Binomial Mixing Model for Premixed Reacting Turbulent Flows Applied to Autoignition

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A turbulent mixing model based on a stochastic process using a binomially distributed random variable is presented and tested in a premixed decaying turbulent flow. Attention is focused on the joint probability density function(PDF) of reactive and inert scalar that are calculated by the PDF transport equation. The numerical work under study is applied to a field similar to autoignition in which the initial medium is composed of partially burnt gas distributed within the fresh mixture. Three dimensional direct numerical simulation has been performed in order to check the prediction capability of the model whose results showed an excellent agreement with the data from numerical experiments. The joint PDF distribution calculated by the binomial model demonstrates that binomial sampling process successfully describes the realistic features of the PDF evolution.

Key Words: Direct Numerical Simulation, Premixed Flame, PDF, Molecular Mixing

1. Introduction

Application of the Probability Density Function(PDF) method has been frequently adopted in the modeling of turbulent combustion . The main objective of this method is choosing the right prediction of the PDF distribution, which, in turn, leads to the evaluation of any moments for scalar quantities. In particular, when using the transport equation for the joint PDF between scalars, one may avoid some closure problems associated with the moment formulations; for example, extension to reactive flow was practical since the highly non-linear chemical reaction term appears in a closed form. If one considers to give a "presumed" shape for the scalar PDF using the first and second moments of the scalar field, closure for the mean reaction rate is required leaving additional closure problem. However, the problem is much more simplified compared to the solution of the PDF transport equation since the governing equations to be solved are very easily formulated especially for the case of isotropic flow. Although, the results obtained by "presumed" PDF have been successful in some case, this approach can not deal with complex PDF distribution that is present in real situation. Furthermore, "guessing" the PDF shape based on only its first two moments may be questioned since usually orders higher than the second order give non-negligible influences on combustion. By contrast, the calculated PDF method is not exposed to that problem due to its complete statistical formulation based on its balance equation. Solving the PDF transport equation governing its evolution for reacting flows was introduced by Dopazo and O'Brien(1974), and then extended by Pope(1981) who derived the evolution of the joint PDF equation for the velocity and non-reactive scalar by a Monte Carlo technique. In this study, the joint PDF of the reactive and inert scalar is emphasized with the Monte Carlo method for the prediction of reactive field where particular attention will be made on a stochastic mixing model used for the closure of the turbulent molecular mixing term appearing in the PDF transport equation.

Until recently, most of the mixing models available in the framework of the PDF method were based on an integral approach using the interac-

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tion of the fluid cells; they are, the LMSE (Least Mean Square Estimations) closure introduced by Dopazo and O'Brien (1974), the closure of Janicka et al. (1978) and the coalescence-dispersion model of Curl (1963). These models were not totally distinct since they could be recovered from the general C/D closure model of Janicka et al. (1978) which was based on a phenomenological process. These models lie in the category of "one-point closure" as they do not take into account the spatial property of turbulence. The scalar mixing frequency, ω_c, present in the turbulent molecular mixing term involves this information. Hence, at one-point level, ω_c must be prescribed by means of external source. More recently, models that are able to provide the spatial information have been addressed thanks to its modeling capability of the multiscale character of turbulent mixing; the linear eddy model of Kerstein (1991) and the Fokker-Planck closure of Fox (1992) lie in this category. Multiscale models however, are far more expensive than a single-point closure. These models are beyond the scope of this paper since time scales must be provided by DNS data. The model of Dopazo and O'Brien (1974) and Curl (1963), though quantitatively gave acceptable evolution of inert scalar, they demonstrated physically wrong behavior of the PDF evolution; the inert scalar PDF did not exhibit a relaxation to an asymptotic gaussian distribution not like experimental evidence suggested (Pope, 1982). The closure of Janicka et al. (1978) reinforces this shortcoming, but, the approach is not quite satisfactory due to the increase of flatness to infinity as time evolves. Beside of these single-point closure models just cited, a Langevin model proposed by Pope (1985) attempted to model the velocity PDF. While the model gave consistent results of velocity field and relaxation to a gaussian scalar PDF, a problem of boundedness of the scalar field appeared. A model introduced by Dopazo and Valiño (1990), which regroups the traditional LMSE model and a stochastic process based on a binomial sampling, is reviewed in detail. The binomial model of Dopazo and Valiño that we will test in our work lies in this category of single point closure where the idea of the proposed binomial sampling was mainly to keep this actual bound of the scalar. The work of Dopazo and Valiño (1990) concerning the PDF of inert scalar showed a qualitatively correct prediction of turbulent mixing process of statistically homogeneous turbulence. In this work, we will try to extend its sensitivity range to the reactive flow. The stochastic model will be applied to a field with finite rate chemistry in a decaying turbulent homogeneous medium where its statistical results will be tested against Direct Numerical Simulation (DNS) data in order to check the validity of the proposed stochastic model.

2. Formulation of the Binomial Mixing Model

We consider here a statistically homogeneous and isotropic turbulent reactive premixed flow system in which a gaseous mixture is consumed by a single step irreversible reaction. It follows then, in the vicinity of constant density flow, the transport equation (Lundgren, 1969) for the fluctuating scalar PDF, $P(\mathbf{C})$ is:

$$\frac{\partial P(\mathbf{C})}{\partial t} = -\frac{\partial}{\partial \mathbf{C}}\left\langle\left[\delta(C-\mathbf{C})\frac{\partial}{\partial x_\alpha}\left(D\frac{\partial C}{\partial x_\alpha}\right)\right]\right\rangle + \frac{\partial}{\partial \mathbf{C}}[-\dot{W}(\mathbf{C})P(\mathbf{C})] \tag{1}$$

C is a 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. $P(\mathbf{C})$ is the PDF of the instantaneous random scalar $\mathbf{C}$ which stands for C in probability space. 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. D is the molecular diffusivity, δ the Dirac delta function, and $\dot{W}$ represents the reaction rate. Modeling of the turbulent molecular mixing term (first term on the RHS) is crucial for the right prediction of the field since the reaction term (second term on the RHS) appears in its closed form leaving no modeling requirement with this PDF transport equation. In the

following work, equations related to the progress variable, C will be added to the work of Dopazo and Valiño (1990) which models the first term on the RHS of Eq. (1).

The binomial approach used for the closure of the mixing term combines the LMSE model of Dopazo and O'Brien (1974) with a stochastic process where binomial sampling is applied to some randomly selected particles out of the total N fluids particles which are N values of discretized $P(C)$ supposed to represent the entire flow field. These particles are subject to the following formulations.

1) The first sub-process affects all N particles by the mixing procedure of LMSE model. The model of Dopazo and O'Brien leads to write the reactive and inert scalar evolution as:

$$C_i(t+\Delta t) = C_i(t) + \frac{1}{2}(\langle C\rangle - C_i)\,\omega_c \Delta t + \dot{W}(C_i)\,\Delta t \tag{2}$$

$$\phi_i(t+\Delta t) = \phi_i(t) + \frac{1}{2}(\langle \phi\rangle - \phi_i)\,\omega_c \Delta t \qquad i=1,\ N \tag{3}$$

where ω_c was evaluated from $\omega_c = 12D/\lambda_c^2$ (λ_c, Corrsin microscale of C field) in the original formulation of LMSE model. Nevertheless, the present paper apply a direct proportionnality between scalar mixing frequency (ω_c) and turbulence frequency (ω) where ω will be prescribed from the result of direct numerical simulation since it allows informations on the turbulent characteristic time τ_t which is nothing but the inverse of ω. It results then $\omega_c = C_D\omega$ where C_D is the constant to be adjusted.

2) A random sampling of $\beta\omega_c \Delta t N$ particles is carried out of the total N particles where selected ones undergo a process using a binomially distributed normalized variable ξ, while $N(1-\beta\omega_c\Delta t)$ particles not selected keep the value derived by LMSE process. The calculation of this process is performed by the Monte Carlo method with a random marching technique similar to the one used by Dopazo and Valiño (1990).

The sampled C_i and ϕ_i then modify their scalar values according to,

$$C_i(t+\Delta t) = \langle C\rangle + \xi_c\sqrt{\langle C'^2\rangle} \tag{4}$$

$$\phi_i(t+\Delta t) = \langle \phi\rangle + \xi_\phi\sqrt{\langle \phi'^2\rangle} \qquad \textit{for}\ \ i=1,\ \beta\omega_c\Delta t N \tag{5}$$

with

$$\xi_\phi = \frac{\eta - MP}{\sqrt{MP(1-P)}} \tag{6}$$

If there are no limitation of the bound, a normalized gaussian variable would be enough for ξ, but the essential point is that gaussianity can not be reached for bounded field. This led Dopazo and Valiño to take advantage of a binomially distributed variable of Eq. (6). β is a positive dimensionless parameter to be adjusted in order to influence the relaxation rate of the PDF field. This sub-process (stochastic events) enhances the boundedness of scalar in the composition space for those randomly selected particles using the property of binomial distribution without altering the $\langle C\rangle$, $\langle\phi\rangle$, $\langle C'^2\rangle$ and $\langle\phi'^2\rangle$ values during the sub-process 2. $\langle\phi\rangle$ and $\langle\phi'^2\rangle$ (as well as $\langle C\rangle$, $\langle C'^2\rangle$) are only affected by sub-process 1 (LMSE process) since ξ_ϕ and ξ_c are defined in a way that its mean and variance are equal to zero and one, respectively. This is achieved by the definition of η. The discrete binomial random variable η, using two parameters (M, P) takes the value between zero and M; $\eta=0$ corresponds to a minimum ϕ value during mixing, and $\eta=M$, to the maximum ϕ value. In fact, η is an integer between 0 and M with the probability:

$$PROB_\eta(X) = \binom{M}{X} P^X (1-P)^{M-X} \tag{7}$$

where mean of η is equal to MP and its variance equal to $MP(1-P)$. Indeed, M and P are defined in a way that ϕ respects well the limited physical bound, and they are:

$$M = \frac{(\langle\phi\rangle - \phi_{\min})\,(\phi_{\max} - \langle\phi\rangle)}{\langle\phi'^2\rangle} \tag{8}$$

$$P = \frac{\langle\phi\rangle - \phi_{\min}}{\phi_{\max} - \phi_{\min}} \tag{9}$$

The more M tends toward infinity, the more ξ_ϕ becomes a normalized gaussian variable. For the calculation of ξ_c, a relation similar to Eq. (6) corresponding to the reactive scalar will not be used but, instead, a correlation coefficient, $\Re$ for

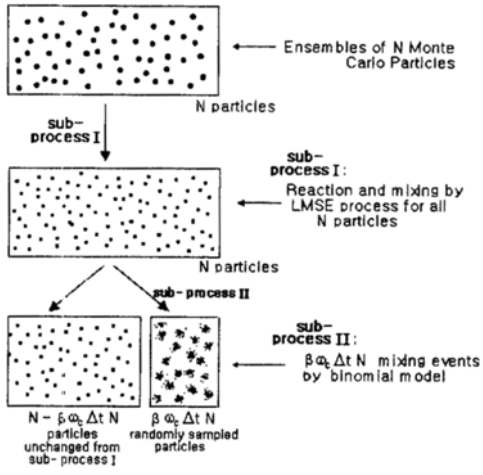


Fig. 1 Mixing process of N Monte Carlo particles used in the binomial model.

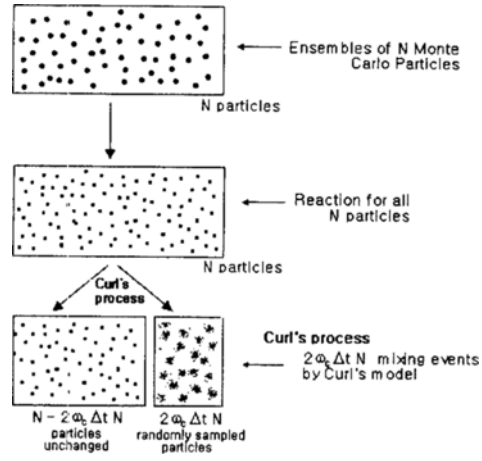


Fig. 2 Mixing process of N Monte Carlo particles used in the Curl's model.

C and ϕ is introduced. The idea is to rely C to ϕ in a realistic way, since there are no evidence that C and ϕ field are independent each other. The correlation for C and ϕ is defined as $\Re=\langle C'\phi'\rangle/\sqrt{\langle C'^2\rangle}\sqrt{\langle\phi'^2\rangle}$. As the variable ξ_c and C, as well as ξ_ϕ and ϕ, are linearly related(Eqs. (4), (5)), and that relations $\langle\xi_c\rangle=\langle\xi_\phi\rangle=0$ and $\langle\xi_c^2\rangle=\langle\xi_\phi^2\rangle=1$ must be satisfied, $\Re$ can also be defined as $\Re=\langle\xi_c'\xi_\phi'\rangle/\sqrt{\langle\xi_c'^2\rangle}\sqrt{\langle\xi_\phi'^2\rangle}$. In addition, giving ξ_c as $\xi_c=\Re\xi_\phi+\sqrt{1-\Re^2}\psi$, in which ψ is a gaussian random variable independent of ξ_ϕ, (i. e., $\langle\xi_\phi\psi\rangle=0$), the zero mean and unity variance of ξ_c are achieved as can be seen by the following relations.

$$\langle\xi_c\rangle=\Re\langle\xi_\phi\rangle+\sqrt{1-\Re^2}\langle\psi\rangle=0 \tag{10}$$

$$\langle\xi_c^2\rangle=\Re^2\langle\xi_\phi^2\rangle+(1-\Re^2)\langle\psi^2\rangle+2\Re\sqrt{1-\Re^2}\langle\xi_c\psi\rangle=1 \tag{11}$$

Figure 1 shows how ensembles of N particles are used in both two sub-processes. It is worthwhile to note that every particle is engaged in mixing at every Δt since LMSE process affects all N particles. This might not be the case with Curl (1963)'s approach whose mixing formulation can lead to a non-negligible number of unmixed particles that are forgotten during the random sampling process as shown in Fig. 2.

3. Autoignition Field of Turbulent Mixture

The reactive field under study is initially composed of partially burnt gas that are randomly distributed within the unburnt premixed gas mixture where these burnt fluid cells will initiate the reaction. This is a representative of autoignition phenomena that we will apply for the test of binomial model with direct numerical simulation. In order to study the very basic dynamic phenomena, we have assumed a simple chemical reaction where one single species F is totally transformed into P species so that only the concentration C of F species needs to be considered. The C field is then bounded between zero and one in which the upper bound, $C=1$, corresponds to the fresh gas concentration. The mean and fluctuation of the initial reactive scalar field are set to $\langle C\rangle_0=0.8$ and $\langle C'^2\rangle_0=0.017$ where $\langle C\rangle_0=0.8$ deviated from $\langle C\rangle=1.0$ results from the presence of partially burnt gas mixture. Figure 3 shows the initial PDF distribution of C formed by a clipped gaussian and a peak at $C=1$, indicating the presence of broad band of concentration due to partially burnt mixture and large amount of fresh gas existing at the initial phase. Figure 4 showing the decrease of $\langle C\rangle$ with time for different levels of $\langle C'^2\rangle_0$, clearly indicates that the initial fluctuation of C influences strongly the autoignition; for $\langle C'^2\rangle_0=0.0075$, one can see that $\langle C\rangle$ demon-

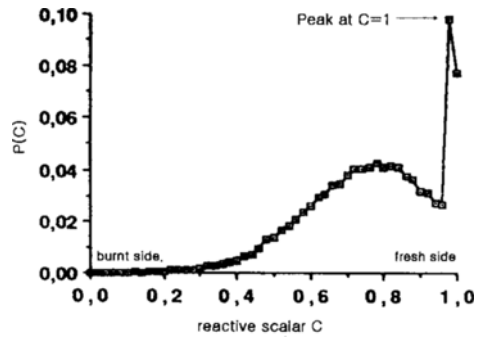


Fig. 3 Profile of the initial PDF distribution of the reactive scalar C; $\langle C\rangle=0.8$, $\langle C'^2\rangle=0.017$.

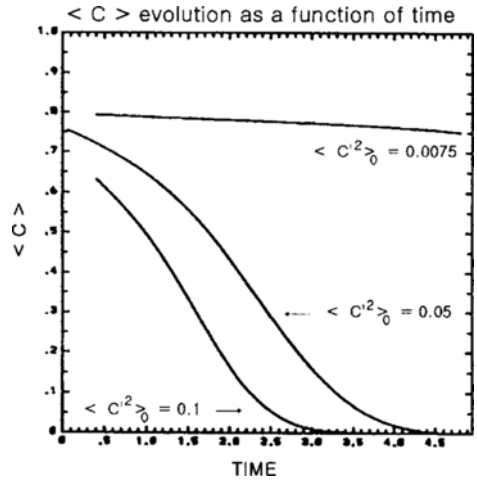


Fig. 4 Time evolution of $\langle C\rangle$ for different levels of $\langle C'^2\rangle$ 'at $D_a=0.66$

strates almost no consumption as time evolves, while drastic decrease of $\langle C\rangle$ is observed for $\langle C'^2\rangle_0=0.05$. Indeed, the chosen $\langle C'^2\rangle_0=0.017$ represents 13% of fluctuations from $\langle C\rangle_0$, and this will be enough to initiate the reaction.

To achieve a well defined comparisons between models and simulation, several assumptions have been made; 3-D statistically homogeneous and isotropic turbulent flow of constant density and Fick's law for the molecular diffusion fluxes are applied. Furthermore, isenthalpic flow condition is used, and unity Lewis number assumption was made to reduce the computational requirements for the temperature in DNS calculation. The reaction rate is the usual Arrhenius type, $\dot{W}\propto -C^{\alpha}\exp(-T_A/T)$ (T_A being the activation temperature), but we will use a simple reaction shown in Borghi et al. (1992) which does not take the temperature T into explicit account and which depends only on one single species C. The modeled $\dot{W}$ is

$$\dot{W}(C)=-\frac{42}{\tau_c}C(1-C)^5 \tag{12}$$

where τ_c is the chemical characteristic time defined by the following relation:

$$\frac{1}{\tau_c}=\int_0^1 \dot{W}(C)\,dC \tag{13}$$

It can be seen that the temperature dependency on $\dot{W}$ is omitted but replaced by $(1-C)^5$, and that the term $1-C$ stands for a non dimensionalized temperature term derived by the isenthalpic flow condition. More complete descriptions of the condition used here are addressed in the work of Borghi et al. (1992).

The governing equations used for DNS are the exact primitive Eulerian balance equations:

$$\frac{\partial u_\alpha}{\partial x_\alpha}=0 \tag{14}$$

$$\frac{\partial u_\alpha}{\partial t}+u_\beta\frac{\partial u_\alpha}{\partial x_\beta}=-\frac{1}{\rho}\frac{\partial p}{\partial x_\alpha}+\nu\frac{\partial^2 u_\alpha}{\partial x_\beta^2} \tag{15}$$

$$\frac{\partial C}{\partial t}+u_\alpha\frac{\partial C}{\partial x_\alpha}=\frac{\nu}{Sc}\frac{\partial^2 C}{\partial x_\alpha^2}+\dot{W}(C) \tag{16}$$

where instantaneous variables are calculated in a cubical domain of 64^3 grid meshes with periodic boundary conditions. ν is the molecular viscosity and Sc the Schmidt number. Pseudospectral collocation method using Fourier transform are used due to its high spatial accuracy for the solution of homogeneous isotropic turbulent flows (Oran and Boris, 1987). The initial turbulent intensity is imposed by prescribing a turbulent kinetic energy spectrum with unity rms and zero mean value for the velocity field. The Reynolds number based on the integral scale takes a value around 50, and it will keep decreasing due to the decay of turbulent motion as time evolves. The length scales and time scales for the scalar field have been taken equal to those of the velocity field.

To investigate the binomial model's applicability, the case of $F+O\rightarrow P$ is considered keeping the assumption of isenthalpy. The fluctuations of

the other reactant O are taken into account in the reaction rate where a new fictitious species, φ defined as $(Y_F - Y_O)/Y_{FM}$, is introduced. Assuming that F and O have the same diffusivity with φ, φ follows a balance equation without the reaction term:

$$\frac{\partial \varphi}{\partial t} + u_a \frac{\partial \varphi}{\partial x_a} = \frac{\nu}{Sc} \frac{\partial^2 \varphi}{\partial x_a^2} \tag{17}$$

The modeled $\dot{W}$ of equation (12) is now a function of C and φ as:

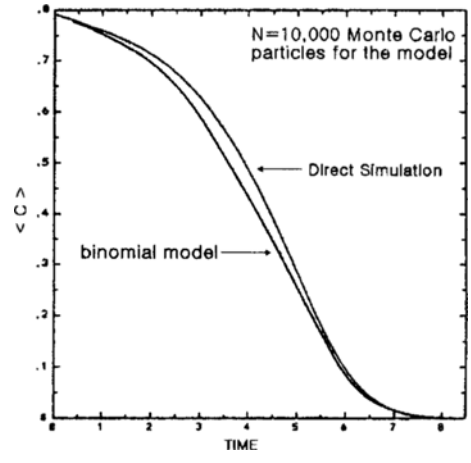
$$\dot{W}(C, \varphi) = -\frac{28}{\tau_c} C(C-\varphi)(1-C)^5 \tag{18}$$

The two reaction rates are both used to see the sensibility of the binomial model, and their results will be discussed in the next section.

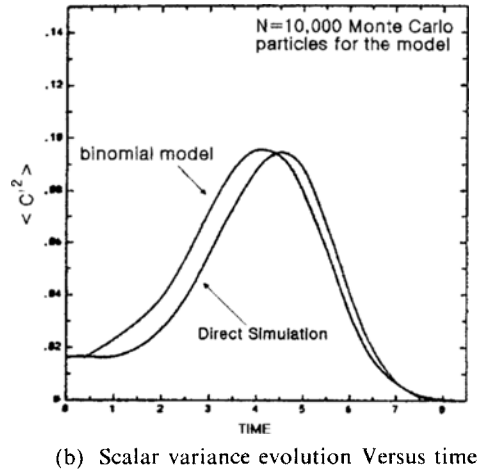
4. Results and Discussion

4.1 Comparisons of models with D. N. S.

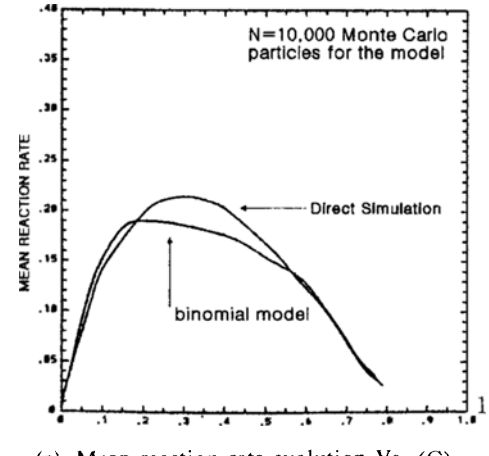
The binomial model results are calculated from the PDF transport Eq. (1) by Monte Carlo simulation of N representative values of the composition variable $C_i (i=1, N)$ which represents the scalar PDF at time t. Results from DNS come from the spatial average of 64^3 instantaneous values evaluated from the exact Eulerian balance Eqs. (14), (15) and (16). For the test of the binomial model, statistical quantities of $\langle C \rangle$, $\langle C'^2 \rangle$ and $\langle \dot{W} \rangle$ evolutions are investigated. Fig. 5 (a) and 5(b) show the temporal evolutions of $\langle C \rangle$ and $\langle C'^2 \rangle$, respectively, and Fig. 5(c) also shows the mean reaction rate evolution as a function of $\langle C \rangle$ computed by the model and DNS. In Fig. 5(b), the variance($\langle C'^2 \rangle$) is strongly increased at the initial phase by the reaction and then decreased after a certain time. This is explained by the fact that the production rate of the scalar fluctuations generated by chemical reaction is stronger than the destruction rate of $\langle C'^2 \rangle$ given by the initial turbulent intensity, and then after some time, the destruction rate of $\langle C'^2 \rangle$ overcomes the reaction. This is expected since the flow is in the regime of moderate Damköhler number where both the chemical and turbulent characteristic time are of same order of magnitude. For the present study, it has been imposed a



(a) Mean scalar evolution Versus time

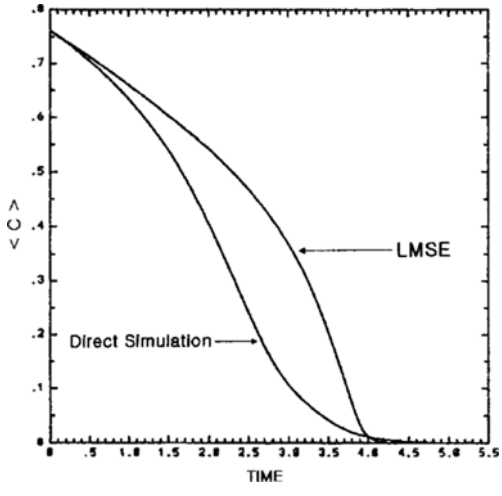


(b) Scalar variance evolution Versus time

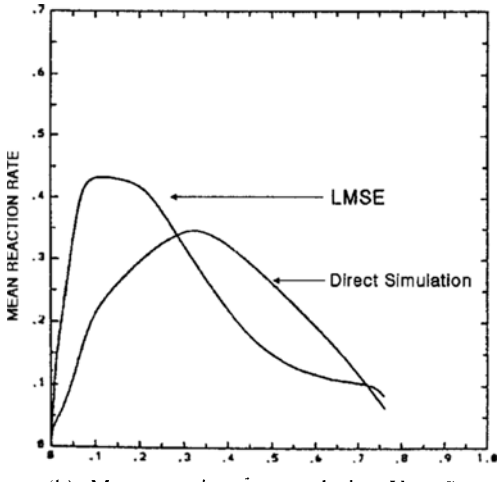


(c) Mean reaction rate evolution Vs. $\langle C \rangle$

Fig. 5 Comparisons between DNS and binomial results of $\langle C \rangle \langle C'^2 \rangle$ and $\langle \dot{W} \rangle$ for $D_a = 0.66$, $C_D = 1.0$.



(a) Mean scalar evolution Versus time



(b) Mean reaction rate evolution Vs. $\langle C \rangle$

Fig. 6 Comparisons between DNS and LMSE model results of $\langle C \rangle$ and $\langle \dot{W} \rangle$ for $D_a=0.66$, $C_D=1.4$.

value of 0.66 for D_a.

The comparisons with DNS results shown in Fig. 5 are in favor of the tested binomial model whose prediction capability is remarkably good. The best agreement was achieved by trimming the constants β and C_D to 0.7 and 1.0, respectively; C_D influences implicitly sub-process 1 and 2 by the presence of ω_c in LMSE process and in $\beta\omega_c \Delta t N$ particles affecting $\langle C \rangle$, $\langle C'^2 \rangle$ and $\langle \dot{W} \rangle$ values. β affects only sub-process 2 which influences the PDF shape by changing the number of stochastic particles undergoing binomial operations. The resolution characteristic of the Monte Carlo method depends on the choice of N. Satisfactory results were obtained with $N=1{,}000$ for $D_a=0.66$, but these amounts were the limit for the prediction of the field. Therefore, $N=10{,}000$ is used for the calculation to keep the margin enough.

In order to see the importance of correct PDF approximation on the modeling of turbulent combustion, a sample result given by the LMSE model is shown in Fig. 6(a), and 6(b). The same results can be obtained from the sub-process 1 of binomial model. Fig. 6(a) shows the decay of $\langle C \rangle$ and Fig. 6(b) shows the mean reaction rate as function of $\langle C \rangle$ for $D_a=0.66$ with C_D adjusted to 1.4. Compared to Fig. 5, the LMSE model results demonstrate a large gap of error with respect to DNS calculation.

4.2 The joint PDF shapes

Time evolution of the joint PDF of reactive and inert scalar calculated by LMSE model, starting initially from $C=\phi$ is presented in Fig. 7. Informations about PDF shape are restricted to the support of the joint PDF without giving any informations about the height of the PDF and its distribution along the curved support represented here by a simple line. Furthermore, both ends of the PDF supports are forgotten during the time evolution. Profiles of the line, $C=\phi$, are bended towards $\langle C \rangle=0$ and $\langle \phi \rangle=0.8$, because the mean value of the inert scalar is conserved whereas the mean value of the reactive scalar moves towards zero simulating mixing and reaction. Figure 8 shows the isoprobability lines representing the joint PDF of reactive and inert scalar calculated in DNS at time $t=2.0$. Comparing Figure 7 and Figure 8, the drawback of LMSE model is evident since its modeling technique do not provide enough information about the joint PDF between reactive and inert scalar. The following figures showing the joint PDF calculated by the binomial model will clarify the right prediction capability of the proposed model. Figure 9(a), 9(b) and 9(c) show the position of N Monte Carlo particles computed from equation (1) in the composition space (C, ϕ) at time $t=0.0$, $t=2.0$

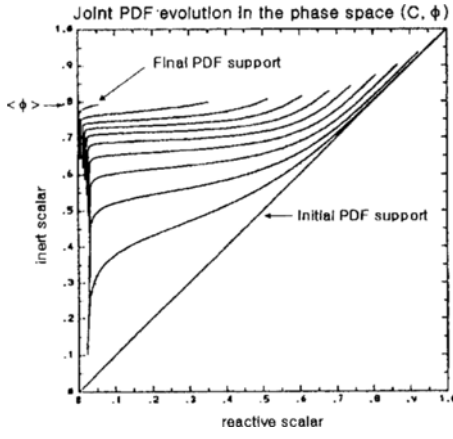


Fig. 7 Time evolution of the joint $P(C, \phi)$ evaluated by the LMSE model for $D_a=0.66$.

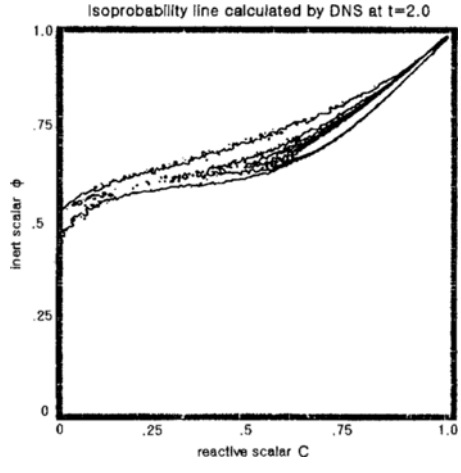
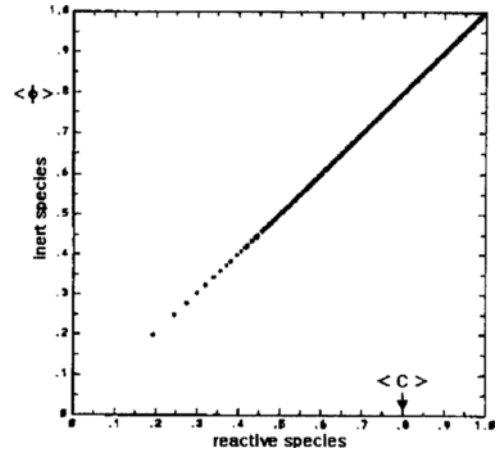
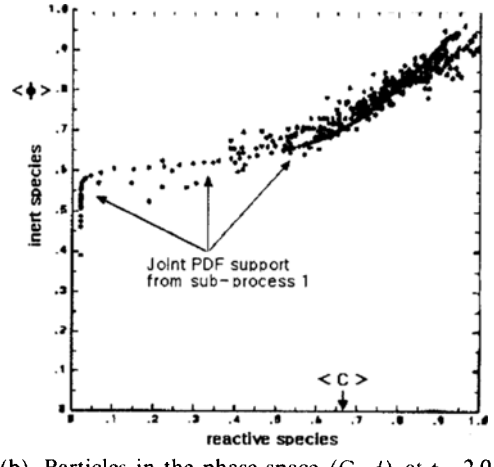


Fig. 8 Isoprobability line of the joint $P(C, \phi)$ evaluated by DNS at $t=2.0$ and $D_a=0{,}66$.

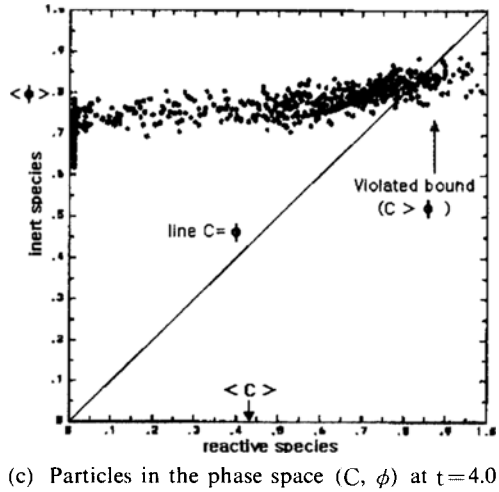
and $t=4.0$, respectively. The joint PDF calculated by the binomial model, which in addition takes an advantage of sub-process 2, clearly shows that unavailable informations from LMSE process are provided by the spreading of N Monte Carlo particles positions giving the width of PDF, and by the density of those particles giving the height of the joint PDF. Looking closely Fig. 9(b) and Fig. 9(c), some particles are regrouped on a support similar to what have been observed in Fig. 7 of LMSE model. This joint PDF support represented by an alignment of dots results from the sub-process 1, and particles(dots) moved and displaced around the support are the



(a) Particles in the phase space (C, ϕ) at t=0.0

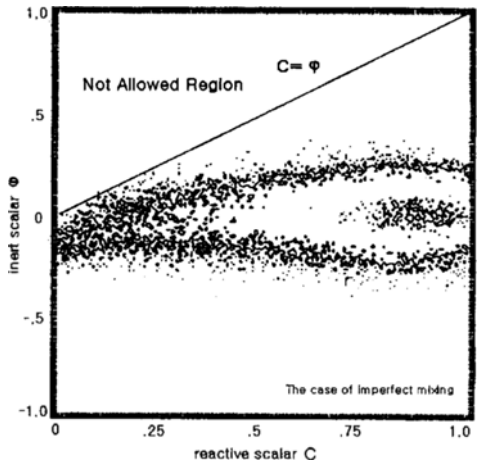


(b) Particles in the phase space (C, ϕ) at t=2.0

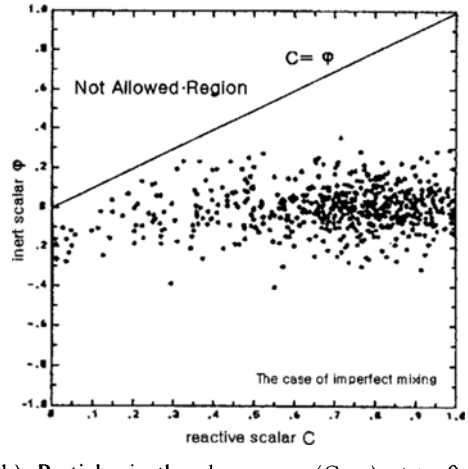


(c) Particles in the phase space (C, ϕ) at t=4.0

Fig. 9 Time evolution of the joint $P(C, \phi)$ evaluated by Monte Carlo particles of the binomial model.



(a) Isoprobability line calculated by DNS at t=0.4



(b) Particles in the phase space(C, φ) at t=0.4

Fig. 10 a): Isoprobability line of $P(C, \varphi)$ by DNS (imperfectly mixed case); b): Monte Carlo particles position for $P(C, \varphi)$ using the binomial model at $t=0.4$.

binomially distributed particles of sub-process 2 that correct the scalar PDF to have an asymptotic gaussian behavior. As a result, these facts explain the excellent quantitative agreement of binomial model with DNS of Figs. 5(a), 5(b) and 5(c).

Figure 10(a) and 10(b) are the joint PDF calculated with the reaction rate of Eq. (18) by DNS and binomial models respectively, where the fluctuations of two reactants are taken into account. As cited earlier φ is a nondimentionalized inert species whose identity is not equivalence ratio but a variable representing the effect of equivalence ratio. The two figures show the evoluted joint PDF shape of C and φ after $t=0.4$ from the initial field where φ and C fluctuations are independently set at initial time in order to simulate an imperfectly premixed field. This represents fluctuations of equivalence ratio that could exist initially in the spatial domain. The initial conditions for both C and φ are $\langle C\rangle_0=0.8$, $\langle C'^2\rangle_0=0.03$, $\langle\varphi\rangle_0=0.0$ and $\langle\varphi'^2\rangle_0=0.015$. The comparison made between Fig. 10(a) and Fig. 10 (b) are in good agreement, in addition, one can remark that both $P(C, \varphi)$'s reside below the line $\varphi=C$ which represents $C_0=0$; this is quite physical since crossing the line $\varphi=C$ simply means that $P(C, \varphi)$ exists in a region of the plane where $C_0<0$. The binomial model, in this applied case, keeps this physical margin as well as its limited bounds.

The model of Dopazo and Valiño which combines a deterministic model with a stochastic process is indeed an appealing model, but a problem of boundedness is observed for C; some particles give physically wrong features as $C>\phi$ (Fig. 9(c)). The reason behind this was because the binomial sampling for the variables C and ϕ have been done independently. Nevertheless, the correct asymptotic Gaussian relaxation of the PDF and the required small amount of computing time(30 minutes on HP730 platform) make the binomial model promising for the prediction of the reactive field, compared to huge memory and time requirement for DNS calculation which usually demands supercomputing environment.

5. Conclusions

A turbulent mixing model used in PDF transport equation has been analyzed and tested against direct numerical simulation results in a premixed isotropic turbulent field of a moderate Damköhler number regime. The binomial model which regroups the traditional LMSE model and a stochastic process based on binomial sampling technique gave a very good agreement of statistical quantities with DNS when the initial fluctuation and turbulent frequency are well prescribed within autoignition field. The direct simulation

for 64^3 resolution was a good candidate for the test tool since it allows the basic phenomena involved in the interaction between chemical reaction and turbulence in a model free basis, thereby, directly providing the turbulent frequency and allowing model test in a well defined conditions. The LMSE model results for the joint $P(C, \phi)$ were investigated and compared to $P(C, \phi)$ of binomial model in order to check the sensibility and the prediction capability of the proposed model. It has been found that the new model was physically more sound and contains much more informations on the PDF distribution, thus allowing better prediction. An extension to the case of imperfectly premixed field is also investigated; the binomial model results demonstrated that the physical bounds are respected. Major advantages of the stochastic model were found to give: 1) correct qualitative PDF evolution, 2) correct asymptotic gaussian behavior of PDF, 3) boundedness imposed for scalar fields. A problem of boundedness of C is reported, but the number of particles out of bounds are small within N, and their influences are negligible. The additional use of binomially distributed normalized variable, ξ for the mixing process in LMSE model, indicates clearly the importance of right PDF approximation in turbulent combustion modeling problems.

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