MODELING SCALAR MIXING PROCESS IN TURBULENT FLOW

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ABSTRACT

The paper accounts for the work in progress: it addresses some issues concerning scalar mixing models to be implemented in the probability density function (PDF) computation of turbulent flow. Basic notions are briefly recalled; a heuristic model that simulates both the effect of turbulent mixing and molecular diffusion in the physical space is presented. A particle model is then proposed that describes an evolution of scalar variable in its sampling space (in the context of the PDF method). The model satisfies a selection of constraints imposed on the general physical modeling.

INTRODUCTION

Scalar mixing has been studied for many years, first rather independently in fluid mechanics, chemical engineering and combustion communities (Villermaux 1986, Villermaux & Falk 1996) and now certain convergence of different approaches is observed. It is an important issue for computation of reactive flows where different species mix at a molecular level to initiate chemical reaction. In the case of turbulent flows, species are first mixed down the smallest turbulent scales (so-called macromixing) and then local non-uniformities of concentration are smoothed out by the action of molecular diffusion (micromixing). Difficulties in modeling are rooted in the proper description of turbulent straining of fluctuating scalar gradients and in the coupling of this effect with molecular mixing.

The issue of an adequate modeling of scalar dynamics in a turbulent flow remains a notoriously difficult problem in traditional moment closures. The reason of this difficulty it (at least) threefold: a closure for scalar convection due to fluctuating velocity is needed; for reactive scalars, source term is not closed; and the molecular diffusion term has to be modeled. The first two difficulties are overcome in the probability density function (PDF) approach; however, the scalar micromixing term is not closed in all one-point closures, including the PDF method.

The motivation for the present study has arisen naturally: the authors have been developing the PDF modeling approach for turbulent free-shear and wall-bounded turbulent flows (Pozorski & Minier 1994, Minier & Pozorski 1999) for some time now, and the PDF method is considered as particularly suitable for turbulent reactive flows (Pope 1990; Fox 1996). Once the difficulties concerning the modeled turbulence equations, statement of boundary conditions, and code validation are overcome, the account for passive and reactive scalars is the next step in this direction.

The main idea of the PDF method (for a review see Pope 1994) is to propose a closed evolution equation for the one-point joint pdf; it can include velocity, turbulent energy dissipation rate and scalar variables (chemical composition, temperature, etc.) The equation is solved by means of the so-called particle representation (Monte Carlo method). In transport equations for inert and/or reactive scalars, convection and source terms are treated without recourse to closure hypotheses. However, the molecular mixing term cannot be represented exactly by one-point PDFs. A variety of modeling proposals have already been put forward (Pope 1990, 1994, and Dopazo 1994 give a review), none of them reveals to be fully satisfying, as far as a number of criteria to be fulfilled by a physically sound model is concerned.

In the present paper, a problem of molecular mixing is stated in the PDF context, the notion of "anti-diffusion" is indicated and related difficulties are distinguished. A simple mechanistic model that accounts for both turbulent (random) and molecular mixing illustrates the physical points. A particle evolution model is then put forward.

GOVERNING EQUATIONS, DIFFUSION AND ANTIDIFFUSION

Consider the evolution of a passive scalar $\phi(\mathbf{x},t)$ in a given velocity field $\mathbf{U}(\mathbf{x},t)$. It is governed by a convection-diffusion equation (we suppose here that there are no scalar sources in the solution domain)

$$\frac{\partial \phi}{\partial t} + \mathbf{U}\nabla\phi = D\nabla^2\phi \qquad (1)$$

where D stands for the molecular diffusivity.

Assuming first that we are interested in features of the diffusion process at small length scales, velocity field at these scales can approximately be considered constant; with no loss of generality it can be taken as zero. With an initial condition $\phi(\mathbf{x}, t = t_0) = \phi_0(\mathbf{x})$ and boundary conditions, a unique solution to the above exists at later times. It is usually written as

$$\phi(\mathbf{x}, t + t_0) = \int \phi_0(\mathbf{y}) K(\mathbf{x},\mathbf{y},t)\, d\mathbf{y} \qquad (2)$$

where

$$K(\mathbf{x},\mathbf{y},t) \sim (Dt)^{-3/2} \exp\left(\frac{-(\mathbf{x}-\mathbf{y})^2}{4Dt}\right) \qquad (3)$$

stands for the kernel function (or propagator) of the diffusion equation. One notices that the solution is linear in ϕ_0; ϕ_0 can be thought of as a sum of weighted Dirac functions (fine-grained distribution). In the language of Monte Carlo method, this is tantamount to simulate (using random walk) certain number of *independent* sources.

In the PDF context, the notion of antidiffusion appears. The equation satisfied by the one-point pdf $f(\psi; t, \mathbf{x})$, i.e. pdf that at time t and location $\mathbf{x}$ the variable $\phi(t, \mathbf{x})$ takes the value ψ, can be obtained from (1); with the assumption of homogeneous turbulence, it writes:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial \psi}[\langle D\nabla^2\phi \,|\, (\mathbf{x},\psi)\rangle f] = D\nabla^2 f - \epsilon_\phi \frac{\partial^2 f}{\partial \psi^2} \quad (4)$$

$\langle Y \,|\, X = x\rangle$ is used to represent the mean value of the random variable Y conditioned on the value $X = x$ and is often directly written as $\langle Y \,|\, x\rangle$. In the above equation, ϵ_ϕ is the mean value of the dissipation rate of the scalar variance $\langle\phi^2\rangle$ conditioned on the value $\phi = \psi$ and $\mathbf{x}$:

$$\epsilon_\phi = D\langle(\nabla\phi)^2 \,|\, (\mathbf{x},\psi)\rangle \qquad (5)$$

The sign before ϵ_ϕ in (4) is negative thus it formally introduces antidiffusion in the phase space of ϕ while there is "normal" diffusion in the physical space of $\mathbf{x}$.

Monte Carlo modeling of the diffusion equation (1) is essentially local; for a review of this approach, see Ghoniem & Sherman (1985). Localness means that random displacement of any notional particle is independent of the actual state of other particles. Only afterwards a mean field (like concentration) is computed.

Now, in the case of antidiffusion, the coefficient in front of $\partial^2 f/\partial\psi^2$ in (4) is negative. Reasoning now in terms of the generic diffusion equation, Eq. (1) with $\mathbf{U} = 0$, with negative D, this corresponds to the inversion of the time arrow ($t \to -t$). Consequently, one finds in (3) a square root of a negative number. This is a simple manifestation of a rigorously proven fact that Eq. (1) with $D < 0$ and a given initial condition represents an ill-posed problem from the mathematical standpoint. Dopazo (1994) alludes to the apparent problems with the numerical solution of this equation. On the other hand, given $\phi(\mathbf{x}, t_0 + t)$, $t > 0$, solution of the antidiffusion equation at the time instant $t_0 + t + t'$ can be found as the solution of the diffusion equation at $t_0 + t - t'$ and, in particular, for $t' = t$ this amounts to finding the initial condition for the diffusion equation, i.e. $\phi_0(\mathbf{x})$ that is governed by its *integral* equation (2). Consequently, an evolution model, possibly stochastic, for notional particles should take into account the actual state of other particles. This is akin to the notion of "self-consistent" field: particle that interacts with others can naturally be considered as placed in a field (or resulting potential) of other particles.

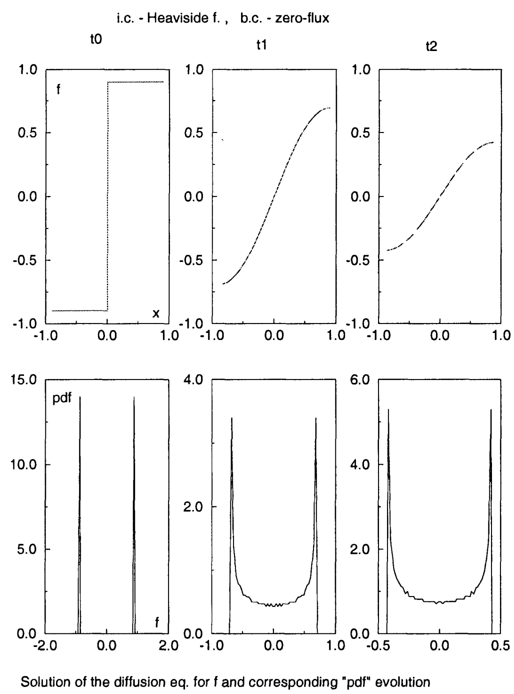

Figure 1: Evolution of a scalar (upper plots) and its quasi-pdf governed by the standard diffusion equation; zero-flux boundary conditions.

The above explains the fact that small-scale scalar mixing is usually modeled in a discrete (or Lagrangian) way with the use of pairs of particles, i.e. two stochastic particles at a time (Dopazo 1994, Pope 1985) and not only one (as in the Langevin equation). Alternatively, information on other (interacting) notional particles is conveyed through the PDF for a range of scalar values; modeled scalar PDF evolution equations are often integral equations.

Now the question arises: how to reconcile the apparent ill-posedness of the antidiffusion equation with real (i.e. existing) physical processes where initial spatial non-uniformity of a certain variable decreases? Looking at the diffusion process, it is readily seen that concentration tends to the uniform, single-valued final state. In fact there is no contradiction: antidiffusion takes place in the phase space, not in the physical one (location space). For the scalar diffusion, the phase space variable is concentration. For the action of viscosity, antidiffusion in the phase space of velocity is a direct consequence of the diffusion of momentum in the physical space.

1D SLAB MODEL

This is a simple mechanistic model that mimics the scalar diffusion process in the field of homogeneous turbulence.

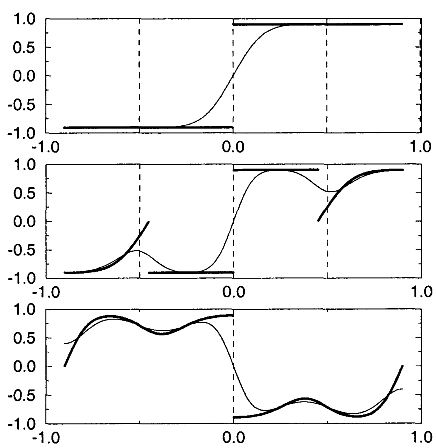

Figure 2: Evolution of a scalar as governed by the diffusion equation and the slab model; zero-flux boundary conditions. Scalar value vs/ x-coordinate at different time instants: thick line at any plot is a rearrangement of the thin line at the plot immediately above it.

The main idea of the "slab" model is to divide the basic interval in 1D of length L_0 into 2^N equal pieces; each of them is further subdivided into 2^M smaller pieces. At time intervals $\Delta t_{N,M}$ the small subintervals are spatially rearranged (mixed). This process is random in a sense that for every slab $(1, 2, \ldots, 2^N)$, its parts $(1, 2, \ldots, 2^M)$ are rearranged in the order $(i_1, i_2, \ldots, i_{2M})$ where a sequence $\{i_k\}$ stands for a randomly-chosen permutation of $(1, 2, 3, \ldots, 2^M)$ indices. The actual simulation goes as follows. After a time $2^{-N} L_0^2/D$, the subintervals are randomly mixed. This mimics the turbulent stirring, i.e. the distortion of the scalar field by turbulent eddies of different length-scales and life times, the distortion by smaller eddies being more frequent than by larger ones. The smallest eddies are characterized by the Kolmogorov length and time scales, and the largest by the basic interval size. Generalisation to the 2D/3D geometry, although not performed yet, is straightforward: subsequent rearrangements of squares (or cubes) are to be considered instead.

Before continuing with the slab model, a simple computer experiment has been performed. One-dimensional diffusion equation (1) has been solved in time on a given interval with a step initial condition (cf. Fig. 1)

$$f(\psi, t{=}0) = 0.5 * [\delta(\psi - 1) + \delta(\psi + 1)]$$

which corresponds to an initially unmixed scalar. Zero-flux boundary conditions are applied. An easy and standard computation using finite differences has been done to forward the solution in time. Then, a less-frequently asked question arises: what is the shape of the quasi-pdf (because a problem is perfectly deterministic) of the solution? The quasi-pdf is defined as the histogram of values of c on the interval, found using bin-counting method.

Figure 1 shows the evolution of $\phi(x,t)$ and the corresponding quasi-pdf $f(\phi, t)$. It is readily seen that the asymptotic evolution of f resembles initial evolution phase of the pdf of a scalar undergoing mixing process. However, contrary to the true pdf, the quasi-pdf stays self-similar and does not relax towards a Gaussian one.

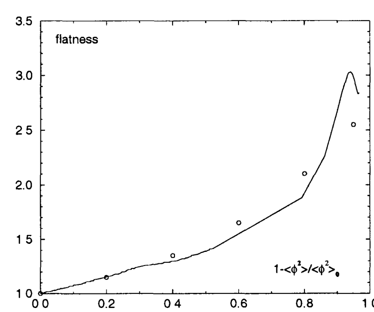

Figure 3: Evolution of a modeled flatness factor in a normalized time; prediction of the slab model. Circles – DNS data of Eswaran & Pope (1988)

Next, we performed another computer experiment with the slab model. To illustrate the idea of random mixing, Fig. 2 shows some subsequent shapes of $\phi(x,t)$ in the simplest rearrangement with $N = 1$, $M = 1$.

Then, a complete simulation result is presented for the flatness factor of the scalar PDF obtained with the model (Fig. 3). A reasonable agreement with the DNS results of Eswaran & Pope (1988) suggests that this simple mechanistic model captures already some physics of the actual mixing process.

It may be worthwhile to mention here that somewhat analogous reasoning has been put forward by Fox (1992). He used analytical solution of the 1D diffusion equation in the context of scalar pdf in lamellar structures to formulate a Fokker-Plank closure. Moreover, the akin idea of the "rearrangement events" is important in the linear eddy modeling (LEM) developed by Kerstein (1991).

PARTICLE MODELS FOR SCALAR MIXING

In the PDF approach, several proposals have been put forward to model the molecular mixing term, but it is extremely difficult to satisfy at a time all imposed criteria of a good model. Concerning only passive and non-reactive scalars, they are as follows (Pope 1994a):
- realisability, i.e. boundedness of scalar values should be preserved,
- variance of scalar concentration should decrease in a prescribed way,
- the scalar pdf evolving in time should be (at least) qualitatively correct,
- the pdf should asymptotically tend to a Gaussian distribution,
- it is preferable for a model to be physically sound.

Now, following the reasoning from the previous section, a tentative idea of a simple antidiffusion model is advanced. It gives an evolution of the initial pdf towards Gaussian distribution. The guiding idea of the model is to consider every stochastic particle (to which a scalar value is attached) in the "field" of other particles, represented by the pdf, at given time instant, in the phase space of the scalar variable.

Model using triangular pdf

Given a certain number (i.e. a discrete representation) of scalar values, $\phi_1, \phi_2, \ldots, \phi_N$, their bounds ϕ_{min}, ϕ_{max} are computed, and an auxiliary variable $\hat{\phi}_i$ is taken, using these scalar bounds and a random number taken from the uniform distribution $\mathcal{U}(0,1)$. In the model, auxiliary triangular pdf on $[\phi_{min}, \phi_{max}]$ with a maximum ϕ_i is used and inversion of its cumulative distribution function (cdf) is the method applied for the purpose.

Then, new values are assigned to scalar variables as follows:

$$\phi_i = \phi_i + \omega(\hat{\phi}_i - \phi_i) \qquad (6)$$

where $0 < \omega < 1$ is a kind of relaxation parameter. The procedure is then repeated for successive iterations.

It should be noted that Eq. (6) differs from both the

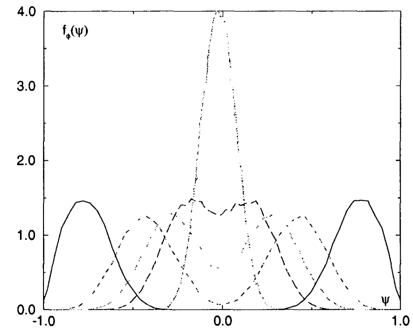

Figure 4: Evolution of a modeled pdf (method using auxiliary triangular pdf).

IEM formula of Dopazo and the improved Curl model (including ordered-pairing improvement by Norris & Pope, 1991). Concerning the IEM formula, it does not change the form of the initial scalar PDF; only its variance is affected. As to the Curl's model, it predicts the asymptotic PDF to differ from Gaussian.

The reason of the different behavior shown by (6) can be stated as follows. The scalar variable ϕ_i is allowed to interact with another notional fluid particle with scalar value $\hat{\phi}_i$, and not only with the mean value $\langle\phi\rangle$ (as in IEM) or another particle from the ensemble ϕ_j (Curl). The point is that scalar values are distributed continuously on the $[\phi_{min}, \phi_{max}]$ interval.

Norris & Pope (1991) state that the necessary condition for the PDF to evolve toward a Gaussian is that the conditional mean $\langle\hat{\phi}_i|\phi_i\rangle$ should be linear in ϕ_i. Taking the formula for the triangular PDF and computing the conditional averages, it is readily checked that this is indeed the case: $\langle\hat{\phi}_i|\phi_i\rangle = \frac{1}{3}(\phi_i + \phi_{min} + \phi_{max}$.

Fig. 5 shows the temporal evolution of the selected moments of the pdf. Variance decreases nearly exponentially and higher order moments tend to their respective Gaussian values. Fig. 4 contains a few plots of the pdf itself (using relaxation parameter $\omega = 0.2$). Pdf is evolving from the initial double-peak distribution towards a Gaussian one.

Finally, in Fig. 6 flatness coefficient of the pdf evolving in a normalized time (defined by the decreasing variance of the pdf) is compared to the DNS data of Eswaran & Pope (1988). Obtained results are (at least) qualitatively correct.

Model using actual pdf

Rather than using somewhat arbitrary triangular pdf (in fact, any other continuous pdf bounded by actual scalar limits ϕ_{min}, ϕ_{max} can be applied), we take the actual scalar pdf computed at a given iteration and inverse its cdf to obtain the auxiliary variable $\hat{\phi}_i$. This is actually the only difference as compared to the previous model. Results are detailed and discussed in the paper. Fig. 8 shows the temporal evolution of the selected moments of the pdf. Variance decreases nearly exponentially and higher order moments tend to their respective Gaussian values. Fig. 7 contains a few plots of the pdf itself (using relaxation parameter $\omega = 0.2$). Pdf is evolving from the initial double-peak distribution towards a Gaussian one. Moreover, in Fig. 9 flatness coefficient of the pdf evolving in a normalized time (defined by the decreasing variance of the pdf) is compared to the DNS data of Eswaran & Pope (1988). Obtained results are (at least) qualitatively correct.

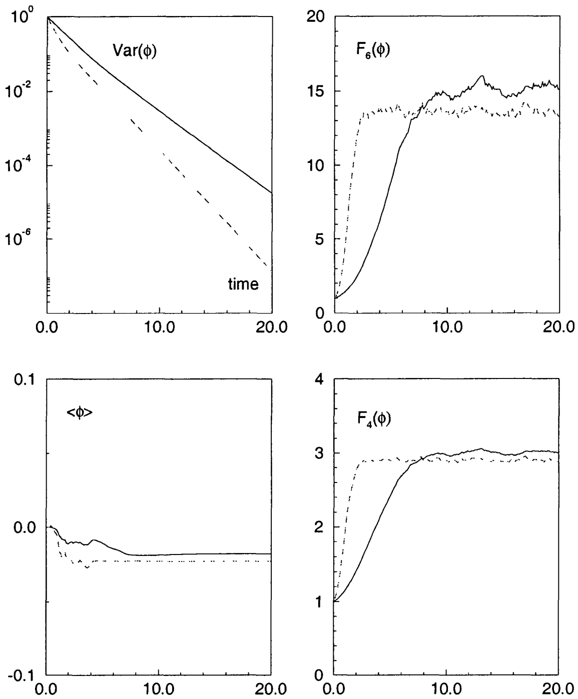

Figure 5: Evolution of chosen moments of the scalar pdf using auxiliary triangular pdf; black (dashed line): $\omega = 0.1$, red (solid line): $\omega = 0.2$.

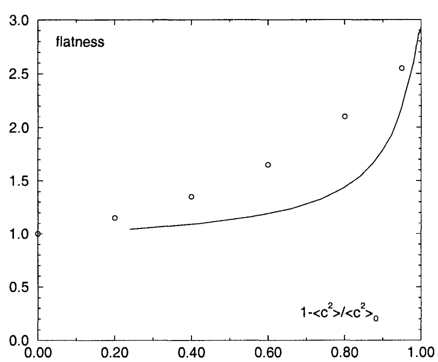

Figure 6: Evolution of a modeled flatness factor in a normalized time (method using auxiliary triangular pdf).

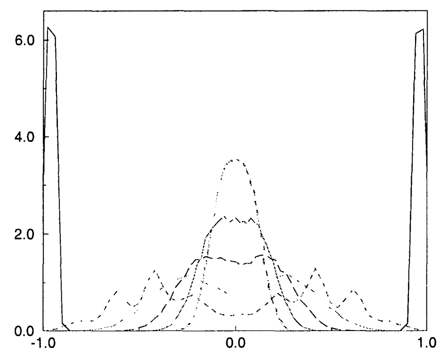

Figure 7: Evolution of a modeled pdf (method using inversion of the cdf).

Both models possess some desirable features:
– scalar bounds $\phi_i \in [\phi_{min}, \phi_{max}]$ are automatically preserved,
– at every iteration all scalar values are modified, contrary to so-called interaction models, as discussed by Pope (1985) and Dopazo (1994), where only a selection of particle pairs are chosen at every time step,
– variance of ϕ decreases exponentially,
– the pdf of ϕ is qualitatively correct, as compared to the available DNS data.

The simple model using inversion of the cdf shows some similarities to the Langevin model, recently proposed by Valiño & Dopazo (1991). However, the difference is that in their model binomial pdf is used whereas in our approach any continuous bounded-support pdf will do. Both naturally give a relaxation towards a final Gaussian distribution.

CONCLUSION

Proposals for models of scalar mixing have been put forward. The models for particle evolution as of particular interest, as they can be directly incorporated in a PDF computation of turbulent flows. Current developments aim also at including multiple scalars (differential diffusion, multispecies reaction) and/or reaction modeling in test diffusion flames, e.g. along the lines of

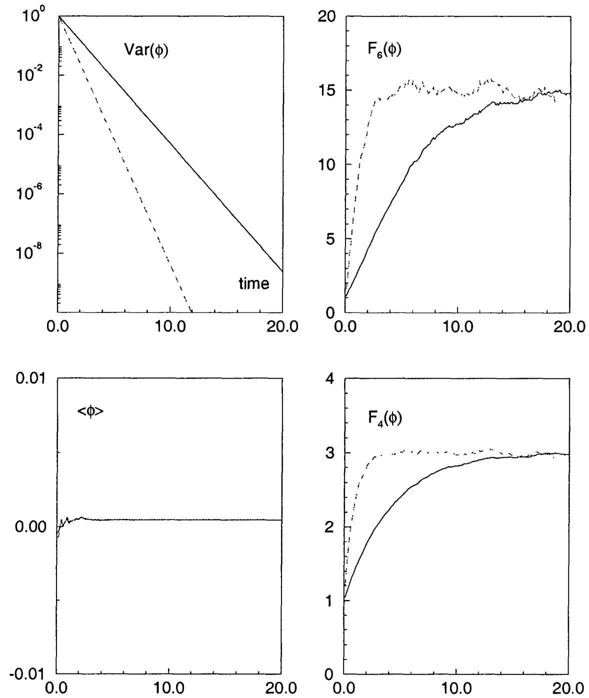

Figure 8: Evolution of chosen moments of the scalar pdf (mean value, variance, flatness, superflatness) using inversion of the cdf; black (dashed line): $\omega = 0.1$, red (solid line): $\omega = 0.2$.

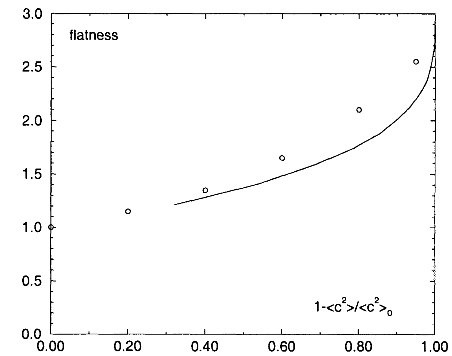

Figure 9: Evolution of a modeled flatness factor in a normalized time (method using inversion of the cdf).

the scheme for (ξ, Y) as considered by Norris & Pope (1991). However, before this is done, the utility of the presented triangular PDF model and its modifications will be tested in the standalone PDF code.

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