EXTENDED LMSE AND LANGEVIN MODELS OF THE SCALAR MIXING IN THE TURBULENT FLOW

V.Sabel'nikov
ONERA/DEFA/EFCA, 91120 Fort de Palaiseau, France
Vladimir.Sabelnikov@onera.fr

M.Gorokhovski
CORIA UMR 6614 CNRS University of Rouen, 76821 Mont-Saint-Aignan, France
Gorokhovski@coria.fr

ABSTRACT

A further developments of the LMSE and Langevin micro-mixing models are proposed in order to account for the entire spectrum of time scales in the turbulent flow. The evolution of these scales are described in the framework of the log-normal stochastic process. The equation for the scalar pdf conditional on the given mixing frequency is derived and numerically solved for each of considered models in the simple case of the statistically homogeneous flow. Then, by integration over all range of the mixing frequency, the unconditional pdf's are obtained and compared against DNS data. It is shown that at late times, the modeled pdf has exponential tails. The model of the forcing mixing with injection of unmixed concentrations is proposed in the last part of the paper.

I.INTRODUCTION

Modern models of reacting turbulent flows are often based on the probability density function (pdf) method since it treats the influence of turbulent fluctuations on the chemistry in closed form [1-4]. The challenging problem in this approach is to describe adequately the molecular mixing in turbulent medium. From both experimental and DNS studies it has been recognized that the scalar mixing scenario is coupled with characteristic time-scales of turbulent eddies. This has led researches to propose several models [5-10] that accounts for the multi-scale nature of the scalar micro-mixing in the turbulent flow. Our primary motivation for the present work was to investigate a new approach which will differ from [5-10] in the following principal feature: the instantaneous relaxation rate (mixing frequency) $\omega(t)=\dfrac{\varepsilon(t)}{k}$ is treated as a stochastic process ($\varepsilon(t)$ - the instantaneous dissipation rate and k - the mean kinetic turbulent energy). Following [11,12], this process is modeled as Ornstein-Uhlenbeck (OU) process [13] for the logarithm of the normalized relaxation rate $\chi(t)=\ln\dfrac{\omega(t)}{\langle\omega\rangle}$. This approach is demonstrated here in its application for two different mixing models, namely, for the LMSE model [2,14] and for the binomial Langevin model [15,16]. In the last one, the binomial stochastic process is replaced by Wiener process.

II.THE EXTENDED LMSE MODEL

II.a Denoting $\langle\ |\omega\rangle$ as a conditional average at the given value of ω, the extended LMSE model writes:

$$dc=-\Omega\,\omega\left(c-\langle c|\omega\rangle\right)dt \qquad (1)$$

where ω is the relaxation rate defined here as a random process and $\langle c|\omega\rangle$ is the mean conditional scalar (instead of mean frequency $\langle\omega\rangle$ and mean scalar $\langle c\rangle$, correspondingly given in the classical LMSE). The coefficient Ω is introduced in such a way that it provides for the known decay rate of $\langle c'^2\rangle$, *i.e.* this coefficient can be determined from the known mean scalar dissipation $\langle\varepsilon_c\rangle$ within one-point approach:

$$\Omega=\frac{\langle\varepsilon_c\rangle}{\left[\left\langle\omega\left(\langle c^2|\omega\rangle-\langle c|\omega\rangle^2\right)\right\rangle\right]} \qquad (2)$$

For example, the DNS data [17] can provide for $\langle\varepsilon_c\rangle$. Note that being a functional of ω, the solution of (1) at the given instant t depends on the all prehistory $\omega(t_1)$, where $t_1\le t$. Complying with general principles stated by Pope [5], the model (1) preserves the constant mean concentration for any random process ω.

II.b Following [11], the OU-process for $\chi(t)$ evolves according to the Ito stochastic differential equation

$$d\chi=-(\chi-m_1)T^{-1}dt+\sqrt{2m_2T^{-1}}\,dW(t) \qquad (3)$$

with $W(t)$ as a Wiener process, the mean $m_1 = \langle \chi \rangle$, the variance $m_2 = \langle (\chi - m_1)^2 \rangle$ and the integral time scale T which is defined to be inversely proportional to the relaxation rate $T^{-1} = C_\chi \langle \omega \rangle$. Similar to [18], the DNS data conducted in [19] suggested: $m_2 = 0.29 \ln Re_\lambda - 0.36$ over the range of the Taylor-scale Reynolds number $Re_\lambda = 38 - 93$.

II.c The evolution equation for the joint pdf $P(c, \chi, t)$ can be obtained from stochastic equations (1) and (3) by standard technique [13]:

$$\frac{\partial P(c,\chi,t)}{\partial t} = \Omega \frac{\partial}{\partial c}\left[\langle \omega \rangle e^{\chi} \left(c - \langle c | \chi \rangle \right) P(c,\chi,t) \right] + \frac{\partial}{\partial \chi}\left[C_\chi \langle \omega \rangle (\chi - m_1) P(c,\chi,t) \right] + \frac{\partial^2}{\partial \chi^2}\left[C_\chi \langle \omega \rangle m_2 P(c,\chi,t) \right] \quad (4)$$

This equation can not be simply reduced to the equation for pdf $P(c,t)$ in the closed form by integration (4) over χ – range. Instead, the equation for conditional pdf $P(c|\chi,t)$ can be derived, which in the case of the stationary Gaussian process for χ (stationary turbulence) is:

$$\frac{\partial P(c|\chi,t)}{\partial t} = \Omega \frac{\partial}{\partial c}\left[\langle \omega \rangle e^{\chi} \left(c - \langle c | \chi \rangle \right) P(c|\chi,t) \right] - C_\chi \langle \omega \rangle (\chi - m_1) \frac{\partial P(c|\chi,t)}{\partial \chi} + C_\chi \langle \omega \rangle m_2 \frac{\partial^2 P(c|\chi,t)}{\partial \chi^2} \quad (5)$$

Then, the unconditional pdf $P(c,t)$ can be found by simple integration:

$$P(c,t) = \int_{-\infty}^{\infty} P(c|\chi,t) P(\chi) d\chi \quad (6)$$

that accounts for the scalar mixing over all range of turbulent time scales. It is worth to note that the knowledge of the joint pdf $P(c,\chi,t)$ allows also to obtain the conditional scalar dissipation $\langle \varepsilon_c | c \rangle$, which plays essential role in the problem of turbulent combustion.

II.d The equation (5) was numerically solved using the 3rd order upwind conservative difference scheme with limiters convection [20]. In order to control the probability zero fluxes at the phase space boundaries, an adaptive grid was specified with a continuous sliding of boundaries simultaneously with evolving pdf's. The initial pdf-distribution in the concentration space was taken from [17] close to a double-delta function for all χ – spectrum. The expression for the variance m_2 was chosen from [19] and the value 1.6 was ascribed for the proportionality constant C_χ as it was suggested in [20]. The solution was compared against DNS [17] of decaying scalar field in homogeneous turbulence. It is shown that at early stages, the predicted pdf's relax from the initial double-delta distribution in the qualitative agreement with the DNS data. The modeled pdf's cover the large spectrum of concentration values. In the Fig. 1, the long-time behavior of normalized pdf's is shown. The time is normalized on the eddy-turnover time l/u. It is seen that at intermediate times (the late times in DNS), the pdf's resemble the Gaussian distribution as it was observed in DNS. However at large times, the computed standardized pdf's expose the exponential tails around the peak at mean value of scalar.

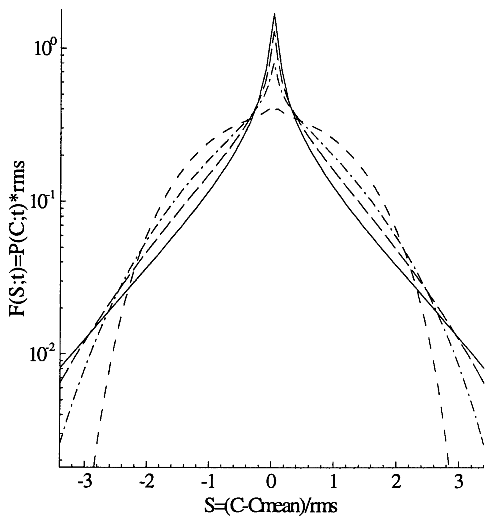


Fig. 1: The standardized pdf's of the scalar at different times for $k_s / k_0 = 1$ and $Re_\lambda = 50$. Lines: --- $tu/l = 2.78$; –-– 3.47; – – 4.13; — 5.

III. THE EXTENDED LANGEVIN MODEL

III.a The extended nonlinear Langevin model writes

$$\begin{cases} dc = -a\Omega\omega\left(c - \langle c|\omega\rangle\right)dt + b\Omega\omega c(1-c)dW \\ a = 1 + d_0\left(\langle c|\omega\rangle - \langle c^2|\omega\rangle\right) \\ b = d_0\left(\langle c^2|\omega\rangle - \langle c|\omega\rangle^2\right) \end{cases} \quad (7)$$

where alongside with notations from II.a and II.b, the arbitrary coefficient d_0 controls the rate of pdf relaxation. This coefficient neither intervenes in the decay of the conditional scalar variance $\left(\langle c^2|\omega\rangle - \langle c|\omega\rangle^2\right)$ nor in the decay of the unconditional one. The time-scale constant Ω is introduced in the same way as in II.a. Here, the distinctions from the Langevin binomial model [15, 16] are:

(i) replacing the mean mixing frequency by the stochastic process (3) thereby accounting for the entire spectrum of time scales;

(ii) replacing the stochastic binomial process by the Winner process; this allows to obtain the pdf equation in the form of Fokker-Planck equation;

(iii) inserting $c(1-c)$ in the diffusion term; this provides for the boundedness of the scalar space. Let us remark that the case $d_0 = 0$ reduces (7) to the extended LMSE model (1).

III.b The evolution equation for the joint pdf $P(c,\chi,t)$ can be obtained from (7) and (3) by usual means [13]. One gets

$$\frac{\partial P(c,\chi,t)}{\partial t} = a\Omega\frac{\partial}{\partial c}\left[\langle\omega\rangle e^{\chi}\left(c-\langle c|\chi\rangle\right)P(c,\chi,t)\right]$$
$$+b\Omega\frac{\partial^2}{\partial c^2}\left[\langle\omega\rangle e^{\chi}c(1-c)P(c,\chi,t)\right] \qquad (8)$$
$$+\frac{\partial}{\partial\chi}\left[C_\chi\langle\omega\rangle(\chi-m_1)P(c,\chi,t)\right]$$
$$+\frac{\partial^2}{\partial\chi^2}\left[C_\chi\langle\omega\rangle m_2 P(c,\chi,t)\right]$$

It can be strictly shown that for the particular case of $\omega = \langle\omega\rangle$ (this corresponds to $P(\chi) = \delta(\chi)$), the asymptotic solution of (8) in the normalized variables is the Gaussian distribution and the coefficient d_0 controls the relaxation rate towards the Gaussian distribution. Similar to II.c, the equation for conditional pdf $P(c|\chi,t)$ yields for the case of the stationary Gaussian process for χ:

$$\frac{\partial P(c|\chi,t)}{\partial t} = a\Omega\frac{\partial}{\partial c}\left[\langle\omega\rangle e^{\chi}\left(c-\langle c|\chi\rangle\right)P(c|\chi,t)\right]$$
$$+b\Omega\frac{\partial^2}{\partial c^2}\left[\langle\omega\rangle e^{\chi}c(1-c)P(c|\chi,t)\right] \qquad (9)$$
$$-C_\chi\langle\omega\rangle(\chi-m_1)\frac{\partial P(c|\chi,t)}{\partial\chi}$$
$$+C_\chi\langle\omega\rangle m_2\frac{\partial^2 P(c|\chi,t)}{\partial\chi^2}$$

Likewise (6), the integration of solved $P(c|\chi,t)$ over entire range of time-scales accounts for the multi-scale nature of the scalar micro-mixing.

III.c The equation (9) was numerically solved (see, II.d) and compared with DNS data of the evolution of scalar field in statistically stationary, homogeneous, isotropic turbulence [17]. In [17], the initial integral length scale of the scalar field is determined by the ratio k_S/k_0 (k_S is the mean wavenumber in the "top-hat" distribution of the initial scalar field and k_0 is the lowest nonzero wavenumber indicated by the geometrical scale). In our computations, the mean scalar dissipation $\langle\varepsilon_c\rangle$ have been chosen according to k_S/k_0. The comparison was performed for two values of k_S/k_0, $k_S/k_0 = 8$ (lower initial length scale) and $k_S/k_0 = 1$ (higher initial length scale). The coefficient d_0 is taken equal to unity $d_0 = 1$. Fig.2 shows an example of standardized scalar pdf in the later period of its evolution. One can see that at large times, the pdf evolves towards an asymptotic form, which is Gaussian at small amplitudes with exponential tails at larger amplitudes. Note that the later times in the model computation have not been reached in DNS [17].

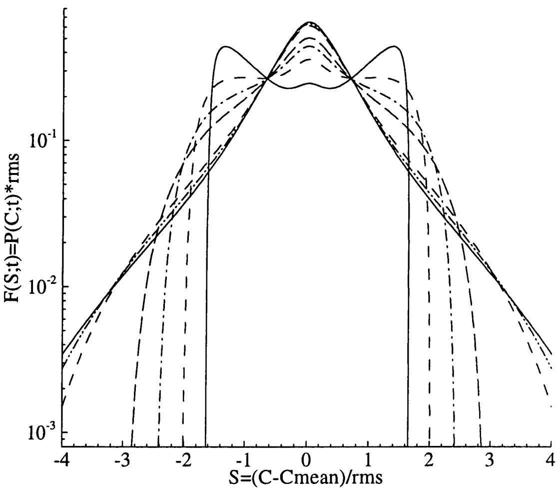
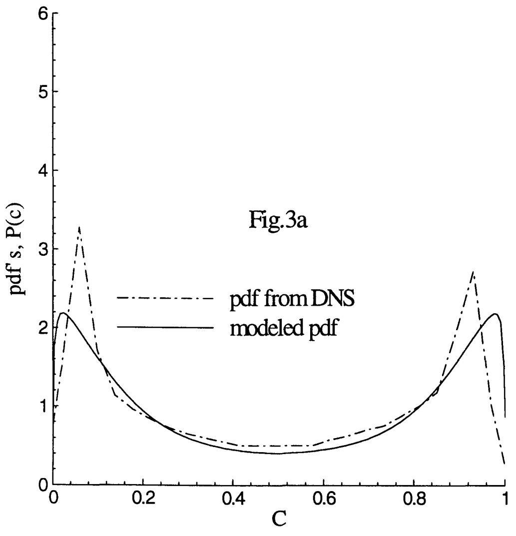
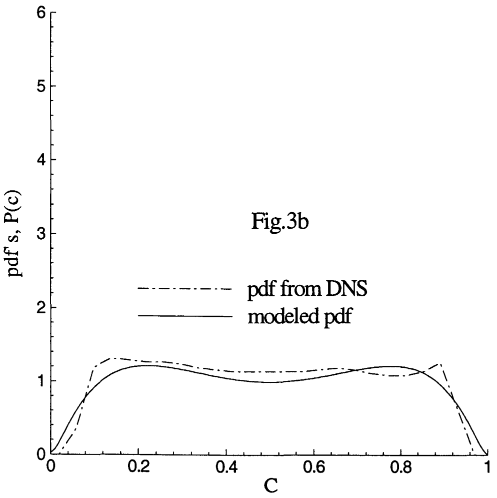


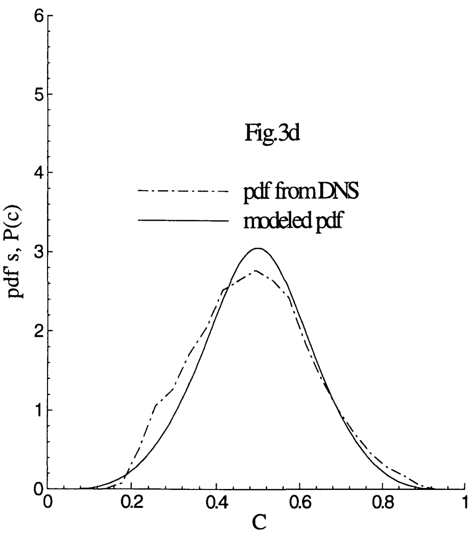
Fig. 2. The standardized pdf's of the scalar at different times for $k_S/k_0 = 1$ and $Re_\lambda = 50$.

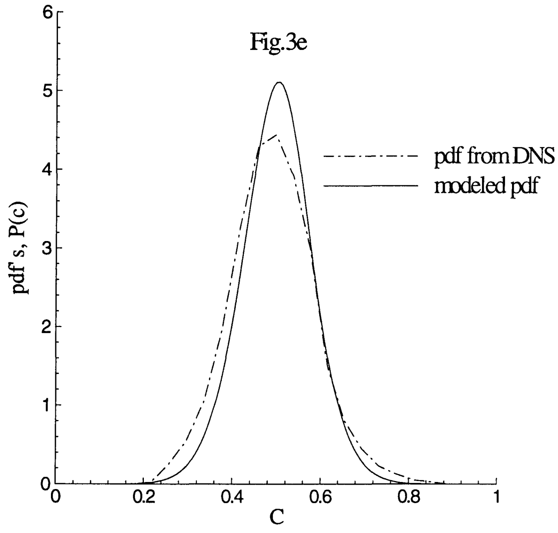
Lines: — tu/l = 1.6; - - 2.4; –·–3.2; – –4; - - 6.4; –··–7.2; — 8

In Fig.3(a-e), the modeled pdf's and those found in DNS [17] are compared at different times for $k_S/k_0 = 1$ and $Re_\lambda = 50$. It is seen that predictions are close to pdf's from DNS.









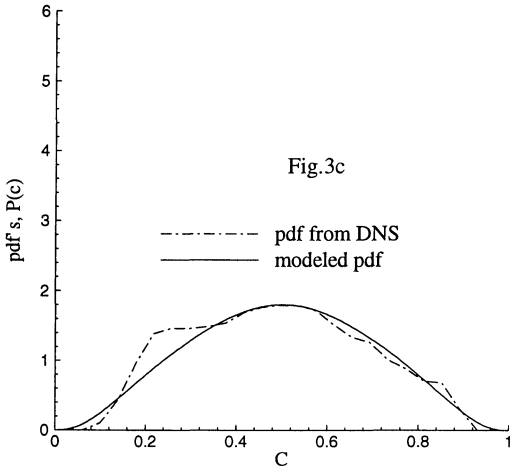


Fig. 3(a-e). Comparison of modeled scalar unconditional pdf's with those found in DNS [17] for $k_S / k_0 = 1$ and $Re_\lambda = 50$ at five different times: $tu / l = 0.22$ (a); 1.49 (b); 2.11 (c); 2.78 (d); 3.47 (e)

IV. THE FORCING MIXING WITH THE INJECTION OF UNMIXED SCALARS

IV.a The last step in the present work concerns the modeling the partially stirred reactor (PaSR) feeded by two inlets, *i.e.* with the injection into reactor of the pure scalar values $c = 0$ and $c = 1$ and with withdrawal at the same time from it of an equal amount of the resulting mixture. In this case, the pdf equation has to be supplemented by an additional inhomogeneous in – and outflow term. Let us assume that the probabilities of observing the values $c = 0$ and $c = 1$ in the injection flow are α and $1-\alpha$, correspondingly (hereafter α is named as injection parameter, for PaSR this parameter is equal to the ratio of the massflow with $c = 0$ to the total injected massflow) , and β_{inj} is a frequency of scalars injection (this frequency is inversely proportional to the residence time). Then this additional inhomogeneous in – and outflow term in the joint pdf equations (4) and (8) is written in the following form:

$$\beta_{inj}\left[\alpha\,\delta(c)P(\chi)+(1-\alpha)\delta(c-1)P(\chi)-P(c,\chi,t)\right]$$

and so far, the equations (5) and (9) for the conditional pdf $P(c|\chi,t)$ will be supplemented also by an additional inhomogeneous forcing term: $\beta_{inj}\left[\alpha\,\delta(c)+(1-\alpha)\delta(c-1)-P(c|\chi,t)\right]$.

Then, making use of the method developed in [21], a smooth function $g(c|\chi,t)$ can be introduced by:

$$P(c|\chi,t)=\left[H(c-0)-H(c-1)\right]g(c|\chi,t),$$

where H is Heaviside function. The equation for this smooth function with boundary conditions at extremities of scalar space can be obtained from (5) and (9) [21]. Let us write this equation for the extended LMSE model while similar modifications can be done for the extended Langevin model, as well. One yields:

$$\frac{\partial g(c|\chi,t)}{\partial t}=\Omega\frac{\partial}{\partial c}\left[\langle\omega\rangle e^{\chi}\left(c-\langle c|\chi\rangle\right)g(c|\chi,t)\right] -C_{\chi}\langle\omega\rangle(\chi-m_1)\frac{\partial g(c|\chi,t)}{\partial\chi} +C_{\chi}\langle\omega\rangle m_2\frac{\partial^2 g(c|\chi,t)}{\partial\chi^2}-\beta_{inj}\,g(c|\chi,t) \qquad (11)$$

with the following boundary conditions:

$$g(c|\chi=0)=\alpha\frac{\beta_{inj}}{\Omega\langle\omega\rangle e^{\chi}\langle c|\chi\rangle}$$
$$g(c|\chi=1)=(1-\alpha)\frac{\beta_{inj}}{\Omega\langle\omega\rangle e^{\chi}\left(1-\langle c|\chi\rangle\right)} \qquad (12)$$

IV.b The computations of (11), (12) and integration (6) of the solution $g(c|\chi,t)$ over all χ have been performed in this paper. An example with symmetric injection of scalars from both sides ($\alpha = 0.5$) is given in Fig.4 for $Re = 100$, $\Omega = 1$, $C_{\chi} = 1$ and $\langle\omega\rangle = 10^{-3}$. The mean mixing-to-injection frequency ratio is taken here as $\langle\omega\rangle / \beta_{inj}$ = 0.5. Initial distribution is chosen as a Gaussian function with $\langle c\rangle = 0.5$ and $\langle c'^2\rangle = 0.01$ for all mixing frequencies. It is seen that the distribution evolves towards the stationary solution of a "flying pdf" with raised wings. Different shapes of the stationary solution have been obtained by changing the injection parameter α.

Fig.5 shows that the asymptotic stationary scalar variance value decreases with increasing of the mixing-to-injection frequency ratio (other conditions are the same as in Fig.4).

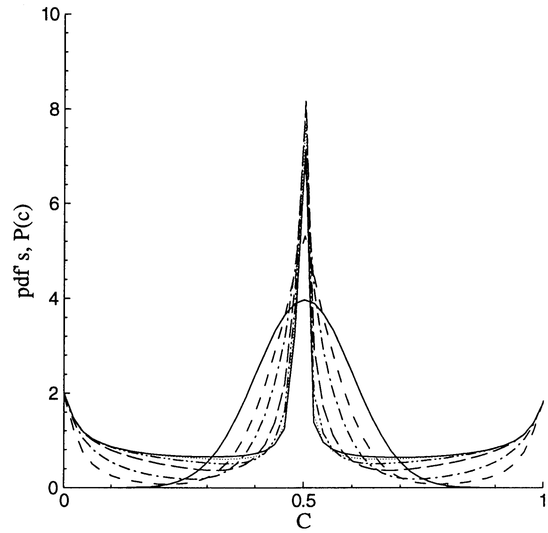


Fig.4. The evolution of unconditional pdf with symmetric injection of unmixed scalars at c=0 and c=1. Lines: — $t\langle\omega\rangle = 0$; - - 0.4; –·– 0.8; – –1.6; –··– 2.4; ... 3.2; — 4.

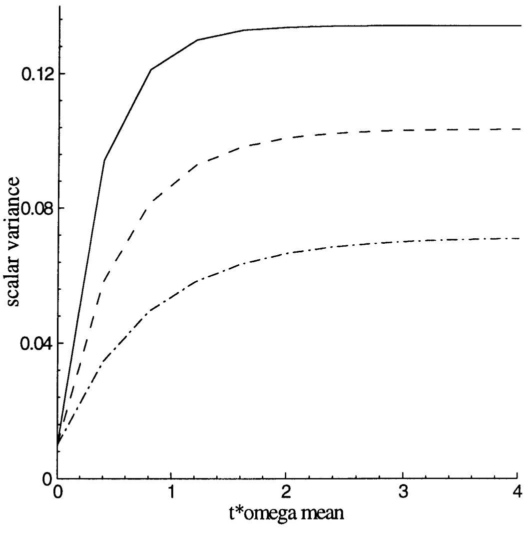


Fig.5. The time evolution of the scalar variance for the case of the symmetric injection of unmixed scalars at c=0 at c=1. Lines: $\langle\omega\rangle / \beta_{inj}$ = : — 0.5; - - 1; –·– 2.

V. CONCLUSION

The modifications of the LMSE and Langevin models are proposed in order to take into account the multi-scale nature of the scalar micro-mixing in the turbulent flow. Following the Pope's and Chen's approach [11], this is done by using the log-normal stochastic process for the mixing frequency. The models are tested against Esweran's and Pope's DNS [17] of decaying scalar field in homogeneous turbulence. Distributions are in the good agreement with the DNS data at intermediate times (normalized on the eddy-turnover time l/u) of the pdf evolution (the late times in DNS). However, at very large evolution times, the computed standardized pdf's expose exponential tails at large amplitudes which were not observed DNS [17]. The models are also extended for the case of the forced mixing with injection of unmixed scalars at $c = 0$ and $c = 1$ values (modeling the partially stirred reactor (PaSR) feeded by two inlets, *i.e.* with the injection into reactor of the pure scalar values $c = 0$ and $c = 1$). Different asymptotic stationary shapes of pdf distribution have been obtained for different values of injection parameter and mixing-to-injection frequency ratio.

References

[1] Frost V.A., Izv. AN SSSR, *Energetika i Transport*, 6, 108 (1973)

[2] Dopazo C., O'Brien E.E., *Acta Astronavtica*, 1, 1239 (1974)

[3] Kuznetsov V.R., Izv. AN SSSR, *Mecanica gidkostej i gazov*, 3, 32 (1977)

[4] Pope S.B., *Combust. Sci. and Tech.*, 25, 159 (1981)

[5] Pope S.B., Prog. Energy Combust. Sci. 11, 119 (1985)

[6] Kerstein A.R., *Combust. Sci. and Tech.*, 60, 391 (1988)

[7] Borghi R. and Gonzalez M., Combust. Flame, 63, 239 (1986)

[8] Fox R.O., Phys. Fluids 7, 1082-1084 (1995)

[9] Fox R.O., Phys. Fluids 7, 2820-2830 (1995)

[10] Fox R.O., Phys. Fluids 8, 2678-2691 (1996)

[11] Pope S.B. and Chen Y.L., Phys. Fluids A 2, 1437-1449 (1990)

[12] Pope S.B., Phys. Fluids A 3, 1947-1957 (1991)

[13] Gardiner C.W., *Handbook of Stochastic Methods* (Springer-Verlag, Second edition, 1985)

[14] O'Brien E.E., in *Turbulent Reacting Flows,* edited by P.A. Libby and F.A. Williams (Springer-Verlag, Berlin, 1980)

[15] Valino L. and Dopazo C., Physics of Fluids A, 2(7), pp.1204-1212 (1990)

[16] Valino L. and Dopazo C., Physics of Fluids A, 3(712), pp.3034-3037 (1991)

[17] Eswaran V. and Pope S.B., Phys. Fluids 31, 506-520 (1988)

[18] Monin A.S. and Yaglom A.M., *Statistical Fluid Mechanics: Mechanics of turbulence* (MIT, Cambridge, MA, 1975),Vol.2

[19] Pyeung P.K. and Pope S.B., J. Fluid Mech., 207, 531-586 (1989)

[20] Jameson A., Int. J. Num. Methods in Fluids, Vol.20, 743-776 (1995)

[21] Kuznetsov V.R., Sabel'nikov V.A., In *Turbulence and Combustion*, Hemisphere (1990)