PDF approach for turbulent scalar field: some recent developments

By Feng Gao

1. Motivation and objectives

The probability density function (PDF) method has been proven a very useful approach in turbulence research. It has been particularly effective in simulating turbulent reacting flows and in studying some detailed statistical properties generated by a turbulent field (see, e.g., Monin & Yaglom 1975, Bilger 1989, Pope 1985 & 1990, Kraichnan 1990, Gao *et al.* 1992).

There are, however, some important questions that have yet to be answered in PDF studies. Our efforts in the past year have been focused on two areas. First, a simple mixing model suitable for Monte Carlo simulations has been developed based on the mapping closure. Secondly, the mechanism of turbulent transport has been analyzed in order to understand the recently observed abnormal PDF's of turbulent temperature fields generated by linear heat sources (Gollub *et al.* 1991, Jayesh & Warhaft 1991).

1.1 Needs for new mixing models in PDF approach

It is well known that the PDF approach provides a closed form representation for the chemical reacting source terms, thus becoming a preferred choice among the available closure models for turbulent reacting flows (O'Brien 1980, Pope 1985). The general argument is that once the PDF of a reacting scalar, ψ, is known, the mean reaction rate, which is the key quantity to be evaluated in reacting flow simulations, can then be readily calculated by

$$\langle S \rangle = \int S(\psi) P(\psi) d\psi.$$

Generally, two approaches have been commonly taken in applying the PDF method, namely, presumed PDF and full PDF methods.

The presumed PDF method assumes a certain form for the PDF with some adjustable parameters, which are supplied by other conventional models (Bray 1980, Borghi 1988, Vervisch 1992). Restricted by the scope of the closure models used (for example $k-\epsilon$ model), the parameters to be adjusted are generally limited to the low order statistics such as mean and variance, thus exposing an important shortcoming of the presumed PDF. In fact, one can construct different PDF's P_1 and P_2 that have the same mean and variance but totally different higher order statistics. If the reaction source term is highly nonlinear (which is true in most cases), the mean reaction rates obtained from P_1 and P_2 may be very different, depending on which PDF form is chosen.

The natural way for obtaining the PDF is the full PDF method which simulates the PDF from its evolution equation. However, a major stumbling block in this approach has been the lack of a proper closure for the diffusion effect (O'Brien 1980, Pope 1985). In order for a model to be accepted in practical simulations, it has to be physically reasonable and numerically easy to implement. Despite the theoretical success the mapping closure enjoys in treating the mixing effect in the PDF approach (Kraichnan 1990, Gao 1991, Pope 1991), it has been shown difficult and computationally intense to implement this closure in simulations (Gao & O'Brien 1991, Valiño & Gao 1992). The most commonly used model for diffusion effect in practical Monte-Carlo simulations remains the LMSE model (Pope 1992) which reads

$$\frac{d\psi_i}{dt} = -\omega(\psi_i - \langle\psi\rangle). \tag{1}$$

It is well known that this model does not relax a PDF. In fact, it can be easily shown that applying this model leads to

$$F_n(t) = \frac{\langle\psi'^n\rangle}{\langle\psi'^2\rangle^{n/2}} = F_n(0),$$

where $\psi' = \psi - \langle\psi\rangle$. Therefore, the PDF so obtained can be very erroneous. This puts us in a rather awkward position. On one hand, we are attempting to use a highly sophisticated approach whose main promise is to provide accurate estimates for mean reaction rates. On the other hand, the PDF could be so contaminated that it does not reflect the true evolution of the fields being considered.

It is, therefore, obvious that in order for the PDF method to live up to its promises, better mixing models which are easy to implement should be developed.

1.2 PDF generated by non-uniform sources

The experiments of Jayesh & Warhaft (1991) and Gollub *et al.*(1991) indicate that the scalar PDF generated by a linear source term exhibits exponential tails. This result is rather surprising because it has generally been believed that the PDF so generated is a Gaussian distribution (Venkataramani & Chevray 1978, Tavoularis & Corrsin 1981). This situation certainly demands a theoretical investigation.

There are three basic processes that determine the distribution of a scalar PDF: the shape of the non-uniform source, the turbulent convection, and the molecular diffusion. A fluid particle leaving the source is convected by the turbulent velocity field to a certain observation point. Because of the chaotic nature of the velocity field, particles from different positions in the source all have certain possibilities of reaching the observation point, thus generating the fluctuations that reflect the characteristics of the source. In the absence of molecular diffusion, the PDF of the scalar is determined by the interaction of the source and the convection.

There are a couple of reasons that justify the neglection of molecular diffusion in search for the mechanism of generating exponential tails. First, it is supported by theoretical arguments and numerical simulations that the molecular diffusion tends to relax a PDF to a Gaussian distribution. Although it has been shown that the interaction between random turbulent advection and molecular diffusion distorts a Gaussian PDF to generate mild non-Gaussian tails (Gao *et al.* 1992), the clear exponential tails observed in these experiments cannot be explained within the frame of this interaction. Secondly, for high Reynolds (Péclet) number flows, the diffusive effect is very small in comparison with the turbulent transport (Taylor 1935) which is responsible for bring around the fluctuations generated by the non-uniform source.

Based on these arguments, the experiments mentioned earlier can be analyzed explicitly under some idealized conditions. This study suggests a mechanism which seems to provide an explanation for the observed tails.

2. Accomplishments

2.1 A mixing model for PDF simulations

In dealing with turbulent reacting flow problems, it is generally accepted to separate the effects of mixing and reaction by time-splitting schemes. Since the reaction term is closed in PDF formulation, we will concentrate on proper modeling for the mixing effect.

The mapping closure maps a known statistical field ϕ (generally chosen as a multi-variate standard Gaussian field) to a surrogate field $X(\phi, t)$ whose statistics resemble those of the true scalar field ψ (Chen *et al.* 1989). Under homogeneous and non-reacting conditions, the mapping relation is governed by

$$\frac{\partial X}{\partial t} = \omega^*(-\phi\frac{\partial X}{\partial \phi} + \frac{\partial^2 X}{\partial \phi^2}), \tag{2}$$

where ω^* is determined by the time scale of turbulent mixing. It has been shown that this model provides an excellent representation for the mixing effect in the PDF approach (Gao 1991a, Pope 1991).

In spite of its good physics, the mapping closure has posed great difficulties for numerical implementation, as pointed out earlier. The problem stems from the necessity that the fields be re-mapped at each time step, which is computationally intense. This problem worsens drastically as the dimension (number of the scalar quantities) involved increases.

In the model we are proposing, the PDF is represented by a group of representative "particles" which advance in time following certain laws, as is generally used in Monte-Carlo simulations. In case of reaction acting alone, for example, each particle is advanced by

$$\frac{d\psi_i}{dt} = S(\psi_i).$$

The task is, therefore, to develop similar models to describe the mixing effect.

One way to generate such models is to use the mapping solution. It is well known that the general solution for (2) is (Gao 1991a, 1991b)

$$X(\phi, t) = \sum_{n=0}^{\infty} a_n H_n(\frac{\phi}{\sqrt{2}})e^{-n\tau}, \tag{3}$$

where $\tau = \int_0^t \omega^* dt$ and H_n are Hermite functions. The expansion coefficients a_n can be determined as

$$a_n = \frac{1}{\sqrt{2\pi}2^n n!} \int_{-\infty}^{\infty} X(\phi, 0) H_n(\frac{\phi}{\sqrt{2}}) \exp(-\frac{\phi^2}{2}) d\phi = \frac{1}{2^{n/2} n!} \langle \frac{\partial^{(n)} X}{\partial \phi^{(n)}} \rangle_{t=0}. \quad (4)$$

Clearly, for reasonably well behaved mapping, a_n tends to zero rapidly. Therefore, we expect that a truncation of the right hand side of (3) at a relatively low order

$$X(\phi, t) = \sum_{n=0}^{m} a_n H_n(\frac{\phi}{\sqrt{2}}) e^{-n\tau} \quad (5)$$

can approximate $X(\phi)$ to a satisfactory degree of accuracy.

A group of surrogate particles can be chosen according to (5) to represent the PDF, and each of these particles evolves according to

$$\prod_{i=1}^{m} (\frac{d}{d\tau} + i)(\psi - \langle \psi \rangle) = 0, \quad (6)$$

where $d/d\tau = d/(\omega^* dt)$ and ω^* can be related to the scalar evolution time scale. In fact, if ω in

$$\frac{d\langle \psi'^2 \rangle}{dt} = -\omega \langle \psi'^2 \rangle$$

can be provided by other models, such as the $k - \epsilon$ model, it can be shown that

$$\omega^* = \frac{\omega}{2} \frac{\sum_{n=1}^{\infty} 2^n n! \mu_{n-1}}{\sum_{n=1}^{\infty} n \cdot 2^n n! \mu_{n-1}}, \quad (7)$$

where $\mu_\alpha = (a_{\alpha+1}/a_1)^2 e^{-2\alpha\tau}$. If the truncated form (5) is used, all μ_α where $\alpha \geq m$ should be set to zero.

μ_α can be related to the certain order moments of the field considered. For example, if $m = 3$, it can be shown that

$$\mu_1 = \frac{\sqrt{2}(1 + 4\mu_1^2 + 24\mu_2^2)^{3/2}}{12 + 144\mu_2 + 32\mu_1^2 + 864\mu_2^2} F_3 \quad (8a)$$

and

$$\mu_2 = \frac{F_4(1 + 4\mu_1^2 + 24\mu_2^2)^2 - 3g(\mu_1, \mu_2)}{48(1 + 48\mu_1^2 + 216\mu_2^2)}. \quad (8b)$$

Here F_i are moment coefficients as defined earlier and

$$g(\mu_1, \mu_2) = 1 + 40\mu_1^2 + 336\mu_2^2 + 5952\mu_1^2\mu_2^2 + 80\mu_1^4 + 17856\mu_2^4.$$

These equations can be solved iteratively, and our tests seem to suggest that μ_α are very small and

$$\omega^* \approx \omega/2 \quad (9)$$

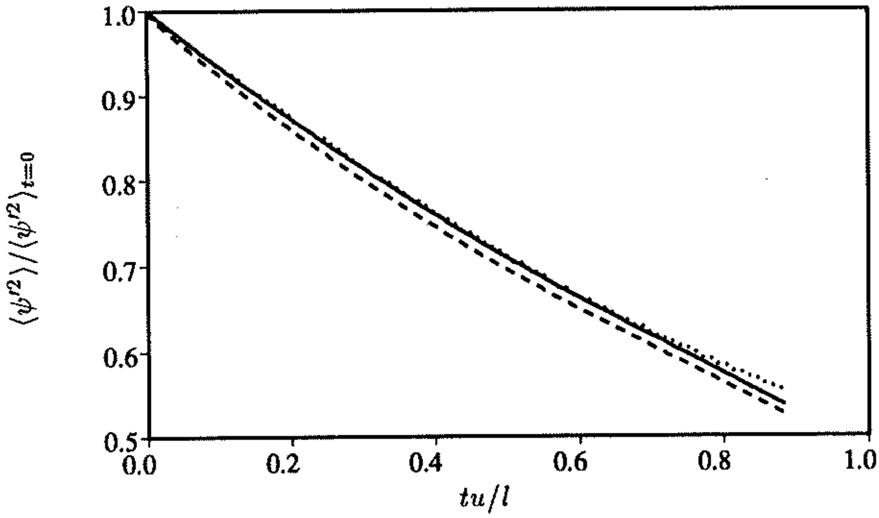

FIGURE 1. Evolution of scalar variance: DNS (dotted line); LMSE (solid line) and current model (dashed line). tu/l is the eddy-turn-over time.

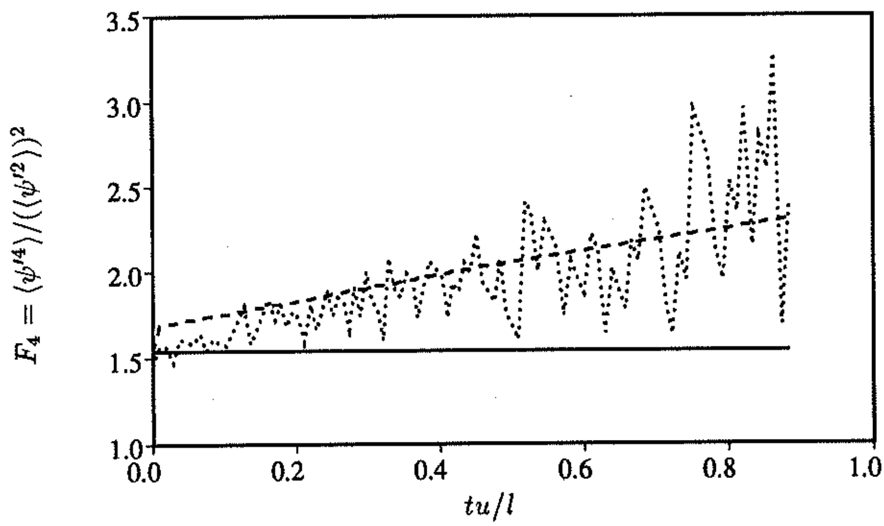

FIGURE 2. Evolution of scalar flatness: DNS (dotted line); LMSE (solid line) and current model (dashed line). tu/l is the eddy-turn-over time.

remains a good approximation. Taking the highly singular double-delta PDF as an example, it can be shown that $\mu_{2\alpha+1} = 0$ (because of symmetry) and $\mu_2 = 1/144$, $\mu_4 = 1/25600$, etc.

It is noticed that if we choose $m = 1$, (6) recovers the equation in the LMSE model (1) and (7) shows that $\omega^* = \omega/2$.

It should be pointed out that in the current model, we are only interested in the

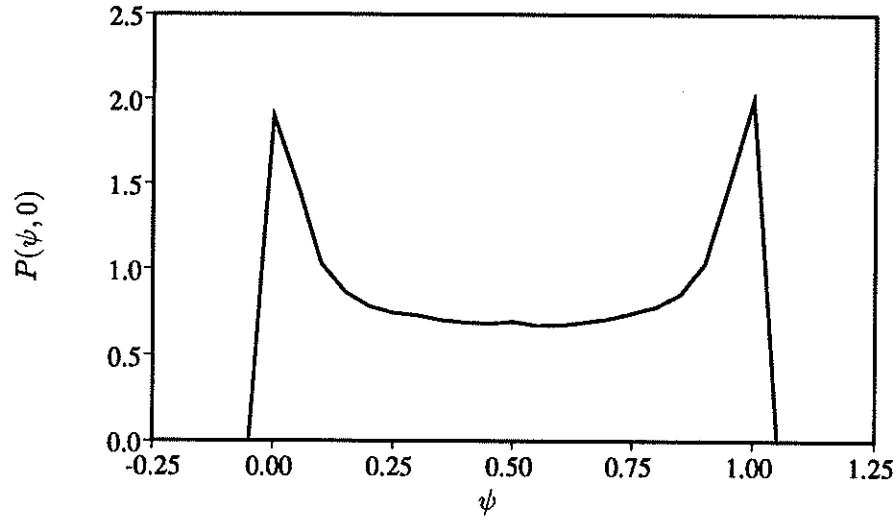

FIGURE 3A. Initial scalar PDF.

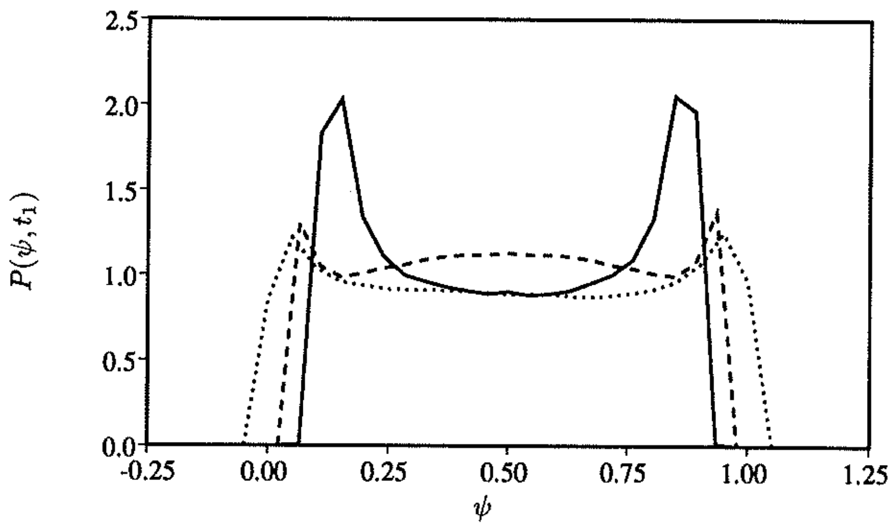

FIGURE 3B. Scalar PDF at $t_1 u/l = 0.178$: DNS (dotted line); LMSE (solid line) and current model (dashed line).

evolution of a group of surrogate particles whose statistics closely resemble those of the true turbulent field. These particles are generally not the fluid particles.

Some tests have been conducted using the model with $m = 3$ and compared with the corresponding cases from DNS and the LMSE model. Figure 1 shows the evolution of scalar variance with ω matched from DNS data. It shows that (8) is indeed a good approximation. Figure 2 exhibits the evolution of the scalar flatness F_4. While the LMSE model clearly does not relax the PDF, the current model catches on the trend of DNS.

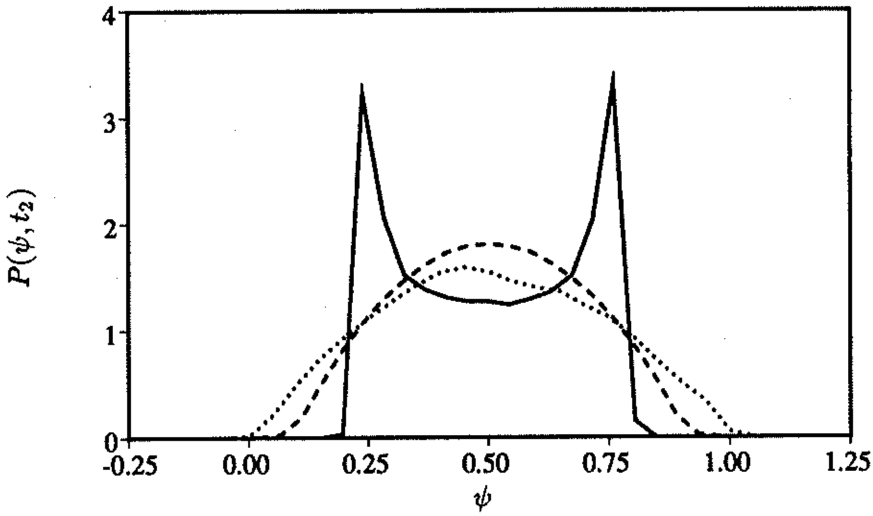

FIGURE 3C. Scalar PDF at $t_2u/l = 0.685$: DNS (dotted line); LMSE (solid line) and current model (dashed line).

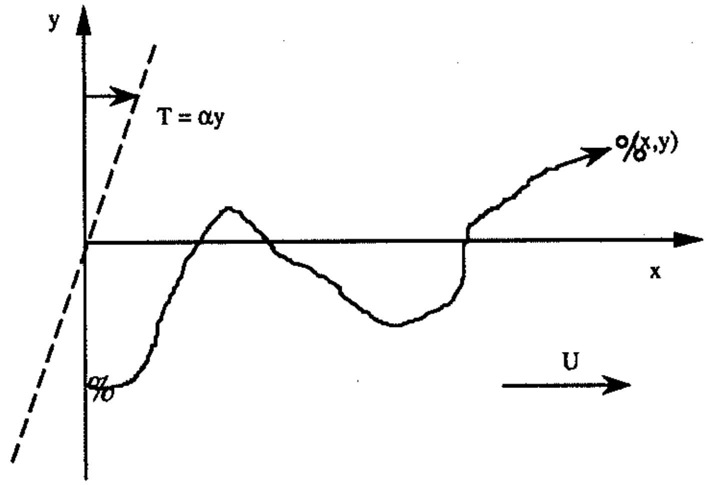

FIGURE 4. Sketch of the system considered.

The plots of PDF evolution perhaps are more revealing. The initial PDF in the model simulations are generated according to that in DNS and normalized in the interval [0,1] (Figure 3(a)). The evolved PDF at two later moments are plotted in Figures 3(b) and 3(c). The improvement achieved by the current model is obvious.

The accuracy of representing the PDF by a collection of surrogate particles depends on the shape of the PDF. Models with better accuracies can be developed along the same line by pushing m higher. However, it is expected that $m = 3$ should suffice for practical simulations.

2.2 PDF of temperature fields generated by a linear heat source

As discussed earlier, the abnormal tails of a scalar PDF are mainly caused by the interaction between the non-uniform source and the random advecting velocity. Let τ_t and τ_d be the time scales of turbulent transport and molecular diffusion, respectively, it is well known that $\tau_d/\tau_t \sim Re$ (Tennekes & Lumley 1973). For high Reynolds number flows, we simply assume that $\tau_d \to \infty$ and $\tau_t \to 0$, namely, neglecting the molecular diffusion and assuming the velocity fluctuation is white in time. The consequences of these simplifications are explained elsewhere (Gao 1992).

Hence, a particle detected at time t at the observation point (x, y) can be traced back to an earlier time τ when it was released from the source at $(0, y_0)$ and acquired the temperature $T(0, y_0; \tau)$ (refer to Figure 4 for a sketch of the system being considered), i.e.

$$x = U(t-\tau) + \int_\tau^t u' dt \qquad \text{and} \qquad y - y_0 = \int_\tau^t u' dt. \tag{10}$$

It can be shown that (Gao 1992)

$$x = U(t-\tau) + \sigma_x \sqrt{t-\tau} r_1 \qquad \text{and} \qquad y - y_0 = \sigma_y \sqrt{t-\tau} r_2, \tag{11}$$

where $\sigma_i^2 = 2u_i L_i$ and r_i are standard independent Gaussian random variables. Here u_i is the variance of velocity and L_i the correlation length in the i direction. The PDF of temperature can be written as

$$P(\hat{T}; x, y, t) = \langle \delta(\hat{T} - T(0, y_0; \tau)) \rangle_{y_0, \tau \le t}, \tag{12}$$

where the average is taken over all possible particles released from the source prior to t.

Consider the case of linear source, i.e.

$$T(0, y_0; \tau) = \alpha y_0.$$

It can be shown that

$$P(T; x, y, t) = F(T; x, y, t) G(T; x, y, t) \tag{13}$$

where

$$F(T) = \frac{\beta}{2\pi\alpha\sigma} \exp[-\frac{U(\gamma - x)}{\sigma^2}] \tag{14}$$

and

$$G(T) = \frac{1}{2\sigma\gamma^2} \int_{-\infty}^{\infty} \frac{x\xi^2 + 2U\gamma(x+\gamma)}{\sqrt{\xi^2 + 4U\gamma}} \exp(-\xi^2/2\sigma^2) d\xi. \tag{15}$$

Here, $\sigma = \sigma_x$, $\beta = \sigma_x/\sigma_y$ and

$$\gamma^2 = x^2 + \beta^2 (\frac{T}{\alpha} - y)^2. \tag{16}$$

It can be demonstrated that

$$\lim_{T\to\infty}\frac{d\ln G}{dT}=0,$$

hence the main contribution to the tails comes from $F(T)$ which decays exponentially as $T \longrightarrow \infty$.

In linear theory, the fluctuation in x (i.e. r_x) is neglected compare with $U(t-\tau)$. This is equivalent to letting $\sigma \longrightarrow 0$ while keeping $\sigma_y = \sigma/\beta$ finite. In this limit, we have $\beta \longrightarrow 0$. It can be easily shown that

$$F(t) \longrightarrow \frac{1}{2\pi\alpha\sigma_y}\exp[-\frac{U}{2x\sigma_y^2}(\frac{T}{\alpha}-y)^2]$$

and

$$G(T) \longrightarrow \sqrt{\frac{2\pi U}{x}}.$$

Hence,

$$P(T)=\frac{\sqrt{U}}{\sqrt{2x\pi}\alpha\sigma_y}\exp[-\frac{U}{2x\sigma_y^2}(\frac{T}{\alpha}-y)^2],$$

which recovers what would be obtained using the traditional method.

However, this approximation seems to be a rather awkward one because in turbulence, β is generally not small. In fact, in a grid generated turbulence, $u' \sim U$ and $v' \sim 0$ near the grid and $u' \sim v'$ in the later stage. It doesn't seem reasonable to neglect the fluctuation in x direction while keeping the terms of similar or lower order of magnitude in the y direction.

For finite β, we therefore should expect exponential tails under turbulent dispersion at not too distant downstream locations. The exponent can be shown as

$$-\frac{U}{\sigma^2}[\sqrt{x^2+\beta^2(\frac{T}{\alpha}-y)^2}-x] \sim -\frac{\beta U}{\alpha\sigma^2}T \quad \text{for} \quad T \gg 1.$$

Another limit can be obtained if we look at far downstream locations and finite temperature range. In this limit, $\beta^2(\frac{T}{\alpha}-y)^2/x^2 \ll 1$, hence,

$$-\frac{U}{\sigma^2}[\sqrt{x^2+\beta^2(\frac{T}{\alpha}-y)^2}-x] \sim -\frac{U}{2x\sigma_y^2}(\frac{T}{\alpha}-y)^2$$

which also recovers the traditional result. This approximation is equally applicable if we have a strong mean scalar gradient. Therefore, if we move the probe to further downstream locations and/or increase the gradient of the scalar source, we will see more Gaussian-like distributions.

Other quantities, such as mean and higher order moments, can be readily calculated. The qualitative features predicted by this idealized model compare favorably with the available experiments. For detailed discussions, please refer to Gao (1992).

3. Future plans

Given the recent exciting developments in large-eddy simulations of turbulent fields (see related reports in this volume), it seems only natural to extend this successful technique to the reacting flow problems. However, despite many attempts, the proper modeling of the reaction source terms remains an unsolved problem. Considering the wide range of different type of reactions encountered in engineering applications, the prospect of developing a suitable sub-grid-scale model for these source terms seems to be grim. The PDF approach can probably be usefully employed to address this problem.

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