Conditional Statistics in Turbulent Scalar Mixing and Reaction

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For more than 30 years, the pioneering hypothesis of Toor (1962) has been utilized for statistical modeling of turbulent reacting flows with nonpremixed reactants. According to this hypothesis, in a chemical reaction of the type "Fuel + Oxidizer → Products" in homogeneous isothermal flows with stoichiometric and (initially) nonpremixed reactants, the temporal decay rate of the "unmixedness" (reactants' covariance) is independent of chemistry and can be related to the standard deviation of the "mixture fraction." This mixture fraction (also referred to as the Shvab-Zeldovich variable (Libby and Williams, 1980)) is a conserved scalar which portrays the mixing behavior of the system under nonreacting but otherwise identical flow conditions (Brodkey, 1975; Toor, 1975). Denoting the concentration of one of the reactants, say fuel by $\mathfrak{F}$, and the mixture fraction by ϕ, Toor (1962) shows that in the limit of infinitely fast chemistry

$$\frac{E\{\mathfrak{F}(t)\}}{E\{\mathfrak{F}(t')\}}=\frac{\sigma(t)}{\sigma(t')}, \tag{1}$$

where $E\{\ \}$ denotes the expectation (ensemble-mean value) and $\sigma^2(t)$ is the variance of the mixture fraction. This mixture fraction, considered a random variable, is defined within the lower and upper bounds: $\phi \in [\phi_l, \phi_u]$. In a spatially homogeneous turbulent flow the statistics are generated by realization and/or space-sampling, thus the decay of the mixture fraction variance and the rate of reactant conversion depend only on time (t).

Determination of the statistics of reacting scalars from those of the mixture fraction continues to be a very challenging issue. Dutta and Tarbell (1989), Frankel et al. (1993), and Frankel (1993) discuss comparative assessments of several turbulence closures for this purpose. In Toor's results portrayed by Eq. 1 the primary assumption is that the probability density function (pdf) of the mixture fraction is Gaussian, and remains Gaussian throughout mixing. In this note we show that Eq. 1 is valid under a less restrictive condition, and that the Gaussian pdf is one special case which satisfies this general condition. This proof is provided by considering the transport equation governing the evolution of the mixture fraction pdf. With this equation, several other important features of scalar mixing are also identified.

The lefthand side of Eq. 1 is determined directly by the pdf of the mixture fraction. By defining $\phi=0$ as the reaction surface (the flame sheet), we have (Libby and Williams, 1980): $E\{\mathfrak{F}(t)\}=\int_0^{\phi_u}\phi P(\phi,t)d\phi$, where P denotes the pdf of ϕ. With the transformation $[\phi,t]\rightarrow[y=\phi/\sigma(t),\sigma(t)]$, Eq. 1 is expressed as

$$\frac{E\{\mathfrak{F}(t)\}}{\sigma(t)}=\int_0^{y_u=[\phi_u/\sigma(t)]} yP[y,\sigma(t)]dy. \tag{2}$$

In order for Eq. 1 to be valid, two conditions must be satisfied: (1) the pdf in the integrand of Eq. 2 must be time-invariant, i.e., $P[y,\sigma(t)]=P(y)$; and (2) the upper limit of the integral must be time-invariant. Here we demonstrate that both of these conditions are satisfied when the "conditional expected diffusion" of the mixture fraction is "linear" in the composition space. For this demonstration, we consider the transport equation for the pdf of ϕ in spatially homogeneous turbulent flows (O'Brien, 1980; Pope, 1985; Dopazo, 1994)

$$\frac{\partial P}{\partial t}+\frac{\partial}{\partial \phi}(E\{\zeta|\phi\}P)=0. \tag{3}$$

Assuming that the molecular diffusion is governed by the Fick's law, $\zeta=\kappa\nabla^2\phi$, κ is the molecular diffusion coefficient. The term $E\{\zeta|\phi\}$ denotes the expectation of the scalar diffusion conditioned (denoted by the vertical bar) on the scalar value ϕ. Equation 3 is alternatively expressed as (O'Brien, 1980; Pope, 1985)

$$\frac{\partial P}{\partial t}+\frac{\partial^2}{\partial \phi^2}(E\{\xi^2|\phi\}P)=0, \tag{4}$$

with $\xi^2=\kappa\nabla\phi\cdot\nabla\phi$ and $E\{\xi^2|\phi\}$ denoting the conditional expectation of the scalar dissipation. At the level of single-point closure, neither of these conditional expectations are known,

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nor is the unconditional expectation of scalar dissipation, $E\{\xi^2\} = \int_{\phi_l}^{\phi_u} P(\phi,t)E\{\xi^2|\phi\}d\phi$. Given the pdf it is possible to determine these conditional expectations (Miller et al., 1993). First, we consider the general family of "exponential pdfs" since this family includes the Gaussian distribution as assumed by Toor, and it also includes other distributions which have been observed in more recent laboratory and numerical experiments (Castaing et al., 1989; Kerstein, 1991; Gollub et al., 1991; Pumir et al., 1991; Jayesh and Warhaft, 1992; Metais and Lesieur, 1992; Lane et al., 1993; Kimura and Kraichnan, 1993)

$$P(\phi,\sigma(t)) = C(\sigma(t),q)\exp\left(-\frac{|\phi-\phi_0|^q}{K[\sigma(t),q]}\right),$$

$$\phi \in [\phi_l,\phi_u] \equiv [-\infty,\infty], \quad (5)$$

where q is a constant parameter; $q=2$ corresponds to Gaussian and $q=1$ implies the Laplace (double exponential) density. Considering distributions with the mean $\phi_0 = E\{\phi\} = 0$ and the variance $\sigma^2 = E\{\phi^2\}$, manipulation of Eqs. 3–4 in the format outlined by Miller et al. (1993) yields

$$\frac{E\{\xi^2|\phi\}}{E\{\xi^2\}} = 1, \quad \frac{E\{\zeta|\phi\}}{E\{\xi^2\}} = -\frac{\phi}{\sigma^2} \quad (6)$$

for the Gaussian density, and

$$\frac{E\{\xi^2|\phi\}}{E\{\xi^2\}} = \frac{1}{2}\left(1+\frac{\sqrt{2}|\phi|}{\sigma}\right), \quad \frac{E\{\zeta|\phi\}}{E\{\xi^2\}} = -\frac{\phi}{\sigma^2} \quad (7)$$

for the Laplace pdf. It is noted that the conditional expectations of diffusion as predicted by these two densities are identical, and are linear in the compositional domain in accord with the least mean-square estimation (LMSE) model (Dopazo, 1994; O'Brien, 1980). Based on this observation, we propose that for all the other members of the family of exponential pdfs, the linear profile is applicable. This proposal is plausible provided that

$$\frac{1}{C}\frac{\partial C}{\partial t} = \frac{E\{\xi^2\}}{\sigma^2}, \quad \frac{1}{K}\frac{\partial K}{\partial t} = -\frac{qE\{\xi^2\}}{\sigma^2}. \quad (8)$$

Manipulation of Eq. 5 shows that $K(\sigma,q) = M(q)\sigma^q$ and $C(\sigma,q) = N(q)\sigma^{-1}$, where $M(q)$ and $N(q)$ are known functions of q. Thus, it is easily verified that Eq. 8 is indeed valid regardless of the magnitude of q.

The general condition under which the conditional expected diffusion is linear for any pdf has been established by Valiño et al. (1994). By considering the characteristic of Eq. 3, they show that with a linear conditional expected diffusion, the pdf of the variable y is time-invariant. Here, we provide a direct means of establishing this condition by substituting the second of Eq. 6 into Eq. 3. Denoting the Fourier transform of the pdf by $\tilde{P}$

$$P(\phi,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\tilde{P}(\Omega,t)\exp(j\Omega\phi)d\Omega, \quad j=\sqrt{-1} \quad (9)$$

we have

$$\frac{\partial\tilde{P}}{\partial t} + \frac{\Omega E\{\xi^2\}}{\sigma^2}\frac{\partial\tilde{P}}{\partial\Omega} = 0. \quad (10)$$

This differential equation has the trial solution

$$\tilde{P}(\Omega,t) = \tilde{f}[\Omega\exp\{h(\sigma,t)t\}], \quad (11)$$

where the function $\tilde{f}$ depends on the initial condition $P(\phi,0)$. With $\sigma(d\sigma/dt) = -E\{\xi^2\}$, this trial solution satisfies Eq. 3 with $h(\sigma,t) = (1/t)\ln[\sigma(t)]$. Thus the unique solution of Eq. 10 is

$$\tilde{P}(\Omega,t) = \tilde{f}[\Omega\sigma(t)]. \quad (12)$$

This solution shows that the transformation $[\phi,t] \rightarrow [y,\sigma(t)]$ is very convenient in portraying the nature of pdf evolution when the conditional expected diffusion is linear. With this transformation Eq. 3 yields

$$P[y,\sigma(t)] = G(y) \quad \text{only}, \quad (13)$$

where the function G is determined by the initial condition and remains the same through mixing. Equation 13 means that for a linear conditional expected diffusion, the pdf of the scalar variable adopts a "self-similar" form in the sense that the pdf of the variable normalized by its standard deviation is time-invariant. This does not imply a "stationary field" as $P(\phi,t)$ can be time-dependent. This self-similarity is, in fact, noticed in direct numerical simulation results (Miller et al., 1993) in which the linearity of the conditional scalar diffusion field is also corroborated. It must be noted that in using the linear conditional diffusion field in LMSE, O'Brien (1980) points to permanency of the initial shape of the pdf when the parameter $\beta = [E\{\xi^2\}(t)]/[\sigma^2(t)]$ is constant. The mathematical procedure adopted here provides a direct means of determining the functional form of the parameter y, as undisguised by Eq. 12. Valiño et al. (1994) and Sinai and Yakhot (1989) suggest this functional form *a priori* by the inspection of numerical simulation data.

Now we consider condition (2) pertaining to the limits of $[y_l(t), y_u(t)] = [\phi_l/\sigma(t), \phi_u/\sigma(t)]$. For a pdf with an "unbounded support" $[y_l, y_u] \equiv [-\infty,\infty]$ condition (2) is satisfied. For the Gaussian pdf, obviously an unbounded support is implied by Toor. For a pdf within a "bounded domain," mixing is accompanied by the migration of the scalar bounds in the composition space as shown by Miller et al. (1993). Notwithstanding the randomness of the scalar bounds, Miller et al. (1993) also show

$$\frac{d\phi_u}{dt} = -\frac{d\phi_l}{dt} = E\{\zeta|\phi_u\} = -E\{\zeta|\phi_l\}. \quad (14)$$

With a linear conditional expected diffusion in Eq. 14 we have

$$\frac{\phi_u(t)}{\sigma(t)} = -\frac{\phi_l(t)}{\sigma(t)} = \text{Constant} = \frac{\phi_u(0)}{\sigma(0)} = C. \quad (15)$$

Equations 13 and 15 indicate that the linearity of the conditional expected diffusion satisfies both conditions (1) and (2); and thus imply the validity of Eq. 1. The Gaussian pdf is one special case which satisfies these conditions, but there are other distributions and/or mixing closures which portray a similar behavior (Givi, 1989). Considering the (approximate) linearity of the conditional diffusion field in several recent numerical and laboratory experiments (Miller et al., 1993; Pope and Ching, 1993; Leonard and Hill, 1991; Kailasanath et al., 1993) in which the pdf is not necessarily Gaussian, it is plausible to assume that Toor's results would be applicable for modeling of equivalent reacting systems. Of course, this would be true if the conditional diffusion remains linear at all times: It is well-established that for initially "segregated" reactants with the initial pdf composed of an exact double-delta function, the assumption is not generally plausible when $t' \rightarrow 0$, $t \neq t'$ (Kosály, 1987; Givi and McMurtry, 1988; Madnia et al., 1992; Frankel et al., 1993) unless the pdf remains double-delta at all times. The transformation of the double-delta pdf to Gaussian (or other) distributions is accompanied by a nonlinear conditional expected diffusion (Miller et al., 1993).

At this point, it is instructive to note that with the same linear conditional diffusion, the conditional expected dissipation can vary depending on the initial form of the pdf. It is useful to note that the self-similarity of the pdf also implies the self-similarity of the conditional dissipation. With the requirements (Miller et al., 1993) $P(\phi_l,t)E\{\xi^2|\phi_l\} = P(\phi_u,t)E\{\xi^2|\phi_u\} = 0$, Eq. 4 gives

$$\frac{E\{\xi^2|y\}}{E\{\xi^2\}} = \frac{-\int_{-C}^{y} y'P(y')dy'}{P(y)}. \qquad (16)$$

The righthand side of Eq. 16, while time-invariant, does depend on the pdf. For the exponential family, for example, Eqs. 3–4 yield, after significant manipulations (Jaberi, 1996)

$$\frac{E\{\xi^2|\phi\}}{E\{\xi^2\}} = \frac{K^{2/q}}{q\sigma^2}\left\{\Gamma\left(\frac{2}{q}\right) - \gamma\left(\frac{2}{q}, \frac{|\phi|^q}{K}\right)\right\}\exp\left(\frac{|\phi|^q}{K}\right), \qquad (17)$$

where Γ and γ denote the gamma function and the incomplete gamma function, respectively. With the identity

$$\Gamma(1+n) - \gamma(1+n,z) = n!\exp(-z)\sum_{k=0}^{n}\frac{z^k}{k!}, \quad n = 0,1,\ldots \qquad (18)$$

the corresponding algebraic relations for the Gaussian density and the Laplace density, Eqs. 6 and 7 are exactly recovered for $q = 2$ and $q = 1$, respectively. For other values of q, Eq. 17 can be evaluated only by numerical means (for $q = 4$ and $q \rightarrow \infty$ the results can be expressed, respectively, in terms of the error function and the exponential integral, both of which still require numerical evaluation). Note that for the Gaussian member ($q = 2$) an analytical expression for the conditional expected dissipation has been previously obtained (Gao, 1991). The results based on Eq. 17 in Figure 1 confirm that if the pdf exhibits tails broader than Gaussian

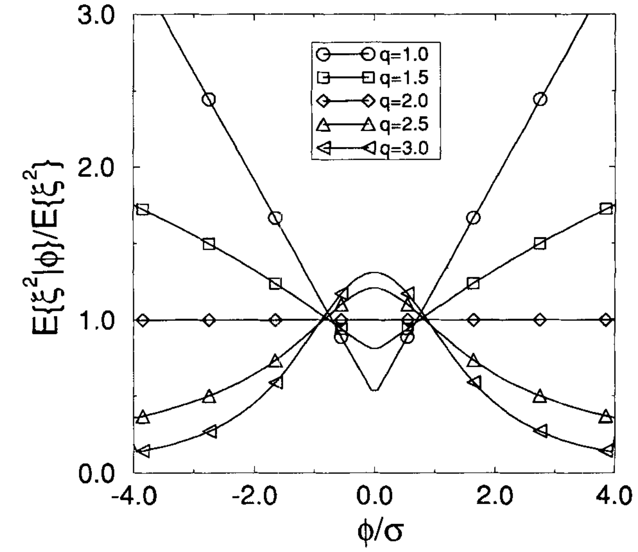

Figure 1. Normalized conditional expected dissipation of the scalar for several members of the exponential pdf.

($q < 2$), the normalized conditional dissipation portrays a "basin" shaped curve (concave up) near the mean scalar value. For pdfs with tails narrower than Gaussian ($q > 2$), the conditional dissipation is "bell" shaped (concave down). For $q = 2$, the profile is a straight line $E\{\xi^2|\phi\} = E\{\xi^2\}$. Only in this case is the conditional scalar dissipation independent of the scalar value (Gao, 1991), for which Eq. 1 was derived by Toor. The relation between the conditional dissipation and broadness (narrowness) of the pdf at its tails was first derived by Sinai and Yakhot (1989) based on a speculation on the asymptotic behavior of scalar mixing in stationary turbulence. Here, Eq. 17 illustrates this relation directly and is very convenient for assessing the results obtained by other closures.

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Notation

C = constant
$E\{|\}$ = conditional expectation
P = PDF
y = normalized scalar variable: $y = \phi/\sigma(t)$

Greek letters

γ = incomplete gamma function
Γ = gamma function
ζ = scalar diffusion
κ = diffusion coefficient
ξ^2 = scalar dissipation
σ = standard deviation of the mixture fraction
ϕ = composition domain

Superscripts

l = lower limit in the composition space
u = upper limit in the composition space

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