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Mapping Closures for Turbulent Mixing and Reaction[1,2]

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I believe in the ultimate possibility of developing general computation procedures based on first principles; and under certain circumstances I believe that it is possible to do this rationally.

J.L. Lumley (1978) on computational modeling of turbulent flows

Abstract. The mapping closure for the one-point pdf of an inert scalar in homogeneous turbulence is explained and developed. It is shown that the pdf's calculated from the closure are in excellent agreement with those obtained from direct numerical simulations. The closure is then extended to many reactive scalars.

1. Introduction

In a turbulent reactive flow, the fluid composition at a point changes with time due to three processes: convection, reaction, and molecular diffusion. In probability density function (pdf) methods (Pope, 1985, 1991) the first two of these processes are treated exactly, but the effects of molecular diffusion have to be modeled. Over the years many models of molecular mixing have been proposed, e.g., Curl (1963), Dopazo (1979), Janicka *et al.* (1979), Pope (1982), Norris and Pope (1991), Chen and Kollmann (1991), and Valiño and Dopazo (1991). These different models have different attributes, but they all share two fundamental shortcomings: none has a sound physical basis; and none yields satisfactory results for the basic test case of a decaying inert scalar field in isotropic turbulence.

Recently Kraichnan and coworkers (Kraichnan, 1989, 1990; Chen *et al.*, 1989) have developed the new formalism of *mapping closures* and have applied it to study scalar mixing in turbulence. In contrast to the models cited above, mapping closures have a sound basis, and yield excellent results for the basic test case.

This paper has two purposes. First, in Sections 2.1–2.4 the simplest mapping closure is explained, so as to make the fundamental concepts accessible to a wider readership. Second, in the remainder of the paper, original contributions are made to extend this closure, in particular to treat many reactive scalars.

[1] Dedicated to Professor J.L. Lumley on the occasion of his 60th birthday.

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2. Mapping Closure for a Single Inert Scalar

2.1. Formulation

We consider the simple case of a single conserved passive scalar $\varphi(\mathbf{x}, t)$ in constant-density homogeneous isotropic turbulence. With $\mathbf{U}(\mathbf{x}, t)$ being the velocity field, and Γ the molecular diffusivity, the evolution equation for φ is

$$\frac{\partial\varphi}{\partial t} + \mathbf{U}\cdot\nabla\varphi = \Gamma\nabla^2\varphi. \tag{1}$$

Initially ($t = 0$) the scalar field $\varphi(\mathbf{x}, t)$ is statistically homogeneous and isotropic, and hence it remains so for all time.

The cumulative distribution function (cdf) of $\varphi(\mathbf{x}, t)$ is defined by

$$F(\psi, t) \equiv \mathrm{Prob}\{\varphi(\mathbf{x}, t) < \psi\}, \tag{2}$$

where ψ is the sample-space variable corresponding to φ. The pdf of $\varphi(\mathbf{x}, t)$ is

$$f(\psi; t) \equiv \frac{\partial F(\psi, t)}{\partial\psi}. \tag{3}$$

Evolution equations for the cdf and pdf can be derived from (1) by standard methods (Pope, 1985). They are

$$\frac{\partial F}{\partial t} + \Gamma\langle\nabla^2\varphi|\psi\rangle\frac{\partial F}{\partial\psi} = 0 \tag{4}$$

and

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial\psi}\{f\Gamma\langle\nabla^2\varphi|\psi\rangle\} = 0, \tag{5}$$

where $\langle\nabla^2\varphi|\psi\rangle$ is the expectation of $\nabla^2\varphi(\mathbf{x}, t)$ conditional on $\varphi(\mathbf{x}, t) = \psi$.

Since $f(\psi; t)$ is the one-point pdf, it contains no gradient information. In particular, $\langle\nabla^2\varphi|\psi\rangle$ is not known in terms of $f(\psi; t)$ and hence (4) and (5) are not closed.

2.2. Mapping from a Gaussian

This subsection serves as a prelude to the next, in which the mapping closure approximation to $\langle\nabla^2\varphi|\psi\rangle$ is developed.

Let φ now denote a random variable with cdf $F(\psi)$ and pdf $f(\psi)$. (For example, φ could be the value of the scalar field at a particular $\mathbf{x}$ and t.) Let θ be a standardized Gaussian random variable—that is, a random variable with zero mean, unit variance, cdf

$$G(\eta) \equiv \mathrm{Prob}\{\theta < \eta\} = \int_{-\infty}^{\eta} \frac{1}{\sqrt{2\pi}}\exp(-\tfrac{1}{2}s^2)\,ds \tag{6}$$

and pdf

$$g(\eta) = \frac{1}{\sqrt{2\pi}}\exp(-\tfrac{1}{2}\eta^2). \tag{7}$$

Note that η is the sample-space variable corresponding to θ.

We now want to determine a function—or *mapping*—X, such that the random variable $X(\theta)$ has the same probability distribution as φ, i.e., such that

$$\mathrm{Prob}\{X(\theta) < \psi\} = \mathrm{Prob}\{\varphi < \psi\}. \tag{8}$$

A smooth mapping exists for the nonpathological case in which

(i) $F(\psi)$ strictly increases continuously from zero to unity,

and it is made unique by the requirement that

(ii) X is a nondecreasing function of its argument.

From condition (ii) we have

$$G(\eta) \equiv \text{Prob}\{\theta < \eta\} = \text{Prob}\{X(\theta) < X(\eta)\}. \quad (9)$$

From (8), replacing ψ by $X(\eta)$, we have

$$\text{Prob}\{X(\theta) < X(\eta)\} = \text{Prob}\{\varphi < X(\eta)\} = F(X(\eta)). \quad (10)$$

Thus the mapping $X(\eta)$ is determined as the solution of the functional equation

$$F(X(\eta)) = G(\eta). \quad (11)$$

A graphical interpretation of (11) is given in Figure 1. It may be seen from Figure 1(d) that for the general pathological case, the mapping exists but is neither unique nor smooth. It is found below that such pathologies are not of concern.

In summary: subject to mild conditions, for the random variable φ, a unique smooth mapping X (given by (11)) exists such that Gaussian random variable θ is mapped to a random variable $X(\theta)$ with the same distribution as φ.

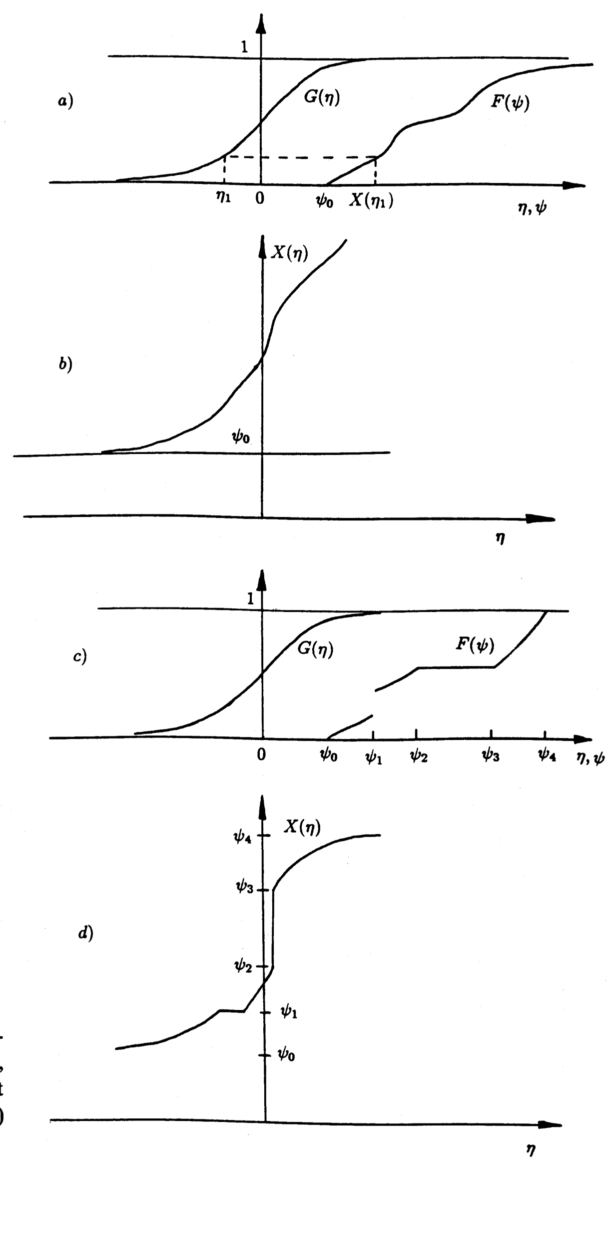

Figure 1. Sketch of cdf's and mappings. (a) Cdf's of standardized Gaussian $G(\eta)$ and of a continuous random variable φ, $F(\psi)$. (b) The corresponding mapping $X(\eta)$. (c) Same as (a) but for pathological random variable φ. (d) The mapping $X(\eta)$ corresponding to (c).

2.3. Turbulent, Gaussian, and Surrogate Fields

The mapping closure approximation given at the end of this subsection is simple to understand, once the definition and significance of three fields is appreciated.

The first is the *turbulent field* $\varphi(\mathbf{x}, t)$, which is only partially known. That is, we assume that we know the one-point pdf $f(\psi; t)$ at time t, and that we want to determine its subsequent evolution. As mentioned above, a knowledge of $f(\psi; t)$ is not sufficient to determine statistics of gradients, in particular, $\langle \nabla^2 \varphi | \psi \rangle$.

The second field is a specified time-independent *Gaussian field* $\theta(\mathbf{z})$, where $\mathbf{z} = \{z_1, z_2, z_3\}$ are spatial coordinates, distinct from $\mathbf{x}$. This is a statistically homogeneous isotropic field that is completely specified by the mean $\langle \theta \rangle$ (taken to be zero), by the variance $\langle \theta^2 \rangle$ (taken to be unity), and by the two-point correlation function

$$\rho(r) \equiv \langle \theta(\mathbf{z}) \theta(\mathbf{z} + \mathbf{e}r) \rangle, \tag{12}$$

where $\mathbf{e}$ is an arbitrary unit vector. In principle we need to specify $\rho(r)$—or equivalently its Fourier transform, the spectral density of the field. But it happens that only the length-scale λ_θ,

$$\lambda_\theta \equiv \left\langle \frac{\partial \theta}{\partial z_i} \frac{\partial \theta}{\partial z_i} \right\rangle^{-1/2}, \tag{13}$$

enters the subsequent analysis. (Note that ∇ is used exclusively to denote gradients in $\mathbf{x}$.)

As an isotropic Gaussian field, $\theta(\mathbf{z})$ has the special property that all the multipoint statistics of θ and its gradients are known in terms of $\langle \theta \rangle$, $\langle \theta^2 \rangle$, and $\rho(r)$ (Lumley, 1970; Panchev, 1971; Adler, 1981). In particular (at any $\mathbf{z}$), the joint pdf of θ, $\partial \theta / \partial z_i$, and $\partial^2 \theta / \partial z_i \, \partial z_j$ is joint normal, from which the following results used below can be deduced:

$$\left\langle \frac{\partial \theta}{\partial z_i} \frac{\partial \theta}{\partial z_i} \middle| \theta = \eta \right\rangle = \left\langle \frac{\partial \theta}{\partial z_i} \frac{\partial \theta}{\partial z_i} \right\rangle = \frac{1}{\lambda_\theta^2}, \tag{14}$$

$$\left\langle \frac{\partial^2 \theta}{\partial z_i \, \partial z_i} \middle| \theta = \eta \right\rangle = -\frac{\eta}{\lambda_\theta^2}. \tag{15}$$

The third field is the *surrogate field* $\varphi^s(\mathbf{x}, t)$ obtained by a mapping of the Gaussian field $\theta(\mathbf{z})$. The independent variable is mapped by a simple time-dependent stretching transformation

$$\mathbf{x} = \frac{\mathbf{z}}{J(t)}, \tag{16}$$

where $J(t) > 0$ is to be specified. The dependent variable φ^s is obtained by a time-dependent mapping $X(\theta, t)$. Thus

$$\varphi^s(\mathbf{x}, t) = X(\theta(\mathbf{x}J(t)), t). \tag{17}$$

With $F(\psi, t)$ and $G(\eta)$ being the cdf's of the turbulent field $\varphi(\mathbf{x}, t)$ and of the Gaussian field $\theta(\mathbf{z})$, the time-dependent mapping satisfies

$$F(X(\eta, t), t) = G(\eta) \tag{18}$$

(cf. (11)). That is (as established in the previous subsection) the mapping is such that $\varphi(\mathbf{x}, t)$ and $\varphi^s(\mathbf{x}, t)$ have the same one-point pdf's.

The statistics of the surrogate field are completely known, since $\varphi^s(\mathbf{x}, t)$ is obtained by a known mapping of a known field. To illustrate this point, we now evaluate the conditional expectation of $\nabla^2 \varphi^s$.

For the first derivative we have

$$\frac{\partial \varphi^s(\mathbf{x}, t)}{\partial x_i} = \frac{\partial}{\partial x_i} X(\theta(\mathbf{x}J(t)), t) = J \frac{\partial \theta}{\partial z_i} X'(\theta, t), \tag{19}$$

where

$$X'(\eta, t) = \frac{\partial X(\eta, t)}{\partial \eta} \tag{20}$$

(and X'' is similarly defined). Thus the Laplacian is

$$\nabla^2 \varphi^s(\mathbf{x}, t) = J^2 \frac{\partial^2 \theta}{\partial z_i\, \partial z_i} X'(\theta, t) + J^2 \frac{\partial \theta}{\partial z_i} \frac{\partial \theta}{\partial z_i} X''(\theta, t). \tag{21}$$

Since the right-hand side of this equation is expressed in terms of θ, it is simplest to take its expectation conditional on $\{\theta(\mathbf{z}) = \eta\}$. In view of the mapping, this is identical to the condition $\{\varphi^s(\mathbf{x}, t) = X(\eta, t)\}$. Thus we obtain

$$\begin{aligned}\langle \nabla^2 \varphi^s(\mathbf{x}, t) | \varphi^s(\mathbf{x}, t) = X(\eta, t) \rangle &= J^2 \left\langle \frac{\partial^2 \theta}{\partial z_i\, \partial z_i} X'(\theta, t) + \frac{\partial \theta}{\partial z_i} \frac{\partial \theta}{\partial z_i} X''(\theta, t) | \theta(\mathbf{z}) = \eta \right\rangle \\ &= \frac{J^2}{\lambda_\theta^2} \{-\eta X'(\eta, t) + X''(\eta, t)\}. \end{aligned} \tag{22}$$

The last line is obtained by substituting (14) and (15) for conditional statistics of θ.

To summarize this result: given λ_θ, $J(t)$, and $F(\psi, t)$, the mapping (17) is known, and hence so also is the right-hand side of (22).

The fundamental mapping-closure assumption is now obvious: *it is assumed that the unknown statistics of the turbulent field are the same as the known statistics of the surrogate field.* Specifically, it is assumed that

$$\langle \nabla^2 \varphi(\mathbf{x}, t) | \varphi(\mathbf{x}, t) = \psi \rangle = \langle \nabla^2 \varphi^s(\mathbf{x}, t) | \varphi^s(\mathbf{x}, t) = \psi \rangle. \tag{23}$$

A discussion of this assumption is postponed until its consequences have been deduced.

2.4. Evolution of the Mapping

The above equations ((22) and (23)) provide a closure to the pdf or cdf equations ((4) and (5)) since they provide a known expression for the unknown $\langle \nabla^2 \varphi | \psi \rangle$. However, it is not a conventional closure approximation in that an explicit model equation for $F(\psi, t)$ or $f(\psi; t)$ is not produced. This is because quantities such as $X''(\eta, t)$ cannot usefully be written explicitly in terms of $F(\psi, t)$. Instead, the implications of the closure can be deduced indirectly, by determining the evolution of the mapping.

The evolution equation for $X(\eta, t)$ can be deduced from the cdf $F(\psi, t)$. Defining

$$\dot{F}(\psi, t) \equiv \frac{\partial F(\psi, t)}{\partial t} \quad \text{and} \quad F'(\psi, t) \equiv \frac{\partial F(\psi, t)}{\partial \psi}, \tag{24}$$

and differentiating (18) with respect to t we obtain

$$\dot{F}(X(\eta, t), t) + F'(X(\eta, t), t) \frac{\partial X(\eta, t)}{\partial t} = 0 \tag{25}$$

(since $G(\eta)$ is independent of t). While the exact evolution equation for $F(\psi, t)$ (equation (4)) is

$$\dot{F}(\psi, t) + F'(\psi, t) \Gamma \langle \nabla^2 \varphi | \varphi(\mathbf{x}, t) = \psi \rangle = 0. \tag{26}$$

Thus, comparing these two equations with the substitution $\psi = X(\eta, t)$, we obtain the exact result:

$$\frac{\partial}{\partial t} X(\eta, t) = \Gamma \langle \nabla^2 \varphi | \varphi(\mathbf{x}, t) = X(\eta, t) \rangle. \tag{27}$$

The closed modeled equation for the mapping is obtained by substituting (22) and (23) into (27). The result is

$$\frac{\partial}{\partial t} X(\eta, t) = \frac{\Gamma J^2}{\lambda_\theta^2} \{-\eta X'(\eta, t) + X''(\eta, t)\} \tag{28}$$

or

$$\left(\frac{\partial}{\partial \tilde{t}} + \eta \frac{\partial}{\partial \eta} - \frac{\partial^2}{\partial \eta^2}\right) X(\eta, \tilde{t}) = 0, \tag{29}$$

where the normalized time $\tilde{t}$ is

$$d\tilde{t} = \frac{dt\, \Gamma J^2}{\lambda_\theta^2}. \tag{30}$$

It may be noted that the specified parameters J and λ_θ affect only the rate at which $X(\eta, t)$ evolves.

2.5. Analytic Solution

For an important special case, the mapping closure can be evaluated analytically, and the results compared with direct numerical simulations (DNS).

Eswaran and Pope (1988) performed DNS of a decaying inert passive scalar field in statistically stationary, homogeneous, isotropic turbulence. For the scalar field, the initial condition approximated blobs of fluid with $\varphi = -1$, and an equal amount of blobs of fluid with $\varphi = 1$. The pdf corresponding to this initial condition is

$$f(\psi; 0) = \tfrac{1}{2}[\delta(\psi + 1) + \delta(\psi - 1)]. \tag{31}$$

In fact, in the DNS, the blobs (and hence the initial pdf) were slightly smeared, so that the resulting field could be resolved numerically.

In the present context, the principal findings of the DNS study are threefold. First, as expected, and in accord with experiments (Warhaft and Lumley, 1978), the smaller the length-scale of the initial scalar field (relative to the scale of the turbulence) the faster the decay of the scalar variance $\sigma(t)^2 = \langle \varphi(\mathbf{x}, t)^2 \rangle$. Second, the shapes adopted by the pdf $f(\psi; t)$ are independent of the initial length scale of the scalar field. That is, at a given stage of decay, characterized by a given value of $\sigma(t)$, the pdf is the same for all initial scalar length scales. These pdf's are shown in Figure 2(a). Third, at large times, as $\sigma(t)$ tends to zero, the pdf tends to a Gaussian.

The mapping corresponding to the initial condition (31) is

$$X(\eta, 0) = 2H(\eta) - 1, \tag{32}$$

where H is the Heaviside function. Thus all points in the Gaussian field with $\theta(\mathbf{z}) < 0$ are mapped to $\varphi(\mathbf{x}, 0) = -1$, while points with $\theta(\mathbf{z}) \geq 0$ are mapped to $\varphi(\mathbf{x}, 0) = 1$. The mapping evolves according to

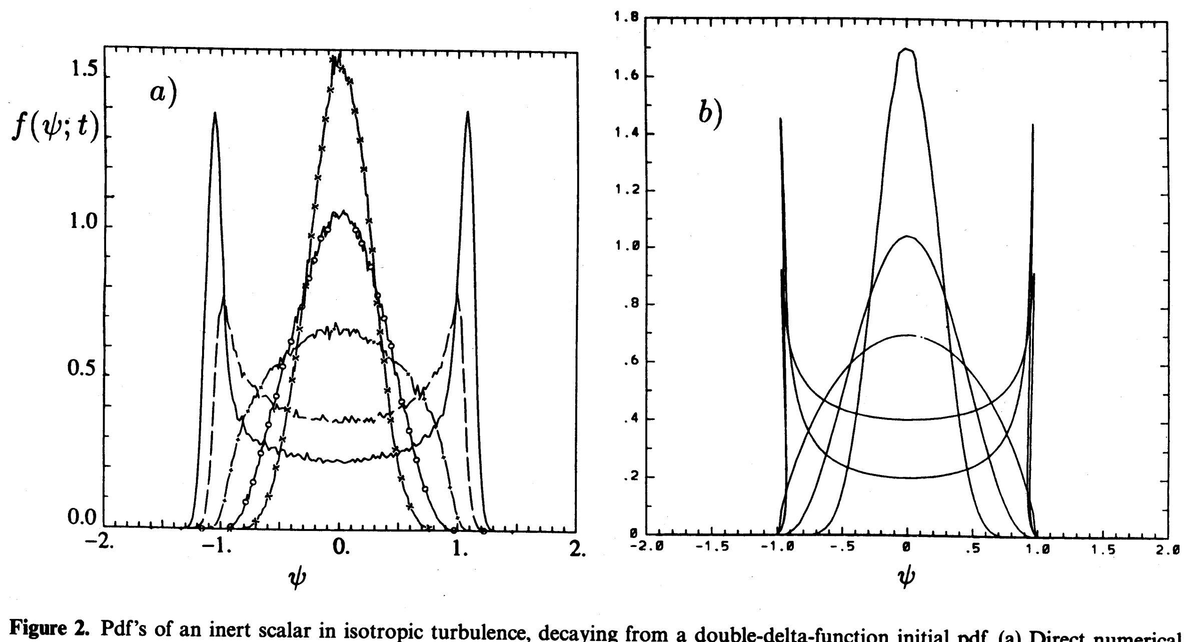

Figure 2. Pdf's of an inert scalar in isotropic turbulence, decaying from a double-delta-function initial pdf. (a) Direct numerical simulations (Eswaran and Pope, 1988). (b) Mapping closure.

(29) which, with the stretching transformation $\tilde{\eta} = \eta \exp(-\tilde{t})$, reduces to the unsteady heat conduction equation. With the given initial condition (32), there is then an analytic solution in terms of the cdf of the standardized Gaussian, G (6). The solution is

$$X(\eta, \tilde{t}) = 2G\left(\frac{\eta}{\Sigma(\tilde{t})}\right) - 1 = \operatorname{erf}\left(\frac{\eta}{\Sigma(\tilde{t})\sqrt{2}}\right), \tag{33}$$

where

$$\Sigma(\tilde{t})^2 = e^{2\tilde{t}} - 1. \tag{34}$$

The corresponding analytic solution for the pdf is obtained, first, by differentiating (18):

$$f(X(\eta, \tilde{t}), \tilde{t})\frac{\partial X(\eta, \tilde{t})}{\partial \eta} = g(\eta), \tag{35}$$

where g is the pdf of a standardized Gaussian (7). Now from (33) we have

$$\frac{\partial X(\eta, \tilde{t})}{\partial \eta} = \frac{2}{\Sigma(\tilde{t})} g\left(\frac{\eta}{\Sigma(\tilde{t})}\right), \tag{36}$$

and hence the solution for the pdf is

$$f(X(\eta, \tilde{t}), \tilde{t}) = \frac{\frac{1}{2}\Sigma(\tilde{t})g(\eta)}{g(\eta/\Sigma(\tilde{t}))} = \tfrac{1}{2}\Sigma(\tilde{t}) \exp\{-\tfrac{1}{2}\eta^2[1 - \Sigma(\tilde{t})^{-2}]\}. \tag{37}$$

It may be observed that the solution depends on time solely through Σ. As t increases from zero to infinity, Σ increases monotonically, and the variance σ^2 decreases monotonically. Thus, in accord with the DNS results, the mapping closure predicts that the pdf shapes are parametrized by the value of the variance. The specified parameters in the mapping closure (λ_θ and $J(t)$) do not affect the pdf shapes, only the rate at which the variance decays.

The pdf shapes given by this analytic solution to the mapping closure are shown in Figure 2(b) for the same values of variance as in the DNS results (Figure 2(a)). The agreement between the figures is remarkable.

At early times, corresponding to $\Sigma(\tilde{t}) < 1$, the pdf is infinite at $\psi = \pm 1$; for $\Sigma(\tilde{t}) = 1$ the pdf is uniform; while for later times ($\Sigma(\tilde{t}) > 1$) the pdf is zero at $\psi = \pm 1$.

For very large times, as $\Sigma(\tilde{t})$ tends to infinity, the mapping becomes linear: an expansion of (33) is

$$X(\eta, \tilde{t}) = \frac{2\eta}{\Sigma\sqrt{2\pi}} + O\left(\left(\frac{\eta}{\Sigma}\right)^3\right). \tag{38}$$

Hence, to leading order, the pdf becomes

$$f(\psi, \tilde{t}) \approx \frac{1}{\bar{\sigma}\sqrt{2\pi}} \exp\left(-\frac{\frac{1}{2}\psi^2}{\bar{\sigma}^2}\right), \tag{39}$$

where

$$\bar{\sigma} \equiv \frac{2}{\Sigma\sqrt{2\pi}}. \tag{40}$$

This approximation is accurate for

$$\frac{\psi}{\bar{\sigma}} \ll \Sigma \approx e^{\tilde{t}}. \tag{41}$$

In other words, for large times the pdf tends to a Gaussian—again in accord with the DNS results.

Analytic solutions have been developed further by F. Gao (private communication).

2.6. Particle Method

In the last decade there have been numerous calculations of inhomogeneous turbulent flows using pdf methods (see Pope (1991) for a review). Nearly all of these calculations have been performed using *particle methods* (or Monte Carlo methods) in which the pdf (e.g., $f(\psi; t)$) is represented indirectly by

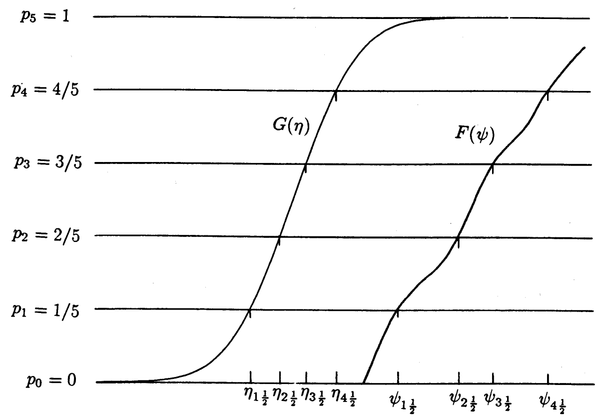

Figure 3. Sketch of cdf's $G(\eta)$ and $F(\psi)$ showing the definitions of $\eta_{i+1/2}$ and $\psi_{i+1/2}$, for $N = 5$.

an ensemble of particles ($\varphi_i(t)$, $i = 1, 2, \ldots, N$). It is natural, therefore, to attempt to develop a particle-method implementation of the mapping closure.

Figure 3 shows the general cdf $F(\psi, t)$ and the standardized Gaussian cdf $G(\eta)$. The horizontal lines correspond to probabilities

$$p_i \equiv \frac{i}{N}, \qquad i = 0, 1, 2, \ldots, N. \tag{42}$$

Then, as shown in the figure, we define $\psi_{i+1/2}$ and $\eta_{i+1/2}$ by

$$F(\psi_{i+1/2}, t) = G(\eta_{i+1/2}) = p_i, \qquad i = 0, 1, 2, \ldots, N. \tag{43}$$

Note that $\eta_{1/2} = -\infty$ and $\eta_{N+1/2} = \infty$.

The ith particle can be taken to represent the fluid with composition $\psi_{i-1/2} \leq \varphi(\mathbf{x}, t) < \psi_{i+1/2}$. Then the value of $\varphi_i(t)$ is appropriately defined as the mean value of φ in this interval:

$$\varphi_i(t) \equiv \frac{\int_{\psi_{i-1/2}}^{\psi_{i+1/2}} \psi f(\psi; t)\, d\psi}{\int_{\psi_{i-1/2}}^{\psi_{i+1/2}} f(\psi; t)\, d\psi}. \tag{44}$$

The integral in the denominator is simply

$$\int_{\psi_{i-1/2}}^{\psi_{i+1/2}} f(\psi; t)\, d\psi = F(\psi_{i+1/2}, t) - F(\psi_{i-1/2}, t) = p_i - p_{i-1} = \frac{1}{N}. \tag{45}$$

The remaining integral can be re-expressed in terms of the Gaussian pdf $g(\eta)$ and the mapping $\varphi = X(\eta, t)$ to yield

$$\varphi_i(t) = N \int_{\eta_{i-1/2}}^{\eta_{i+1/2}} X(\eta, t) g(\eta)\, d\eta. \tag{46}$$

The evolution of $\varphi_i(t)$ is determined by differentiating this equation with respect to t (or $\tilde{t}$) and substituting (29) for $\partial X/\partial \tilde{t}$. Thus

$$\frac{d\varphi_i}{d\tilde{t}} = N \int_{\eta_{i-1/2}}^{\eta_{i+1/2}} g(\eta) \left\{ -\eta \frac{\partial X(\eta, \tilde{t})}{\partial \eta} + \frac{\partial^2 X(\eta, \tilde{t})}{\partial \eta^2} \right\} d\eta. \tag{47}$$

Now in view of the Gaussian property

$$\frac{dg(\eta)}{d\eta} = -\eta g(\eta), \tag{48}$$

(47) can be evaluated as

$$\frac{d\varphi_i}{d\tilde{t}} = N \int_{\eta_{i-1/2}}^{\eta_{i+1/2}} \frac{\partial}{\partial \eta} \left\{ g(\eta) \frac{\partial X(\eta, \tilde{t})}{\partial \eta} \right\} d\eta = N \left[g(\eta) \frac{\partial X(\eta, \tilde{t})}{\partial \eta} \right]_{\eta_{i-1/2}}^{\eta_{i+1/2}}. \tag{49}$$

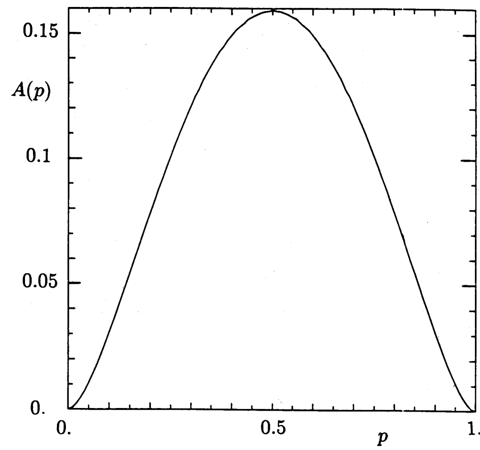

Figure 4. The function $A(p)$.

We now introduce the only approximation in this development, which is to use a finite-difference approximation for $\partial X/\partial\eta$:

$$\left(Ng(\eta)\frac{\partial X(\eta,\tilde{t})}{\partial\eta}\right)_{\eta_{i+1/2}} \approx \frac{Ng(\eta_{i+1/2})[X(\eta_{i+1},\tilde{t}) - X(\eta_i,\tilde{t})]}{[\eta_{i+1}-\eta_i]}$$
$$= (\varphi_{i+1}(\tilde{t}) - \varphi_i(\tilde{t}))B_{i+1/2}, \qquad i = 1, 2, \ldots, N-1, \tag{50}$$

where

$$B_{i+1/2} \equiv \frac{Ng(\eta_{i+1/2})}{[\eta_{i+1}-\eta_i]}, \qquad i = 1, 2, \ldots, N-1. \tag{51}$$

At the lower limit $\eta_{1/2} = -\infty$ and at the upper limit $\eta_{N+1/2} = \infty$, $g\,\partial X/\partial\eta$ is zero. Thus, the particle-property evolution equation (49) becomes

$$\frac{d}{d\tilde{t}}\varphi_1 = B_{3/2}(\varphi_2 - \varphi_1),$$
$$\frac{d}{d\tilde{t}}\varphi_i = B_{i+1/2}(\varphi_{i+1} - \varphi_i) - B_{i-1/2}(\varphi_i - \varphi_{i-1}), \qquad i = 2, 3, \ldots, N-1, \tag{52}$$
$$\frac{d}{d\tilde{t}}\varphi_N = -B_{N-1/2}(\varphi_N - \varphi_{N-1}).$$

These equations show that each particle is drawn to its neighbors at the rates $B_{i\pm1/2}$. For large N, $B_{i+1/2}$ tends to a limit

$$B_{i+1/2} \to N^2 A\left(\frac{i+\frac{1}{2}}{N}\right),$$

where the function $A(p)$ is shown in Figure 4. It may be seen that the rates $B_{i+1/2}$ decrease toward the edges of the distribution.

2.7. Stochastic Process

In the terminology of Pope (1985), the particles $\varphi_i(t)$ introduced in the previous section are *conditional particles*. Their rate of change with time is the conditional rate of change of fluid particles:

$$\frac{d\varphi_i}{dt} = \left\langle \frac{D\varphi}{Dt} \middle| \varphi = \varphi_i \right\rangle. \tag{53}$$

Thus $\varphi_i(t)$ does not contain the random behavior of fluid particles. Stochastic processes have long been used to model properties following fluid particles in turbulence (Taylor, 1921; Novikov, 1963; Haworth and Pope, 1986; Pope and Chen, 1990; Girimaji and Pope, 1990). These models are based on diffusion processes, the simplest of which is the Uhlenbeck–Ornstein (UO) process (Karlin and Taylor, 1981). If $\theta^*(t)$ is a standardized UO process of time scale T, then: (at any time t) $\theta^*(t)$ is a standardized Gaussian; the autocorrelation of $\theta^*(t)$ is $\rho(s) = \exp(-|s|/T)$; and, the finite-dimensional joint distribution of $\theta^*(t)$ at different times is joint normal.

Since the stochastic process $\theta^*(t)$ is a standardized Gaussian (at each t), the mapped process

$$\varphi^*(t) \equiv X(\theta^*(t), t) \tag{54}$$

has the pdf $f(\psi; t)$. In other words, $\varphi^*(t)$ is a stochastic process with the same one-time pdf as $\varphi(\mathbf{x}, t)$. Consequently, $\varphi^*(t)$ can be taken as a model for the value of $\varphi(t)$ following a fluid particle.

The stochastic differential equation (sde) for $\varphi^*(t)$ has an interesting form. Allowing T to be time dependent, the sde for θ^* is

$$d\theta^*(t) = -\frac{\theta^*(t)\,dt}{T} + \left(\frac{2}{T}\right)^{1/2} dW, \tag{55}$$

where $W(t)$ is a Wiener process. Applying the Ito transformation (Karlin and Taylor, 1981), from the above two equations we obtain

$$d\varphi^*(t) = \dot{X}\,dt + \frac{dt}{T}(-\theta^* X' + X'') + X'\left(\frac{2}{T}\right)^{1/2} dW, \tag{56}$$

where X is written for $X(\theta^*(t), t)$, etc. Now, defining

$$\tau \equiv \frac{\lambda_\theta^2}{\Gamma J^2}, \tag{57}$$

the evolution equation for the mapping $X(\eta, t)$ is (28)

$$\dot{X}(\eta, t) = \frac{1}{\tau}(-\eta X' + X''). \tag{58}$$

Hence the sde for $\varphi^*(t)$ is

$$d\varphi^*(t) = \left(\frac{1}{\tau} + \frac{1}{T}\right)(-\theta^* X' + X'')\,dt + X'\left(\frac{2}{T}\right)^{1/2} dW. \tag{59}$$

It may be observed that, as T tends to infinity, the randomness dissappears, and the sde (59) reverts to the standard evolution equation for the mapping (28).

As observed by Fox (1990), the pdf equation corresponding to (59) is a Fokker–Planck equation with nonlinear drift and diffusion coefficients.

3. Mapping Closure for Several Inert Scalars

The mapping closure is now extended to a set of σ compositions $\varphi(\mathbf{x}, t) = \{\varphi_1(\mathbf{x}, t), \varphi_2(\mathbf{x}, t), \ldots, \varphi_\sigma(\mathbf{x}, t)\}$. While the development parallels that of the previous section, there are significant technical and conceptual differences.

The field $\varphi_\alpha(\mathbf{x}, t)$ $(\alpha = 1, 2, \ldots, \sigma)$ is statistically homogeneous and isotropic and evolves according to

$$\frac{\partial \varphi_\alpha}{\partial t} + \mathbf{U}\cdot\nabla\varphi_\alpha = \Gamma_\alpha \nabla^2 \varphi_\alpha, \tag{60}$$

where the diffusivity Γ_α may be different for each scalar. (Greek sufficies are excluded from the summation convention.)

We introduce the notation

$$[\varphi]_\alpha \equiv \{\varphi_1, \varphi_2, \ldots, \varphi_\alpha\}, \qquad \alpha = 1, 2, \ldots, \sigma, \tag{61}$$

to indicate a partial set of compositions. The joint pdf of $[\varphi(\mathbf{x}, t)]_\alpha$ is denoted by $f_\alpha^J([\psi]_\alpha; t)$ where ψ_α

is the sample-space variable corresponding to φ_α. By definition, the pdf of φ_α conditional on $[\varphi]_{\alpha-1}$ is

$$f_\alpha^c([\psi]_\alpha; t) \equiv \frac{f_\alpha^J([\psi]_\alpha; t)}{f_{\alpha-1}^J([\psi]_{\alpha-1}; t)}, \tag{62}$$

with the convention that $f_1^c = f_1^J$ is the marginal pdf of φ_1.

By repeated use of (62), the joint pdf of all the scalars can be written as

$$f_\sigma^J([\psi]_\sigma; t) = \prod_{\alpha=1}^{\sigma} f_\alpha^c([\psi]_\alpha; t). \tag{63}$$

That is, the joint pdf is the product of the (appropriately defined) conditional pdf's.

Corresponding to the conditional pdf's, we define the conditional cumulative distribution functions (ccdf's) by

$$F_\alpha([\psi]_\alpha, t) \equiv \int_{-\infty}^{\psi_\alpha} f_\alpha^c([\psi]_{\alpha-1}, \psi'_\alpha; t)\, d\psi'_\alpha. \tag{64}$$

A set of σ independent, statistically homogeneous, isotropic, standardized Gaussian fields $\theta_\alpha(\mathbf{z})$ ($\alpha = 1, 2, \ldots, \sigma$) is specified, each with its own length scale λ_α. Thus

$$\langle\theta_\alpha\rangle = 0, \qquad \langle\theta_\alpha\theta_\beta\rangle = \delta_{\alpha\beta}, \qquad \left\langle\frac{\partial\theta_\alpha}{\partial z_i}\frac{\partial\theta_\beta}{\partial z_i}\right\rangle = \frac{\delta_{\alpha\beta}}{\lambda_\alpha^2}. \tag{65}$$

The pdf of $\theta_\alpha(\mathbf{z})$ is $g(\eta_\alpha)$ and its cdf is $G(\eta_\alpha)$, where η_α is the corresponding sample-space variable.

The σ surrogate fields are specified by the mappings

$$\begin{aligned}\varphi_1^s(\mathbf{x}, t) &= X_1(\theta_1(J_1(t)\mathbf{x}), t),\\ \varphi_2^s(\mathbf{x}, t) &= X_2(\theta_1(J_1\mathbf{x}), \theta_2(J_2\mathbf{x}), t),\\ \varphi_\alpha^s(\mathbf{x}, t) &= X_\alpha([\theta(J\mathbf{x})]_\alpha, t).\end{aligned} \tag{66}$$

For each Gaussian field there is a different stretching $J_\alpha(t)$ of the independent variable. Note that X_1 maps θ_1 to φ_1^s, X_2 maps θ_1 and θ_2 to φ_2^s, and so on, so that φ_α^s depends on θ_β for all $\beta \le \alpha$.

Derivatives of the mappings are denoted by

$$X_{\alpha,\beta}([\eta]_\alpha, t) \equiv \frac{\partial}{\partial\eta_\beta} X_\alpha([\eta]_\alpha, t). \tag{67}$$

We want the surrogate fields $[\varphi^s]_\alpha$ to have the same joint pdf as the turbulent fields $[\varphi]_\alpha$. It is now shown that this is achieved if the mappings are such that

$$F_\alpha([X(\eta, t)]_\alpha, t) = G(\eta_\alpha) \tag{68}$$

(cf. (11)), where

$$[X(\eta, t)]_\alpha = \{X_1([\eta]_1, t), X_2([\eta]_2, t), \ldots, X_\alpha([\eta]_\alpha, t)\}. \tag{69}$$

As in the single-scalar case, we require X_α to be a strictly increasing function of η_α. Differentiating (68) we obtain

$$\frac{\partial F_\alpha}{\partial\eta_\alpha} = X_{\alpha,\alpha} f_\alpha^c([X(\eta, t)]_\alpha, t) = g(\eta_\alpha), \tag{70}$$

which shows that indeed $X_{\alpha,\alpha} > 0$, provided that the conditional pdf f_α^c is strictly positive.

The mapping condition (68) is now established. A necessary and sufficient condition for the equality in one-point distributions of $[\varphi(\mathbf{x}, t)]_\alpha$ and $[\varphi^s(\mathbf{x}, t)]_\alpha$ is that their ccdf's be identical. That is, for all α, we require

$$\begin{aligned}F_\alpha([\psi]_\alpha, t) &\equiv \mathrm{Prob}\{\varphi_\alpha(\mathbf{x}, t) < \psi_\alpha \mid [\varphi(\mathbf{x}, t)]_{\alpha-1} = [\psi]_{\alpha-1}\}\\ &= \mathrm{Prob}\{\varphi_\alpha^s(\mathbf{x}, t) < \psi_\alpha \mid [\varphi^s(\mathbf{x}, t)]_{\alpha-1} = [\psi]_{\alpha-1}\}.\end{aligned} \tag{71}$$

Replacing ψ_α by $X_\alpha([\eta]_\alpha)$, and substituting the mapping $X_\alpha([\theta]_\alpha)$ for φ_α^s (66), equation (71) becomes

$$F_\alpha([X(\eta)]_\alpha) = \mathrm{Prob}\{X_\alpha([\theta]_\alpha) < X_\alpha([\eta]_\alpha) \mid [X(\theta)]_{\alpha-1} = [X(\eta)]_{\alpha-1}\}, \tag{72}$$

where, for brevity, **x**, **z**, and t are not shown explicitly. Now since the mapping between $[\eta]_{\alpha-1}$ and $[X(\eta)]_{\alpha-1}$ is one-to-one, the condition in (72) is the same as the condition $[\theta]_{\alpha-1} = [\eta]_{\alpha-1}$. With $[\eta]_{\alpha-1}$ fixed by this condition, since X_α is an increasing function of η_α, the inequality in (72) is the same as $\{\theta_\alpha < \eta_\alpha\}$. Thus, (72) becomes

$$F_\alpha([X(\eta)]_\alpha) = \mathrm{Prob}\{\theta_\alpha < \eta_\alpha | [\theta]_{\alpha-1} = [\eta]_{\alpha-1}\} = \mathrm{Prob}\{\theta_\alpha < \eta_\alpha\} = G(\eta_\alpha). \tag{73}$$

The last line follows since θ_α is independent of θ_β ($\beta \neq \alpha$), and hence the conditional and unconditional probabilities are the same. Thus we have established that the surrogate fields φ^s_α obtained via the mappings X_α (66) have the same one-point distribution as the turbulent fields φ_α, providing that the mappings are determined by (68).

Having established the mapping between $\theta(\mathbf{z})$ and $\varphi^s(\mathbf{x}, t)$, we can now evaluate derivatives of the surrogate field. From (66) we obtain

$$\frac{\partial \varphi^s_\alpha(\mathbf{x}, t)}{\partial x_i} = \sum_{\beta=1}^{\alpha} X_{\alpha,\beta}([\theta(J(t)\mathbf{x})]_\alpha, t) J_\beta \frac{\partial \theta_\beta}{\partial z_i}, \tag{74}$$

and, with abbreviated notation,

$$\nabla^2 \varphi^s_\alpha = \sum_{\beta=1}^{\alpha} X_{\alpha,\beta} J^2_\beta \frac{\partial^2 \theta_\beta}{\partial z_i\, \partial z_i} + \sum_{\beta=1}^{\alpha} \sum_{\gamma=1}^{\alpha} X_{\alpha,\beta\gamma} J_\beta J_\gamma \frac{\partial \theta_\beta}{\partial z_i} \frac{\partial \theta_\gamma}{\partial z_i}. \tag{75}$$

Now taking the expectation of (75) conditional on $[\theta]_\alpha = [\eta]_\alpha$ we obtain

$$\begin{aligned}\langle \nabla^2 \varphi^s_\alpha | [\varphi^s]_\alpha = [X(\eta)]_\alpha \rangle = &\sum_{\beta=1}^{\alpha} X_{\alpha,\beta}([\eta]_\alpha, t) J^2_\beta \left\langle \frac{\partial^2 \theta_\beta}{\partial z_i \partial z_i} \middle| [\theta]_\alpha = [\eta]_\alpha \right\rangle \\ &+ \sum_{\beta=1}^{\alpha} \sum_{\gamma=1}^{\alpha} X_{\alpha,\beta\gamma}([\eta]_\alpha, t) J_\beta J_\gamma \left\langle \frac{\partial \theta_\beta}{\partial z_i} \frac{\partial \theta_\gamma}{\partial z_i} \middle| [\theta]_\alpha = [\eta]_\alpha \right\rangle. \end{aligned} \tag{76}$$

For the term in $\partial^2 \theta_\beta / \partial z_i\, \partial z_i$, given the independence of the Gaussian fields, only the conditioning on θ_β is relevant. Thus we obtain

$$\left\langle \frac{\partial^2 \theta_\beta}{\partial z_i\, \partial z_i} \middle| [\theta]_\alpha = [\eta]_\alpha \right\rangle = \left\langle \frac{\partial^2 \theta_\beta}{\partial z_i\, \partial z_i} \middle| \theta_\beta = \eta_\beta \right\rangle = -\frac{\eta_\beta}{\lambda^2_\beta} \tag{77}$$

(cf. (15)). Similarly, for the other term the result is

$$\left\langle \frac{\partial \theta_\beta}{\partial z_i} \frac{\partial \theta_\gamma}{\partial z_i} \middle| [\theta]_\alpha = [\eta]_\alpha \right\rangle = \frac{\delta_{\beta\gamma}}{\lambda^2_\beta}. \tag{78}$$

Thus the conditional expectation (76) is

$$\langle \nabla^2 \varphi^s_\alpha | [\varphi^s]_\alpha = [X(\eta)]_\alpha \rangle = \sum_{\beta=1}^{\alpha} \frac{J^2_\beta}{\lambda^2_\beta} \{X_{\alpha,\beta\beta} - \eta_\beta X_{\alpha,\beta}\}. \tag{79}$$

A very important observation about the surrogate fields is that for $\beta \le \alpha$

$$\langle \nabla^2 \varphi^s_\beta | [\varphi^s]_\alpha = [\psi]_\alpha \rangle = \langle \nabla^2 \varphi^s_\beta | [\varphi^s]_\beta = [\psi]_\beta \rangle. \tag{80}$$

That is, the conditioning on φ^s_ε, $\varepsilon > \beta$, is irrelevant. This is so because the surrogate field φ^s_β is synthesized solely from θ_γ and F_γ, $\gamma \le \beta$, and hence is completely unaffected by θ_ε and F_ε, $\varepsilon > \beta$. (The corresponding statement does not apply to the turbulent fields.)

We are now in a position to derive the evolution equations for the mappings. As before, this is achieved by comparing two different evolution equations for the ccdf's. The first is obtained by differentiating (73):

$$\dot{F}_\alpha([X(\eta)]_\alpha, t) + \sum_{\beta=1}^{\alpha} \frac{\partial X_\beta([\eta]_\beta, t)}{\partial t} F_{\alpha,\beta}([X(\eta)]_\alpha, t) = 0, \tag{81}$$

where

$$\dot{F}_\alpha([\psi]_\alpha, t) \equiv \frac{\partial}{\partial t} F_\alpha([\psi]_\alpha, t) \tag{82}$$

and

$$F_{\alpha,\beta}([\psi]_\alpha, t) \equiv \frac{\partial}{\partial \psi_\beta} F_\alpha([\psi]_\alpha, t). \tag{83}$$

The second equation is derived, ultimately, from the evolution equation for φ_α (60). The evolution equation for the joint pdf of $[\varphi]_\alpha$ is

$$\frac{\partial}{\partial t} f_\alpha^J([\psi]_\alpha; t) + \sum_{\beta=1}^{\alpha} \frac{\partial}{\partial \psi_\beta} (f_\alpha^J \Gamma_\beta \langle \nabla^2 \varphi_\beta | [\varphi]_\alpha = [\psi]_\alpha \rangle) = 0. \tag{84}$$

From this, and from the relation $f_\alpha^c = f_\alpha^J / f_{\alpha-1}^J$, the equation for the conditional pdf is deduced to be

$$\begin{aligned} \frac{\partial f_\alpha^c}{\partial t} + \frac{\partial}{\partial \psi_\alpha}(f_\alpha^c \Gamma_\alpha \langle \nabla^2 \varphi_\alpha | [\psi]_\alpha \rangle) &= \frac{f_\alpha^c}{f_{\alpha-1}^J} \sum_{\beta=1}^{\alpha-1} \frac{\partial}{\partial \psi_\beta} (f_{\alpha-1}^J \Gamma_\beta \{ \langle \nabla^2 \varphi_\beta | [\psi]_{\alpha-1} \rangle - \langle \nabla^2 \varphi_\beta | [\psi]_\alpha \rangle \}) \\ &\quad - \sum_{\beta=1}^{\alpha-1} \Gamma_\beta \langle \nabla^2 \varphi_\beta | [\psi]_\alpha \rangle \frac{\partial f_\alpha^c}{\partial \psi_\beta}. \end{aligned} \tag{85}$$

The mapping-closure assumption is now invoked, namely that the statistics of φ_β are the same as those of φ_β^s. When this is done, the first term on the right-hand side of (85) vanishes, because of (80). Similarly, in the last term, the conditioning on $[\psi]_\alpha$ can be replaced by the conditioning on $[\psi]_\beta$. With these substitutions, (85) can be integrated with respect to ψ_α (from $-\infty$ to ψ_α) to yield

$$\dot{F}_\alpha([\psi]_\alpha, t) + \sum_{\beta=1}^{\alpha} \Gamma_\beta \langle \nabla^2 \varphi_\beta^s | [\varphi^s]_\beta = [\psi]_\beta \rangle F_{\alpha,\beta}([\psi]_\alpha, t) = 0. \tag{86}$$

Comparing (81) and (86) (with $[\psi]_\beta = [X(\eta)]_\beta$) and making use of (79) we obtain, for all α,

$$\frac{\partial}{\partial t} X_\alpha([\eta]_\alpha, t) = \Gamma_\alpha \langle \nabla^2 \varphi_\alpha^s | [\varphi^s]_\alpha = [X(\eta)]_\alpha \rangle = \Gamma_\alpha \sum_{\beta=1}^{\alpha} \frac{J_\beta^2}{\lambda_\beta^2} \{ X_{\alpha,\beta\beta} - \eta_\beta X_{\alpha,\beta} \}. \tag{87}$$

Or, alternatively,

$$\left\{ \frac{\partial}{\partial t} - \Gamma_\alpha \sum_{\beta=1}^{\alpha} \frac{J_\beta^2}{\lambda_\beta^2} \left(\frac{\partial^2}{\partial \eta_\beta \, \partial \eta_\beta} - \eta_\beta \frac{\partial}{\partial \eta_\beta} \right) \right\} X_\alpha = 0. \tag{88}$$

Thus each mapping X_α evolves independently in its α-dimensional sample space according to this convective–diffusive equation.

We close this section by making a few observations about the mapping closure that has been developed.

(i) At this level, the mapping closure is not useful in giving the rate at which each variance decays. Rather, given the scalar dissipation rates

$$\chi_\alpha(t) \equiv \Gamma_\alpha \langle \nabla \varphi_\alpha \cdot \nabla \varphi_\alpha \rangle, \tag{89}$$

the stretching $J_\alpha(t)$ can be determined from the relation

$$\chi_\alpha = \Gamma_\alpha \sum_{\beta=1}^{\alpha} \left(\frac{X_{\alpha,\beta} J_\beta}{\lambda_\beta} \right)^2, \tag{90}$$

which is obtained from (74).

(ii) For the first variable φ_1 (i.e., $\alpha = 1$), (87) is identical to the equation for a single scalar (28).

(iii) If initially φ_α is independent of φ_β for all $\beta < \alpha$, then again (87) for X_α reduces to (28).

(iv) In the case of equal diffusivities ($\Gamma_\alpha = \Gamma$, all α), suppose that initially φ_α is linearly dependent on $[\varphi]_{\alpha-1}$. Then it can readily be shown from (87) that this linear dependence is preserved—as it is by the exact equations. Conversely, if the diffusivities differ the linear dependence is not preserved. Whether or not this prediction of differential diffusion is quantitatively correct remains to be shown.

(v) For the case of equal diffusivities, (87) admits a solution in the form of a product of α one-dimensional mappings:

$$X_\alpha([\eta]_\alpha, t) = \prod_{\beta=1}^{\alpha} Y_\beta(\eta_\beta Q_\beta(t), t), \tag{91}$$

where

$$Q_\beta(t) \equiv \exp\left\{\int_0^t -\Gamma \frac{J_\beta^2}{\lambda_\beta^2}\, dt\right\}, \tag{92}$$

and each mapping evolves according to the unsteady heat conduction equation

$$\dot{Y}_\beta = \Gamma\left(\frac{J_\beta Q_\beta}{\lambda_\beta}\right)^2 Y_\beta''. \tag{93}$$

(vi) It appears that the mapping closure violates the linearity and independence principles outlined by Pope (1983). Consider the case of equal diffusivities with statistically dependent initial fields $[\varphi]_\sigma$. The mapping closure can be applied in $\sigma!$ different ways—one for each ordering of the fields. It appears likely that the subsequent evolution of the pdf given by the mapping closure will be different for each ordering, in clear violation of the linearity and independence principles.

This violation can be viewed as a manifestation of the inadequacy of the level of closure (Kraichnan, private communication).

4. Mapping Closure for Several Reactive Scalars

We now extend the development to reactive scalars by considering the fields evolving according to

$$\frac{\partial \varphi_\alpha}{\partial t} + \mathbf{U}\cdot\nabla\varphi_\alpha = \Gamma_\alpha \nabla^2 \varphi_\alpha + S_\alpha, \tag{94}$$

where $S_\alpha(\mathbf{x}, t)$ is the rate of increase of φ_α due to chemical reactions. In general, if φ determines the thermochemical state of the fluid, then the source terms are known functions of φ, i.e.,

$$S_\alpha(\mathbf{x}, t) = \hat{S}_\alpha(\varphi(\mathbf{x}, t)) \tag{95}$$

(see, e.g., Pope, 1985).

The procedure developed in the previous section can be applied to determine the evolution of the mappings X_α corresponding to (94). The result is exactly the same equation as before ((87) or (88)), but with the additional source term (on the right-hand side)

$$R_\alpha \equiv \langle S_\alpha(\mathbf{x}, t) | [\varphi^s(\mathbf{x}, t)]_\alpha = [X]_\alpha \rangle. \tag{96}$$

This source can be determined from (95) and from the conditional pdf's, since we have

$$\langle S_\alpha | [\psi]_\alpha \rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \hat{S}_\alpha(\psi) \prod_{\beta=\alpha+1}^{\sigma} f_\beta^c([\psi]_\beta)\, d\psi_{\alpha+1}\, d\psi_{\alpha+2}\cdots d\psi_\sigma. \tag{97}$$

It follows, then, that the mapping closure does indeed provide a closure even with reaction.

Equation (97) appears intractable both analytically and numerically. But there is an important special case in which (96) simplifies. Suppose the reaction scheme is such that $\hat{S}_\alpha$ only depends on φ_β, $\beta \le \alpha$ (for some ordering of the scalars). For this case we have

$$S_\alpha(\mathbf{x}, t) = \hat{S}_\alpha([\varphi(\mathbf{x}, t)]_\alpha) \tag{98}$$

(in place of (95)), and hence the source in the equation for X_α is (from (96)) simply

$$R_\alpha = \hat{S}_\alpha([X]_\alpha). \tag{99}$$

Even though the special requirement of (98) is very restrictive, there are some important examples of its applicability: we cite just one. Consider the production of NO is nonpremixed combustion. A standard approach is to characterize the thermochemistry by three scalars: the mixture fraction φ_1 (usually denoted by ξ); a reaction progress variable φ_2; and the mass fraction of NO, φ_3. Then the source terms are of the form

$$S_1 = 0, \qquad S_2 = \hat{S}_2(\varphi_1, \varphi_2), \qquad S_3 = \hat{S}_3(\varphi_1, \varphi_2), \tag{100}$$

thus satisfying (98).

5. Discussion

The principal contributions of this paper are to demonstrate the excellent agreement between the mapping closure and direct numerical simulations and to extend the formalism to many reactive scalars.

The mapping closure can be applied at a higher level than considered here. In particular, it can be applied to the joint pdf of φ and $\nabla\varphi$. In spite of the apparent success of the closures considered here, there are some intrinsic defects at the level of closure of the pdf of φ alone. For example, for the case of a scalar field with a Gaussian pdf, the closure implies that the pdf of the derivative $\partial\varphi/\partial x_1$ is Gaussian. Whereas it is known (Eswaran and Pope, 1988) that $|\nabla\varphi|$ is log-normal.

A second defect is that (at this level of closure) there is no description of the processes that generate the term to be modeled, i.e., $\nabla^2\varphi$. It is sobering to realize that, for homogeneous fields, the pdf equation for φ, and hence the mapping closure, are the same whatever the nature of the velocity field $\mathbf{U}(\mathbf{x}, t)$. In particular, the mapping closure is the same for the heat conduction equation (i.e., $\mathbf{U} = 0$) as it is for homogeneous turbulence. Another manifestation of the same defect is that the closure cannot distinguish between flamelet and distributed reaction (Pope, 1991).

It is expected that the development of mapping closures for the joint pdf of φ and $\nabla\varphi$ will be a profitable area of research, with the potential of overcoming the above-mentioned defects.

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