

# Extended LMSE Mixing Model With Chemical Reaction and Injection of Unmixed Concentrations.

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I. It is well-known that in the modeling of turbulent reacting flows, the probability density function (pdf) approach provides the non-linear chemical reaction term in the closed form. The challenging problem in this approach is to describe adequately the molecular mixing in turbulent medium. Although various ideas and analytical frameworks have been proposed to assess the micro-mixing process, the problem of micro-mixing modeling still remains open. The simplest and perhaps the most frequently used micro-mixing model is the LMSE closure developed by O'Brien and Dopazo. In terms of the particle scalar value this closure without chemistry reads<sup>1</sup>

$$\frac{dc}{dt} = -\Omega \langle \omega \rangle (c - \langle c \rangle) \quad (1)$$

where the mean quantity is denoted by angled brackets and the mean mixing frequency is defined as an inverse magnitude of the turbulence time scale,  $\langle \omega \rangle = \frac{\langle \varepsilon \rangle}{k}$ ,

where  $\langle \varepsilon \rangle$  and  $k$  are averaged viscous dissipation and turbulent energy, correspondingly. Here  $\Omega$  is a coefficient that can be defined from the known scalar dissipation computed from DNS to match one-point statistics. The well-known shortcoming of the LMSE model is that the initial shape of pdf (in homogeneous turbulence) does not relax alongside with the evolving process of the scalar fluctuations decay. Several ways to modify the LMSE and others mixing models have been proposed to remedy this principal deficiency. The developments of micro-mixing models are reviewed by Pope<sup>2</sup> and later by Dopazo<sup>3</sup> and Fox<sup>4</sup>. To recapitulate, one can essentially emphasize two LMSE improvements: a) the multi-scale model for the mixing frequency<sup>5,6,7</sup> and b) the joint-scalar-velocity model<sup>2,8,9</sup> in which  $\langle c \rangle$  in (1) is replaced by the mean value conditional on the velocity  $\langle c|v \rangle$ . In our paper in<sup>10</sup>, a new extension of the LMSE model is proposed. Similarly to the multi-scale model<sup>5,6</sup>, this modification accounts for the entire spectrum of time scales in the turbulent flow which is ranging from the integral scale  $k/\langle \varepsilon \rangle$  down to the Kolmogorov micro-scale  $\tau_K = \sqrt{\nu/\langle \varepsilon \rangle}$ . However, alternatively to the multi-scale model<sup>5,6</sup> the proposed in<sup>10</sup>

model treats the instantaneous relaxation rate  $\omega(t) = \frac{\varepsilon(t)}{k}$  as a stochastic process.

Here, the extended LMSE model<sup>10</sup> is applied for the mixing of reacting scalars. The case when unmixed gases (pure burnt, or fresh) are injected in the reactor at a certain frequency, is considered as well.

II. Denoting  $\langle | \omega \rangle$  as a conditional average at the given value of  $\omega$ , the extended LMSE model writes<sup>10</sup>:

$$dc = -\Omega \omega (c - \langle c|\omega \rangle) dt \quad (2)$$

where the relaxation rate  $\omega(t)$  is to be a random process and  $\langle c|\omega \rangle$  is the mean conditional scalar (instead of the mean frequency  $\langle \omega \rangle$  and the mean scalar  $\langle c \rangle$ , correspondingly given in the classical LMSE). Following Pope and Chen<sup>11</sup> and Pope<sup>12</sup>, the stochastic process for  $\omega(t)$  can be modeled by Ornstein-Uhlenbeck (OU)-process<sup>13</sup> for the logarithm of the normalized relaxation rate  $\chi(t) = \ln \frac{\omega(t)}{\langle \omega \rangle}$  with mean

$m_1 = \langle \chi \rangle$  and variance  $m_2 = \langle (\chi - m_1)^2 \rangle$  that are related through  $m_2 = -2m_1$ <sup>14</sup>.

Likewise, the Taylor-scale Reynolds number dependence for the variance  $m_2$  is taken according to<sup>15</sup> as:  $m_2 = 0.29 \ln Re_\lambda - 0.36$ .

Note that being a functional of  $\omega$ , the solution of (2) at the given instant  $t$  depends on the all prehistory  $\omega(t_1)$ , where  $t_1 \leq t$ . Complying with general principles stated by Pope<sup>2</sup>, the model (2) preserves the constant mean concentration for any random process  $\omega$ .

In the case of the stationary Gaussian process for  $\chi$ , the evolution equation for the conditional scalar pdf  $P(c|\chi, t)$  is derived as:

$$\begin{aligned} \frac{\partial P(c|\chi, t)}{\partial t} = & \Omega \frac{\partial}{\partial c} [\langle \omega \rangle e^\chi (c - \langle c|\chi \rangle)] P(c|\chi, t) - \frac{\partial}{\partial c} [\mathcal{R}(c) P(c|\chi, t)] - \\ & - C_\chi \langle \omega \rangle (\chi - m_1) \frac{\partial P(c|\chi, t)}{\partial \chi} + C_\chi \langle \omega \rangle m_2 \frac{\partial^2 P(c|\chi, t)}{\partial \chi^2} \end{aligned} \quad (3)$$

where  $\mathcal{R}(c)$  is the chemical rate and the proportionality constant  $C_\chi$  for the inverse of integral time scale is to be 1.6 as was suggested in<sup>11</sup>. So far, having obtained the solution of (3), one can get the unconditional pdf  $P(c, t)$ :

$$P(c, t) = \int_{-\infty}^{\infty} P(c|\chi, t) P(\chi) d\chi \quad (4)$$

which accounts for the scalar mixing over all range of turbulent length scales and

$$P(\chi) = \frac{1}{\sqrt{2\pi m_2}} \exp\left(-\frac{(\chi - m_1)^2}{2m_2}\right) \quad (5)$$

**III.** First, the equation (3) was numerically solved for the simple case of the inert ( $\mathcal{R}=0$ ) scalar mixing in homogeneous turbulent flow. The 3rd order upwind conservative differencing scheme with limiters convection<sup>16</sup> was used in the computation. 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<sup>17</sup> close to a double-delta function for all  $\chi$ -spectrum and the coefficient  $\Omega$  was fitted from the DNS data<sup>17</sup>. Fig.1 shows an example of the evolution of unconditional pdf. It is seen that pdf's cover the large interval of intermediate concentrations instead of the symmetric movement of two  $\delta$ -peaks towards the mean concentration, as it would be done in the case of the classical LMSE model. Results were compared to those found by DNS.<sup>17</sup> It was shown that at the early stages of the evolution of  $P(c, t)$ , the extended LMSE model predicts forms which are not far from those obtained by DNS.<sup>17</sup>. At the same time, in the long-time limit, the predicted standardized pdf's do not evolve towards a Gaussian as it makes

think from results of DNS study. Instead, at later times, the computed pdf's display the sharp exponential tails around the peak located at the mean scalar value.

The case with the chemical reaction is demonstrated in Fig.2. Initially, the concentration of fresh gas is taken as eight times more than the concentration of burnt one. These unmixed gases are mixing in a turbulent way and reacting. The chemical source is taken here as in <sup>18</sup>:  $\bar{W}(c) = 42 \cdot (1-c)^5 c / \tau_{ch}$  (burnt and fresh gases are ascribed correspondingly to  $c = 0$  and  $c = 1$ ; and  $\tau_{ch}$  is the chemical time). The coefficient  $\Omega$  is taken here equal to unity. It is seen that the initial delta peak at  $c = 0$  disappears in time and as time progresses further, the probabilities for intermediate concentrations arise due to the mixing. In sequel, the rate of chemical reaction is increasing and the peak of pdf at the side of burnt gas ( $c = 1$ ) is growing.

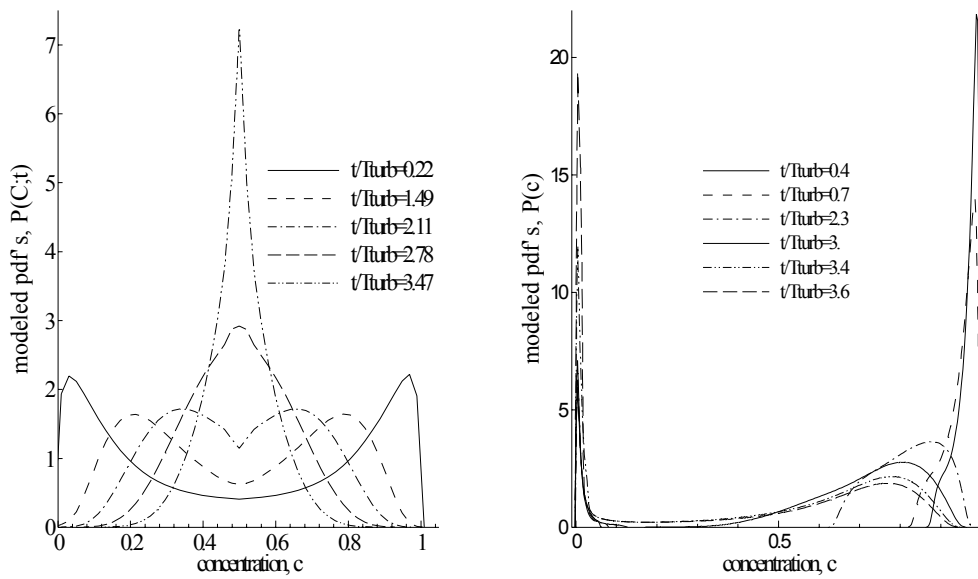


Fig. 1. Evolution of the scalar pdf without chemical reaction (the parameters are taken from DNS <sup>17</sup>:  $Re_\lambda = 50$ ,  $k_s / k_0 = 1$ )

Fig. 2. The pdf with chemical reaction ( $Re_\lambda = 100$ ;  $\tau_{ch} = 0.001$ ;  $T_{turb} = 0.001$ ;  $\Omega = 1$ )

**IV.** Next step in the present work concerns the modeling of the mixing of reacting scalars when unmixed gases (pure burnt,  $c = 0$ , or fresh,  $c = 1$ ) are injected in the reactor at a certain frequency  $\beta_{inj}$  with simultaneous withdrawal of the same mass of mixture from reactor. Let us assume that the probabilities of observing the values  $c = 0$  and  $c = 1$  in the injection flow are  $\alpha$  and  $1 - \alpha$ , correspondingly. Using the method developed in <sup>19</sup>, an equation for the smooth function  $g(c|\chi)$  with boundary conditions can be derived:

$$\frac{\partial g(c|\chi, t)}{\partial t} = \Omega \frac{\partial}{\partial c} [\langle \omega \rangle e^{\chi} (c - \langle c|\chi \rangle)] g(c|\chi, t) - \frac{\partial}{\partial c} [\bar{W}(c) g(c|\chi, t)] - C_\chi \langle \omega \rangle (\chi - m_1) \frac{\partial g(c|\chi, t)}{\partial \chi} + C_\chi \langle \omega \rangle m_2 \frac{\partial^2 g(c|\chi, t)}{\partial \chi^2} - \beta_{inj} g(c|\chi, t) \quad (6)$$

$$\text{with } g(c=0|\chi) = \frac{\alpha \beta_{inj}}{\langle \omega \rangle \langle c|\chi \rangle \exp(\chi)} \quad \text{and} \quad g(c=1|\chi) = \frac{(1-\alpha) \beta_{inj}}{\langle \omega \rangle (1 - \langle c|\chi \rangle) \exp(\chi)} \quad (7)$$

The case with  $\alpha = 0$  is shown in Fig. 3 where an evolution of the value

$\tau_{ch} \cdot \int_0^1 \bar{W}(c)P(c,t)dc$  for different ratio of injection-to-integral time scale is presented.

It is seen that the turbulent combustion rate is increasing at early stages due to the turbulence/chemistry interaction and further is decreasing due to dilution of partially mixed gases by the pockets of fresh gas. The analysis of pdf distributions is given in the paper for different cases of scalars injection.

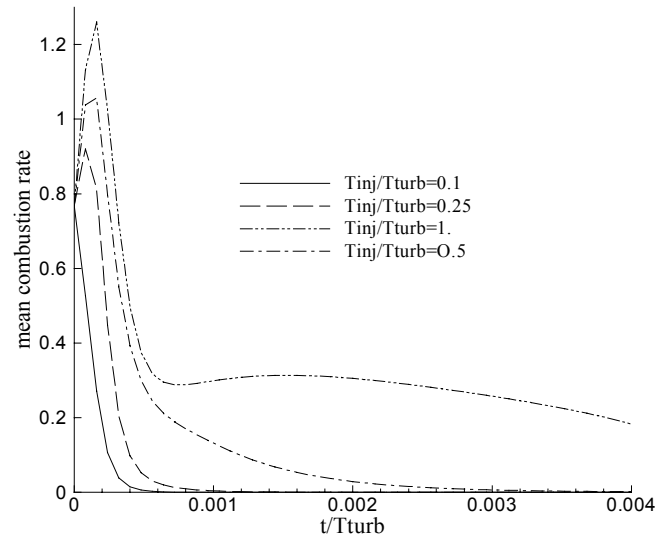


Fig.3. The influence of the injection-to-integral time scale ratio on the mean combustion rate.

## References

- <sup>1</sup> E.E. O'Brien, in *Turbulent Reacting Flows*, edited by P.A. Libby and F.A. Williams (Springer-Verlag, Berlin, 1980)
- <sup>2</sup> S.B. Pope, Prog. Energy Combust. Sci. 11, 119 (1985)
- <sup>3</sup> C. Dopazo in *Turbulent Reacting Flows*, edited by P.A. Libby and F.A. Williams (Springer-Verlag, Berlin, 1994)
- <sup>4</sup> R.O. Fox, *Revue de l'Institut Français du Pétrole*, 51, 215-243 (1996)
- <sup>5</sup> R. Borghi and M. Gonzalez, Combust. Flame, 63, 239 (1986)
- <sup>6</sup> R.O. Fox, Phys. Fluids 7, 1082-1084 (1995)
- <sup>7</sup> R.O. Fox, Phys. Fluids 7, 2820-2830 (1995)
- <sup>8</sup> R.O. Fox, Phys. Fluids 8, 2678-2691 (1996)
- <sup>9</sup> S.B. Pope, J. Fluid Mech. 359, 299-313 (1998)
- <sup>10</sup> V. Sabel'nikov and M. Gorokhovski, TSFP-2, June 27-29, 2001, Stockholm, 6 p.
- <sup>11</sup> S.B. Pope and Y.L. Chen, Phys. Fluids A 2, 1437-1449 (1990)
- <sup>12</sup> S.B. Pope, Phys. Fluids A 3, 1947-1957 (1991)
- <sup>13</sup> C.W. Gardiner, *Handbook of Stochastic Methods* (Springer-Verlag, 1985)
- <sup>14</sup> A.S. Monin and A.M. Yaglom, *Statistical Fluid Mechanics: Mechanics of turbulence* (MIT, Cambridge, MA, 1975), Vol.2
- <sup>15</sup> P.K. Yeung and S.B. Pope, J. Fluid Mech., 207, 531-586 (1989)
- <sup>16</sup> A. Jameson, Int. J. Num. Methods in Fluids, Vol.20, 743-776 (1995)
- <sup>17</sup> V. Eswaran and S.B. Pope, Phys. Fluids 31, 506-520 (1988)
- <sup>18</sup> J.P. Chollet, A. Picart, 12<sup>th</sup> IMACS World Congress, Paris, 18-22 July 1988
- <sup>19</sup> V. Kuznezov and V. Sabel'nikov, *Turbulence and Combustion* (Hemisphere, 1990)