Probability density function approach and related closures for turbulent scalar fields

By Feng Gao

1. Motivation and objectives

Turbulent flows are characterized by highly irregular flow patterns and, therefore, require statistical descriptions (Monin & Yaglom 1975; Tennekes & Lumley 1973). The probability density function (PDF) of a turbulent field provides complete statistical properties of the quantity concerned.

The PDF approach is especially useful when applied to complicated statistical behavior of turbulent fields, such as intermittency (Kraichnan 1990a, 1990b), and highly nonlinear reacting flow problems (O'Brien 1980, Pope 1985, Bilger 1989). Intermittency refers to the "bursting" signal that is frequently observed in a turbulent flow. Its presence is normally represented by long tails of the velocity or scalar gradient PDF (non-Gaussian tails). The application of the PDF method to this problem seems to be natural. For reacting flow problems, the chemical source terms are usually nonlinear and have to be modeled if the traditional moment method is employed. Given the fact that there are many different types of reactions, these models, if they can be constructed, are very likely to be problem oriented and do not have widespread applicability. On the other hand, the PDF approach provides a closed form for the reacting source terms, which makes it an attractive method in dealing with turbulent reacting flows (Pope 1990).

However, the PDF method is not without its setbacks: the major difficulty associated with the PDF method has been the unclosedness of Fickian diffusion terms in the PDF formulation. Recently, the mapping closure was formulated to address this difficulty (Chen *et al.* 1989, Gao & O'Brien 1991, Pope 1991). It has been shown that this closure model captures major characteristics of the scalar PDF's (Gao 1991a, 1991b; Pope 1991). The mapping closure has been used to study some fundamental problems in turbulence, such as the intermittency of the velocity and scalar gradient fields (Kraichnan 1990, Gao *et al.* 1991).

Our current study generally concerns the development of PDF methodology in turbulence research. More specifically, our efforts have been focused on various aspects of the mapping closure models in PDF approach. The results of mapping closure are tested against the available direct numerical simulation (DNS) data to further validate the model. Encouraged by the success of single scalar mapping closure, we have extended the same idea to cases with more than one species, which is a rather natural step because most reactions involve many reacting species.

It should be pointed out that any single-point PDF only provides local information of the concerned field. In other words, the interactions between different points in a turbulent field cannot be properly described by a single-point PDF. The mapping closure model, being a one-point closure model, certainly cannot be exempted from this shortcoming. There have been two ways to cure this problem. The first one is to introduce two-point PDF's. But this method does not solve the problem at all because three-point information would be needed to close the two-point PDF and this hierarchy would continue to higher level. Also, this method complicates the problem by doubling the dimension of the problem, which makes numerical simulation very difficult (Pope 1990). The second method, which is widely accepted, is to characterize the effects of turbulence by a time scale. Other turbulence models are used to determine this time scale.

In the second method, the scalar PDF in a turbulent field would evolve in the same way as in the pure diffusion case with a modified time. As a consequence of this argument, an initial Gaussian scalar PDF remains a Gaussian distribution. However, recent DNS and experimental results have shown that this may not be the case (Kraichnan, private communication). Figure 1(B) shows the PDF of a scalar field evolved from an Gaussian initial state (Figure 1(A)) in a stationary turbulence field in a 64^3 direct simulation. The development of non-Gaussian tails is obvious. Similar simulations are performed for the pure diffusion case with essentially the same initial field (the only difference being that a different random seed is used in generating the initial field) by turning the velocity field off. As expected, the PDF in this case remains Gaussian (Figure 1(C)). Our analysis suggests that the representation of the turbulent effect may have over-simplified the problem (Gao *et al.* 1991). W. C. Reynolds and P. A. Durbin have also pointed out on different occasions that the structure of the turbulence field should be reflected in the PDF formulation. Hence, an attempt has been made to study detailed interaction between scalar and velocity fields.

2. Accomplishments

3.1. Mapping closure for multispecies Fickian diffusion

We seek mappings

$$\psi_1 = X(\phi_1, \phi_2, t), \tag{1.a}$$

$$\psi_2 = Y(\phi_1, \phi_2, t), \tag{1.b}$$

where ϕ_1 and ϕ_2 are standard independent Gaussian reference fields, and $\psi_1(\vec{x}, t)$ and $\psi_2(\vec{x}, t)$ are governed by

$$\frac{\partial X}{\partial t} = D_1[\nabla^2 \psi_1]_{c:\psi_1\psi_2}, \tag{2.a}$$

$$\frac{\partial Y}{\partial t} = D_2[\nabla^2 \psi_2]_{c:\psi_1\psi_2}. \tag{2.b}$$

It can be shown (Gao & O'Brien 1991a) that X and Y satisfy

$$\frac{\partial X}{\partial t} = D_1(\hat{L}_1 + \hat{L}_2)X, \tag{3.a}$$

$$\frac{\partial Y}{\partial t} = D_2(\hat{L}_1 + \hat{L}_2)Y, \tag{3.b}$$

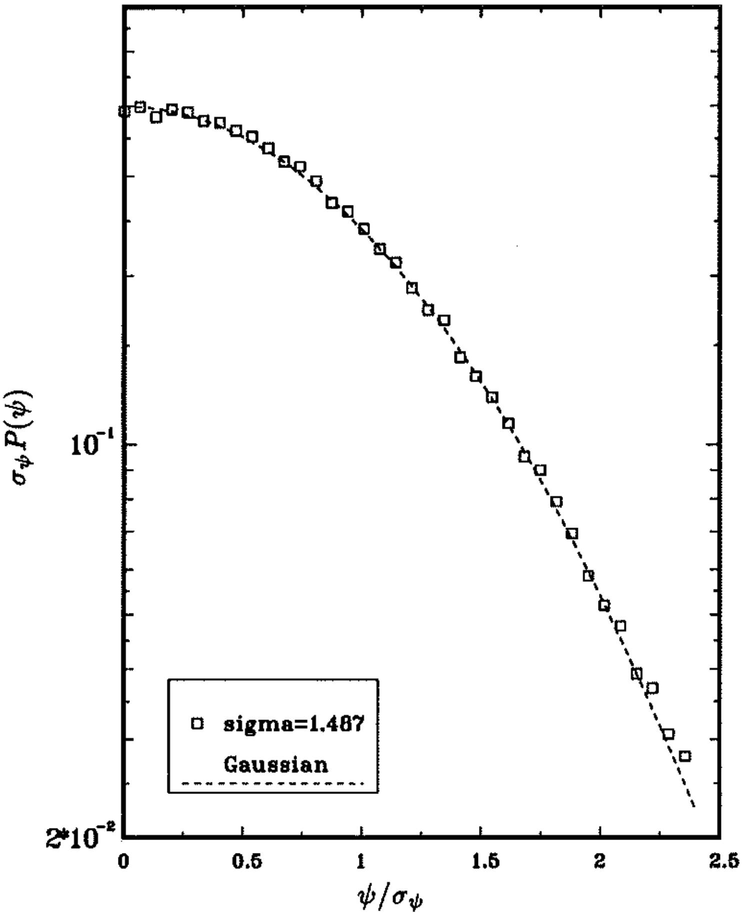

FIGURE 1(A). Normalized initial scalar PDF. $\sigma_\psi(0) = 1.487$ (symbol) and standard Gaussian distribution (dashed line).

where

$$\hat{L}_i = -\lambda_i \phi_i \frac{\partial}{\partial \phi_i} + \frac{\partial^2}{\partial \phi_i^2}, \qquad (i = 1, 2)$$

and $\lambda_i \quad (i = 1, 2)$ are the time scales to be determined.

The solutions of equation (3) are

$$X = \int\int_{-\infty}^{\infty} \frac{du_1 du_2}{4\pi a_1 a_2} \{X(u_1, u_2, 0) \exp[-\frac{(\phi_1 e^{-D_1\tau_1} - u_1)^2}{4a_1^2} - \frac{(\phi_2 e^{-D_1\tau_2} - u_2)^2}{4a_2^2}]\}, \qquad (4.a)$$

$$Y = \int\int_{-\infty}^{\infty} \frac{du_1 du_2}{4\pi b_1 b_2} \{Y(u_1, u_2, 0) \exp[-\frac{(\phi_1 e^{-D_2\tau_1} - u_1)^2}{4b_1^2} - \frac{(\phi_2 e^{-D_2\tau_2} - u_2)^2}{4b_2^2}]\}, \qquad (4.b)$$

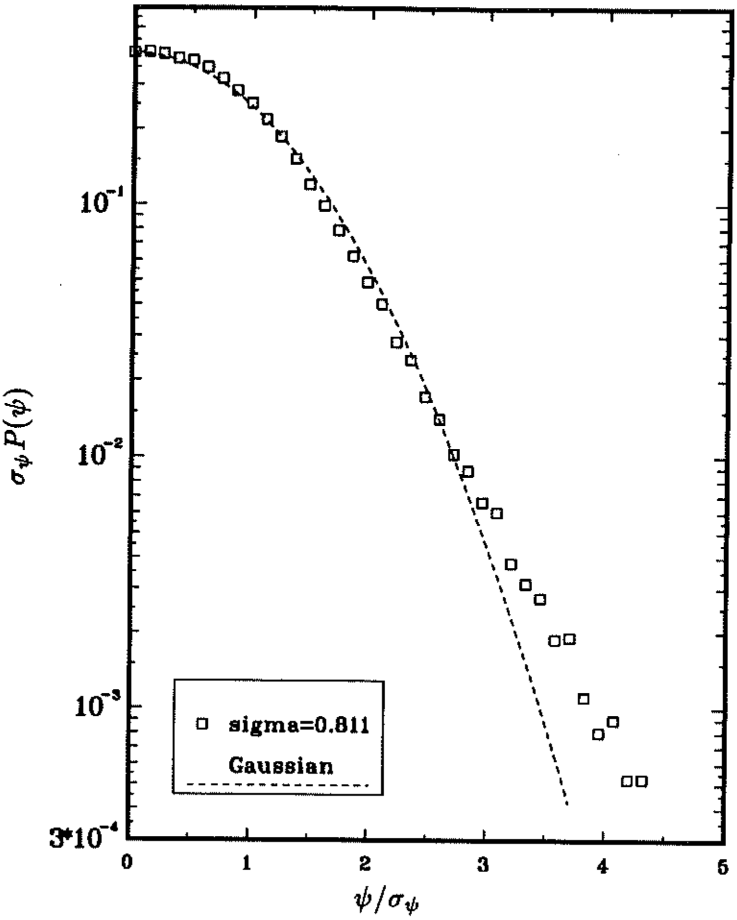

FIGURE 1(B). Normalized scalar PDF at a later time ($\sigma_\psi = 0.811$) in a turbulence field.

where $\tau_i = \int_0^t \lambda_i dt \quad (i = 1, 2)$,

$$a_i^2(t) = \int_0^t \exp(-2D_1\tau_i)dt \qquad \text{and} \qquad b_i^2(t) = \int_0^t \exp(-2D_2\tau_i)dt.$$

Clearly, solutions (4) preserve two important features of the scalar PDF: 1) if the initial scalar fields are bounded, the subsequent fields remain bounded, and 2) the leading terms in the solution relax to Gaussian distributions (Gao & O'Brien 1991a). It is also obvious that the above procedure can be applied to cases with more scalar fields involved.

3.2. Test of amplitude mapping against DNS results

For an initially double-delta PDF

$$P(\psi, 0) = \frac{1}{2}[\delta(\psi) + \delta(\psi - 1)], \tag{5}$$

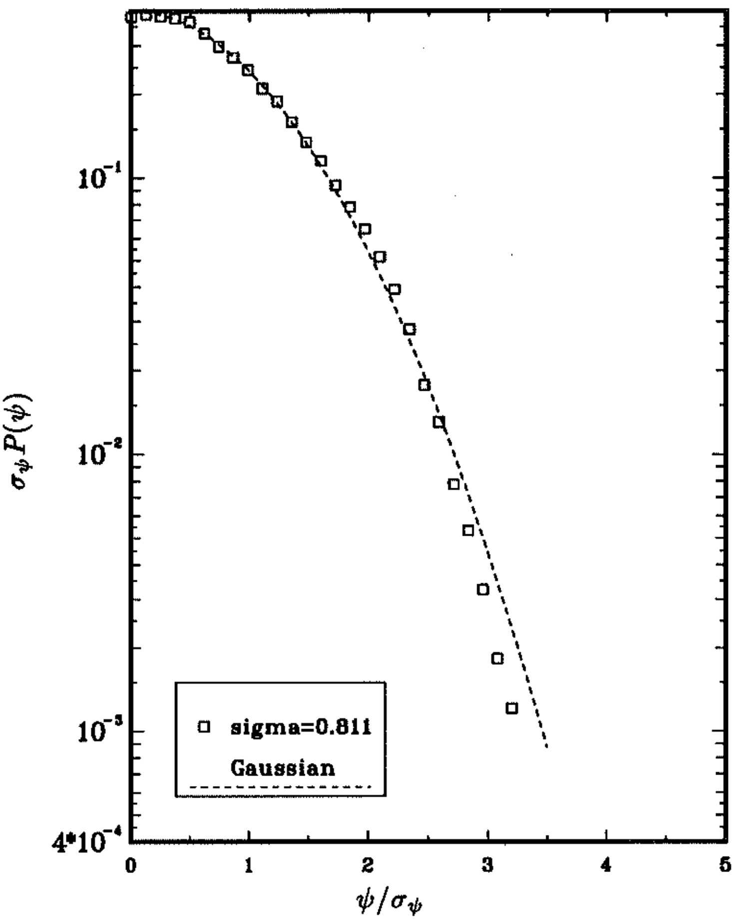

FIGURE 1(C). Normalized scalar PDF at a later time ($\sigma_\psi = 0.811$) for pure diffusion case.

the mapping solution can be shown (Gao 1991a, Pope 1991) to be

$$X(\phi, t) = \frac{1}{2}(1 + \text{erf}[\phi e^{-\tau}/\sqrt{2}a(\tau)]), \tag{6}$$

where τ is the rescaled time and $a^2 = 1 - e^{-2\tau}$. Consequently, the conditional dissipation rate of the scalar field $E\{(\nabla\psi)^2|\psi\} = E(\psi, t)$ can be derived for this case (O'Brien, private communication) as

$$E(\psi, t)/E(0.5, t) = \exp\{-2[\text{erf}^{-1}(2\psi - 1)]^2\}. \tag{7}$$

This result provides a perfect test case for the mapping closure because any error that may be introduced by time rescaling has been ruled out. Direct numerical simulations are performed for this specific case and the results are plotted in Figure 2. It shows that the mapping prediction are in excellent agreement with the DNS data.

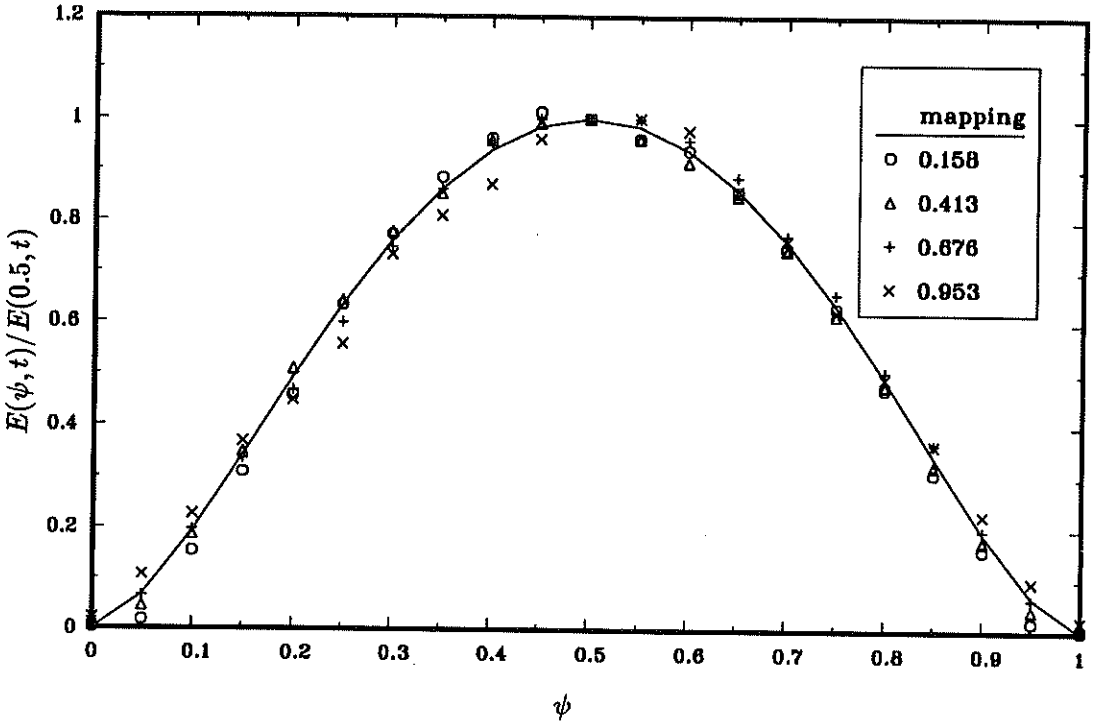

FIGURE 2. $E(\psi,t)/E(0.5,t)$ for an initially double delta PDF at different times. Solid line: mapping closure; symbols: DNS data (taken at eddy-turn-over times $tu/l = 0.158$; 0.413; 0.676 and 0.953).

3.3 *Persistence of scalar PDF non-Gaussianity*

An interesting observation can be made about Figure 2: the relative shape of the conditional dissipation rate does not change with time. Recalling the fact that the PDF of a homogeneous scalar field is a Gaussian distribution if and only if the conditional dissipation rate $E\{(\nabla\psi)^2|\psi\}$ is independent of the scalar field ψ (Gao 1991b), Figure 2 suggests that some of the non-Gaussian properties of a scalar field persist during the scalar evolution process.

It is well known that scalar gradient fields become intermittent in turbulence and their PDF's develop non-Gaussian tails (e.g. Monin & Yaglom 1975; Kraichnan 1990). However, it has been generally believed that the PDF of a homogeneous scalar field relaxes to a Gaussian distribution. Figure 2 definitely casts some doubts about this conclusion and needs to be explained.

The amplitude mapping solution can be written in an expansion form (Gao 1991b)

$$X(\phi,t) = \sum_{n=0}^{\infty} b_n H_n(\phi/\sqrt{2})e^{-n\tau}, \tag{8}$$

where H_n is the Hermite function. It is obvious from (8) that in the course of time, H_1, which is a linear function of ϕ, becomes the leading term. In this sense, the scalar PDF relaxes to a Gaussian distribution. However, the higher order terms survive for large ϕ even at later times, which means that the tails of the scalar PDF continue to be influenced by the initial and boundary conditions. Thus, non-Gaussianity of a scalar field persists, most noticeably in the tails of its PDF and in the high order moments of the scalar amplitude (Gao 1991b).

3.4 Effect of turbulence on the evolution of scalar PDF's

As has been pointed out earlier, an initially Gaussian scalar field develops a non-Gaussian PDF under the action of turbulence. To understand this phenomenon, let us start with an ensemble of scalar fields which has a Gaussian distribution. Under the action of a certain velocity field, the scalar PDF remains Gaussian, but the decaying rate of the scalar variance is determined by scalar diffusivity and the advecting velocity field $\vec{v}$. i.e.

$$P_c(\psi, t|[\vec{v}]) = \frac{1}{\sqrt{2\pi}\sigma([\vec{v}], t)} \exp(-\frac{\psi^2}{2\sigma^2([\vec{v}], t)}),$$

where $[\vec{v}]$ indicates a functional of velocity field and P_c is the PDF of scalar ψ conditioned on a given $\vec{v}$. Hence, we have

$$P(\psi, t) = \int P_c(\psi, t|[\vec{v}])P([\vec{v}], t)d[\vec{v}]. \tag{9}$$

Obviously, $P(\psi, t)$ given by (9) has longer tails than a Gaussian distribution (Gao & O'Brien 1991b).

The above analysis can be formulated by introducing J, which represents the stretching produced by the velocity field. The J-analysis was first proposed by Kraichnan, who used a heuristic non-stochastic J-model to explained the intermittency (exponential-like tails in velocity gradient PDF) in Burgers' turbulence (1990a, 1990b). For a passive scalar field, J is generally a random functional of the advecting velocity field. Therefore, a stochastic J-model is needed for turbulent scalar fields.

The mapping analysis can be readily carried out if we consider a one-dimensional case with random uniform stretching velocity field $u = a(t)x$. For an initial Gaussian scalar field, the mapping solution yields

$$\psi = \phi e^{-\tau} = \phi \exp(-D \int_0^t J^2 dt), \tag{10}$$

where J measures the stretching of length scale by a certain velocity field and this defines τ. Therefore,

$$\xi = \frac{\partial \psi}{\partial x} = J\xi_0 e^{-\tau}. \tag{11}$$

J is generally a functional of the velocity field and is random in time. A Stratonovich type stochastic differential equation

$$dJ = -\alpha J^3 dt + \sqrt{2\beta} J dW_t \tag{12}$$

can be written for J if the stretching velocity field $a(t)$ is replaced by a white noise process in time. Here $\alpha \propto D$, β is determined by velocity stretching and W_t is a standard Wiener process.

The Fokker-Planck equation for the PDF of J can be easily written as

$$\frac{\partial P}{\partial t} = \alpha \frac{\partial}{\partial J}(J^3 P) + \beta \frac{\partial}{\partial J}[J \frac{\partial}{\partial J}(JP)]. \tag{13}$$

It is shown that (13) represents both limits of pure diffusion and of pure convection cases (Gao *et al.* 1991). The stationary solution for (13) can also be easily written as

$$P(J) \sim \frac{1}{J} \exp(-\frac{\alpha}{2\beta} J^2). \tag{14}$$

It should be noted that (14) does not apply as $J \to 0$, where unsteady effects remain important. The scalar PDF $P(\psi)$, given $\psi \approx \phi \exp(-cJ^2)$, can be derived from (14) as

$$P(\psi) = \int P_G(\phi) P(J) dJ,$$

where P_G is the standard Gaussian distribution. A typical scalar PDF so obtained is plotted in Figure 3. It shows similar non-Gaussian scalar PDF as those observed in the DNS results (Figure 1(B)).

The PDF of the scalar gradient ξ can also be obtained from (11) and (14) as

$$P(\xi) \sim \frac{1}{|\xi|} \exp(-|\xi| / \sqrt{\frac{\beta}{\alpha}}). \tag{15}$$

This clearly demonstrates the exponential-like tails for the scalar gradient PDF, similar to that derived by Kraichnan for velocity gradient in Burgers' turbulence (1990a, 1990b). These tails indicate the expected intermittency of the scalar gradient field and are widely observed in experiments and DNS. 64^3 DNS have been conducted for both turbulent and pure diffusion cases. It is shown by the DNS that while the scalar gradient remains a Gaussian distribution for the pure-diffusion case (Figure 4(A)), the gradient of a turbulent scalar field clearly develops exponential-like tails (Figure 4(B)).

3.5 Implementation of mapping for reacting flows

A scheme has been developed for implementing the mapping closure model for single-scalar turbulent reacting flows. The results are in excellent agreement with the DNS data. For more details, see the report by L. Valiño in this volume.

4. Future plans

It is important to find practical schemes for implementing the available closure models, especially for multispecies reacting cases. Three issues are involved.

First, the dimension of the problem increases with increasing species number, thus making numerical calculations of multispecies PDF very difficult using the

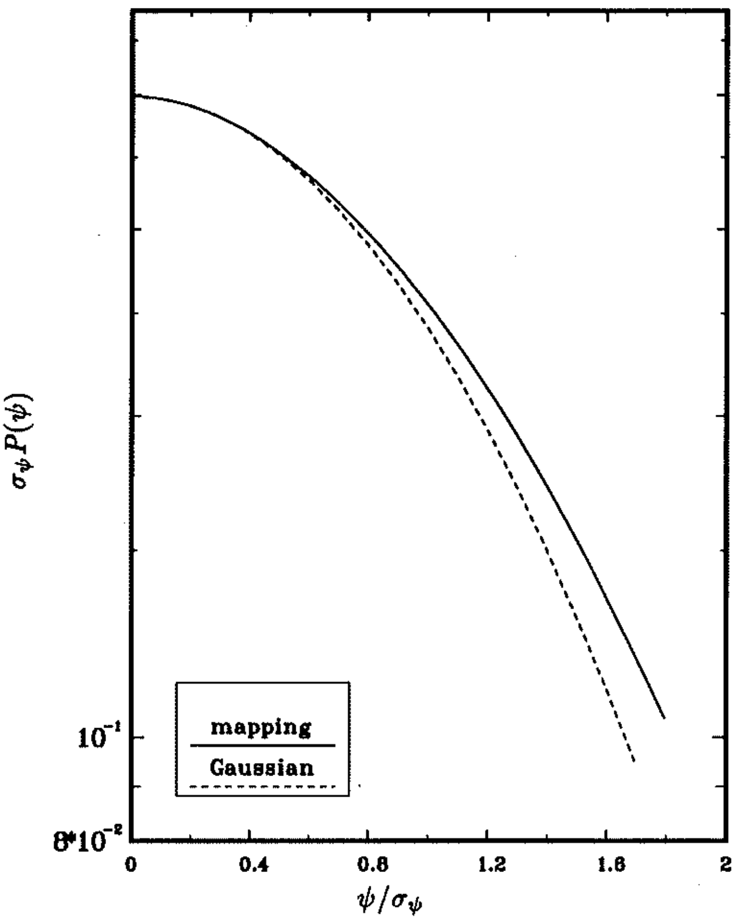

FIGURE 3. A typical PDF of a scalar field (initially Gaussian distributed) in a turbulence field.

traditional finite-difference method (Pope 1990). The Monte-Carlo technique is suggested to carry out such calculations. Preliminary results show this may be a feasible technique.

Second, the time scale of scalar evolution process under turbulence advection must be modeled for practical problems. More detailed studies will be conducted to answer two questions: 1) How does turbulence affect the scalar evolution? and 2) Does representing the turbulent effect by a single time scale cause much error in calculating terms that are of practical interest? Both of these questions concern turbulent mixing theory, and the second question is related to the application of the PDF approach to study of turbulent reacting flows. Our results show that the low order statistics, which are of interest in practical problems, are not greatly affected by the "tail" effects. Thus, detailed interactions between velocity and scalar fields, although theoretically of great interest, may not render substantial practical improvement. If this is true, our implementation of the PDF approach will be much

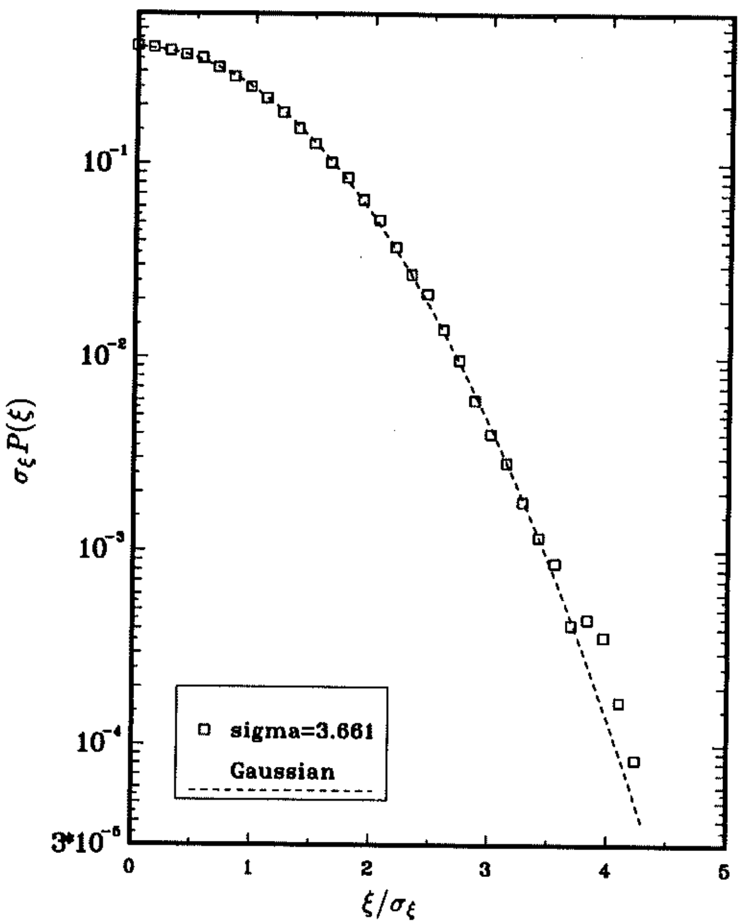

FIGURE 4(A). Normalized PDF of a scalar gradient developed from an initially Gaussian distribution ($\sigma_\xi(0) = 5.263$) under pure-diffusion. $\sigma_\xi = 3.661$.

simpler.

Third, to deal with problems of turbulent combustion, the current research should be extended to more general cases involving several scalar fields in non-homogeneous turbulence. The key issue is to develop methods that are workable under available resources at relatively low cost compared with the DNS method. The feasibility of mapping closure to such complicated cases is not obvious and will be investigated.

Acknowledgment

The non-Gaussian tails of the scalar PDF in a turbulence field was first pointed out by Dr. Y. Kimura. The theoretical study of this problem is an on-going collaboration among Dr. R. H. Kraichnan, Dr. Kimura and myself.

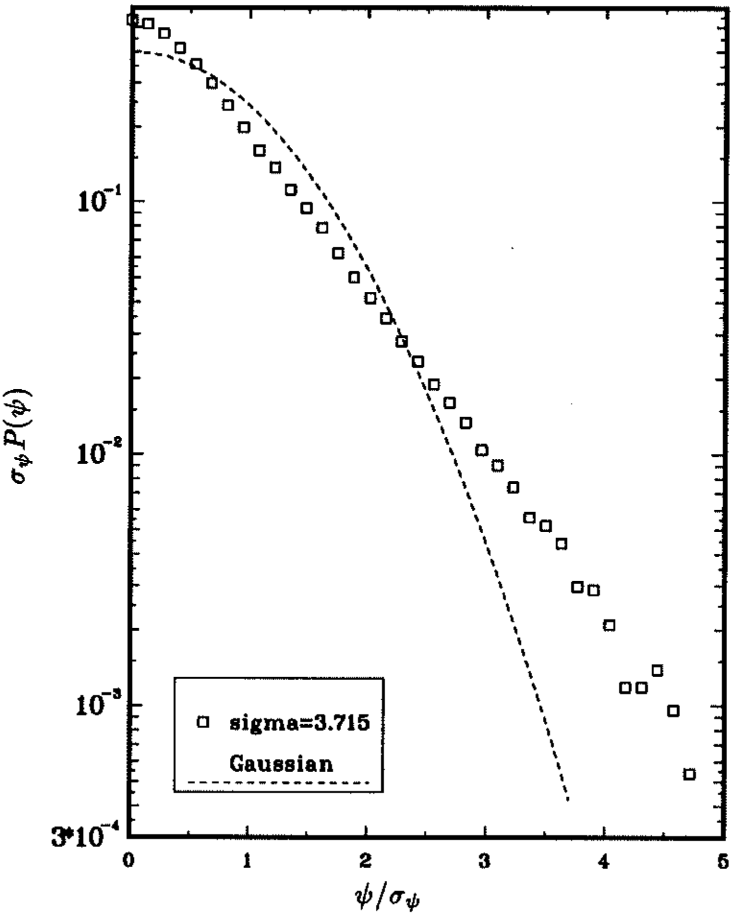

FIGURE 4(B). Normalized scalar gradient PDF in homogeneous turbulence (developed from a similar initial field as in 4(A), $\sigma_\xi(0) = 5.263$). $\sigma_\xi = 3.715$.

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