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Study of stochastic mixing models for combustion in turbulent flows

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Abstract

This study evaluates several mixing models for the prediction of combustion within a Partially Stirred Reactor (PaSR). The models considered are the Interaction by Exchange with the Mean (IEM) model, the extended IEM, Langevin and extended Langevin models. The degree of mixing and of reaction and their influence on the thermochemical properties in a combustion process are investigated. Since these mixing models involve stochastic terms, their implementation is performed by the Monte Carlo method using numerical schemes which solve the stochastic differential equations.

This study consists, first, on the presentation and assessment of those mixing models in a situation in which a single scalar field is considered in the presence of a homogeneous and isotropic turbulent field. The evolution of the probability density function and the main properties for a single scalar field are studied for each mixing model. Numerical results are compared with direct numerical simulation, showing excellent qualitative and quantitative agreements.

Then, the mixing models are used for numerical simulation of a PaSR where the mixing and reactive processes occur. The PaSR is used to assess the mixing model influence on the thermochemical properties of the mixture in a premixed combustion process, which is modeled using a reaction progress variable. The results obtained with the different mixing models are compared in several operating regimes of the PaSR showing that, when mixing is fast and reaction is intense, the different models lead to similar results. However, when mixing is slow and reaction is mild, important differences are observed between the models' results.

Keywords: Partially stirred reactor; Probability density function; Stochastic differential equations; Monte-Carlo technique

1. Introduction

One of the most important challenges in the study of combustion in turbulent flows is the development of models that are able to accurately describe the interaction between chemical reaction, turbulence and mixing. When models that consider the transport of the Probability Density Function (PDF) of the flow properties are used,

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the chemical production term appears in closed form, however, micro-mixing requires closure assumptions [1,2], since the underlying physical process governing mixing cannot be described by single-point statistical techniques.

In the past decades, several models were proposed and used in order to represent this mixing process, ranging from the classical Curl [3] and Interaction by Exchange with the Mean (IEM) [4,5] models, to more elaborate ones, such as Langevin models [1,6], the Mapping Closure Mode model [7], models based on Euclidean minimum spanning trees [8] or on reference scalar fields [9]. More recently, Sabel'nikov and Gorokhovski [10] have proposed new scalar stochastic mixing models. The extended IEM model substitutes the single time scale used on the IEM model by a stochastic description of the frequency of the turbulent motion, thus allowing for a relaxation of the PDF of an inert scalar to a shape which is different from the initially prescribed one. The Langevin model includes a PDF dissipation term to the IEM model PDF transport equation which leads to a decorrelation of phase space trajectories while ensuring the boundedness of the scalar. Finally, the extended Langevin model incorporates the turbulent frequency description of the extended IEM (EIEM) model to the Langevin model. Note that the IEM model can be viewed as limiting case of these stochastic models. These new mixing models have been evaluated against Direct Numerical Simulation (DNS) data [11,12], but only the EIEM model has been successfully compared to other models in a combustion situation [13].

The present work is devoted to the study of the stochastic scalar mixing models developed by Sabel'nikov and Gorokhovski [10] in a simple system which is representative of the practical application of such models, i.e., the Partially Stirred Reactor (PaSR). In this system, the outcome of the combustion process is governed by the competition between the characteristic time scales of chemical reaction, mixing and the residence time of the gases within the PaSR. Since an analytical solution is available only for the case of the IEM model [14], and the direct solution of the corresponding PDF transport equation meets with difficulties associated to the specification of boundary conditions and to the stiffness of the chemical source term, the equivalent system of stochastic differential equations (SDE) is solved. This solution is achieved using a classical Monte-Carlo technique. However, since both the chemical source term and the PDF diffusion term involve non-linearities, a new, fully implicit, numerical method is used for the discretisation of the SDE system [15]. The solutions obtained for the case of the decay of an inert scalar are compared to Direct Numerical Simulation (DNS) data [16]. Then, the steady-state PDF of the reactive scalar within the PaSR is analyzed in situations corresponding to fast mixing and reaction and to slow mixing and reaction. Finally, a parametric study of the influence of the characteristic times of mixing and chemical reaction and of the model parameters on the averaged scalar properties within the PaSR is presented.

2. Mathematical formulation

This section describes the mathematical formulation for the reactive scalar transport within a PaSR where an exothermical chemical reaction and mixing occur between reactants and combustion products. The chemical process is described by a single-step Arrhenius reaction involving a single scalar field, the reaction progress variable, $c = (T - T_0)/(T_{ad} - T_0)$, where T, T_0 and T_{ad} are the temperature, the reactor inlet temperature and the adiabatic combustion temperature, respectively.

The stochastic mixing models considered in this work are the Interaction by IEM model and the models recently developed by Sabel'nikov and Gorokhovski [10], i.e., the Extended IEM (EIEM) model, the Langevin Model (LM) and the Extended Langevin Model (ELM). The transport equation of the joint Probability Density Function (PDF) of the reactive scalar and of the logarithm of the turbulent frequency, χ, reads

$$\begin{aligned}\frac{\partial P_{c,\chi}(\theta,\varphi;t)}{\partial t^*} &= \left[\delta(\theta)P_{0,\chi} - P_{c,\chi}(\theta,\varphi;t)\right] \\ &+ \mathscr{L}\left\{\frac{\partial}{\partial\theta}\left[a\Omega e^{\varphi}(\theta - \langle c \mid \varphi\rangle)P_{c,\chi}(\theta,\varphi;t)\right]\right. \\ &+ \frac{\partial^2}{\partial\theta^2}\left[b\Omega e^{\varphi}\theta(1-\theta)P_{c,\chi}(\theta,\varphi;t)\right] \\ &+ \frac{\partial}{\partial\varphi}\left[C_\chi(\varphi - m_1)P_{c,\chi}(\theta,\varphi;t)\right] \\ &+ \left.\frac{\partial^2}{\partial\varphi^2}\left[C_\chi m_2 P_{c,\chi}(\theta,\varphi;t)\right]\right\} \\ &- \mathscr{Y}\frac{\partial}{\partial\theta}\left[\dot{\mathscr{S}}(\theta)P_{c,\chi}(\theta,\varphi;t)\right], \end{aligned} \quad (1)$$

where, $t^* = t/\tau_r$ is the non-dimensional time, τ_r is the residence time of the mixture within the PaSR. The sample space variables of c and χ are θ and φ, respectively. In this equation, the left-hand side represents the transient evolution of the joint PDF $P_{c,\chi}$. The logarithm of the turbulent frequency, χ, is described by an Orstein–Uhlenbeck stochastic process [17,18]. The entrance–exit processes of the gases are represented by the first and second terms of the right-hand side. Note that the fresh gases that enter the reactor are characterized by an initial distribution of turbulence frequency, $P_{0,\chi}$. The remaining terms describe, in order, the diffusive–dissipative process of c and χ and the chemical source term, which is given by

$$\dot{\mathscr{S}}(c) = (1-c)\exp\left(\beta\frac{c}{c+1/\alpha}\right), \tag{2}$$

where $\alpha = (T_{ad} - T_0)/T_0$ is the reduced heat of reaction and $\beta = E/RT_0$ is the reduced activation energy. The ratio between the mean residence time and the characteristic turbulence time is $\mathscr{Z} = \tau_r/\tau_t$. Hence, for a value of $\mathscr{Z} \to \infty$ the Perfectly Stirred Reactor (PSR) is obtained. In the case when $\mathscr{Z} = 0$, mixing is absent and the steady solution of the PaSR is reduced to an ensemble of Plug Flow Reators (PFR). When $\mathscr{Z}$ is finite, fast mixing cases are those for which the value of the averaged reaction progress variable within the PaSR is close to that obtained within the PSR whereas, for slow mixing, large deviations from the PSR behavior are observed. The parameter $\mathscr{Y} = \tau_r/\tau_c$ represents the Damköhler number based on the residence time and the characteristic time scale of the chemical process, $\tau_c \propto \exp(\beta)$ [14]. Note that the usual definition of the Damköhler number is $Da = \tau_t/\tau_c = \mathscr{Y}/\mathscr{Z}$. The limit $\mathscr{Y} \to \infty$ correspond to chemical equilibrium, when reaction is intense, whereas the mild reaction regime is obtained as $\mathscr{Y} \to 0$. The values of a, b and Ω are given by

$$a = 1 + d_0\frac{\langle c(1-c) \mid z\rangle}{\sigma_M^2}, \tag{3}$$

$$b = d_0\frac{\langle c^2 \mid z\rangle - \langle c \mid z\rangle^2}{\sigma_M^2}, \tag{4}$$

$$\Omega = \frac{\sigma^2\mathscr{X}}{\langle z(\langle c^2 \mid z\rangle - \langle c \mid z\rangle^2)\rangle}, \tag{5}$$

where $\mathscr{X} = \tau_r/\tau_m$, $\tau_m^{-1} = \langle\omega_c\rangle$ is the average scalar mixing frequency. In Eqs. (3)–(5), z represents the stochastic model of the non-dimensional turbulent frequency

$$z = \tau_r\langle\omega\rangle e^{\chi} = \mathscr{Z}e^{\chi}, \tag{6}$$

where ω and $\langle\omega\rangle$ are the turbulent frequency and its mean. Note that ω is described by a log-normal distribution [18]. It can be shown that $\langle\omega_c\rangle = \Omega\langle\omega\rangle$, and thus $\mathscr{X} = \Omega\mathscr{Z}$ [11]. In addition, in Eq. (1), m_1 and m_2 are the mean and the variance of the stochastic process φ, and $C_\chi = 1.6$ [18,11]. Since χ is normally distributed, $m_1 = -m_2/2$. Yeung and Pope [19], based on DNS results, propose $m_2 = 0.29\ln Re_\lambda - 0.36$, for $38 \leqslant Re_\lambda \leqslant 96$, where Re_λ is the Reynolds number based on the Taylor length scale. The correct decay of the scalar variance, $\sigma^2 = \langle\theta - \langle c\rangle\rangle^2$, coherent with exact equation in the homogeneous turbulence case [11], $\sigma^2 = \sigma_0^2\exp(-2\langle\omega_c\rangle t)$, is ensured by the choice of Ω in Eq. (5). Finally, $\sigma_M^2 = \langle c\rangle(1-\langle c\rangle)$ is defined as the maximum value of the scalar variance and d_0 is a constant which controls the relaxation rate of the PDF [11,12]. In the chemically inert case, the PDF evolution at large times is independent of d_0.

The set of Eqs. (1)–(5) represents the generalized case in the formulation of the stochastic mixing models to be considered in this work. Note that if one choses to use $d_0 = 0$ the third term of the right-hand of Eq. (1) vanishes and the Extended IEM model is obtained. When the PDF of the stochastic variable ω is $P(\omega) = \delta(\omega - \langle\omega\rangle)$, one obtains $\chi = 0$, $\Omega = 1$, and thus $\mathscr{Z} = \mathscr{X}$ [11,12]. In addition, the conditional means in Eqs. (3)–(5) are reduced to inconditional ones, consequently, the fourth and fifth terms on the right-hand side of Eq. (1), which describe the PDF evolution in frequency space, are removed and the Langevin model (LM) is recovered. Finally, if simultaneously $d_0 = 0$ and $z = cte$, it is possible to obtain the PaSR model that obeys the classic IEM model [14].

These mixing models (EIEM, LM and ELM) respect the boundedness property. In the case of the Langevin models, this property is enforced through the limiting function $\theta(1-\theta)$ as a factor of the PDF diffusion term.

The PDF transport equation used in this work, Eq. (1), doess not have a known analytical solution, with the exception of the case when the IEM model is adopted [14]. Furthermore, contrarily to the chemically inert case, where a direct numerical solution of this equation has been obtained [11], the chemical source term poses difficulties in specifying boundary conditions at the vicinity of $c = 1$ [14]. Therefore, the classical technique of solving the equivalent stochastic differential equation (SDE) system in accordance with the Itô representation is adopted [17]

$$dc = \left[-\mathscr{Z}a\Omega e^{\chi}(c - \langle c \mid \chi\rangle) + \mathscr{Y}\dot{\mathscr{S}}(c)\right]dt^* + \left[2\mathscr{Z}b\Omega c(1-c)\right]^{1/2}dW_c, \tag{7}$$

$$d\chi = -\mathscr{Z}C_\chi(\chi - m_1)dt^* + \left(2\mathscr{Z}C_\chi m_2\right)^{1/2}dW_\chi, \tag{8}$$

where dW_c and dW_χ are independent variations of c and χ that obey a standard Wiener process with zero mean and variance equal to dt [17]. The initial condition for these equations are fresh gases ($c = 0$) and a turbulent frequency ω which is either constant and equal to $\langle\omega\rangle$, in the case of the IEM and the LM, or log-normally distributed, i.e., χ is prescribed as having a normal distribution, when extended models (EIEM and ELM) are used.

3. Numerical method of solution

Equations (7) and (8) are nonlinear SDE that represent the evolution of c and χ within the PaSR. This nonlinearity is associated both to the stochastic mixing and to the chemical source terms. The numerical solution of this system requires the use of numerical methods that may cope with stiff stochastic differential equations. Classical time-explicit integration schemes, such

as the Euler–Maruyama [17], are not adequate choices, since boundedness of the scalar field cannot be guaranteed.

The numerical scheme considered in this work for the solution of Eqs. (7) and (8) is the Implicit Milstein Taylor Method [15]. The general formulation of a stochastic differential equation describing the evolution of a variable, ϕ subjected to a one dimensional Wiener process, using the Itô representation, is [17]

$$\begin{aligned} &\mathrm{d}\phi(t) = A[\phi(t),t]\,\mathrm{d}t + B[\phi(t),t]\,\mathrm{d}W, \\ &\phi(t_0) = \phi_0, \quad t \in [t_0, T], \end{aligned} \tag{9}$$

where $A[\phi(t),t]$ and $B[\phi(t),t]$ are the drift and the diffusion coefficients, respectively, and $\mathrm{d}W$ is the increment of a Wiener process. The discretized form of Eq. (9) using the Implicit Milstein Taylor Method [15] reads

$$\begin{aligned} \phi_{n+1} = \phi_n + A\left[\phi_{n+1}, t_{n+1}\right]\Delta t + B\left[\phi_{n+1}, t_{n+1}\right]\Delta W_n \\ - \frac{1}{2}(BB')\left[\phi_{n+1}, t_{n+1}\right]\left[(\Delta W_n)^2 + \Delta t\right], \end{aligned} \tag{10}$$

where $B' = \mathrm{d}B/\mathrm{d}\phi$, Δt and ΔW_n represent the time and discretized Wiener process increments, respectively, and the subscripts n and $n+1$ denote successive times. This method, which is implicit both on the drift and the diffusion terms and exhibits a strong convergence of order 1, is also adopted due to its good stability properties, when compared to other numerical methods available for the solution of SDEs [15], and because of the simplicity in its implementation. This is the first known implementation of the Implicit Milstein Taylor Method for the solution of a combustion problem. Equations (7) and (8), discretized using Eq. (10), are solved by a classical Monte-Carlo technique [1]. At each time-step fresh gases enter the reactor. The value of turbulent frequency of the incoming gases is either $\langle\omega\rangle$, in the case of the IEM model and the LM, or, when extended models are used, prescribed according to a log-normal distribution with given values of m_1 and m_2.

4. Results and discussion

In this section are presented and discussed the results obtained with the different stochastic mixing models. First, a pure mixing situation is considered. Then, an analysis of the evolution of the probability density function of the reactive scalar within the PaSR is presented for two representative situations, i.e., fast mixing and reaction and slow mixing and reaction. Finally, a parametric study of the influence of the controlling parameters of the models on the first two moments of the PDF is presented.

4.1. Scalar mixing in homogeneous turbulence

This section presents the results obtained for the chemically inert case, i.e., $\mathscr{Y} = 0$ in Eq. (1), considering the different mixing models [10], which have been solved in the case of the decay of a homogeneous turbulence passive scalar field. In such a case, the reactor is closed and thus the entrance–exit term in Eq. (1) vanishes. The initial PDF considered is a Beta function with average $\langle c\rangle = 0.5$ and variance, $\sigma^2 = 0.15$, the value of Re_λ adopted is 50. This distribution, generated with 4^7 stochastic particles, represents the PDF of the Direct Numerical Simulation of Eswaran and Pope [16], which was used by Soulard et al. [11] as basis of comparison for their direct solution of the PDF transport equation. In order to allow for such a comparison, the scalar dissipation rate, $\langle\varepsilon_c\rangle$, was prescribed using the evolution obtained by Eswaran and Pope [16] and, instead of Eq. (5), Ω reads

$$\Omega = \frac{\langle\varepsilon_c\rangle}{\left\langle \omega\left(\langle c^2 \mid \omega\rangle - \langle c \mid \omega\rangle^2\right)\right\rangle}. \tag{11}$$

In Fig. 1 are presented comparisons of the PDF evolution obtained with the LM, EIEM and the ELM models with the results obtained by Eswaran and Pope [16] by means of DNS. The chosen value of d_0 for the Langevin models (LM and ELM) is 1.0. These results shows a good agreement, during the early stages of mixing, among

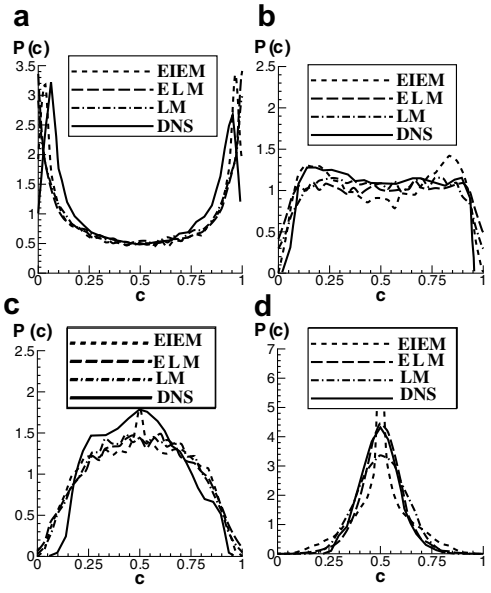

Fig. 1. Comparisons of PDFs of a modelled scalar with the DNS results. $(\langle\omega\rangle t, \sigma/\sigma_0) = (0.22,\ 0.99)$ (a); (1.49, 0.73) (b); (2.11, 0.55) (c) and (3.47, 0.27) (d). The initial PDF is a Beta distribution with $\langle c\rangle = 0.5$ and $\sigma_0^2 = 0.15$.

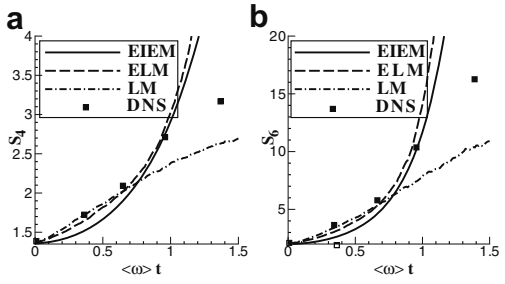

Fig. 2. Comparisons of the Flatness and Hyperflatness witn the DNS results. (a) Flatness; (b) Hyperflatness. The initial PDF is a Beta distribution with $\langle c \rangle = 0.5$ and $\sigma_0^2 = 0.15$.

the PDFs obtained by the mixing models and to those issued by the DNS. This good agreement can also be observed in Fig. 2 for the flatness factor S_4 and the hyperflatness factor S_6 for $\langle \omega \rangle t < 1$. For larger mixing times, only the LM exhibits values of S_4 and S_6 that asymptotically reach to the Gaussian ones ($S_4 = 3$ and $S_6 = 15$), whereas the EIEM and the ELM models show a divergent behavior which is not consistent with the DNS. Note that Soulard et al. [11] have obtained similar results, not shown here for the sake of brevity. The results shown in Figs. 1 and 2 indicate that the developed computational model adequately solves the stochastic mixing models LM, EIEM and ELM.

4.2. PaSR simulation

The results presented in this section were obtained for the PaSR considering the IEM and the stochastic mixing models developed by Sabel'nikov and Gorokhovski [10]. A study of the influence of the parameter d_0 and of the non-dimensional characteristic time scales $\mathscr{X}$ and $\mathscr{Y}$ on the combustion process will be presented.

In all the results presented, which were obtained via a stochastic simulation of the PaSR by the Monte Carlo method, $N_p = 4^6$ stochastic particles are considered. At each non-dimensional time step, Δt^*, $N_{\text{sub}} = 4^3$ particles are withdrawn from the reactor. These values were chosen in order to minimize the statistical error while maintaining the computational time to a reasonable value. Thus, the mean residence time is

$$\tau_r = \frac{N_p \Delta t}{N_{\text{sub}}}, \tag{12}$$

and the non-dimensional time-step $\Delta t^* = \Delta t/\tau_r = N_{\text{sub}}/N_p$ is 4^{-3}. At the beginning of the simulation all the stochastic particles contain only fresh gases, i.e., $P[c(t=0)] = \delta(c)$. Concerning the description of the chemical source term, the non-dimensional values of the heat release, α, and activation energy, β, employed are 0.8 and 15, respectively. These values, which were used in previous works [14], represent a moderate heat release, high activation energy, reaction.

4.2.1. Fast mixing with intensive reaction regime

The first situation examined is the one when mixing and chemistry evolutions are fast with respect to the residence time within the PaSR. The set of non-dimensional parameters used, which is characteristic of such a situation, is $\mathscr{X} = 2$ and $\mathscr{Y} = 0.167$, which control, respectively, the micromixing and reaction processes.

Figure 3 shows histograms of the steady-state PDF of the reaction progress variable, $P(c)$, obtained with the models IEM, LM, EIEM and ELM. For reference purposes, the solid line always represents the semi-analytic solution of PDF corresponding to the IEM model [14]. This figure clearly shows that the PaSR contains mostly burned gases in such a situation.

Figure 3a shows that the PDF obtained with the IEM model exhibit an excellent agreement with the semi-analytic steady-state solution, whereas the other models yield PDFs which pres-

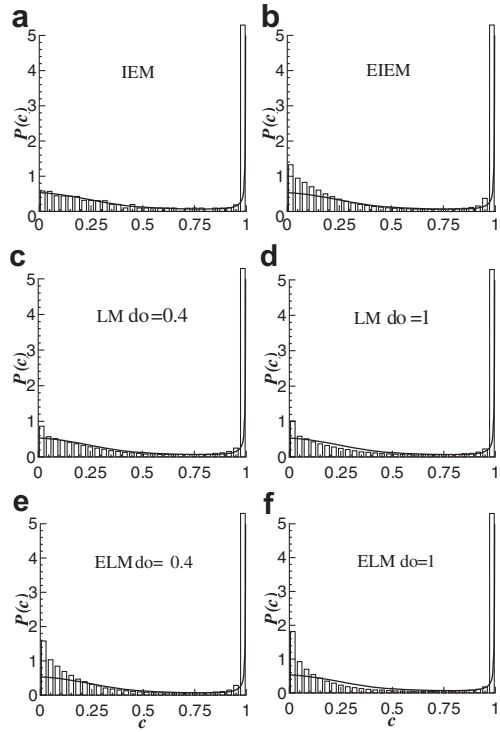

Fig. 3. Comparisons between semi-analytical solution of the IEM model (line) and simulated (histograms) steady-state PDFs of c for $\mathscr{X} = 2$ and $\mathscr{Y} = 0.167$ using the (a) IEM; (b) EIEM; (c) LM with $d_0 = 0.4$; (d) LM with $d_0 = 1$; (e) ELM with $d_0 = 0.4$ and (f) ELM with $d_0 = 1$. This regime correspond to an intensive combustion with high mixing frequency.

ent rather small deviations from this baseline solution for the IEM model. These deviations are perceptible at the vicinity of the unburned gases, $c = 0$, where a slight increase on the value of $P(c)$ is observed. Note, also, that the value of d_0 does influence the steady-state solution, which is a departure from the pure mixing behavior [11]. However, these changes will be shown not to influence the statistical moments of the PDF in such a fast mixing, fast chemistry situation. Indeed, in such a situation the PaSR could be approximated by a PSR, since mostly burned gases exist within the reactor.

4.2.2. Slow mixing with mild reaction regime

This section presents results obtained with the different models in a situation where mixing and chemistry are slow with respect to the residence time. The representative set of reactor parameters chosen is $\mathscr{X} = 0.5$ and $\mathscr{Y} = 0.042$. Figure 4 shows, by comparison with Fig. 3, that the bi-modal nature of the PDF is increased when both mixing and chemistry are progressively slower. Thus, the probability for finding fresh gases $P(c \to 0)$ is larger than in the case of intensive combustion

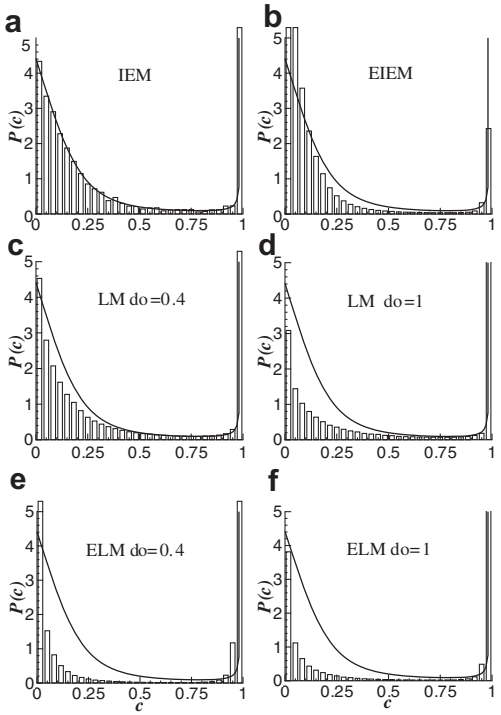

Fig. 4. Comparisons between semi-analytical solution of the IEM model (line) and simulated (histograms) steady-state PDFs of c for $\mathscr{X} = 0.5$ and $\mathscr{Y} = 0.042$ using the (a) IEM; (b) EIEM; (c) LM with $d_0 = 0.4$; (d) LM with $d_0 = 1$; (e) ELM with $d_0 = 0.4$ and (f) ELM with $d_0 = 1$. This regime correspond to an mild combustion with low mixing frequency.

regime, which in turn should lead to a decrease of $\langle c \rangle$. In Fig. 4a an excellent agreement is observed between the semi-analytic (solid line) and the Monte-Carlo (histogram) solutions for the IEM model [14]. This semi-analytic solution is used when the other models are considered, for reference purposes only, since these models do not possess a known analytical solution.

Figure 4b allows to verify that, when the turbulence mixing frequency is described by the log-normal distribution considered here, the amount of unburned gases increases within the PaSR, i.e., $P(c \to 0) > P(c \to 1)$. The average value of the reaction progress variable is thus expected to decrease with respect to the value computed with the IEM model. Furthermore, the absolute value of $\mathrm{d}P(c)/\mathrm{d}c$ on the vicinity of $c = 0$ is larger, in the case of the EIEM model, than in the case of the IEM model, thus indicating that mixing is faster in the case of the extended model's result.

In the case of the Langevin models, which results are shown in Fig. 4c–f, the evolution of the PDF for small values of the progress variable, i.e., when the chemical source term is small when compared to mixing, clearly shows that an increase on the value of d_0 leads to an augmented curvature of $P(c \to 0)$, $|\mathrm{d}^2 P(c)/\mathrm{d}c^2|$. This could be expected, since higher values of d_0 correspond to a larger weight given to the reactive scalar mixing process, when compared to reaction. Furthermore, in contrast to the intensive combustion regime, the choice of the value of d_0 strongly influences the PDF shape. Indeed, for a given model choice, increasing the value of d_0 always leads to a decrease of the probability of finding unburned gases within the PaSR, and should lead to an increase of the averaged reaction progress value $\langle c \rangle$. Also, higher values of d_0 always increase the segregation between fresh and burnt gases, thus enhancing the bi-modal nature of the PDF. However, for a given choice of d_0, the passage from the LM to the ELM yields higher absolute values $\mathrm{d}P(c)/\mathrm{d}c$ and a smaller probability of finding unburned gases within the PaSR.

4.2.3. Parametrical study of the choice of the mixing models on $\langle c \rangle$ and σ

This section presents the results of a parametrical study of the choice of the stochastic mixing model on the average, $\langle c \rangle$, and on the standard deviation, σ, of the reaction progress variable for two values of $\mathscr{X}$, 0.5 and 2, which correspond to slow and fast mixing processes, respectively. A broad range of chemical time scales is covered, $0.03 \leqslant \mathscr{Y} \leqslant 1$, ranging from mild to intensive reaction regimes.

Figure 5 presents a comparison of the values of $\langle c \rangle$ and σ obtained with the IEM model and with the LM when $d_0 = 0.4$ and $d_0 = 1$ are used. Figure

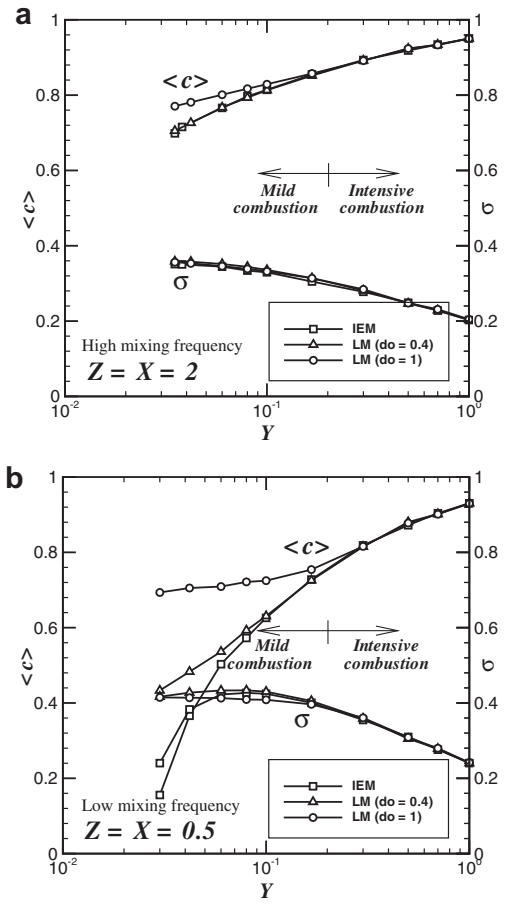

Fig. 5. Comparisons of the mean and standard deviation of c in a PaSR operation using the IEM and LM model, for the (a) High mixing frequency and (b) low mixing frequency.

5a, which depicts the case of fast mixing ($\mathscr{Z} = \mathscr{X} = 2$), shows that $\langle c \rangle$ is nearly identical for the IEM and LM with $d_0 = 0.4$ in the range of $\mathscr{Y}$ analyzed in this work. When the LM with $d_0 = 1$ is used larger values of $\langle c \rangle$ are obtained in the mild combustion regime ($\mathscr{Y} < 0.2$). However, the difference observed among the models is at most 8%. The standard deviation values are similar in all the combustion regimes, discrepancies smaller than 2% are observed.

A different picture results for the slow mixing case shown in Fig. 5b. On the one hand, values of $\langle c \rangle$ and σ computed using the IEM model and LM model with $d_0 = 0.4$ and 1 are practically identical in the case of an intensive combustion regime ($\mathscr{Y} > 0.2$). On the other hand, as the chemical reaction process slows, the choice of the mixing model substantially influences the $\langle c \rangle$ and σ values. Indeed, for $\mathscr{Y} = 0.030$ and $\mathscr{Z} = \mathscr{X} = 0.5$, which represents a mild reaction, slow mixing case, the values of $\langle c \rangle$ obtained by the IEM, LM with $d_0 = 0.4$ and 1 are, 0.1556, 0.4332 and 0.6935, respectively – note that the IEM model is the limit case of the LM with $d_0 = 0$. In other words, the IEM model predicts a virtually extinct PaSR, whereas the LM with $d_0 = 1$ leads to a combustion which is almost as intense as if mixing were fast. This demonstrates that there exists a significant influence of the choice of d_0 over $\langle c \rangle$. Figure 5b also shows that the standard deviation is affected to a lesser extend by the aforementioned choice of models. Nevertheless, when $\mathscr{Y} < 0.06$, the value of σ predicted by the IEM model is substantially smaller than the computed with the LM. It can also be verified in this figure that the value of σ obtained by the LM model seems to stabilize at a value close to 0.4 as d_0 is increased. This tendency accompanies the evolution of the shape of the PDF toward a bimodal shape.

The results obtained with the use of the extended models, shown in Fig. 6, exhibit a still

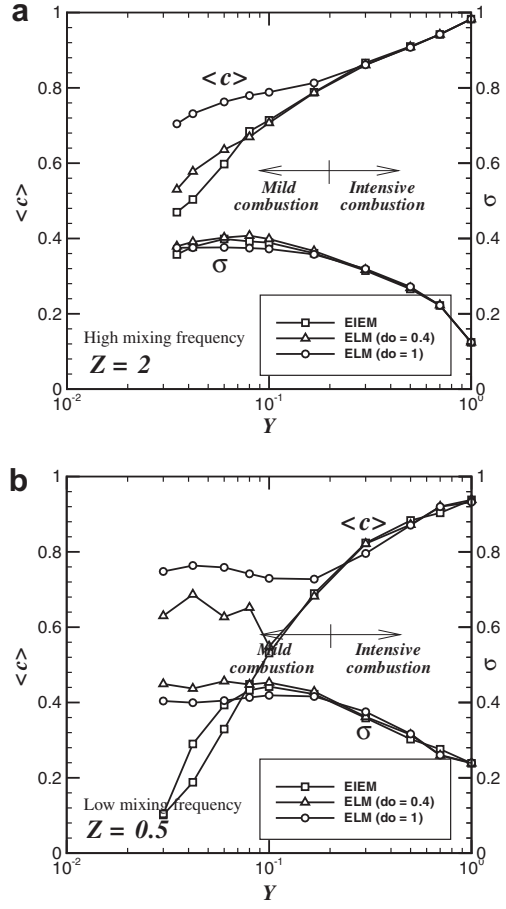

Fig. 6. Comparisons of the mean and standard deviation of c in a PaSR operation using the EIEM and ELM model, for the (a) High mixing frequency and (b) low mixing frequency.

larger sensitivity to the choice of the model and of the parameter d_0. Indeed, this figure shows that, for the chosen values of $\mathscr{L}$, a good agreement between these extended models is only obtained when $\mathscr{Y} > 0.3$. Also, as d_0 is increased (when $d_0 = 0$ the EIEM model is recovered from the ELM), the corresponding value of $\langle c \rangle$ always increases. This tendency is in agreement with the classical increase with the scalar dissipation rate of the progress variable reaction rate [20]. Figure 6 also shows that the value of σ computed with the ELM is only slightly affected by the choice of d_0, the trends observed are analogous to those obtained with the IEM model and the LM.

Further insight on the behavior of the Langevin models could be gained by examining the evolution of the parameter $(a-1)$ [Eqs. (3) and (4)]. This parameter, which expresses the contribution of the scalar dissipation model to the increase of the mixing frequency, is found to increase as $\mathscr{Y}$ is decreased. For values of $\mathscr{Y} \approx 1$, $(a-1) \approx 0$, which confirms that the dissipation process influence on combustion is negligible in this limit. When $\mathscr{Y}$ approaches values close to the extinction limit, the contribution of the dissipation model to the PDF drift term reaches 10–20%, i.e., $(a-1) \approx 0.1 - 0.2$. Note that $(a-1)$ exhibits a sub-linear increase with d_0 and is practically invariant with respect to $\mathscr{L}$.

A comparison of Figs. 5 and 6 reveals that the adoption of a log-normal description of the turbulent frequency, characteristic of the extended models, influences in a non-trivial manner the computed averaged values of the reaction progress variable. Some of the results exhibit an increase of $\langle c \rangle$, whereas a decrease is found to occur in other situations. A thorough examination of this question is out of the scope of the present paper, and should be performed on the light of carefully designed Direct Numerical Simulations or experiments.

5. Conclusions

This work presented the results of a comparison of stochastic mixing models on the simulation of mixing and combustion. This simulation was performed using a Monte-Carlo technique to yield the solution of stochastic differential equations equivalent to the joint transport equation of scalar-frequency probability density function. Due to the nonlinearities involved on the mixing and the chemistry description, it was necessary to adopt a newly developed, time-implicit, numerical method. First, the case of an inert scalar evolution subjected to homogeneous turbulent fluctuations was addressed. During the early stages of mixing the scalar PDFs computed by the different models agreed well with direct numerical simulation results. For large mixing times, only the Langevin model yielded self-similar scalar PDFs consistent with a Gaussian shape, whereas the models which contained a description of the turbulent frequency led to a divergent, super-Gaussian, behavior. Then, a partially stirred reactor was simulated using the classical IEM and the stochastic mixing models. The qualitative evolution of the PDF was examined for situations characteristic of fast mixing and reaction and of slow mixing and reaction. In the former case, the shape of the steady-state of PDF is only slightly modified by the choice of mixing model. When the PaSR is operating in a slow reaction and mixing regime, differences between the computed PDF shapes are found to occur, mostly at the vicinity of the unburned gases. The extended models, which contain a log-normal description of the turbulent frequency, are found to enhance mixing, whereas Langevin models promote reaction via an increase of scalar dissipation. Finally, a parametric analysis of the behavior of the first two moments of the reactive scalar within the PDF was performed. This analysis shows that, in the intense combustion regime, i.e., when the ratio of residence time to chemical time is larger than 0.3, all the studied mixing models lead to equivalent results. However, in the mild combustion regime, large differences are found to occur. In general, Langevin models lead to larger average values of the reactive scalar $\langle c \rangle$ within the PasR, whereas the extended models may lead either to an increase or to a decrease of $\langle c \rangle$. The results obtained for the Langevin models (LM and ELM) in the reactive case also show a dependence on the parameter that controls the reactive scalar dissipation. In particular, an increment of this parameter leads to an increment of $\langle c \rangle$. This behavior is consistent with the increment of the averaged reaction rate with the scalar dissipation rate which corresponds to the classic modeling of the premixed turbulent combustion. Further work will be directed to the comparison between these models in more complex situations. It can be expected that the Extended Langevin Model, that includes a stochastic description of turbulent frequency fluctuations and requires the prescription of the parameter d_0, should be more successful in describing experimental results or DNS data.

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