A Modeling Study of Local Equivalence Ratio Fluctuation in Imperfectly Premixed Turbulent Flames

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The effect of fluctuation of Equivalence Ratio (ER) in a turbulent reactive field has been studied in order to check the global combustion characteristics induced by the local fluctuation. When the flow is premixed on a large scale, closer examination on a small scale reveals that local fluctuations of ER exist in an imperfectly premixed mixture, and that these fluctuations must be considered to correctly estimate the mean reaction rate. The fluctuation effect is analyzed with DNS by considering the joint PDF of reactive scalar and ER, followed by modeling study where an extension of stochastic mixing models accounting for the ER fluctuation is reviewed and tested. It was found that models prediction capability as well as its potential is in favor to this case accounting the local ER fluctuation. However, the effect of local fluctuation did not show any notable changes on the mean global characteristics of combustion when statistical independence between the reactive scalar and ER field is imposed, though it greatly influenced the joint PDF distribution. The importance of taking into account the statistical dependency between ER and combustible at the initial phase is demonstrated by testing the modeled reaction rate.

Key Words : Equivalence Ratio Fluctuation, PDF Balance Method, Small Scale Mixing Model, Turbulent Combustion

1. Introduction

Considering that most combustion devices (operating under non-premixed or premixed regime) demand for local mixing event before combustion, the value of the Equivalence Ratio (ER) is undoubtedly a critical parameter for performance analysis (Lee et al., 2002a). If one considers a premixed flame subjected to a turbulent medium, it is evident that a good mixing process is crucial for preparing a perfectly mixed mixture. However, perfect mixing at the molecular level is not always evident, and very often, we refer to the terminology "rich in fuel" or "lean in fuel" for defining the mixture degree, which is just the mean value of the ER in the fuel-air mixture. Studies on the variation of the mean value of ER is beyond our scope of interest; rather, this study is focused on the local ER fluctuation effect existing in the spatial domain in order to investigate whether these ER fluctuations have great impact on turbulent combustion characteristics. Indeed, this is true in reality by the fact that there may be local imperfections of mixture composition in the actual engines prior to ignition. Special attention will be paid also on the performance of proposed mixing models by comparing model results with DNS results. Two mixing models, the integral model (Curl, 1963; Pope, 1982; Pope, 1985a) and the binomial model (Valiño and Dopazo, 1990; Moon, 1998) in the framework of Probability Density Function (PDF) method used in

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the gas phase combustion will be dedicated in this modeling study in order to analyze if these models can capture the effect of ER fluctuation where spray vaporization effect is omitted keeping the condition of isenthalpy. This is because relatively few studies and few models accounting for spray vaporization are available, and also because these upper assumptions would let us concentrate our interests solely on ER fluctuation effect, though Reveillon and Vervisch (2000) and Demoulin and Borghi (2002b) have recently proposed to include the major effects of spray vaporization on the equivalence ratio fluctuation. Therefore, an imperfectly premixed mixture with a non-homogeneous ER distribution at the initial phase is considered in a statistically isotropic turbulence field. The flow field condition is similar to the one earlier presented in the work of Moon (1998) where a stochastic model for micromixing (small scale mixing) was tested and concluded to be a potential model due to the physically sound basis; additionally, possibility of the model application toward the ER effect was briefly introduced in the earlier work. If the previous work (Moon, 1998) was devoted to the stochastic mixing model development for the closure of the turbulent molecular mixing term, the present work is an extension of the model's application toward the fluctuation of ER. Objectives of this study are to check the validity range of mixing models, and to analyze whether ER fluctuations produce an important effect on the combustion process. In the sections 2 and 3, modeling procedure accounting for the ER fluctuation in a simple global reaction is introduced, followed by the results of mixing models that are compared with DNS results in the section 4. A critical examination of the results obtained in the section 4 indicates possible improvement of the modeling.

2. Reaction Rate Modeling for Imperfect Mixture

2.1 The proposed global reaction rate

Single-step irreversible chemical reaction of the type $F+vO \rightarrow P$ is adopted with the following reaction rate:

$$\dot{\omega}_F = -kY_F Y_O (T-T_0)^5 \quad (1)$$

where k is a constant, v, the mass stoichiometric coefficient, and T_0 the initial temperature ($T > T_0$). Note that the usual exponential part in Arrhenius form is replaced by the power law. Defining a coupling parameter Z as $Z = Y_F - \frac{1}{v} Y_O$ and with the assumption of equal mass diffusivity between F and O, Z is a conserved scalar for which the following relation holds:

$$\dot{\omega}_Z = \dot{\omega}_F - \frac{1}{v}\dot{\omega}_0 = 0 \quad (2)$$

From Shvab-Zeldovich energy equation with unity Le number, and assuming constant c_p in an isenthalpic flow, the mixture enthalpy h is also a conserved scalar leading Eq. (1) to be a function of Y_F, Z and h/c_p. Defining $\dot{\omega}_c = \dot{\omega}_F / Y_{FM}$ and $c = Y_F / Y_{FM}$, the Eq. (1) can be written as follows:

$$\dot{\omega}_c = -kY_{FM}(\Delta T Y_{FM})^5 c\left(c - \frac{Z}{Y_{FM}}\right)(1-c)^5 \quad (3)$$

where Y_{FM} is the maximum fuel mass fraction in the mixture, and c the progress variable having the value between 0 and 1. The term $kY_{FM}{}^6 \Delta T^5$ that depends on the chemical kinetic is modeled under the form Cst/τ_c in a way that τ_c, the chemical characteristic time is the inverse of the integral of reaction rate for the domain of the progress variable (see Borghi (1985b) for details)

$$\frac{1}{\tau_c} = \int_{-\infty}^{+\infty} \dot{\omega}_c dc \quad (4)$$

To rely the effect of ER fluctuation on the reaction rate, we set $\phi = Z/Y_{FM}$ and Eq. (3) finally becomes

$$\dot{\omega}_c = -(kY_{FM}{}^6 \Delta T^5)\, c(c-\phi)(1-c)^5 \quad (5)$$

If the flame is perfectly premixed, ϕ will be constant in space. Furthermore, ϕ will be equal to zero when stoichiometry is considered, i.e., the equivalence ratio of the flow field will be equal to 1 with no spatial fluctuation in the field. We then obtain for the reaction rate

$$\dot{\omega}_c = -(kY_{FM}{}^6 \Delta T^5)\, c^2 (1-c)^5 \quad (6)$$

For more complete descriptions of the appro-

ach used here, the work of Moon (1991) should be consulted.

2.2 Generation of initial ER field

Let us define the ER as $\varphi = vY_F/Y_O$ where v is the stoichiometric coefficient based on mass of the global reaction. ϕ then can be represented as:

$$\phi = \frac{Z}{Y_{FM}} = \times \frac{Y_F}{Y_{FM}} - \frac{Y_F}{Y_{FM}} \frac{1}{\varphi} \tag{7}$$

and, we end up to a simple relation between ϕ and ER,

$$\phi = c\left(1 - \frac{1}{\varphi}\right) \tag{8}$$

where ϕ becomes a parameter describing the extent of ER. Note that the parameter ϕ is conserved during combustion, and the value combined with the progress variable provides the local ER value. In order to impose fluctuations of ER in the flow field, the model requires the knowledge of the mean and the variance of ϕ. The link between ϕ and φ can be modeled as follows:

i) Usually the degree of mixture is defined before combustion, i.e., the statistics of ϕ at $t=0$ are necessary. This case corresponds to $c=1$, and it yields $\varphi_0 = (1-\phi_0)^{-1}$ where the subscript 0 refers to the initial state. We can then relate ϕ with φ by

$$\overline{\varphi_0'^2} = \int_{-\infty}^{+\infty} \left(\frac{1}{1-\phi_0} - \bar{\varphi}_0\right)^2 P(\phi_0)\, d\phi_0 \tag{9}$$

$$\bar{\varphi}_0 = \int_{-\infty}^{+\infty} \frac{P(\phi_0)}{1-\phi_0}\, d\phi_0 \tag{10}$$

with the probability density function of ϕ at the initial stage, $P(\phi_0)$.

ii) Meanwhile, if the fluctuation of ER is weak, there exists a direct link between $\overline{\phi}$ and $\bar{\varphi}$ as well as between $\overline{\phi'^2}$ and $\overline{\varphi'^2}$. From the relation $\phi_0\varphi_0 = \varphi_0 - 1$, we can derive

$$\overline{\phi} = \frac{\bar{\varphi}_0 - 1}{\bar{\varphi}_0} \quad \text{and} \quad \overline{\phi_0'^2} = \left(\frac{1-\overline{\phi}}{\bar{\varphi}_0}\right)^2 \overline{\varphi_0'^2} \tag{11}$$

neglecting the second order term. If $\overline{\phi}=0$ (stoichiometry), this will lead $\bar{\varphi}=1$ and $\overline{\phi'^2} = \overline{\varphi'^2}$. In other words, depending on the values of $\overline{\phi}$ and $\overline{\phi'^2}$, one may simulate the required intensity of ER fluctuation. Figure 1 shows the domain of existence of the joint PDF, $P(c, \phi)$, which does not cover the whole plan (c, ϕ). The maximum allowable value of ϕ is unity while α defined as

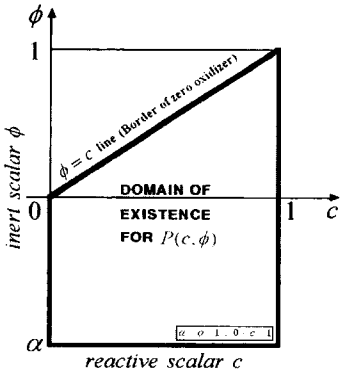


Fig. 1 The allowed domain of existence for the joint PDF of reactive species and ER, $P(c, \phi)$: $\alpha < \phi < 1$, $0 < c < 1$

$$\alpha = -\frac{Y_{OM}}{vY_{FM}} \tag{12}$$

is the minimum value of ϕ allowed in the mixture. Y_{OM} is the maximum mass fraction of oxidizer in the mixture, e.g., for air, Y_{OM} would be around 0.23. The line $\phi = c$ represents the border when $Y_O = 0$. This implies that ϕ cannot be greater than c; otherwise this causes the value of Y_O to be negative. Figure 2 shows the isoprobability line of the joint PDF, $P(c, \phi)$, at initial stage calculated by DNS where the fluctuation of ER is taken into account with an imposed value of $\overline{\phi}_0 = 0.0$ and $\overline{\phi_0'^2} = 0.015$. These values correspond to $\bar{\varphi}_0 = 1$ and $\overline{\varphi_0'^2} = 0.015$ which are the mean ER and variance of ER, respectively. The fluctuation rate from the mean value will then be about 12% ($\sqrt{\overline{\phi_0'^2}} \cong 12$ %), and this condition is kept throughout the present work to satisfy the weak ER fluctuation assumption. Tests with $\overline{\phi_0'^2} = 0.025$ (representing 16% of deviation from the mean ER) did not show noticeable difference with respect to the case of $\overline{\phi'^2_0} = 0.015$ where a higher value than $\overline{\phi'^2_0} = 0.025$ would violate the weak ER fluctuation assumption. Besides, in Fig. 2, it should be noted that the line $\phi = c$ is not violated and that isoprobability lines are distributed with a certain extent from $\phi = 0$ line.

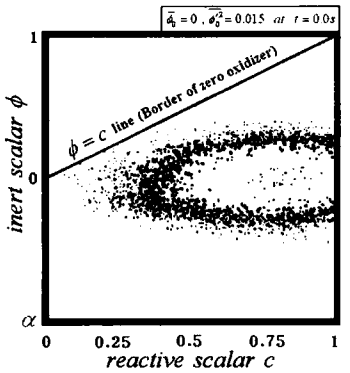


Fig. 2 Imposed fluctuations of equivalence ratio at the initial stage in the phase space (c, ϕ) represented by the isoprobability line (iso-PDF) of $P(c, \phi)$ from DNS. ($\bar{c}_0$=0.78, $\overline{c_0'^2}$=0.03, $\bar{\phi}_0$=0.0, $\overline{\phi_0'^2}$=0.015)

3. Given Flow Field

3.1 Governing equations

The field of interest is a statistically homogeneous and isotropic three-dimensional flow field where chemical reaction takes place between two scalars that are initially premixed with a certain degree of ER fluctuation. The turbulent intensity is decaying as time evolves ; we have imposed for the initial turbulent characteristic time, τ_t=2.0s with zero mean value for the velocity field. The gaseous turbulent mixture is generated with a randomly distributed local ER (more exactly ϕ) in order to initiate the effect of fluctuation triggered by the imperfection of the pre-mixture. The flow is assumed to have a constant density and be isenthalpic. The computational domain is a cubical box in an unconfined space in order to separate any interference that might influence the flow by the geometrical constraints. The field is computed concurrently by DNS and by PDF balance method for joint scalar PDF. The former solves instantaneous equations for continuity, Navier-Stokes and the conservation equations for the reactive species and ϕ (representing a scalar variable for ER) whereas the latter solves PDF transport equations (Pope, 1981) for c and ϕ with the use of mixing model (integral or binomial) for the unclosed small scale mixing term. The reason for adopting these two models is because the prediction capability of both the integral and binomial mixing models already have been validated for turbulent combustion (Valiño and Dopazo, 1990 ; Moon et al., 1997) with an acceptable fit with DNS data. The governing equations used in the DNS are the following instantaneous equations solved in the physical space :

$$\frac{\partial u_i}{\partial x_i}=0 \tag{13}$$

$$\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}=-\frac{1}{\rho}\frac{\partial p}{\partial x_i}+\nu\frac{\partial^2 u_i}{\partial x_j^2} \tag{14}$$

$$\frac{\partial c}{\partial t}+u_i\frac{\partial c}{\partial x_i}=D\frac{\partial^2 c}{\partial x_i^2}+\dot{\omega}(c) \tag{15}$$

$$\frac{\partial \phi}{\partial t}+u_i\frac{\partial \phi}{\partial x_i}=D\frac{\partial^2 \phi}{\partial x_i^2} \tag{16}$$

with a pseudo-spectral collocation method (see Picart et al. (1988) for details). The governing equations used in the PDF balance method are the following averaged equations (Eqs. 17 and 18) representing the evolution of the probability distribution of the reactive and inert scalars in the probability space.

$$\begin{aligned}&\frac{\partial P(C)}{\partial t}+\frac{\partial}{\partial x_i}\overline{u_i\delta(c-C)}\\&=-\frac{\partial}{\partial C}\overline{\left[\delta(c-C)\frac{\partial}{\partial x_i}\left(D\frac{\partial C}{\partial x_i}\right)\right]}\\&\quad+\frac{\partial}{\partial C}[-\dot{\omega}(C)P(C)]\end{aligned} \tag{17}$$

$$\begin{aligned}&\frac{\partial P(\Phi)}{\partial t}+\frac{\partial}{\partial x_i}\overline{u_i\delta(\phi-\Phi)}\\&=-\frac{\partial}{\partial C}\overline{\left[\delta(\phi-\Phi)\frac{\partial}{\partial x_i}\left(D\frac{\partial \Phi}{\partial x_i}\right)\right]}\end{aligned} \tag{18}$$

$P(C)$ is the PDF of the random variable C that can be generated from the progress variable c and from the single point fine grained density defined as $p(C\,;\,x,\,t)=\delta(c(x,\,t)-C)$ with the Dirac delta function δ. The instantaneous random scalar C stands for c in probability space, while random scalar Φ represents ϕ in probability space. These equations introduced in the field of classical turbulence were extensively used by Pope and Anand (1984) and Dopazo et al. (e.g., see Dopazo (1979)) for the inherent advantage,

in which the term containing the mean reaction rate appears in a closed form. The first term in the RHS is the molecular mixing term for the closure of which in this study integral and binomial mixing models are applied.

3.2 Models for small scale mixing term used in PDF transport equation

The integral model originally comes from the Coalescence-Dispersion model of Curl (1963) where mixing event is stochastically modeled. It assumes that two fluid particles with concentrations c_1 and c_2 will coalesce and disperse, giving two fluid particles to have the same concentration of the mean value between c_1 and c_2. This model provides the following equations:

$$\begin{cases} c_1(t+\Delta t)=[c_1(t)+c_2(t)]/2 \\ \quad \text{for } C_m\dfrac{\Delta tN}{\tau_t} \text{ particles out of } N \text{ particles} \\ c_2(t+\Delta t)=[c_1(t)+c_2(t)]/2 \end{cases} \tag{19}$$

to some of the randomly selected particles $C_m \frac{\Delta tN}{\tau_t}$. C_m is an empirical constant to be adjusted, and N, the total number of fluid particles (representing the total fine grained PDF). This widely used model, however, has disadvantage of physical non-relevance by the fact that the PDF of inert scalar does not relax to Gaussian distribution in decaying turbulence (Janicka, 1978). This unphysical characteristic led Valiño and Dopazo (1990) to introduce a binomial stochastic model whose inert PDF distribution relaxed to Gaussian distribution by the use of a binomially distributed discrete random variable. The stochastic mixing process is composed of two successive sub-processes where small scale mixing is simulated with the following equations:

$$c(t+\Delta t)=c(t)+\frac{1}{2}(\bar{c}-c)\,C_m\frac{\Delta t}{\tau_t} +\dot{\omega}(c)\Delta t \quad \text{for all N particles} \tag{20}$$

$$c(t+\Delta t)=\bar{c}+\xi_c\sqrt{<c'^2>} \quad \text{for } C_m\frac{\Delta tN}{\tau_t} \text{ particles} \tag{21}$$

where ξ_c is a binomially distributed variable. The same rule as shown above applies to ϕ without the reaction term. These two models are completely described in Moon et al. (1997) and Valiño and Dopazo (1990). Here, these models will be used to build a joint PDF, $P(c, \phi)$ that will be served for the present study on ER fluctuation.

4. Results and Discussion

The evolution of the joint $P(c, \phi)$ is concurrently simulated by both DNS and PDF balance method using Monte Carlo simulation. The reaction rate of Eq. (5) is taken with the following initial conditions for the reactive scalar and the inert scalar representing the distribution of ER:

$$\bar{c}=0.78,\ \overline{c'^2}=0.03,\ \bar{\phi}=0.0,\ \overline{\phi'^2}=0.015$$
$$\tau_t=2.0\text{s},\ \tau_c=0.5\text{s}$$

This corresponds to the case of stoichiometry ($\bar{\phi}=0$) with a given low intensity of fluctuating ER ($\overline{\phi'^2}=0.015$) in the spatial domain where initially the two scalars, c and ϕ are not correlated. Instead, we have prescribed randomly and independently distributed c and ϕ fields. The turbulent characteristic time starts from $\tau_t=2.0$s, and it will increase as time evolves since the field is subjected to free evolving turbulent field. Figure 3a to 3d show the isoprobability line formed by the joint PDF, $P(c, \phi)$ found by DNS for different times. At the early stage of combustion ($t=0.38$s), the cloud formed by $P(c, \phi)$ clearly shows that the particle c and ϕ are spread out in all the allowed domain of the mixture. Furthermore, note that at any given value of c, several ϕ particles are associated. This represents the spatial imperfection of the mixture. It can be seen that the joint PDF retracts in the direction of $\phi=0$ and elongates in order to concentrate toward $c=0$. Although the fluctuations of c and ϕ were initially set independent, the independency could not be kept, and a particular correlation appears. This evidence demonstrated by DNS results implies that the assumption of initial independency between c and ϕ might not be the best one for modeling the initial ER fluctuation field. These phenomena are, of course, primarily due to mixing for ϕ, and mixing and reaction for c.

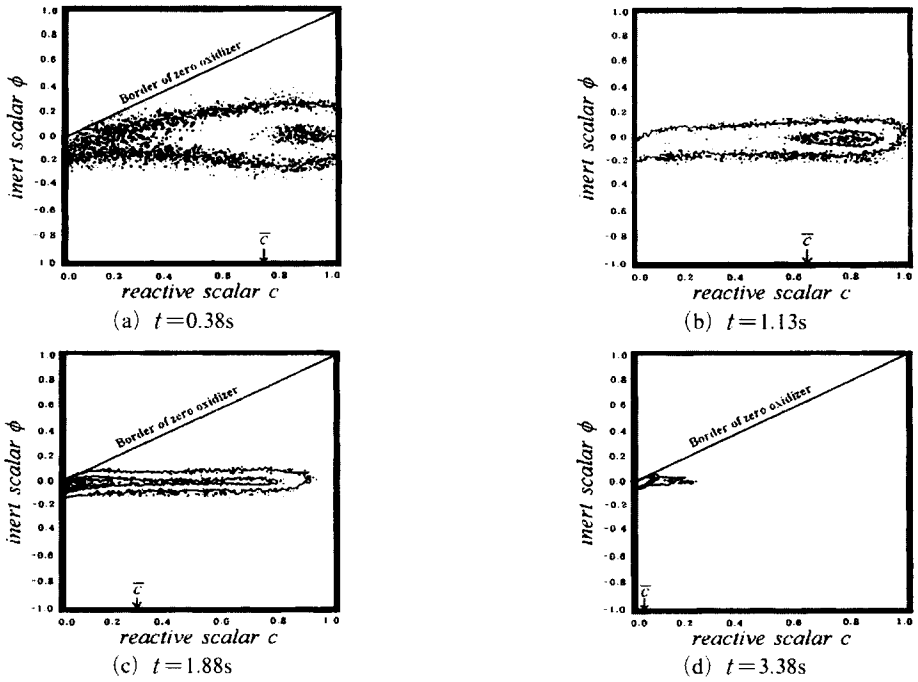


Fig. 3 Time evolution of the joint $P(c, \phi)$ evaluated by DNS during combustion from t=0.38s to t=3.38s

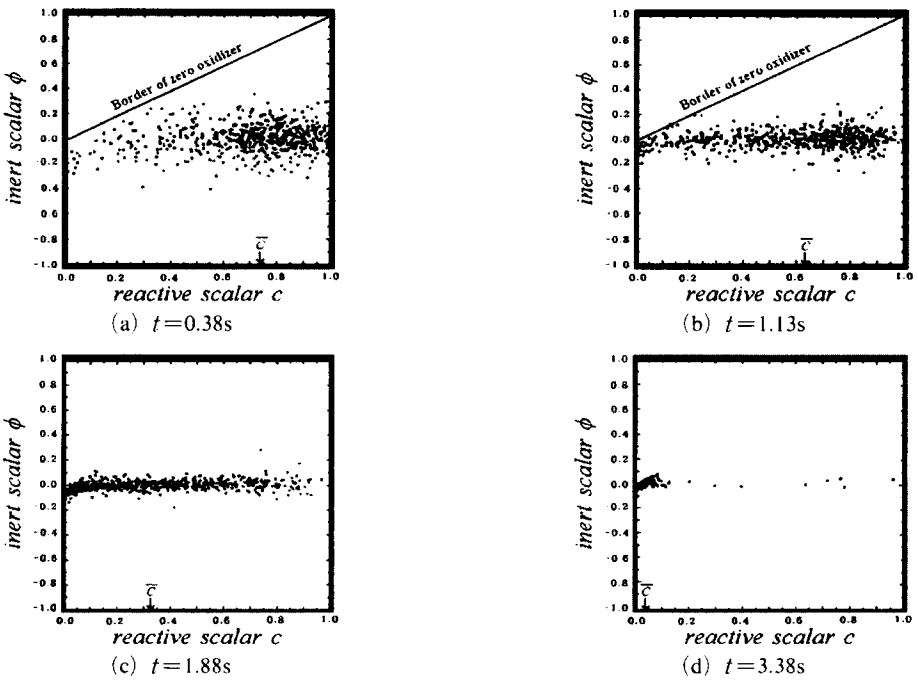


Fig. 4 Time evolution of the joint $P(c, \phi)$ evaluated by Monte Carlo particles using the integral model from t=0.38s to t=3.38s (The width of $P(c, \phi)$ is represented by the spreading of dots, while its height by the density of dots)

4.1 The sensibility of PDF balance method

$P(c, \phi)$ evolutions shown in Figs. 4 and 5 are computed by the Monte Carlo simulation with the integral model and with the binomial model, respectively. The width of $P(c, \phi)$ is represented by the spreading of dots, while the height of $P(c, \phi)$ is represented by the accumulation (density) of dots, which are regrouped in the phase space (c, ϕ). The dots represent the position of stochastic particles used in the mixing model where for this study 10,000 sampled fine grained PDFs are considered. The joint PDF evaluated by these models respects well the bounds of c and ϕ, and furthermore, shows a time evolution that is very close to the evolution calculated by the DNS. In addition, it should be noted that the site where

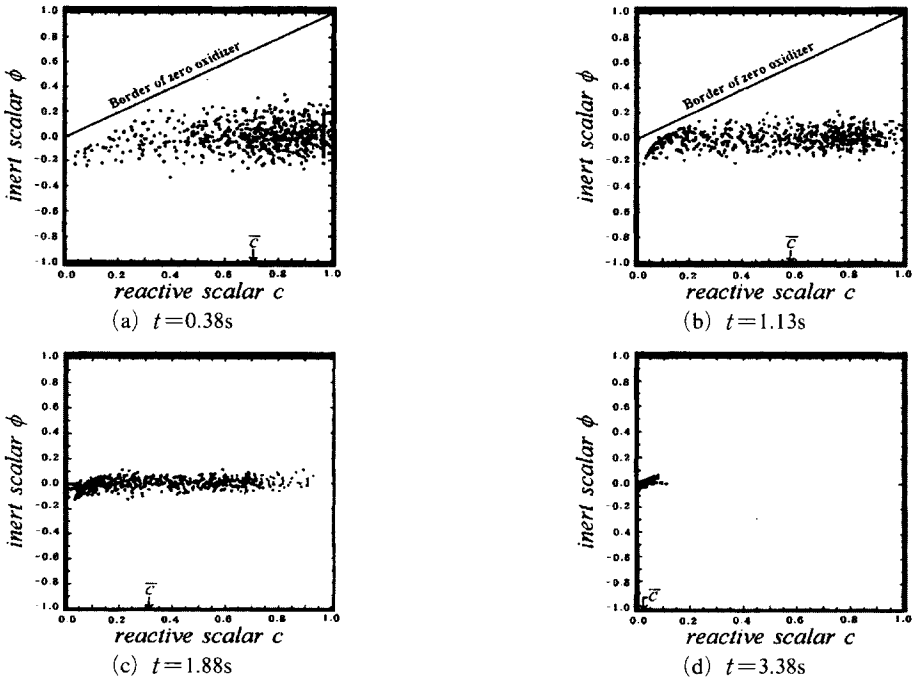
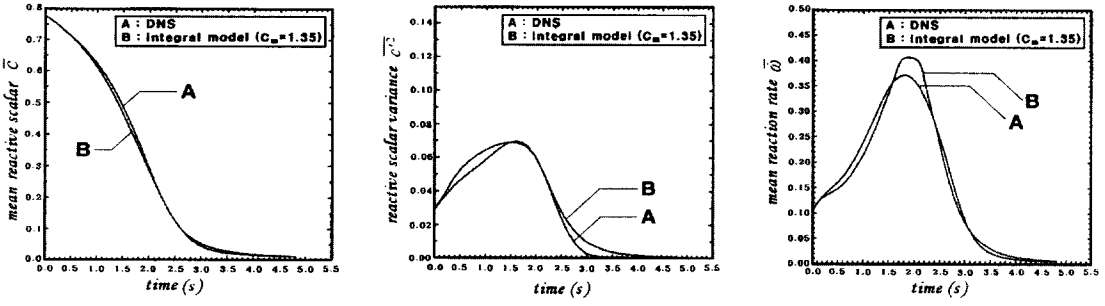
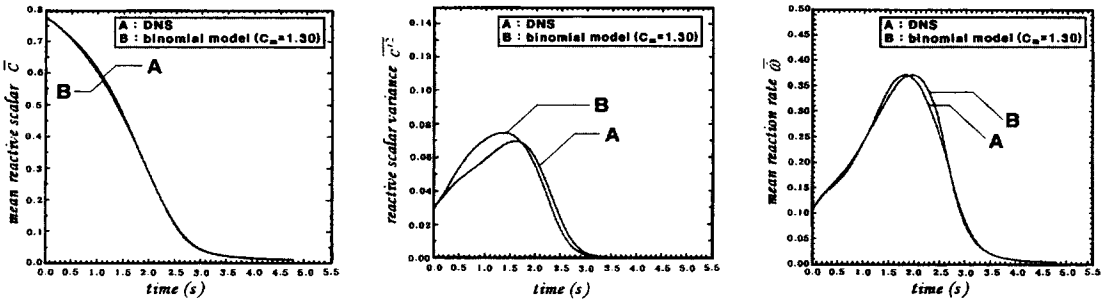


Fig. 5 Time evolution of the joint $P(c, \phi)$ evaluated by Monte Carlo particles using the binomial model from t=0.38 s to t=3.38s (The width of $P(c, \phi)$ is represented by the spreading of dots, while its height by the density of dots)



(a) Decay of mean reactive scalar (b) Time evolution of scalar variance (c) Time evolution of mean reaction rate

Fig. 6 Comparisons of statistical moments between DNS and PDF balance method using integral model for c_m=1.35 in the event of ER fluctuation (A : DNS data, B : Monte Carlo simulation with integral model)



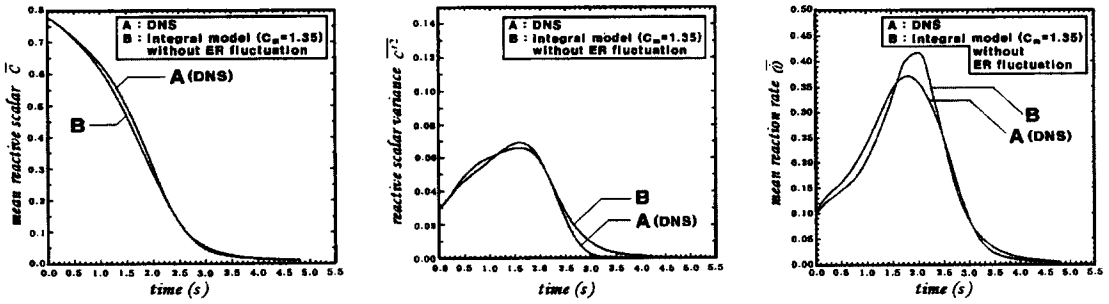
(a) Decay of mean reactive scalar (b) Time evolution of scalar variance (c) Time evolution of mean reaction rate

Fig. 7 Comparisons of statistical moments between DNS and PDF balance method using binomial model for C_m=1.30 in the event of ER fluctuation (A : DNS data, B : Monte Carlo simulation with binomial model)

dots are concentrated matches to that of high isoprobability line of DNS within the acceptable range. In view of this fact, the advantage of PDF balance method can be clearly seen if we refer to the "Presumed" PDF method (for instance, see Borghi (1988) and Moon et al. (1992)) whose modeled probability distribution cannot build such a sophisticated PDF shape. To investigate quantitative behavior of the PDF balance method, statistics of c, ϕ and the reaction rate are reviewed in Figs. 6 and 7. Figure 6 and 7 show the comparisons of the evolution of the statistical moments between DNS and Monte Carlo simulation using the integral model and the binomial model, respectively. While Figs. 6a and 7a show the decrease of the mean progress variable (first moment) during combustion for the two mixing models, Figs. 6b and 7b show the time evolution of the variance (second moment) predictions of which are not as precise as those of the first moment. This also applies to the time evolution of the mean reaction rate prediction (Figs. 6c and 7c). Though in the mixing model, an empirical constant C_m is engaged and trimmed for fitting the DNS evolution, it is remarkable that the results of the PDF balance method demonstrates good agreement with the DNS results in this study where local ER fluctuation is considered. In fact, this agreement with DNS was not really expected even though models predicative capability previously demonstrated in the earlier work of Moon (1998) showed good comparisons with much simpler reaction rate without the effect of ER. Based on the above analysis, we can partially conclude that extensions of these models to the case of imperfectly premixed flame pose no significant problem. The best concordance was found with the value of the constant, C_m=1.35 for the integral model, and C_m=1.3 for the binomial model.

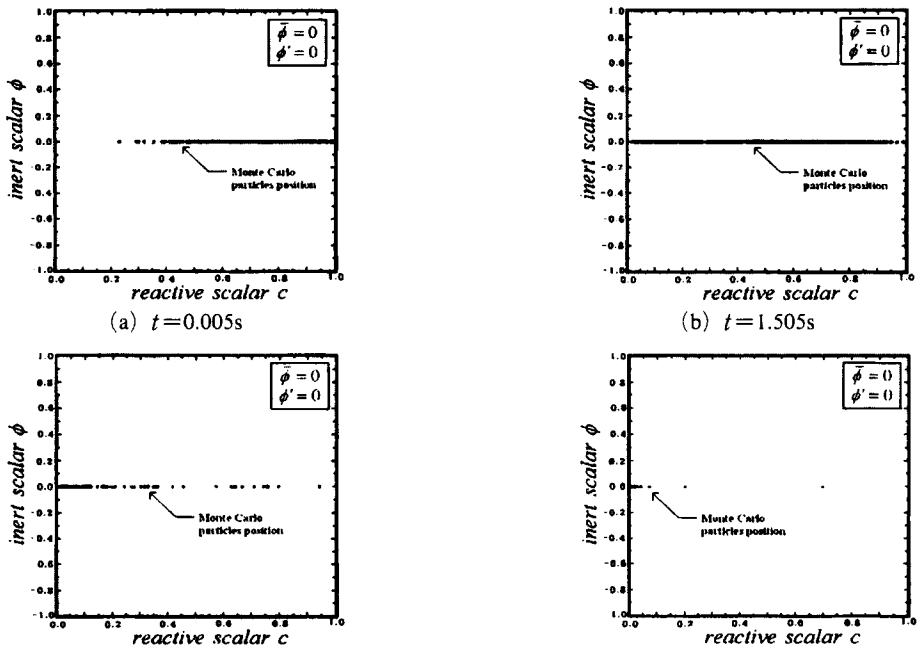
4.2 The ER fluctuation effect

It would be interesting now to see whether the existence of ER fluctuation distributed at every local point has a notable impact on the global characteristics of turbulent combustion. For this, time evolutions of $\bar{c}$, $\overline{c'^2}$ and $\bar{\omega}$ calculated by both the DNS and PDF balance method in the case of ϕ=0 (zero fluctuation of ER) for all particles are presented in Figs. 8a, 8b and 8c, respectively. This is the case of stoichiometry without any instantaneous ER fluctuation in the whole domain of the flow field where the reaction rate corresponds to the one presented in Eq. (6). Considering the sensibility of models, evolutions computed by Monte Carlo method with stochastic model (integral model) compared quite well the DNS evolution as expected. Meanwhile, comparisons of DNS results observed between Figs. 8 and 6 were unattended. It turns out that results of DNS shown in Fig. 8 ($\bar{\phi}$=0, $\overline{\phi'^2}$=0) are nearly identical to the DNS results shown in Fig. 6 ($\bar{\phi}$=0, $\overline{\phi'^2}$ ≠0) which takes into account the presence of ER fluctuations (ϕ≠0 in the spatial domain). In-



(a) Decay of mean reactive scalar (b) Time evolution of scalar variance (c) Time evolution of mean reaction rate

Fig. 8 Comparisons of statistical moments between DNS and PDF balance method using integral model without ER fluctuation (A : DNS data, B : Monte Carlo simulation with integral model)



(a) t=0.005s (b) t=1.505s

(c) t=3.005s (d) t=4.505s

Fig. 9 Time evolution of the joint $P(c, \phi)$ evaluated by Monte Carlo particles using the integral model without ER fluctuation (note : Monte Carlo particles position are concentrated on the line, ϕ=0)

deed, the time evolution of the mean reaction rate, the mean scalar decay or even the rms of scalar responded very slightly to the fluctuation of ER. This observation is beyond our expectation since a significant difference was somewhat anticipated. To verify results of Fig. 8, the time evolution of the joint PDF $P(c, \phi)$ for $\bar{\phi}$=0 and $\overline{\phi'^2}$=0 is plotted in Fig. 9. It is clearly seen that the joint PDF respects the initial condition ϕ=0 during the whole time, and keeps the uni-dimensional distribution. As a consequence, the local fluctuations of equivalence ratio that exist in the spatial domain have negligible influence on the global mean combustion characteristics ($\bar{c}$, $\overline{c'^2}$, $\bar{\omega}$), at least, in the case when scalar c and ϕ are independently distributed at the initial phase. To analyze the reason of these resemblances between Figs. 6 and 8, the mean of $\dot{\omega}_c$ described in Eq. (5)

is decomposed as follows:

$$\overline{\dot{\omega}_c}(c,\phi) = -\overline{\frac{Cst}{\tau_c} c(c-\phi)(1-c)^5} = -\frac{Cst}{\tau_c}\left[\overline{c^2(1-c)^5} - \bar{\phi}\,\overline{c(1-c)^5} - \overline{c\phi'(1-c)^5}\right] \quad (22)$$

In the third term at the RHS, the term $\overline{c\phi'(1-c)^5}$ povides the cause of the similitude found between Figs. 6 and 8. This is because independency (hence uncorrelation) between c and ϕ leads the third term to vanish. Whether ϕ' exists or not, Eq. (22) becomes the mean of Eq. (6) as far as the flow field keeps the stoichiometry condition ($\bar{\phi}=0$). This fact implies that a certain degree of correlation between the combustible and ER at the initial phase should be taken into account before combustion for more concrete analysis of the imperfection of mixture.

5. Conclusions and Perspective

This work is devoted to the modeling of local equivalence ratio fluctuation in an imperfectly premixed turbulent flame existing in a generic combustor. Numerical analysis using DNS and modeled PDF transport equation is conducted in order to clarify these instantaneous fluctuation effects on the global combustion characteristics. The main objective of this work is to evaluate the effect of ER fluctuation that usually exists on a small scale basis in the spatial domain, and that may have a considerable influence on turbulent combustion interactions. Concurrently, two small scale mixing models in the context of the PDF approach have been proposed for predicting the local ER effect. It was found that the integral as well as the binomial model used for the closure of the small scale mixing term of the PDF transport equations can be extended from the previous work that dealt simple reaction rate without local ER effect. The models were tested by comparisons with DNS data; the joint PDF of reactive scalar and ER, $P(c, \phi)$, found by mixing models showed realistic agreement with DNS, and offered a good prediction capability for the mean reaction rate as well as for the scalar variance. Meanwhile, present numerical studies revealed that local fluctuations of equivalence ratio existing in the spatial domain have minor effect on the global mean combustion characteristics when zero correlation between c and ϕ is imposed. Results from DNS showed that the assumption of independent spatial distribution between the initial concentrations of fluctuating fuel and oxidizer is not sufficient to demonstrate any notable influence on the mean progress variable and the mean reaction rate. These observations led us to conclude that the initial ER fluctuation field should be linked to the initial reactive scalar field in a way that the local fuel concentration must be correlated to the local equivalence ratio. This conclusion is quite realistic when the equivalence ratio is not homogeneous in the pre-mixture, and thus demands additional investigation for correlated case. These studies are in progress, and further works on local ER effect with rich and lean cases besides stoichiometry are also anticipated in the near future.

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