Investigations of turbulent scalar fields using probability density function approach

By F. Gao

1. Motivation and objectives

1.1. Background

Scalar fields undergoing random advection have attracted much attention from researchers in both the theoretical and practical sectors (Chen *et al.* 1989, Pope 1990, Bilger 1989). Research interest spans from the study of the small scale structures of turbulent scalar fields to the modeling and simulations of turbulent reacting flows (Pope 1985, Lin & Pratt 1987).

The probability density function (PDF) method is an effective tool in the study of turbulent scalar fields, especially for those which involve chemical reactions. It has been argued that a one-point, joint PDF approach is the one to choose from among many simulation and closure methods for turbulent combustion and chemically reacting flows based on its practical feasibility in the foreseeable future for multiple reactants (Pope 1990).

Taking chemical species advected by an incompressible fluid as an example, the governing equations can be written as

$$\frac{\partial \vec{\phi}}{\partial t} + \vec{u} \cdot \nabla \vec{\phi} = D \nabla^2 \vec{\phi} + \vec{S}(\vec{\phi}), \tag{1}$$

where $\vec{\phi} = (\phi_1, \phi_2, ..., \phi_\sigma)$ are the mass fractions of the different chemical species and S_α is the reaction source term for species α. For simplicity, the Fickian diffusion coefficients have been assumed to be same for all species.

Defining the fine-grain density function

$$\rho(\vec{x}, t) = \delta(\vec{\phi}(\vec{x}, t) - \vec{\psi}),$$

the PDF equation corresponding to (1) can be derived (O'Brien 1980, Pope 1985)

$$\frac{\partial P(\vec{\psi})}{\partial t} + < \vec{u} \cdot \nabla \rho > = -\frac{\partial}{\partial \vec{\psi}} < D \rho \nabla^2 \vec{\phi} > - \frac{\partial}{\partial \vec{\psi}} [\vec{S}(\vec{\psi}) P(\vec{\psi})] \tag{2}$$

where $< \bullet >$ indicates ensemble average and $\frac{\partial}{\partial \vec{\psi}}$ is the gradient operator in the composition space.

Equation (2) shows that the reaction source term is expressed in a closed form, which distinguishes PDF approach from the traditional moment method. It should also be pointed out that if the joint PDF of the velocity and scalars is employed, the convective terms are also closed. Both of these properties are highly desirable.

However, the weakness of the PDF method is also obvious – it only provides the local information, thus the interaction between neighboring points has to be modeled, i.e. the term representing molecular diffusion has to be treated by *ad hoc* assumptions.

To deal with the interactions between different points in the flow field, multi-point PDF's are introduced (e.g. Jiang 1990). Unfortunately, the inclusion of more points does not resolve the diffusion closure problem and increases the dimension of the problem drastically. It is normally very difficult to solve a differential equation of many variables numerically. Thus the application of multi-point PDF is likely to be quite limited. Another problem with multi-point PDF is that it is not a suitable quantity to handle the small scale structures of the scalar field. Let ψ_1 and ψ_2 be the values of scalar $\phi(\vec{x})$ at points $\vec{x}_1$ and $\vec{x}_2$ respectively, the two-point PDF of ϕ has the property

$$\lim_{\vec{x}_2 \to \vec{x}_1} P_2(\psi_1, \psi_2; \vec{x}_1, \vec{x}_2, t) = P_1(\psi_1; \vec{x}_1, t)\delta(\psi_2 - \psi_1).$$

The numerical solutions of a multi-point PDF may encounter significant errors when applied to the points that are very close to each other.

The major advantage of the PDF method is that it avoids having to close both the convective and the highly nonlinear reaction terms. But the problems with modeling molecular diffusion have not been properly resolved. To model the diffusion term correctly, it is important for us to understand the small scale structures of the scalar fields, which are described by the statistical properties of the scalar gradient. This can be easily seen if we rewrite the diffusion term in (2) under homogeneous conditions as

$$< \rho \nabla^2 \phi >= \frac{\partial}{\partial \psi}[E\{(\nabla \phi)^2 | \psi\} P(\psi)],$$

where $E\{A|B\}$ is the expectation of A conditional on a given B.

1.2. Objectives

Instead of the multi-point PDF, we suggest introducing the joint PDF of a scalar and its gradient which represents the roles of both scalar and scalar diffusion. It is hoped that this study will lead to a proper closure model for the molecular diffusion term in the PDF equation.

Another direction in this research is to study the mapping closure method that has been recently proposed to deal with the PDF's in turbulent fields (Chen *et al.* 1989, Kraichnan 1990a). This method seems to have captured the physics correctly when applied to diffusion problems (Gao 1990). However, if the turbulent stretching is included, the amplitude mapping has to be supplemented by either adjusting the parameters representing turbulent stretching at each time step or by introducing the coordinate mapping. This technique is still under development and seems to be quite promising.

The final objective of this project is to understand some fundamental properties of the turbulent scalar fields and to develop practical numerical schemes that are capable of handling turbulent reacting flows.

2. Previous work

The following results concern the joint PDF of a scalar and its gradient and have been presented elsewhere (Gao & O'Brien 1990a). They are briefly outlined here in order to provide a clue for the future works in this direction.

Since scalar gradient is mainly affected by the small scale structures of the scalar field, we are, therefore, hopeful for two things. First, the isotropic conditions may be applied if the local isotropy condition is correct (Monin & Yaglom 1975). Under this condition, the joint PDF of ψ and $\vec{\xi} = (\xi_1, \xi_2, \xi_3)$, $\hat{P}(\psi, \vec{\xi})$, can be expressed by the joint PDF of ψ and ξ_1, $P(\psi, \xi)$ (Gao 1990a)

$$\hat{P}(\psi, \xi_1, \xi_2, \xi_3) = -[\frac{1}{2\pi\xi}\frac{\partial P(\psi, \xi)}{\partial \xi}]_{\xi=\sqrt{\xi_1^2+\xi_2^2+\xi_3^2}}.$$

Secondly, the universality of the scalar spectrum at small scales may be reflected in the PDF of the scalar gradient. It is argued that the PDF of ξ_1 conditional on a given ψ is a near Gaussian distribution (Gao & O'Brien 1990a). Hence, the conditional PDF $P(|\vec{\xi}|^2|\psi)$ is a χ^2-distribution with three degrees of freedom. Noticing that χ^2 is a special γ-distribution, our result is consistent with the *ad hoc* γ-distribution model for the scalar dissipation, which is used to investigate the intermittency effects of the scalar fields (Andrews & Shivamoggi 1990).

In the spectral space, the scalar is represented by the scalar spectrum $E_\phi(k)$ which is mostly distributed in the small k domain, while the scalar gradient is expressed by the dissipation spectrum $D_\phi(k)$ which is concentrated in the large k domain (see, e.g. Tennekes & Lumley 1973). Figure 1 shows such spectra schematically. When Péclet number is large, these two spectra are widely separated so that ψ and $\vec{\xi}$ are weakly correlated. This conclusion is in agreement with direct numerical simulation results (Rogers 1990).

To further investigate the joint PDF of a scalar and its gradient, the conditional PDF of ξ_1 is expanded according to the Gram-Charlier expansion,

$$P(\xi|\psi) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{\xi^2}{2\sigma^2}}\sum_{n=0}^{\infty} a_n(\psi)H_n(\frac{\xi}{\sqrt{2}\sigma}), \tag{3}$$

where H_n's are the Hermite functions and

$$\sigma^2(\psi) = E\{(\frac{\partial\phi}{\partial x})^2|\psi\},$$

$$a_n = \frac{1}{2^n n!}\int_{-\infty}^{\infty} P(\xi|\psi)H_n(\frac{\xi}{\sqrt{2}\sigma})d\xi.$$

The expansion coefficients can be evaluated as $a_0 = 1$ and $a_2 = 0$, and under isotropic conditions,

$$a_{2n+1} = 0.$$

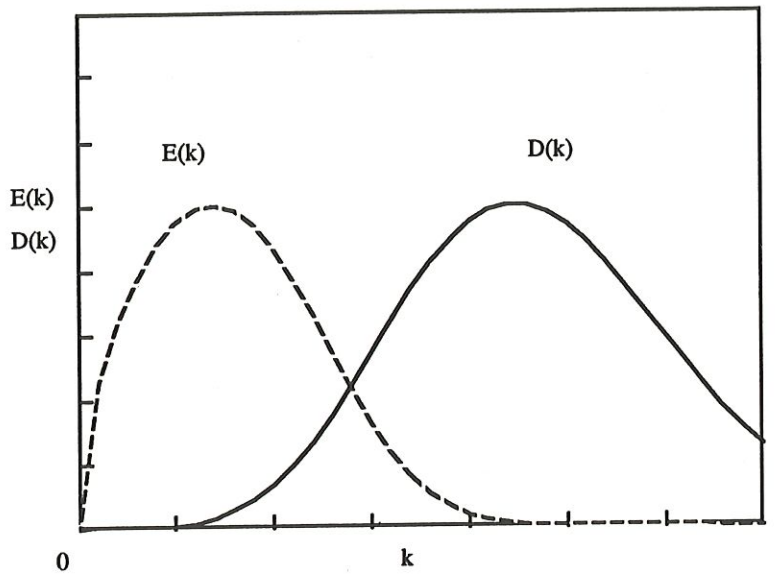

FIGURE 1. Sketch of the Spectra for Ψ, E(k), and ξ, D(k).

Direct numerical simulation (DNS) results are used to evaluate a_n and $\sigma(\psi)$. Primary results show that a_4 is of the same order of magnitude as a_1 and a_3, indicating that a_n is small for higher n, thus a Gaussian distribution is a good approximation for $P(\xi|\psi)$. DNS results also show that $\sigma(\psi)$ is almost a constant throughout most of the ψ domain and drops to zero rapidly as ψ approaches ψ_{max} and ψ_{min}, which is consistent with theoretical predictions.

The database available at the Center for Turbulence Research will be used to evaluate a_n and $\sigma(\psi)$ further under different flow conditions. The details will be outlined in Section 4.

3. Accomplishments

3.1. Mapping closure for PDF

In a different spirit, Chen *et al.* (1989) derive the governing equation for scalar PDF using a Liouville type of equation in the composition space. They then propose a closure method which maps the scalar field to a multivariate Gaussian reference field. This method is subsequently generalized to include the PDF's of various quantities such as that of velocity gradient, etc. (Kraichnan 1990a, 1990b).

Two types of mapping have been considered and both have given some encouraging results. The coordinate mapping has been used by Kraichnan to investigate the PDF of the velocity gradient in Burger's equation. Strong intermittency effects have been demonstrated (Kraichnan 1990a, 1990b). As for the amplitude mapping, the general mapping equation for a turbulent scalar field has been solved analytically (Gao 1990b). The amplitude mapping technique is subsequently generalized

to deal with the joint PDF of multispecies under Fickian diffusion (Gao & O'Brien 1990b).

3.2. Amplitude mapping

Suppose a one-to-one mapping is established between ψ and the reference field ψ_0, $\psi = X(\psi_0, t)$, the mapping equation can be written as (Chen *et al.* 1989)

$$\frac{\partial X}{\partial t} = S(X) + D < \xi_0^2 > (-\frac{\psi_0}{< \psi_0^2 >}\frac{\partial X}{\partial \psi_0} + \frac{\partial^2 X}{\partial \psi_0^2}), \tag{4}$$

where $\xi_0^2 = |\nabla \psi_0|^2$. It corresponds to the scalar evolution equation (1) for single scalar case.

When $S = 0$, the general solution of equation (4) can be written

$$X(\psi_0, t) = \frac{1}{\sqrt{2\pi}a}\int_{-\infty}^{\infty} X(u, 0)\exp[-\frac{(\phi e^{-\tau} - u)^2}{2a^2}]du, \tag{5}$$

where $\phi = \psi_0/\sqrt{< \psi_0^2 >}$, $\tau = D< \xi_0^2 >t/< \psi_0^2 >$ and

$$a^2 = 1 - e^{-2\tau}.$$

The probability density function can then be calculated according to the mapping relation

$$P(\psi, t) = P_0(\psi_0)(\frac{\partial X}{\partial \psi_0})^{-1},$$

where P_0 is a Gaussian distribution. Figure 2 demonstrates the evolution of an initially double-delta PDF

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

Two properties of the scalar fields which have been difficult to recover using the traditional closure models (Pope 1985) now can be readily derived from (5). First, the boundedness of the scalar field is preserved as it can be easily seen that

$$[X(\psi_0, 0)]_{\min} \leq \psi = X(\psi_0, t) \leq [X(\psi_0, 0)]_{\max}.$$

Second, the relaxation to Gaussian of any scalar PDF under Fickian diffusion is captured since

$$X(\psi_0, t) \longrightarrow \alpha(t)\psi_0 \qquad \text{when} \qquad t \gg 1.$$

When n scalars are involved, it has been shown that mapping relations can be established between these scalars and n independent, multivariate Gaussian reference fields. The equations governing these mapping relations can be solved formally (Gao & O'Brien 1990b). This procedure is useful when time-splitting schemes are used to integrate the evolution of the scalar transport equations where the effects of convection, diffusion and chemical reaction can be treated independently.

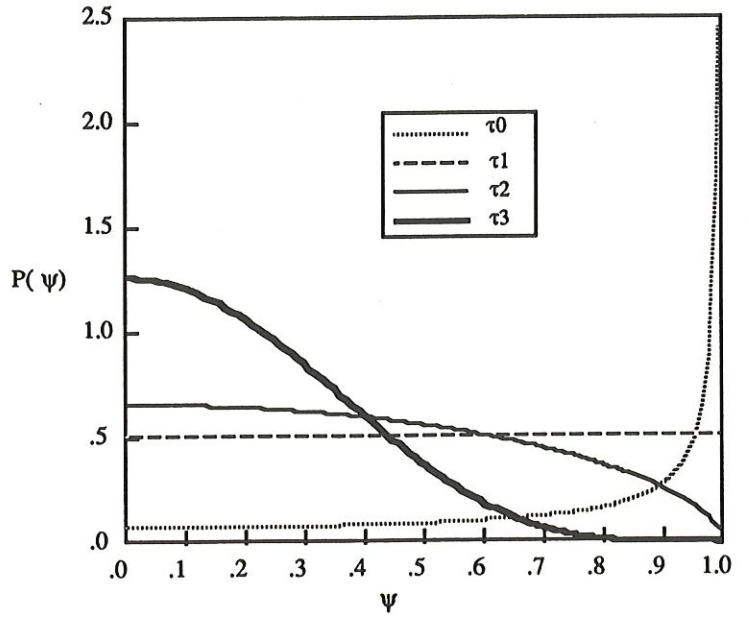

FIGURE 2. Evolution of an Initially Double-Delta PDF.

4. Future plans

The goal of this research is to develop a practical scheme to simulate turbulent reacting flows and combustion. According to Pope (1990), PDF method seems to be a prominent candidate among the available methods for this purpose. It has been identified that the major difficulty one would encounter in the PDF formulation is to close the diffusion term. The results presented above are aimed at addressing this problem. Since these results are mostly obtained from theoretical arguments, our first task will be to test them against experimental and/or numerical data. At the current stage, it is planned to use the extensive DNS data available at CTR for the following purposes.

1) To identify the role of the higher order terms in expansion (3), the coefficients a_n will be further evaluated under different flow conditions. It is hoped that two questions will be answered. First, is local isotropy a good approximation for the turbulent scalar fields? Second, are the higher order terms important?

2) To find out the statistical inter-dependency between a scalar and its gradient. An important quantity to calculate for this purpose is $\sigma^2 = E\{(\nabla\phi)^2|\phi\}$ if the higher order terms in the Gram-Charlier expansion are indeed negligible. Besides, proper modeling of the diffusion term also depends on our knowledge about this quantity.

3) To compare the scalar PDF's obtained from DNS with those derived from the mapping closure in order to determine the applicability of the mapping closure to the reacting flow problems. In this case, the amplitude mapping will be used with the parameter representing turbulent stretching effects being adjusted at each time step.

It is hoped that this research will lead to proper closure models for the PDF equations, which can be used to simulate practical problems in combustion and chemically reacting flows. This will be the first phase of this work.

The second phase of this research will be to explore the possibility of constructing a numerically efficient scheme for the reacting and combustion problems by using the closures obtained from the first phase. There are certain difficulties for this task, especially in the case of combustion where the heat release and temperature variation effects are strong and the diffusion and reaction are closely coupled. DNS results are expected to be used to investigate these problems.

Study on the joint PDF of a scalar and its gradient will also be pursued by using the amplitude and coordinate mappings with the hope that it will help us to better understand the structures of turbulent scalar fields as well as the interactions between the scalar and velocity fields.

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