDF and reactive scalar PDF in the event of
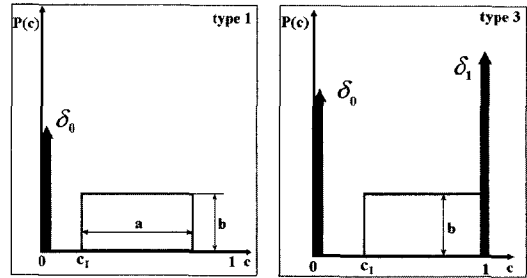   local ignition

steps, followed by $\bar{c}$ and $\overline{c'^2}$ calculations that will serve for evaluating three parameters that define the PDF shape.

4. Results and Discussion

4.1 The time evolution of the progress variable

In order to evaluate the prediction capability of the present model, the model results were compared with DNS (Direct Numerical Simulation) from the spatial average of 64^3 instantaneous values representing a cubical box in a three-dimensional isotropic decaying turbulent field. Spectral collocation method with a periodic boundary condition is applied to the turbulent field with a simple chemical reaction. The flow is assumed to have a constant density and be isenthalpic where the enthalpy of the mixture is linear with respect to temperature. Qualitative and quantitative comparison is made by inspecting the time evolution of the spatial average of the progress variable, $\bar{c}$, the variance, $\overline{c'^2}$ and the mean reaction rate as a function of the mean progress variable, $\bar{\omega}(\bar{c})$. Figure 8 shows one of the earlier comparisons with DNS of Moon (1991b) using the PDF model of Borghi (1988a) and PDF model using a beta function. Figure 8 and 9 correspond to the case of $D_a=3.3$ where the Damköhler number Da is defined as the ratio between initial turbulent characteristic time and chemical characteristic time. The above value
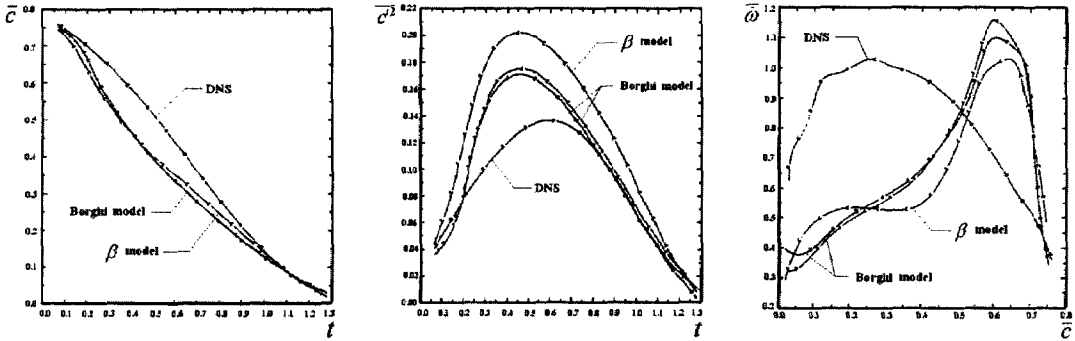
Fig. 8 Comparisons of $\bar{c}$, $\overline{c'^2}$ and $\bar{\omega}$ evolutions between DNS and classical presumed PDF models for $Da=$ 3.3 (reproduced from Moon (1991))
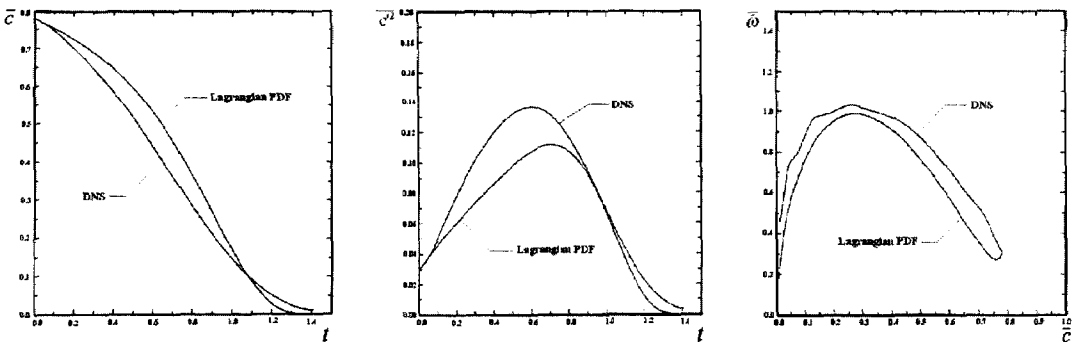

Fig. 9 Comparisons of $\bar{c}$, $\overline{c'^2}$ and $\bar{\omega}$ evolutions between DNS and Lagrangian PDF model with the dissipation rate closure $\tau_{ex} \propto \tau_t$ for $Da=3.3$

implies that the turbulent flame of interest is in the thickened-wrinkled flame regime where both the turbulent characteristic time and chemical characteristic time are of same order. It was concluded that these models that do not account for the local chemistry information, predict the reactive field within 30% of deviation from the DNS results; however, the mean reaction rate computed by the model did not demonstrate acceptable evolution by the fact that the reaction rate at the cold gas side was too strong when compared with the DNS results. Figure 9 shows the same flame regime with the Lagrangian PDF model, and it can be seen that the prediction of the model is much better than that of the old model when the time evolution of $\bar{c}$ is considered, which demonstrates a much less deviation from the result of DNS. In addition, the results of mean reaction rate clearly shows that the present model result follows the trend observed by DNS. This

explains the closer resemblance of the time evolution of $\bar{c}$ computed by Lagrangian PDF model with respect to the one by DNS.

4.2 The PDF and the dissipation rate

In order to clarify the right quantitative concordance of the model with DNS data, a comparison of PDF shape obtained by the model and DNS has been checked. Figure 10a to 10c show the non-dimensionalized time evolution of the PDF form calculated by DNS at $t=0$, 0.4 and 0.8 respectively. It is found that the shape of PDF shows a hollow between the peak at $c=0$ and the Gaussian part for the case $t=0.4$ (Fig. 10b) and $t=0.8$ (Fig. 10c). These PDFs match to the case of $\tau_{ex} > \tau_l$ corresponding to the line number 1 in the schematic of Fig. 3 where the points I and S are far apart between them. The PDF at $t=0$ match to the case of $\tau_{ex} < \tau_l$ corresponding to the line number 3 in the schematic of Fig. 5 where the

points I and S are very close. If the former case models the abrupt ignition event, the latter case agrees the case when the mixing event is predominant over the weak local reaction rate. It is shown that the PDF shape at $t=0$ looks like a clipped Gaussian shape with a peak at the fresh gas side $(c=1)$. This implies that the proposed assumed shape of PDF is in qualitative agreement with the PDF computed by DNS, justifying the right prediction of the mean progress variable, as well as the mean reaction rate evolution plotted in Fig. 9. The inclusion of the aforementioned parameter, c_I in constructing the shape of the PDF of Fig. 7, clearly shows that the present Lagrangian modeling formulation accounting for the local chemistry information has physical evidence when $\tau_{ex} > \tau_I$. It should also be accented that the use of parameter, c_I, explicitly provides additional information in reshaping the PDF dis-

tribution than the classical "presumed" PDF model. The fact that τ_{ex} varies in a decaying turbulent field, this model will have the privilege to use either the assumed shape defined in Fig. 1 or the modified shape shown in Fig. 7.

It is interesting now, to check if the PDF shape really allowed the good concordance with DNS data. For this, we have used another dissipation rate model depending on the ratio $k^{0.5}/U_L$ (see Said et al. (1988b) for details) that usually showed much more realistic results relatively to the case using Eq. (4). The empirical formula for the modeled dissipation rate of Said et al. (1988b) is

$$\varepsilon_c = C_d \frac{\overline{c'^2}}{\tau_t}\left[1 + \frac{4.4}{0 + 3.2 k^{0.5}/U_L}\right] \qquad (9)$$

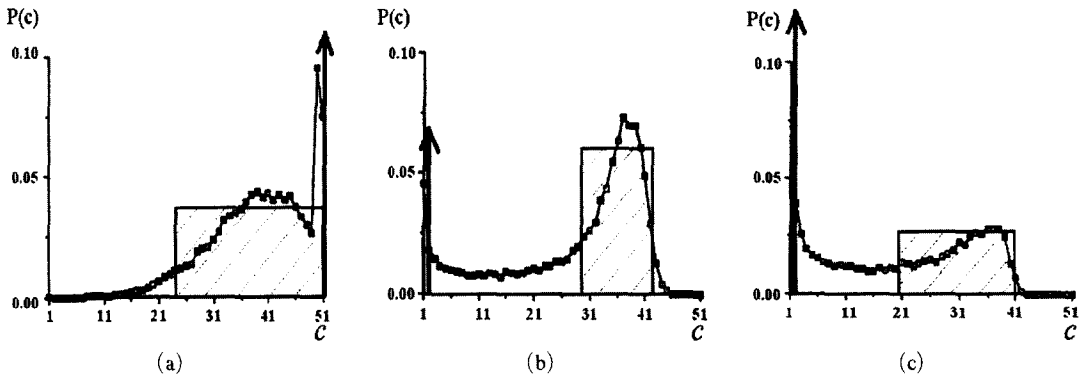where C_d is an empirical constant. Figure 11 shows the result obtained by the Lagrangian PDF

Fig. 10   PDF of the progress variable deduced from DNS during combustion ; 10a : PDF distribution at non-dimensionalized time $t=0.0$, 10b : PDF distribution at $t=0.4$, 10c : PDF distribution at $t=0.8$
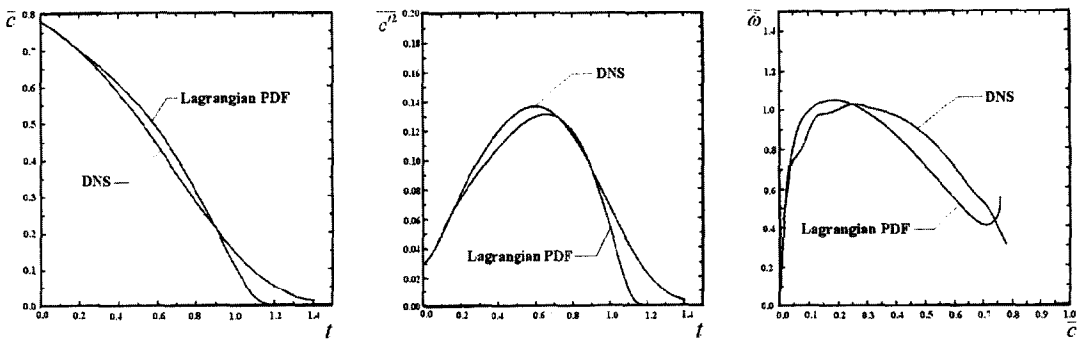

Fig. 11   Comparisons of $\bar{c}$, $\overline{c'^2}$ and $\bar{\omega}$ evolutions between DNS and Lagrangian PDF model with the dissipation rate closure of Said (1988b) for $Da=3.3$

model with the dissipation rate model of Said et al. (Eq. (9)). Comparing these statistical quantities of the reactive species with those of Fig. 9 which use the classical closure for ε_c(Eq. (4)), no noticeable qualitative difference can be found, i.e., evolutions of $\bar{c}$, $\overline{c'^2}$ and $\bar{\omega}$ by the closure of Said et al. (1988b) merely show any improvement over the classical closure though some quantitative difference is observed with the result of Fig. 11. Through these calculations, the constant, C_d, was trimmed in order to have the best concordance with the result of DNS. The constant C_d ranged from unity to two for most simulations. However, with the classical presumed PDF model based solely on the first and second moments, even trimming the C_d value, the model had limitation on finding the best concordance with the result of DNS as can be seen through the comparison shown in Fig. 8.

5. Conclusions

A Lagrangian based "presumed" PDF method is proposed for turbulent premixed flames subjected in a decaying turbulent field. The model prediction capacity is tested and compared to DNS data in order to analyze the model applicability and performance. The new PDF approach which is a blended model with the Lagrangian method is dependent not only on the first and second moments of the reactive scalar, but also on a parameter derived from the Lagrangian tracking method. The proposed approach offered realistic PDF distributions, and this has been in part confirmed by comparing the PDF extracted from DNS results (Fig. 10). It has been found that the time evolution of the mean scalar, the variance and the mean reaction rate are strongly influenced by the additional parameter, c_l which contains local reaction effect via the Lagrangian trajectories. This implies that the newly constructed PDF shape is refined by the local chemistry information, and depends more explicitly on the chemical term than the conventional PDF model which depends solely on the first two moments of the reactive scalar. The test is conducted for a moderate Damköhler number

range in which both the turbulent characteristic time and chemical characteristic time are of same order. The new results showed good agreement with the DNS results (Fig. 9): evolutions of statistical quantities such as mean reaction rate, scalar variance and mean progress variable predicted by the model closely follow the trend simulated by DNS without critical deviation. The precision of the proposed method can be clearly seen if Fig. 9 is compared with Fig. 8 which shows the result obtained with the classical PDF method. Moreover, the proposed PDF model could construct various PDF shapes by the use of instantaneous equations in the Lagrangian model. However, extension of the proposed PDF model toward complex chemistry would be a challenging problem.

Acknowledgment

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