

# 난류연소 유동장에서의 확률밀도함수 전달방정식을 이용한 난류혼합 모델링

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## Modeling of Turbulent Molecular Mixing by the PDF Balance Method for Turbulent Reactive Flows

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Key Words : mixing model, turbulent combustion, direct numerical simulation, probability density function

### Abstract

A review of probability density function(PDF) methodology and direct numerical simulation for the purpose of modeling turbulent combustion are presented in this study where particular attention is focused on the modeling problem of turbulent molecular mixing term appearing in PDF transport equation. Existing mixing models results were compared to those evaluated by direct numerical simulation in a turbulent premixed medium with finite rate chemistry in which the initial scalar field is composed of pockets of partially burnt gases to simulate autoignition. Two traditional mixing models, the least mean square estimations(LMSE) and Curl's model are examined to see their prediction capability as well as their modeling approach. Test calculations report that the stochastically based Curl's approach, though qualitatively demonstrates some unphysical behaviors, predicts scalar evolutions which are found to be in good agreement with statistical data of direct numerical simulation.

### Nomenclature

$\langle C \rangle$	: mean of $C$	$\langle C^2 \rangle$	: variance of $C$
$C$	: progress reactive variable	$c$	: random variable of $C$
$D$	: diffusion coefficient	$k$	: wavenumber
$k$	: turbulent kinetic energy	$\tau_c$	: chemical time
$l_t$	: turbulent integral scale	$L_c$	: reactive scalar integral scale
$N$	: total number of particles	$p$	: pressure
$u_i$	: velocity components	$P(C)$	: probability density function of $C$
$\langle \dot{W} \rangle$	: mean reaction rate	$\omega_c$	: turbulent frequency
$\epsilon$	: turbulent dissipation rate	$\epsilon_c$	: reactive scalar dissipation rate
$Y$	: mass fraction of reactive species	$S_c$	: Schmidt number
$\tau_{tc}$	: reactive scalar characteristic time	$\tau_t$	: turbulent characteristic time
$E(k)$	: turbulent kinetic energy spectrum	$C_c$	: Mixing Constant
$D_a$	: Damköhler number	$\nu$	: molecular viscosity
$\rho$	: density	$R_e$	: Reynolds number based on $l_t$

## 1. Introduction

The modeling problems of the turbulent flames that take place in most of the combustion equipments are especially difficult to handle due to interactions existing between chemical reactions, turbulence and heat release in highly variable geometrical characteristics. The chemistry itself is very complex, and is not well understood particularly in turbulent medium where the temperature as well as the concentrations of chemical species do fluctuate due to turbulence. This paper deals the prediction method of flame characteristics using Probability Density Function(PDF) approach by its transport equation whose main stumbling block is the right prediction of turbulent molecular mixing term appearing in the equation. We will review some existing probabilistic molecular mixing models that have been proposed so far, and test these with the results of numerical experiments. Some of these assumptions have been tested against experiments, but only to a small extent. Computational experiments based on Direct Numerical Simulation (DNS) have proven very useful in evaluating the capability of several closures [1] since the computational capabilities of nowadays allow quite sufficient resolution at least for a moderate Reynolds number. After a brief review of PDF methodology section 3 will present the cases under study for the DNS, and section 4 for the applied mixing models. Section 5 will present results of comparisons and discussions about them in a turbulent premixed medium.

## 2. Review of basic equations and problems

The basic transport equations for the approximation of turbulent non-reacting and reacting flow are the usual mean conservation equations; conservation of mass, momentum, chemical species and of energy, where

thermo-fluid properties of the system are decomposed into its average and fluctuation to give a set of coupled partial differential equations. Whether density-weighted (Favre) or not, the formulation of these equations are similar. Our intention is not to write and discuss all those equations, but to focus our discussion on the mean chemical species transport equation:

$$\frac{\partial}{\partial t} \bar{\rho} Y_i + \frac{\partial}{\partial x_a} (\bar{\rho} \tilde{u}_a Y_i) = \frac{\partial}{\partial x_a} (-\bar{\rho} \tilde{u}'_a \tilde{Y}'_i) + \bar{\rho} \tilde{W}_i \quad (1)$$

whose predictions for the averaged quantities,  $\tilde{Y}_i$ ,  $\tilde{W}_i$  are the main objectives of the statistical investigation.  $Y_i$  is the mass fraction of species  $i$  defined as  $Y_i = \bar{\rho} \tilde{Y}_i / \bar{\rho}$ , and the mean combustion rate,  $\tilde{W}_i$  represents chemical reaction interacting with the turbulent fluctuations. This equation contains two terms which are not directly related to the mean quantities, and which need to be modeled before equation (1) can be solved. One of them, the turbulent diffusion flux term on the RHS (dominant with respect to molecular diffusion flux, here neglected for a large Peclet number,  $k^{1/2} l_i / D_i$ ) can be tackled with the definition of a turbulent diffusion coefficient. Modelisation of diffusion fluxes will be beyond our scope since this paper deals isotropic field. Another closure problem arise from mean reaction rate term,  $\tilde{W}_i$ , which is highly non-linear and very difficult to predict in turbulent transport. Even though its nature is based on chemistry, it must take into account for the fluctuations of concentration and temperature resulted from the turbulent reactive field. Several approach exist for the closure of non-linear reaction, however, the most prominent approach seems to be the use of the probability density function (rather than moments method) of scalar variables since, the mean reaction rates can be elegantly solved by the joint PDF of

fluctuations of species. The main advantage of this method is that, at least with the knowledge of the PDF distribution, it allows exact calculation of non-linear reaction terms. Especially, PDF derived from its transport equation, contains all the information on high order moments whose influences are not negligible at all, but gives important impact on turbulent combustion. The philosophy of this approach is to consider the thermo-fluid quantities as random variables where we follow the transport of their PDF rather than their finite moments. The main reason for using PDF method for turbulent combustion is due to its fundamental property that can evaluate any mean quantities (e.g., mean reaction rate) from the probabilistic distribution as:

$$\bar{W}_i = \int_{-\infty}^{+\infty} W_i P(Y_i, T) dY_i dT \quad \text{where } P(Y_i, T) \text{ is the}$$

PDF of  $Y_i$  and  $T$  at a given point. On the other hand, if we refer to the commonly used moments method, it uses a modeled transport equations of any existing correlation between the fluctuating scalar component, present in the equation for the mean values (first moment). This approach is an explicit description of the transport equations at one level higher than its precedent, namely the mean transport equation. Of course, the resulting second order equation still needs a closure due to the appearance of third and higher order correlation leaving another modeling problem. However, the main advantage of moment method is its ease of use in engineering application. For instance, most of models can be implemented quite simply into the computer code developed for fluid dynamics subjected to turbulence. A lot of commercially available software computing the reactive flow problem is based on these method which allows to engineers a general approximation to the combustion phenomena. The weak point with that method is the change of model for each

specific case; there is no unique model for many different sets of flow conditions. The physical constants appearing in the equations should adapt themselves to the problems by changing their values. Nevertheless, the ability and possibility of applying these moment closure to a broad field of industrial applications is its major advantage.

### 3. Numerical Simulation

#### 3.1 Flow field

The progress of computing power that allows fine resolution of flame structures have led to a better representation of detailed chemistry and turbulent combustion process in recent years. Direct numerical simulation of turbulent reacting flow have contributed considerably not only to the understanding of the interaction between chemistry and turbulence but also to the testing of various combustion models. Inspecting the sensibility of those models with laboratory experiments results was not usually evident. Therefore, numerical experiment has been a good candidate in evaluating the prediction capabilities of new models proposed due to its ability of handling the transport equation in a model free basis.

Three dimensional statistically homogeneous and isotropic field subjected to a decaying turbulence with chemical reaction is considered in this study. Two scalars are initially premixed and their molecular diffusion fluxes are assumed to follow Fick's law with Lewis number being equal to unity. The ignition is simulated by considering a random distribution of several pockets of partially burned mixture within the flow field at the initial phase to represent autoignition. Constant density and isenthalpic flow is assumed where the enthalpy of the mixture is linear with respect to the temperature. In order to understand the basic phenomena involved in the interactions between

chemical reaction and turbulence, we have chosen a cubical box in an infinite space for the computational domain so that no geometrical constraints do influence the existing physico-chemical interaction of the reactive field. Chemistry is simulated by a single step irreversible reaction where the reaction rate,  $\dot{W}(C)$  which consumes the scalar  $C$  is chosen by:

$$\dot{W}(C) = -42 \frac{C(1-C)^{\alpha}}{\tau_c} \quad (2)$$

$C$  is the reacting progress variable representing the degree of reactant consumption by the chemistry defined as  $C = Y_F / Y_{FM}$ , where  $Y_F$  is the fuel mass fraction in the mixture with  $Y_{FM}$  being its maximum value. The Damköhler number can be prescribed by changing the value of  $\tau_c$  which is a chemical characteristic time defined as:

$$\frac{1}{\tau_c} = \int_0^1 \dot{W}(C) dC \quad (3)$$

The  $C(1-C)^{\alpha}$  in  $\dot{W}(C)$  simulates the temperature effect on the reaction, and the exponential in Arrhenius law is replaced by a power law. Fig. 1 shows the reaction rate simulated with different values of  $\alpha$ . We will use  $\alpha=5$  for the present study.

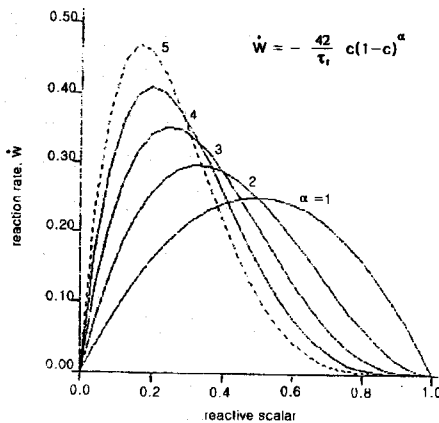


Fig. 1 Reaction rate simulated with different values of  $\alpha$  for the reactive field

### 3.2 Basic equations

The governing instantaneous equations to be used in DNS for the evolution of passive scalars are the continuity, Navier-Stokes and the conservation equation for the species:

$$\frac{\partial u_a}{\partial x_a} = 0 \quad (4)$$

$$\frac{\partial u_a}{\partial t} + u_\beta \frac{\partial u_a}{\partial x_\beta} = -\frac{1}{\rho} \frac{\partial p}{\partial x_a} + \nu \frac{\partial^2 u_a}{\partial x_\beta^2} \quad (5)$$

$$\frac{\partial C}{\partial t} + u_a \frac{\partial C}{\partial x_a} = \frac{\nu}{Sc} \frac{\partial^2 C}{\partial x_a^2} + \dot{W}(C) \quad (6)$$

where  $\nu$  is the molecular viscosity,  $p$  the pressure, and  $\nu/Sc$  the diffusion coefficient. The turbulent kinetic energy spectrum applied to the flow field is set to  $E(k) = k^4 \exp(-2k^2/16)$ ;  $k$  represents the wavenumber vector in the spectral space, and we have imposed for the velocity field, zero mean and unity rms values where the initial Reynolds number based on the integral scale has a value around 50. The spectrum of initial scalar field takes also the same form but different mean and rms is applied. The numerical method used for the calculation of equations (4), (5), (6) are based on pseudospectral collocation method with periodic boundary conditions on a  $64^3$  grid meshes. The intensive use of pseudospectral method among spectral simulation of turbulent reactive flows is due to its treatment of nonlinear term in physical (rather than spectral) space, thus avoiding huge computational requirements of Fourier transformed convolution term resulted from the nonlinear product. The spectral accuracy is achieved only in evaluating spatial derivatives. The choice of  $64^3$  grid meshes is possible because the flow under investigation has a moderate range of Reynolds number ( $Re_\tau=50$ ); it should be noticed that for reactive flows, spectral simulations of  $64^3$  and  $128^3$  resolutions are routine since the current

computational capacity restricts the Reynolds number but also the resolution requirements which are proportional to  $Re^{9/4}$  for three dimensional flows. For more complete description of spectral method, Reference [1] [2] should be consulted.

## 4. Turbulent Mixing models

### 4.1 Governing equation for the Monte Carlo

#### PDF method

Solving PDF transport equation governing its evolution for reacting flows was introduced by Dopazo and O'Brien [3], and then extended by Pope who derived the evolution of joint PDF equation for velocity and non-reactive scalar by a Monte Carlo technique [4]. In this study, we will deal the joint PDF of reactive and inert scalar with Monte Carlo method where particular attention will be made on the stochastic mixing models.

PDF transport equation comes from the early work of classical turbulence. The systematic way of solving directly a transport equation of PDF evolution is more accurate than the presumed PDF method, which predicts the PDF distribution only by means of scalar moments. The transport equation for  $p(c;x,t)$  of the random variable  $c$  is derived from the balance equation for  $C(x,t)$  by relating the PDF of  $c$  in terms of Dirac delta function :

$$p(c;x,t) = \delta(C(x,t) - c)$$

The probability density,  $P(c;x,t)$  is constructed from  $P(c;x,t) = \langle p(c;x,t) \rangle$ ;  $p(c;x,t)$  is just a representation of a Monte Carlo particle used in stochastic process where  $P(c;x,t)$  is its expected value. By limiting the formulation to that of constant density flow,  $P(c;x,t)$  transport equation in the probability space will have the following form :

$$\frac{\partial P(c)}{\partial t} + \frac{\partial}{\partial x_a} \langle U_a \delta(C-c) \rangle = \frac{\partial}{\partial c} [-\dot{W}(c)P(c)]$$

$$- \frac{\partial}{\partial c} \langle [\delta(C-c) \frac{\partial}{\partial x_a} (D \frac{\partial C}{\partial x_a})] \rangle \quad (7)$$

The constant density assumption can be true for reactive flow if the reactants in the medium are dilute from which the heat release can be neglected. The dependence of space,  $x$  and time,  $t$  is omitted in the upper equation for simplicity. If the major advantage of PDF approach using its transport equation is the appearance of reactive term (first term on the RHS) in its closed form, the major drawback would be the difficulty in the description of the molecular mixing term (second term on the RHS) which implicitly encloses the action of turbulent stretching on the fluctuating scalar gradient. For a field subjected to a homogeneous and isotropic turbulence, the modeling problem reduces to the correct prediction of the molecular mixing term. In the following parts, we will present in more details the existing knowledge concerning the question of molecular mixing (micromixing) modeling in premixed combustion.

### 4.2 Modeling of molecular mixing term

Models applied in this study are based on probabilistic approach where their calculations are performed by Monte Carlo method since they use stochastic modeling to handle the mixing process. These models lie in the category of "one-point closure" as they do not take into account the spatial properties of turbulence. There are models that are able to provide the spatial information; the recent linear eddy model of A. Kerstein [5] and the Fokker-Planck closure of Fox [6]. However in this study, we will deal models that are in the context of "one-point closure".

The majority of models frequently used for molecular mixing is the C/D (coalescence/dispersion) model of Curl [7], which simulates the effects of molecular action in the form of collisions between fluids particles. Using

the original Curl's closure, often called "integral model", the evolution of the probability in a homogeneous field is given by:

$$\frac{\partial P(c)}{\partial t} = 2 \omega_c \left[ \int_{c'} \int_{c''} P(c'') P(c') \delta \left( c - \frac{c' + c''}{2} \right) \times \right. \\ \left. dc'' dc' - P(c) \right] - \frac{\partial}{\partial c} [ W(c) P(c) ] \quad (8)$$

where  $\omega_c$  is the appropriate turbulence frequency to be prescribed. The first RHS refers to the modeling term of molecular mixing which destroys the fluctuations in probability space where  $c'$  and  $c''$  are the scalar values interacting to give the value at  $c$ . More precisely,  $c'$  and  $c''$  are two fluid particles of different concentration that collide each other with a frequency  $\omega_c$  to produce two fluid particles of concentration  $c$ . This model uses a random sampling of  $2\omega_c \Delta t N$  particles (the  $p(c, x, t)$ s) out of  $N$  particles representing the whole  $C$  field at an arbitrary time  $t$  in which the sampled  $2\omega_c \Delta t N$  particles are mixed according to Curl's procedure. Fig. 2 shows how ensembles of  $N$  particles undergo mixing and reaction.

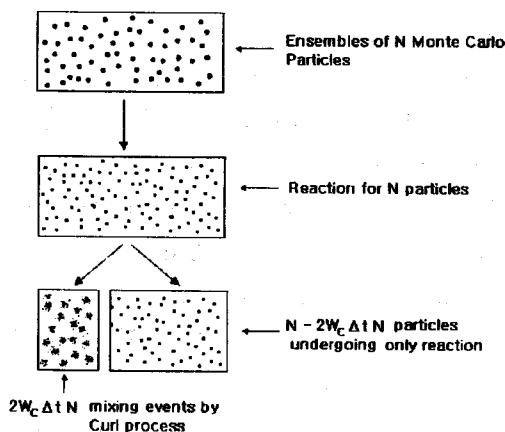


Fig. 2 Ensembles of  $N$  particles used in stochastic process of Curl's model

Besides Curl's model, there are the LMSE (Least Mean Square Estimations) closure of Dopazo and O'Brien [3] which is probably the earliest mixing

model proposed and numerous version of C/D model derived from Curl's original formulation. The closure proposed by Janicka et al. [8] and Pope [9] can be viewed as a general C/D closure since both Curl and LMSE model can be recovered from it. The LMSE closure models the molecular mixing in term of two point PDF:

$$\frac{\partial}{\partial c} \left( P(c) \lim_{x^* \rightarrow x} \frac{\partial}{\partial x^*} D \frac{\partial}{\partial x^*} \right) \\ \times \int c^* P_c(c^*/c) dc^* \quad (9)$$

where  $P_c(c^*/c)$  is the conditional PDF that the concentration at  $x^*$  tends toward  $c^*$ , while at  $x$ , the concentration corresponds to  $c$ . This approach is rather deterministic in contrast to C/D model whose formulation involves a stochastic process. The PDF evolution then obeys the following transport equation:

$$\frac{\partial P(c)}{\partial t} = \frac{1}{2\tau_{tc}} \frac{\partial}{\partial c} [(c - \langle c \rangle) P(c)] - \frac{\partial}{\partial c} [ W(c) P(c) ] \quad (10)$$

$\tau_{tc}$  is the reactive scalar characteristic time which is the inverse of  $\omega_c$  and it can be evaluated from

$1/\tau_{tc} = 12D/\lambda_c^2$  where  $\lambda_c$  is the Corrsin microscale of  $c$  field. The LMSE model by its simplicity could be quite attractive but its inability to change the PDF shape during the time evolution is the main drawback as shown in Fig. 3. The high  $P(c)$  situated at the fresh gas side ( $C=0.9$ ) existing at the initial phase ( $t=0.75$ ) keeps traveling along the  $C$  axis during combustion when calculated by LMSE model (represented by dots). This is not the case of  $P(c)$  evaluated by DNS, here shown by solid line. Moreover as reported in [8], each models described above have a critical flaw; the PDF of inert scalar calculated by both models do not relax toward a gaussian distribution during mixing. These unphysical features led Janicka et al. [8], Pope [9] and Dopazo [10] to introduce an extension of Curl's

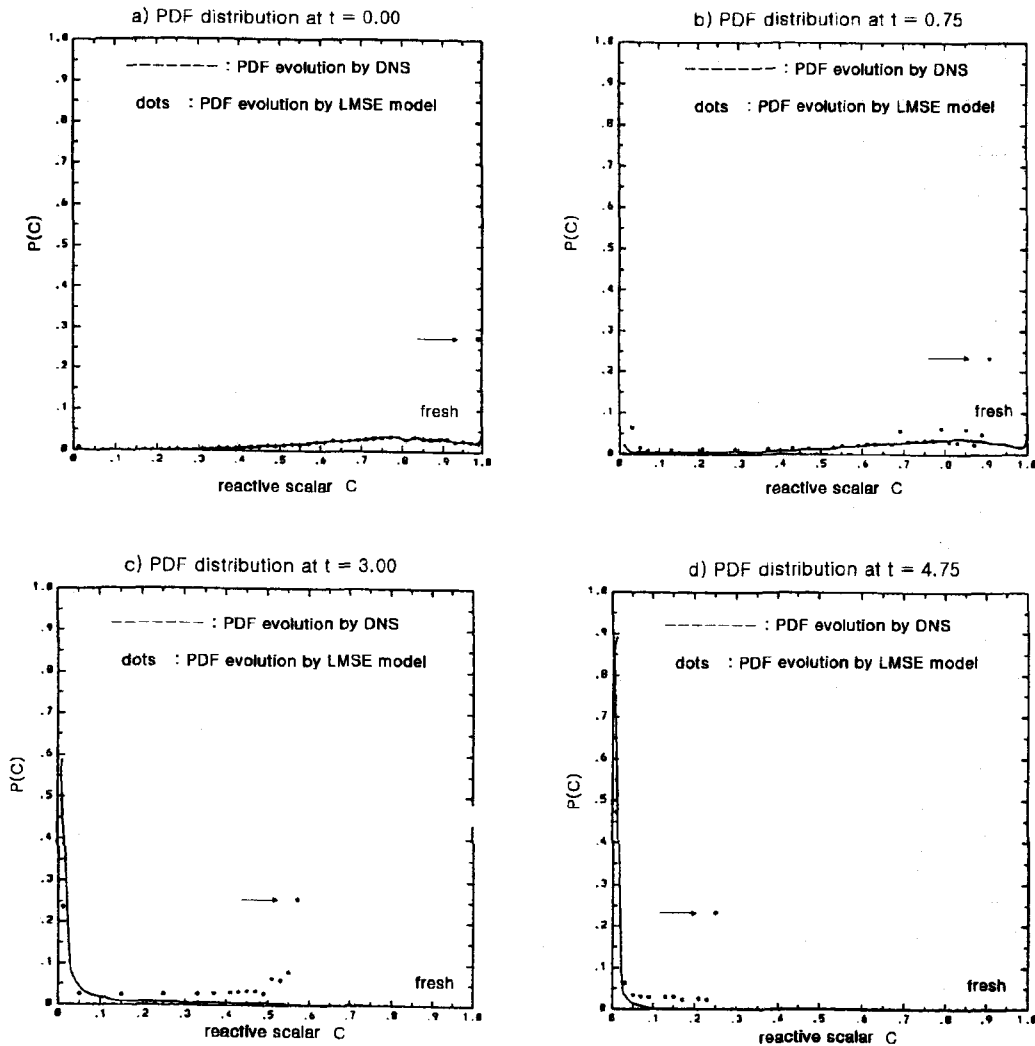


Fig. 3 Time evolution of PDF shape evaluated by DNS(solid line) and LMSE(dots) for Da=0.66

closure that allows gaussian relaxation of PDF. The final and general form of equation using C/D closure yields:

$$\frac{\partial P(c)}{\partial t} = 2\omega_c \left[ \int_c \int_{c'} \int_0^1 A(a) P(c'') P(c') \delta(c - (1-a)c' - a \frac{c' + c''}{2}) da dc'' dc' - P(c) \right] - \frac{\partial}{\partial c} [ \bar{W}(c) P(c) ] \quad (11)$$

$\alpha$  is a parameter controlling the extent of mixing of fluid elements, and takes values between 0 and 1 with probability density  $A(\alpha)$ . All the mixing models commented in this section as well as various C/D model in the literature can be

reproduced from the equation (11) depending on the distribution of  $A(\alpha)$ , i.e., the LMSE closure of Dopazo and O'Brien and Curl's model are recovered. The model of Janicka et al. and of Dopazo [10] has a value of unity for  $A(\alpha)$ . Curl's original C/D model correspond to  $A(\alpha) = \delta(1-\alpha)$ . Representing the mixing term of equation (11) in the form of stochastic process where  $C_1$  and  $C_2$  are the particles participating collision, their concentration after a time step  $\Delta t$  will be:

$$C_1(t + \Delta t) = (1-\alpha)C_1(t) + \frac{\alpha}{2} (C_1(t) + C_2(t)) \quad (12)$$

$$C_2(t + \Delta t) = (1 - \alpha)C_2(t) + \frac{\alpha}{2} (C_1(t) + C_2(t)) \quad (13)$$

It can be seen that  $\alpha=1$  corresponds to a complete binary collision of two random particles which result in two new particles having the mean value of their predecessors. Equation (12) and (13) represent then the mixing process of Curl's model. On the other hand,  $\alpha=0$  implies no mixing event that has occurred for the particles  $C_1$  and  $C_2$ . The effort made to predict a correct qualitative behavior of PDF evolution of this general C/D closure, however, is not quite satisfactory due to the increase of flatness to infinity as time evolves. This is the major drawback of particle interaction model except for the LMSE model who preserve the shape of the initial PDF.

The question of the asymptotic form of the scalar PDF in homogeneous turbulence has been addressed in a number of recent modeling studies. The PDF evolution generated by the mapping closure of reference [11] was in good agreement with DNS results. Dopazo and Valino introduced a model [12] based on a binomially distributed random sampling of scalar variables where PDF demonstrates correct asymptotic gaussian behavior and qualitatively acceptable evolution. The idea was to combine the LMSE model with a stochastic process where binomial random sampling is applied to an ensemble of particles out of the total particles representing the scalar PDF field. As cited earlier, it should be pointed out that the LMSE and Curl model (which are the main models compared to DNS results in this paper) correspond to "one-point closure". Since at single point level, the PDF approach do not requires spatial scale, information on turbulence intensity is only provided via turbulent characteristic time,  $\tau_t$ . This quantity, present in the molecular mixing term can be either evaluated by  $k-\epsilon$  model or

extracted from DNS results. The PDF model calculation results showed almost no difference for each  $\tau_t$  considered above for our decaying homogeneous and isotropic turbulent field; this is achieved when the model constant,  $c_2$  of dissipation equation of the velocity field,  $d\epsilon/dt = -c_2 \epsilon/\tau_t$ , has been slightly adjusted to 1.39 from the default value ( $c_2=1.92$ ) commonly used in the classical two equations model. This lowered  $c_2$  value is mainly due to moderate Reynolds number of the field under consideration. Nevertheless, in this study,  $\tau_t$  extracted from DNS will be used since the main scope of the paper deals the PDF based model validity and the sensibility of molecular mixing models.

## 5. Results

### 5.1 Setting the flow field

The mean value of the initial scalar concentration,  $C_0$  is set to 0.8 since the initial reacting field includes some pockets of partially burnt gases;  $C_0=1$  implies a complete fresh mixture of unburnt gas whereas  $C_0=0$  corresponds to burnt mixture in the whole region. The fluctuation of the initial scalar field is set by giving the variance of  $C$  as  $\langle C_0^2 \rangle = 0.017$  whose intensity will be enough to initiate autoignition generated by randomly distributed burnt pockets in the medium. The turbulent characteristic time,  $\tau_t$ , given by the turbulent kinetic energy spectrum starts from a value of 2.0 and will keep increasing due to the decay of turbulent motion as time evolves. For the modeling of  $\tau_{tc}$ , a direct proportionality with respect to  $\tau_t$  is assumed as usually done in turbulent combustion modeling. The relation  $\omega_c = 1/\tau_{tc} = C_d/\tau_t$  will be used during the calculation, however, this particular assumption



will be discussed later on. The calculation of the reactive field by PDF method is performed with LMSE and Curl model. Especially, Monte Carlo simulation for the stochastic solution of Curl model is performed in the composition space for the reaction and mixing process with the use of  $N$  representative values of the composition variable  $C_i (i=1, N)$ . The choice of  $N$  influences the resolution characteristics of Monte Carlo method, and satisfactory results can be obtained with  $N=1,000$  for  $Da=0.66$  and  $N=5,000$  for  $Da=3.3$ . These amount were the limit for the calculation of the field, nevertheless we have used  $N=10,000$  particles for  $Da=0.66$  to keep enough margin. The number of particles participating mixing as cited earlier for the Curl model was  $2\omega_c \Delta t N$  where now the number of mixing particles become  $2C_c / \tau_c \Delta t N$ . We can see that depending on the value of  $\tau_c$  and the adjusted value of  $C_c$ , the mixing events vary.  $C_c$  will be constant during the whole calculation whereas  $\tau_c$  given by DNS calculation is changed at every  $\Delta t$ . For the test of mixing models, the same initial conditions of direct numerical simulation and Monte Carlo PDF model calculation will be applied.

## 5.2 Tests of mixing models with DNS

A sample results of a reactive flow with moderate chemistry ( $Da=0.66$ ) given by LMSE and Curl model are shown in Fig. 4 and Fig. 5 respectively. Fig. 4a shows the decay of  $\langle C \rangle$  during combustion and Fig. 4b the mean reaction rate evolution with respect to  $\langle C \rangle$ . The constant  $C_c$  has been adjusted to 1.4 for the best concordance with DNS results. Except the early and end phase of scalar evolution, LMSE model results demonstrate a rough concordance to DNS

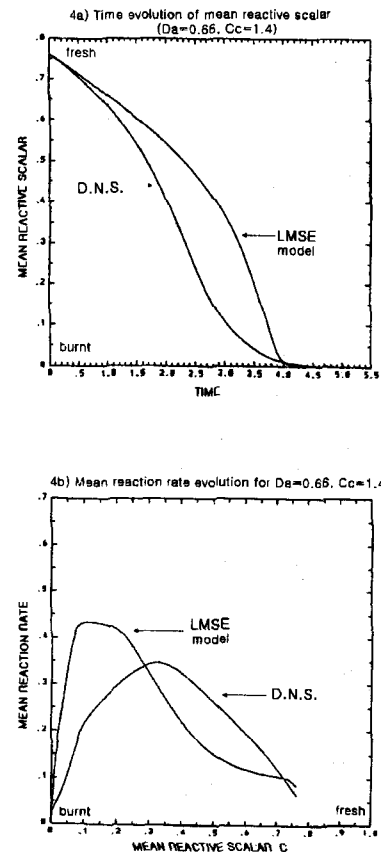


Fig. 4 Comparisons between DNS and LMSE model for the mean scalar and  $\langle \dot{W} \rangle$  for  $Da = 0.66$ ,  $C_c = 1.4$

calculation. This is mainly due to the fact that the PDF of reactive scalar can not change its initial PDF shape as explained earlier and seen in Fig. 3. Looking at the calculations conducted with Curl model shown in Fig. 5, the agreement with DNS looks excellent for  $\langle C \rangle$ ,  $\langle C^2 \rangle$  and  $\langle \dot{W} \rangle$  with  $C_c = 1.25$ . Fig. 6 shows the comparison of Curl model results with DNS for the case of faster reaction ( $Da = 3.3$ ) with  $N = 10,000$  and  $C_c$  fixed to 2.5. The first moments of reactive scalar,  $\langle C \rangle$  shown in Fig. 6a follows quite well the DNS results but the second moments ( $\langle C^2 \rangle$ ) of Fig. 6b demonstrates rather a gap when compared to the results obtained with the case of  $Da = 0.66$  for the evolution of second moments (Fig. 5b). If we examine closely the joint PDF of reactive and

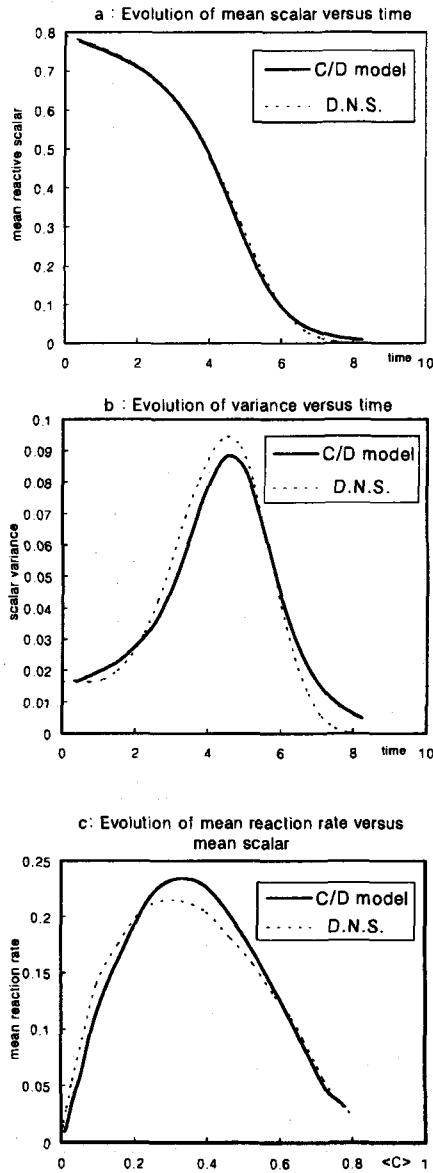


Fig. 5 Comparisons between DNS and C/D model of  $\langle C \rangle$ ,  $\langle C^2 \rangle$  and  $\langle \dot{W} \rangle$  for  $Da=0.66$ ,  $N=10,000$ ,  $Cc=1.25$

inert scalar of both models, it is clear why the prediction capability of LMSE model is weak in contrast to Curl's stochastic approach. Fig. 7 represents the joint PDF evolution computed by Curl, and Fig. 8 those resulted from LMSE model. Fig. 7 shows the positions of some of the 10,000 particles of the Monte Carlo simulation of Curl model while Fig. 8 shows the support of the joint PDF that can be calculated by LMSE model. Due

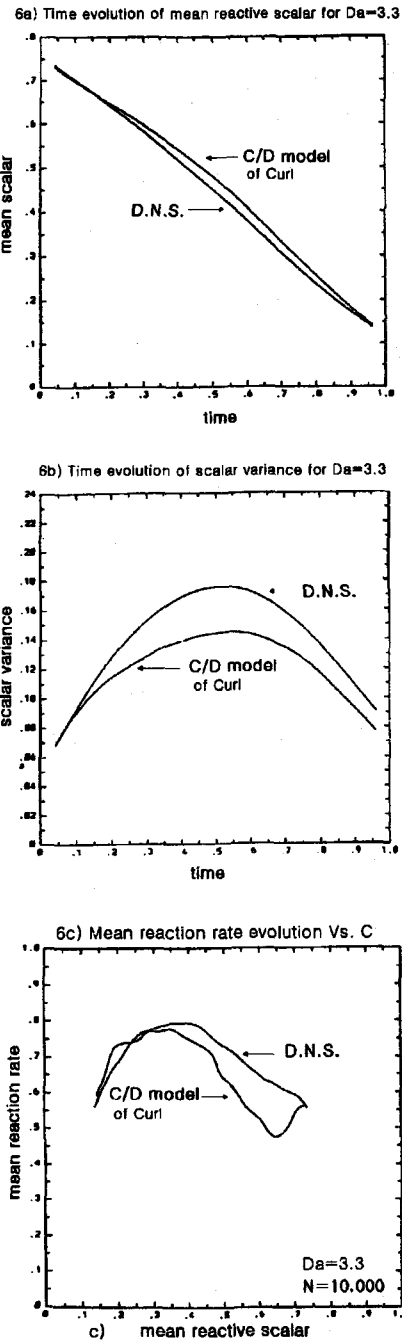


Fig. 6 C/D model predictions of  $\langle C \rangle$ ,  $\langle C^2 \rangle$  and  $\langle \dot{W} \rangle$  for  $Da=3.3$ ,  $N=10,000$ ,  $Cc=2.5$

to its deterministic nature, the LMSE model can only reproduce the skeleton of probability distribution without giving any information concerning the height of PDF. At the contrary, the positions of some of 10,000 particles in the  $(C, \phi)$  space of Curl model are spread out or regrouped to show the range of PDF distribution where the spreading corresponds to the width of PDF and

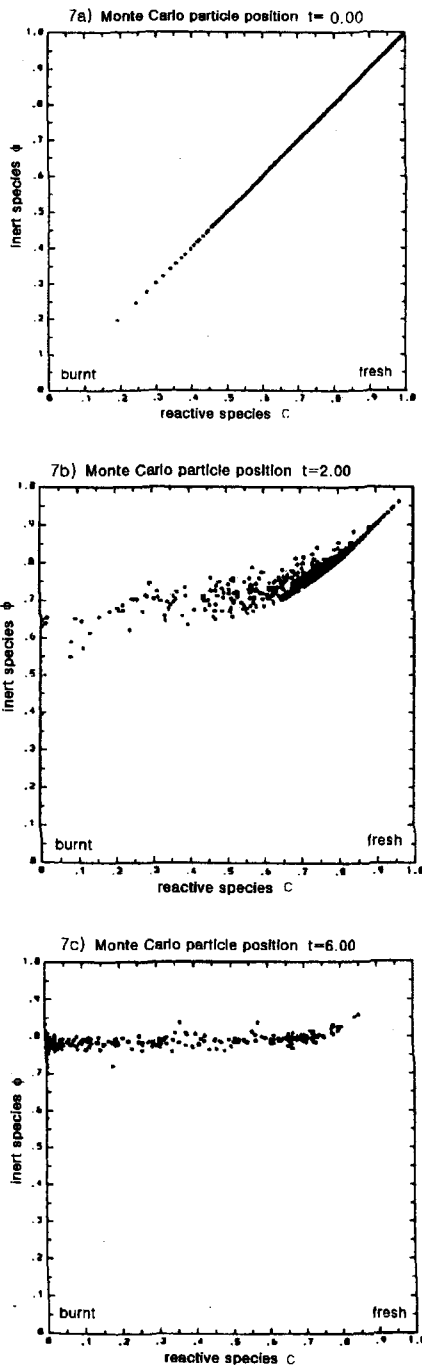


Fig. 7 Time evolution of  $P(C, \phi)$  evaluated from Monte Carlo particles for  $Da = 0.66$ , using Curl's closure

the regrouping to the density of PDF which represents the height of PDF. It is seen that as time evolves, the mean value of the inert scalar is conserved while the mean value of the reactive scalar moves toward zero simulating mixing and reaction. Indeed, all the joint PDF calculated by

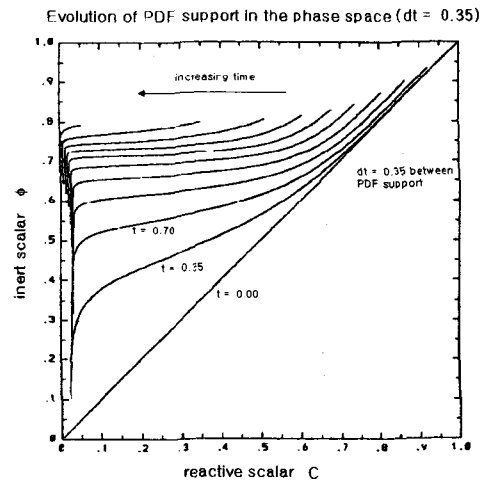


Fig. 8 Time evolution of the joint  $P(C, \phi)$  evaluated by LMSE model for  $Da=0.66$  with  $C_c$  adjusted to 1.25

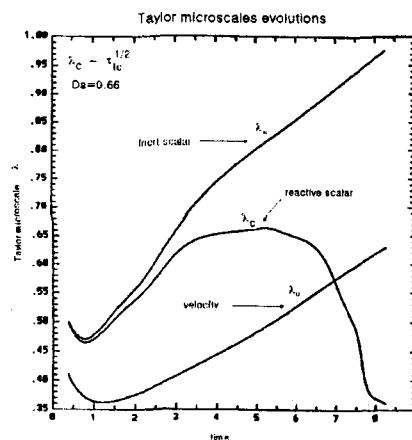


Fig. 9 Variations with time of  $\lambda_c, \lambda_u$  (the Taylor microscales,  $\approx \tau_{tc}^{1/2}$ ), computed with DNS for  $Da = 0.66$

Curl's C/D model possess much more information than the LMSE model on scalar quantities. This remark, in fact, has been expected since LMSE is the earliest proposed mixing model that relies on simple basis. The Curl model is also not fully satisfactory; the PDF relaxation to gaussian form is not obtained, and still the bi-collision assumption is questionable. However, the comparison with DNS results can address a proper direction for modeling problems.

## 6. Concluding Remarks

The numerical investigations carried in this study gave us informations concerning the validity and sensitivity of Curl and LMSE mixing models. Models were used for the closure of the balance equation of PDF where PDF of scalar is used as a key quantity for the calculation of scalar field. The direct comparisons of models results with DNS support analytical and experimental work since DNS can extract easily statistical quantities which are not measurable in the experiments. Though the results made by the Curl's closure are encouraging, its range of validity for different flame types as well as for the nonhomogeneous reactive field must be covered. Application of the PDF balance method to nonhomogeneous flow requires the modeling of turbulent convection term(second term on the LHS of eq. (7)); the use of diffusion coefficient for  $P(C)$  in the probability space is possible as usually done for the diffusion process in the physical space. However, relating the turbulence by means of a usual turbulent diffusivity is not yet straightforward. The most promising approach for the closure of the turbulent convection term seems to be the use of the joint PDF of velocity and scalar quantities,  $P(V,C)$ , as it solves directly the convective term appearing in the PDF transport equation thus avoiding the use of the diffusion coefficient. Some related topics are given in reference [9].

The constant  $C_c$ (which was kept constant during the time evolution) has been adjusted to assess those correct comparisons for different Damköhler number. In reference [13], it was found that the value of  $C_c$  for any proposed models differs and should change its value depending on  $D_a$  number to have a correct scalar evolution. This was due to the fact that in a turbulent reactive flow, the ratio  $\tau_{ic}/\tau_t$  (the  $1/C_c$ ) varies not only for different  $D_a$  but also during the time evolution. A

review of time scales and length scales cited in [14] shows this evidence(see Fig. 9). The usual assumption made in many literature for  $\tau_{ic}$  being proportional to  $\tau_t$  fails and seems to indicate that  $\tau_{ic}/\tau_t$  has to be a function of  $D_a$  in this case of moderate Damköhler number. Hence Damköhler number dependency on  $C_c$  should be tackled. Nevertheless, those comparisons show excellent agreement with DNS when we refer to previous works in which the comparisons made with presumed PDF [15] did not follow DNS results even with tuning the constant  $C_c$ .

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