

The Application of PDF Transport Equations to Turbulent Reactive Flows

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Abstract

The transport equation for the probability density function (pdf) of scalars is useful in the modelling of turbulent reactive flows because the effects reaction appear in closed form. Monte Carlo calculations of the pdf transport equation are shown to be in good agreement with experimental data for two flows. In order to avoid the gradient diffusion assumption for turbulent transport, the equation for the joint pdf of velocity and scalars is also considered. As in the equation for the pdf of scalars alone, non-linear reaction schemes can be treated without approximation. The advantage of considering the joint pdf equation is that convection (by both the mean and fluctuating velocities) appears in closed form. Closure approximations are presented for the terms involving the fluctuating pressure and viscous and diffusive mixing. These models can be expected to be reliable since they are compatible with accurate and proven Reynolds-stress models. The resulting modelled transport equation for the joint pdf can be solved by the Monte Carlo method for inhomogenous flows with complex reactions.

Introduction

A major problem in the theoretical treatment of turbulent reactive flows arises due to the coupling between random turbulent fluctuations and non-linear reaction rates. This problem can be circumvented by considering the probability density function (pdf) of the chemical and thermodynamic variables [1, 2]. In the transport equation for this scalar pdf, the effects of reaction appear in closed form although models are required for turbulent transport and mixing. At first sight, the pdf transport equation appears extremely difficult to solve because the dimensionality of the pdf can be large. However, the equation can be solved by a Monte Carlo method [3].

In the next section of this paper, previous work [3, 4] on the scalar pdf equation is summarized. Good agreement is found between measurements and Monte Carlo calculations both for an inert mixing layer and for a premixed turbulent flame.

The great advantage of solving the transport equation for the scalar pdf by the Monte Carlo method is that non-linear reactions can be handled without approximation. This is demonstrated by the premixed flame calculations. But the method has weaknesses – gradient diffusion is assumed; the effects of reaction on the turbulence are ignored; and, a separate turbulence model (e. g. the k- ϵ model [5]) is needed to determine the velocity and turbulence fields. In the second section of this paper, the probability approach is extended to the joint pdf equation of the velocity $\mathbf{U} = U_1, U_2, U_3$ and the scalars $\vec{\Phi}$. This equation, which can be solved by the Monte Carlo method, does not suffer from the above-mentioned weaknesses of the scalar pdf equation.

The joint pdf of \mathbf{U} and $\vec{\Phi}$ is $f(\mathbf{V}, \vec{\psi}; \mathbf{x}, t)$ where $\mathbf{V} = V_1, V_2, V_3$ is the velocity space and $\vec{\psi}$ is the composition space. In the transport equation for $f(\mathbf{V}, \vec{\psi})$, reaction appears in closed form and so also does the convective transport. Consequently, the gradient-diffusion assumption is avoided. In addition, since $f(\mathbf{V}, \vec{\psi})$ contains all the statistical information about the velocity at each point, a turbulence model to determine the Reynolds stresses is not needed. However, since $f(\mathbf{V}, \vec{\psi})$ is a one-point statistic it contains no length-scale information – this must be supplied, either directly or through the standard modelled equation for the rate of dissipation ϵ .

The transport equation for $f(\mathbf{V}, \vec{\psi})$ is derived and examined to determine the effect of each term. The modelling of the unknown terms is considered.

There have been several contributions to the modelling of the scalar pdf equation in recent years [1, 2, 6]. Also, Lundgren [7] considered the velocity pdf equation and proposed simple relaxation models for the unclosed terms.

1. The scalar pdf equation

At any point in a turbulent reactive mixture of gases, the state of the fluid can be characterised by the velocity \mathbf{U} , the pressure p , the specific enthalpy h , and the mass fraction of each species \mathbf{m} . Since the mass fractions and the enthalpy obey the same form of transport equation, it is convenient to define the set of scalars $\vec{\Phi} = \Phi_1, \Phi_2 \dots \Phi_\sigma$ as

$$\Phi_\alpha = m_\alpha, \quad \alpha = 1, 2 \dots \sigma - 1, \quad (1)$$

$$\Phi_\sigma = h. \quad (2)$$

Thus with $\sigma - 1$ species there are σ scalars in $\vec{\Phi}$. In a low Mach number flow, the equations of conservation of mass, momentum and the scalars are

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} \rho U_i = 0, \quad (3)$$

$$\frac{\partial}{\partial t} \rho U_j + \frac{\partial}{\partial x_i} \rho U_i U_j = - \frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial p}{\partial x_j} + \rho g_j, \quad (4)$$

and

$$\frac{\partial}{\partial t} \rho \Phi_\alpha + \frac{\partial}{\partial x_i} \rho U_i \Phi_\alpha = - \frac{\partial J_i^\alpha}{\partial x_i} + \rho S_\alpha, \quad (5)$$

where \mathbf{g} is the gravitational acceleration, τ_{ij} is the viscous stress tensor and \mathbf{J}^α is the diffusive flux of Φ_α . The density ρ and S_α — the rate of creation of Φ_α — can be expressed as functions of $\vec{\Phi}$,

$$\rho = \rho(\vec{\Phi}), \quad S_\alpha = S_\alpha(\vec{\Phi}). \quad (6)$$

The joint pdf of the scalars is defined by

$$p(\vec{\psi}; \mathbf{x}, t) = \langle p'(\vec{\psi}; \mathbf{x}, t) \rangle, \quad (7)$$

where angled brackets indicate an ensemble mean and

$$p'(\vec{\psi}; \mathbf{x}, t) = \prod_{\alpha=1}^{\sigma} \delta(\Phi_\alpha(\mathbf{x}, t) - \psi_\alpha). \quad (8)$$

The independent variables $\vec{\psi}$ form the composition space: a particular location $\vec{\psi} = \vec{\psi}^*$, corresponds to a gas composition $\vec{\Phi} = \vec{\psi}^*$. It follows from the above definitions that for any function $Q(\vec{\Phi})$,

$$\langle Q(\vec{\Phi}) \rangle = \int Q(\vec{\psi}) p(\vec{\psi}) d\vec{\psi}, \quad (9)$$

where the integration ($d\vec{\psi} = d\psi_1 d\psi_2 \dots d\psi_\sigma$) is over the whole of composition space.

In variable-density flows the use of density-weighted averages has advantages both theoretically and practically. Density-weighted averages, denoted by a tilde, are defined by

$$\tilde{Q}(\Phi(\mathbf{x}, t)) \equiv \langle \rho(\mathbf{x}, t) Q(\vec{\Phi}(\mathbf{x}, t)) / \langle \rho \rangle \rangle. \quad (10)$$

And from the definition of the density-weighted joint pdf

$$\tilde{p}(\vec{\psi}; \mathbf{x}, t) \equiv \rho(\vec{\psi}) p(\vec{\psi}; \mathbf{x}, t) / \langle \rho \rangle, \quad (11)$$

it follows

$$\tilde{Q}(\vec{\Phi}) = \int \tilde{p}(\vec{\psi}; \mathbf{x}, t) Q(\vec{\psi}) d\vec{\psi}. \quad (12)$$

A transport equation for $\tilde{p}(\vec{\psi})$ can be obtained from the conservation equation for Φ_α , equation (5). If the turbulent transport is modelled by simple gradient diffusion (with the turbulent diffusion coefficient being $\Gamma_T(\mathbf{x}, t)$), the equation for $\tilde{p}(\vec{\psi})$ is

$$\frac{\partial \tilde{p}(\vec{\psi})}{\partial t} + \tilde{U}_i \frac{\partial \tilde{p}(\vec{\psi})}{\partial x_i} + \frac{\partial}{\partial \psi_\alpha} (\tilde{p}(\vec{\psi}) S_\alpha(\vec{\psi})) = \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_i} \Gamma_T \frac{\partial \tilde{p}(\vec{\psi})}{\partial x_i} + E(\vec{\psi}; \mathbf{x}, t). \quad (13)$$

Summation is over repeated indices (i and α) and $E(\vec{\psi}; \mathbf{x}, t)$ represents the effect of molecular mixing. The terms on the left-hand side are exact whereas those on the

right are modelled or (in the case E) need to be modelled. The two leading terms represent the rate of change of $\tilde{p}(\vec{\psi})$ along a density-weighted streamline; the third term represents the transport of $\tilde{p}(\vec{\psi})$ in composition space due to reaction. It is noteworthy that, in this formulation, chemical reactions – however complicated the scheme – can be treated without approximation.

A number of models for the molecular mixing term E have been proposed [2, 8, 9, 10], but none is entirely satisfactory. Here Curl's model [10] is employed since it alone is applicable to an arbitrary number of quantities (i.e., any σ) and can be expected to produce qualitatively correct results. Accordingly, we take

$$E(\vec{\psi}; \mathbf{x}, t) = 2^\sigma \omega \int \tilde{p}(\vec{\psi} + \vec{\psi}') \tilde{p}(\vec{\psi} - \vec{\psi}') d\vec{\psi}' - \omega \tilde{p}(\vec{\psi}), \quad (14)$$

where $\omega(\mathbf{x}, t)$ is the appropriate turbulent frequency.

In order to complete the closure, the turbulent diffusion coefficient Γ_T and mixing frequency ω need to be determined. In the calculations reported below, the $k - \epsilon$ turbulence model [5] was used to determine the turbulent viscosity ν_T . Then in order for the modelled pdf equation (13) to be consistent with the standard model equation for $\langle \Phi'^2 \rangle$ [11], we require

$$\Gamma_T = \rho \nu_T / \sigma_\Phi, \quad (15)$$

and

$$\omega = 2C_\Phi \epsilon / k, \quad (16)$$

where the constants σ_Φ and C_Φ take the values 0.7 and 2.0.

The pdf equation (13) has been solved by the Monte Carlo method for two flows. The first is an inert turbulent mixing layer which was measured by Batt [12]. There was a small temperature difference between the two streams so that the normalised temperature Φ is a conserved, passive scalar. The pdf equation was solved for this flow along with the mean velocity equations and the $k - \epsilon$ turbulence model equations (see [3] for details). Figure 1 shows the resulting pdf's of ψ at seven cross-stream locations at an axial location where the mixing layer is self-preserving. It may be seen that, in general, the agreement is good: for the five central pdf's, the locations of the peaks* and the shapes and spreads of the distributions are closely matched. (The measurements at the extreme locations are suspicious: in neither case does the pdf integrate to unity and, from similar data [13], a spike resembling an exponential decay can be expected at the bounds $\psi = 0$ and $\psi = 1$.)

The second flow for which the scalar pdf equation has been solved by the Monte Carlo method is the premixed propane/air flame studied by Robinson and Kovitz [14]. These flames were stabilized behind a plate, perforated with 1/4" diameter holes in a 4" diameter tube. The homogenous propane/air mixture was supplied at a temperature of 590 K, a pressure of 5×10^5 Pa and equivalence ratios of 0.635, 0.725 and 0.825. In order to study the flame, the Monte Carlo method was used to solve the equation for the joint pdf of the mass fractions of C_3H_8 , CO and NO (see [4] for details).

* The comparisons between measured and calculated pdf's have been made where the mean values are the same. Consequently, it is not surprising that the peaks nearly coincide.

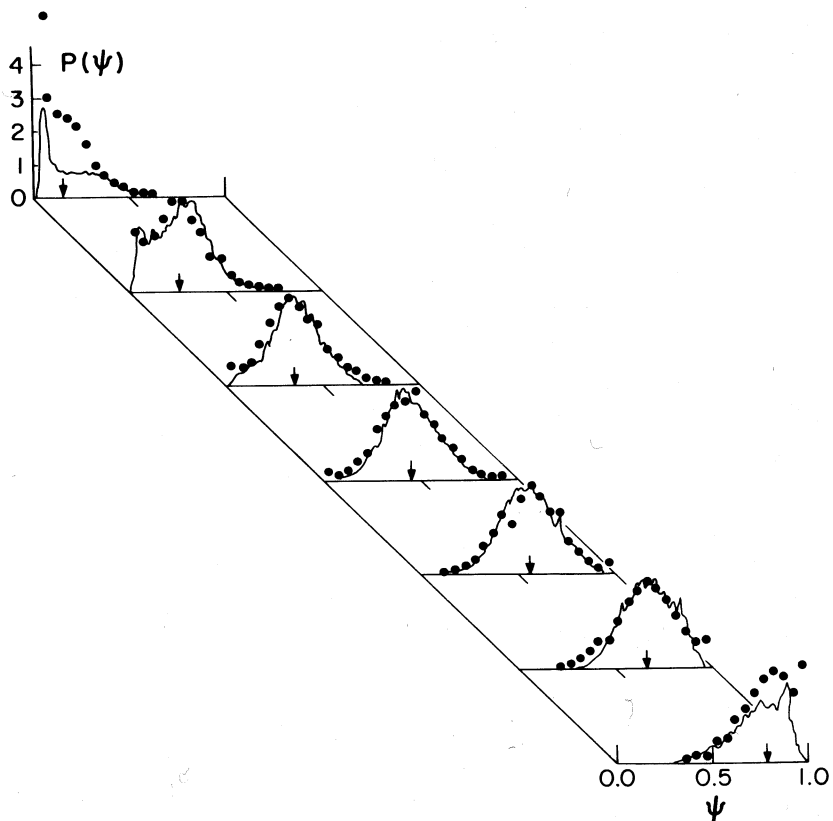


Fig. 1: Probability density functions of temperature in a mixing layer: $p(\psi)$ against ψ .
 (Arrows show position of means.)
 ● Monte Carlo calculations
 ~~~~~ Measurements of Batt (1977)

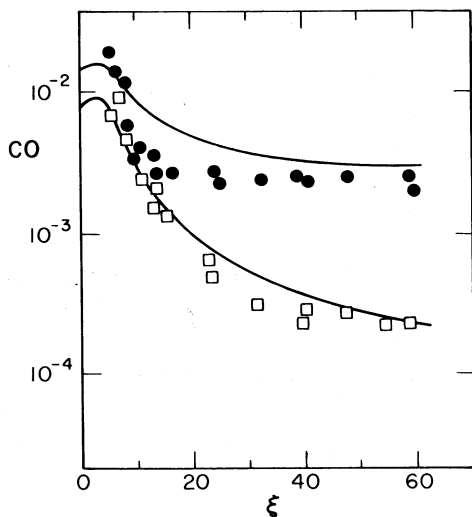


Fig. 2: Mole fraction of CO against axial distance;  $s = 0.815$ .  
 ●  $\Phi = 0.845$  } data of Robinson [14].  
 □  $\Phi = 0.635$  }  
 — calculations

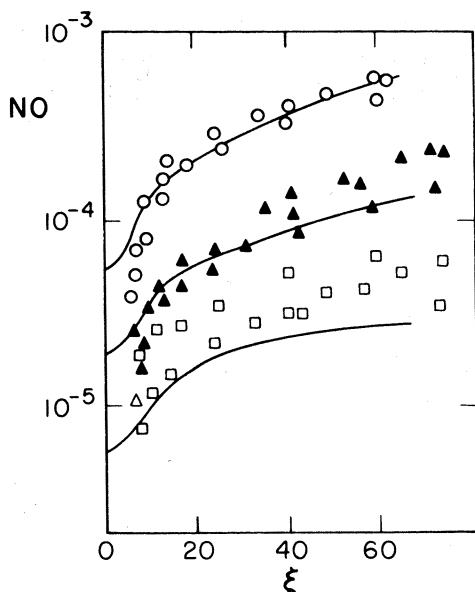


Fig. 3: Mole fraction of NO against axial distance;  $s = 0.815$ .

$\circ \Phi = 0.845$   
 $\blacktriangle \Phi = 0.725$   
 $\square \Phi = 0.635$

} data of Robinson [14].  
 — calculations

Figures 2 and 3 show a comparison between measured and calculated CO and NO concentrations against the normalized axial distance  $\xi$ . It may be seen that in general the agreement is good. Since the oxidation of CO and the formation of NO are strongly influenced both by finite-rate non-linear kinetics and by turbulence, this level of agreement is testament to the ability of the pdf equation to handle these cases accurately.

For both the flows reported, the computer requirements of the Monte Carlo method were modest. In each case, the CPU time on a VAX 11/780 was about  $2\frac{1}{2}$  minutes at a cost of \$5.00.

## 2. The joint pdf equation

While the calculations based on the scalar pdf equation are very encouraging, modelling deficiencies are evident. In particular, the gradient-diffusion assumption is suspicious especially for reacting flows. Consequently, we now consider the extension of the approach to the joint pdf of velocity and scalars which removes the need for the gradient-diffusion assumption.

The joint pdf of the velocities and scalars is defined by

$$f(\mathbf{V}, \vec{\psi}; \mathbf{x}, t) \equiv \langle f'(\mathbf{V}, \vec{\psi}; \mathbf{x}, t) \rangle, \quad (17)$$

where

$$f'(\mathbf{V}, \vec{\psi}; \mathbf{x}, t) \equiv \prod_{j=1}^3 \delta(U_j(\mathbf{x}, t) - V_j) \prod_{\alpha=1}^{\sigma} \delta(\Phi_{\alpha}(\mathbf{x}, t) - \psi_{\alpha}). \quad (18)$$

The independent variables  $\mathbf{V} = V_1, V_2, V_3$  and  $\vec{\psi} = \psi_1, \psi_2, \dots, \psi_\sigma$  form the velocity space and the composition space: a particular location  $\mathbf{V}^*, \vec{\psi}^*$  corresponds to a fluid velocity  $\mathbf{U} = \mathbf{V}^*$  and a gas composition  $\vec{\Phi} = \vec{\psi}^*$ . Infinitesimal hypervolumes in these spaces are denoted by

$$d\mathbf{V} = dV_1 dV_2 dV_3, \quad (19)$$

and

$$d\vec{\psi} = d\psi_1 d\psi_2 \dots d\psi_\sigma. \quad (20)$$

From these definitions, the following basic properties of the joint pdf can be deduced:

$$f(\mathbf{V}) = \int f(\mathbf{V}, \vec{\psi}) d\vec{\psi}, \quad (21)$$

$$f(\vec{\psi}) = \int f(\mathbf{V}, \vec{\psi}) d\mathbf{V}, \quad (22)$$

$$1 = \int \int f(\mathbf{V}, \vec{\psi}) d\mathbf{V} d\vec{\psi}, \quad (23)$$

and for any function  $Q(\mathbf{U}, \vec{\Phi})$ ,

$$\langle Q(\mathbf{U}, \vec{\Phi}) \rangle = \int \int f(\mathbf{V}, \vec{\psi}) Q(\mathbf{V}, \vec{\psi}) d\mathbf{V} d\vec{\psi}. \quad (24)$$

$f(\mathbf{V})$  and  $f(\vec{\psi})$  are the separate pdf's of velocity and scalars, and the integrations are performed over the whole of the spaces.

The transport equation for  $f(\mathbf{V}, \vec{\psi})$  is obtained from the definition of  $f$  and from the transport equations for  $\mathbf{U}$  and  $\vec{\Phi}$ . Differentiating eq. (18) we obtain

$$\frac{\partial f'}{\partial t} = - \frac{\partial f'}{\partial V_j} \frac{\partial U_j}{\partial t} - \frac{\partial f'}{\partial \psi_\alpha} \frac{\partial \Phi_\alpha}{\partial t}, \quad (25)$$

where summation is implied over repeated suffices ( $j$  and  $\alpha$ ). With a similar expression for the spatial derivative, substituting for  $\partial U_j / \partial t$  and  $\partial \Phi_\alpha / \partial t$  from eqs. (4) and (5) and averaging, we obtain the equation for  $f$ :

$$\begin{aligned} \rho(\vec{\psi}) \left( \frac{\partial}{\partial t} + V_i \frac{\partial}{\partial x_i} \right) f &= \frac{\partial}{\partial V_j} \{ \langle f' \frac{\partial p}{\partial x_j} \rangle - f \rho(\vec{\psi}) g_j + \langle f' \frac{\partial \tau_{ij}}{\partial x_i} \rangle \} + \\ &\quad (a) \qquad (b) \qquad (c) \qquad (d) \\ &+ \frac{\partial}{\partial \psi_\alpha} \{ - f \rho(\vec{\psi}) S_\alpha(\vec{\psi}) + \langle f' \frac{\partial J_1^\alpha}{\partial x_i} \rangle \}. \end{aligned} \quad (26)$$

(e) \qquad (f)

Before examining the above equation term by term, several general comments can be made. First it should be remembered that  $f$  is a function of the independent variables  $\mathbf{V}, \vec{\psi}, \mathbf{x}$  and  $t$ : thus  $\rho(\vec{\psi})$  is the local density – local, that is, in  $\vec{\psi}$ -space. Similarly,  $\mathbf{V}$  is the local velocity in  $\mathbf{V}$ -space. The derivative with respect to  $V_j$  in terms (b), (c) and (d) indicates that the terms represent transport of  $f$  in  $\mathbf{V}$ -space: the terms dis-

appear when the equation is integrated over the whole of  $\mathbf{V}$ -space to form the equation for  $f(\vec{\psi})$ . Similarly, terms (e) and (f) represent transport of  $f$  in  $\vec{\psi}$ -space. Before equation (26) can be solved, the three terms involving correlations with  $f'$  (terms (b), (d) and (f)) need to be modelled. Each of these terms can be reexpressed as a conditionally expected value; for example

$$\langle f' \frac{\partial p}{\partial x_j} \rangle = f E \left( \frac{\partial p}{\partial x_j} \mid \mathbf{V}, \vec{\psi} \right). \quad (27)$$

The first term in eq. (20) (term a) is the local density times the rate of change of  $f$  along a local particle path. That is,

$$\left( \frac{\partial}{\partial t} + V_i \frac{\partial}{\partial x_i} \right) f(\mathbf{V}, \psi; \mathbf{x}, t) = \frac{\partial}{\partial t} f(\mathbf{V}, \psi; \mathbf{y}(t), t), \quad (28)$$

where

$$\frac{d\mathbf{y}}{dt} = \mathbf{V}. \quad (29)$$

This term accounts for the convection by both the mean and fluctuating velocities. In moment formulations, convection by the fluctuating velocity appears as an unknown correlation that is usually modelled by gradient diffusion. While the gradient-diffusion assumption for turbulence has never had a firm foundation, recently both theoretical [15] and experimental [16] studies have shown that the assumption can be grossly in error for reactive flows. In the present joint pdf formulation, the convective term appears in closed form and so there is no need for a gradient-diffusion assumption. This is a major reason for considering  $f(\mathbf{V}, \vec{\psi})$  rather than  $f(\vec{\psi})$ .

The usefulness of the equation for  $f(\vec{\psi})$  in reactive flows stems from the fact that the effects of reaction appear in closed form, irrespective of the complexity and nonlinearity of the reaction scheme. The same is true in the equation for  $f(\mathbf{V}, \psi)$ : term (e) in eq. (26) shows that the effect of reaction (which appears in closed form) is to transport  $f$  in composition space.

Term (f) also transports  $f$  in composition space, in this case as a result of molecular diffusion. The form of the term is readily seen if, for the single scalar  $\Phi$ , we assume simple gradient diffusion

$$J_i = -\Gamma \partial \Phi / \partial x_i, \quad (30)$$

where  $\Gamma$  is the diffusive coefficient. Then term (f) can be decomposed as

$$\frac{\partial}{\partial \psi} \langle f' \frac{\partial J_i}{\partial x_i} \rangle = \frac{\partial}{\partial x_i} \Gamma \frac{\partial f}{\partial x_i} - \frac{\partial^2}{\partial \psi^2} \langle f' \Gamma \frac{\partial \Phi}{\partial x_i} \frac{\partial \Phi}{\partial x_i} \rangle. \quad (31)$$

The first term on the right-hand side (which is negligible at high Reynolds number) is the molecular transport of  $f$ . The second term is minus the second derivative of a positive correlation. It is simply shown [2] that such a term does not affect the



mean  $\langle \Phi \rangle$  but tends to decrease the second moment  $\langle \Phi'^2 \rangle$ . Thus the effect of diffusion is to transport  $f$  in composition space so that  $\langle \Phi \rangle$  is unchanged while  $\langle \Phi'^2 \rangle$  tends to decrease.

The effect of molecular viscosity (term d) is exactly analogous to the effect of diffusion: it transfers  $f$  in  $\mathbf{V}$ -space, tending to decrease the turbulent kinetic energy while not affecting the mean velocity. In spite of the known shortcomings, it is suggested here to model both the diffusive and viscous mixing terms with Curl's model [10]. Thus,

$$\frac{\partial}{\partial \psi_\alpha} \langle f' \frac{\partial J_i^\alpha}{\partial x_i} \rangle = 2C_\Phi \rho(\vec{\psi}) \frac{\epsilon}{k} \{ 2^\sigma \int f(\mathbf{V}, \vec{\psi} + \vec{\psi}') f(\mathbf{V}, \vec{\psi} - \vec{\psi}') d\vec{\psi}' - f(\mathbf{V}, \vec{\psi}) \}, \quad (32)$$

and

$$\frac{\partial}{\partial V_j} \langle f' \frac{\partial \tau_{ij}}{\partial x_i} \rangle = 2\rho(\psi) \frac{\epsilon}{k} \{ 8 \int f(\mathbf{V} + \mathbf{V}', \psi) f(\mathbf{V} - \mathbf{V}', \psi) d\mathbf{V}' - f(\mathbf{V}, \psi) \}. \quad (33)$$

The rate of dissipation  $\epsilon_{jk}$  of the Reynolds stresses  $\langle u_j u_k \rangle$  is generally assumed to be isotropic, i.e.,

$$\epsilon_{jk} = \frac{2}{3} \epsilon \delta_{jk}. \quad (34)$$

However, multiplication of equation (33) by  $V_j V_k$  and integrating yields,

$$\epsilon_{jk} = \epsilon \langle u_j u_k \rangle / k = \frac{2}{3} \epsilon \delta_{jk} + \frac{\epsilon}{k} (\langle u_j u_k \rangle - \frac{2}{3} k \delta_{jk}). \quad (35)$$

Thus Curl's model results in isotropic dissipation plus some redistribution. This observation is used below.

In addition to molecular viscosity, gravity and the pressure gradient transport  $f$  in  $\mathbf{V}$ -space. The buoyancy term (c) is in closed form and needs no further comment. The pressure gradient term (b), on the other hand, is the major unknown in the equation. In order to examine the effects of the term, we note that it can be re-expressed as

$$\frac{\partial}{\partial V_j} \langle f' \frac{\partial p}{\partial x_j} \rangle = \underbrace{\frac{\partial f}{\partial V_j} \frac{\partial \langle p \rangle}{\partial x_j}}_{(bi)} + \underbrace{\frac{\partial^2}{\partial x_j \partial V_j} \langle f' p' \rangle}_{(bii)} + \frac{1}{2} \underbrace{\frac{\partial^2}{\partial V_j \partial V_k} \langle f' p' (\frac{\partial U_k}{\partial x_j} + \frac{\partial U_j}{\partial x_k}) \rangle}_{(biii)}, \quad (36)$$

where  $p'$  is the fluctuating pressure,

$$p' = p - \langle p \rangle. \quad (37)$$

The first two terms, having derivatives in both physical and velocity spaces, represent transport of  $f$  in these spaces due to the mean and fluctuating pressure gradients.

Bray and Libby [15] have attributed the cause of counter-gradient diffusion to the mean pressure gradient affecting different density fluid differently. In this formulation the effect appears in closed form.

Term (bii) which represents the transport of  $f$  by the fluctuating pressure contains the unknown correlation  $\langle f' p' \rangle$ . An obvious model is

$$\langle f' p' \rangle = C_1 f(\vec{\psi}) v_i v_i - \langle \rho u_i u_i \rangle, \quad (38)$$

where

$$v_i = V_i - \langle U_i \rangle,$$

and

$$u_i = U_i - \langle U_i \rangle. \quad (39)$$

A value of  $C_1 = -1/5$  makes the model compatible with Lumley's model [17] for the pressure velocity correlation.

The final term in equation (36) contains the pressure-rate-of-strain  $p'(\partial U_k/\partial x_j + \partial U_j/\partial x_k)$  that is familiar to Reynolds-stress modellers. Because of the second derivative, the term does not affect the mean velocity. In constant-density flow (where  $\partial U_i/\partial x_i$  is zero), the term also leaves the turbulent kinetic energy unaffected. It serves therefore to redistribute energy in velocity space. In Reynolds-stress closures, the term is usually [18] modelled in two parts: the first is a linear return to isotropy, and the second is the mean velocity gradient multiplied by a tensor function of the Reynolds stresses. For the pdf equation, there are equivalent models for both parts, which are discussed in detail elsewhere [19].

The linear return to isotropy is simulated directly in the Monte Carlo method by a random reorientation of energy in velocity space [19]. This, combined with the effect of Curl's model (equation (35)), produces the required amount of redistribution.

The second part, which we denote by  $\langle f' \partial p^{(2)}/\partial x_j \rangle$ , is modelled by

$$\langle f' \frac{\partial p^{(2)}}{\partial x_j} \rangle = -2\rho(\vec{\psi}) \frac{\partial \langle U_e \rangle}{\partial x_m} v_q C_{qmej} f, \quad (40)$$

where the fourth-order tensor  $C$  is a function of the Reynolds stresses. This tensor can be chosen to be compatible with any of the current Reynolds-stress models [19].

### 3. Conclusion

Monte Carlo calculations of the transport equation for the pdf of scalars have been shown to be in good agreement with measurements in an inert mixing layer and in a premixed turbulent flame. However, in order to avoid the gradient diffusion assumption in the scalar pdf equation, the equation for the joint pdf of velocity and scalar  $f(\mathbf{V}, \vec{\psi}; \mathbf{x}, t)$  has been considered. Each term in the equation represents transport of  $f$  in  $\mathbf{x}$ ,  $\mathbf{V}$  or  $\vec{\psi}$  space. The terms representing convection, the effect of gravity, the mean pressure gradient and reaction appear in closed form.

In order to close the joint pdf equation, models are required for the terms involving the fluctuating pressure and viscous and diffusive mixing. Such models have been provided. The models pertaining to the fluctuating pressure and viscous mixing are compatible with current Reynolds-stress models. Consequently, the Reynolds stresses calculated by the joint pdf equation can be expected to be more accurate than those calculated by a Reynolds-stress model, since Reynolds-stress closures require additional models for the triple correlations. As far as the scalar field is concerned, reaction and convection (by both mean and fluctuating velocities) appear in closed form – only diffusive mixing requires modelling. Curl's coalescence/dispersal model is suggested. The Monte Carlo method can be used to solve the joint pdf equation for inhomogeneous flows with complex reactions.

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## Discussion

Professor Dwyer: There are many problems where this type of approach will be very successful, but there are also some problems with statistical techniques. Let me make an analogy. There is no question that the Boltzmann equation describes propagation of the pdf for molecules. Now, there is the Knudsen-number, which is the ratio of the characteristic distance of molecules to the scales. The Boltzmann equation is very useful as long as the Knudsen number is low. When the Knudsen number becomes high, it means that the pdf is determined more by what is happening by the initial condition than by what is happening by the boundaries. So the phenomenon inside the region you are solving is not so important. It is clear to me that in certain turbulent flows where some of the eddies might be determined by initial conditions or the eddies are being determined by the shape of the boundaries, in this situation you don't want to take a statistical approach. It may not be that valuable. You may want to take a more causal approach. I am not saying that there are a lot of problems with history of the initial conditions and the boundary conditions. It might not be dominant. You will be able to calculate the pdf from phenomena inside the region, but there is this other region important too.

Professor Pope: I guess your comment is that there are flows in which boundary conditions (other than those that you can impose on the statistical quantities you have) are going to influence the flow. Of course, you are right.

Professor Dwyer: What I am saying is the shape of the boundaries and the quality of the flow in the initial conditions have a long history and unless you know exactly, you have a very difficult time calculating the flow.

Professor Pope: The basic idea of a statistical approach is, as far as I see it, to get rid of information. We have all the information we need in the conservation equations, but it is too much for us to handle. So the idea of the statistical approach is to throw away this information. Now, that being the case, you don't have a full description of the flow. There will always be flows that you can't calculate. However, I think that considering the joint pdf of velocity and scalars is considering by orders of magnitude more than other statistical approaches are considering. That is why the applicability of this equation would be greater than any other.

Professor Dwyer: The point of my discussion is, can we find some sort of parameter like the Knudsen number for turbulent flows? Somehow, to define what type of initial conditions and boundary conditions will take a long time to lose their history.

Professor Pope: People have tried that, I tried to work out conditions under which a given model will work. The conditions are always fairly vague. For example, one can work out an effective diffusivity from measurements across the mixing layer with coherent structures and it seems to be constant. Whereas any argument based on mixing length theories, where the Knudsen number comes in, obviously cannot be justified. Still, the model seems to work.

Professor Elghobashi: Do you think that by removing the need of the  $k-\epsilon$  model you still have to model the decay rate of  $f$ ? How would you model the dissipation rate?

Professor Pope: The equation contains no scale information, you must have a separate means of providing that.

Professor Elghobashi: To me, in the  $k-\epsilon$  model or in the Reynolds-stress model, the weakest point is the  $\epsilon$ -equation.

Professor Pope: No, I think there are several weak points. For example, in the  $k-\epsilon$  model, you are assuming an isotropic viscosity.

Professor Elghobashi: Yes, but with the Reynolds-stress you will eliminate this difficulty. But still the weakest point is the  $\epsilon$ -equation.

Professor Pope: It depends on what you are dealing with. If you are dealing with an equilibrium flow, like a free shear layer, then it is really not a problem.

Professor Elghobashi: To me, that still needs a lot of work, just  $\epsilon$  by itself. What about the economy of the Monte Carlo method? You show the solution of the ID-flow.

Professor Pope: The machine I use is a VAX 11/780 which is about one tenth as fast as a CDC 7600. To perform one of the calculations of the premixed flame with three species, one spatial dimension and time, it took  $2\frac{1}{2}$  minutes at a cost of \$5.00.

Professor Elghobashi: How many grid points across?

Professor Pope: There were 20 grid points.

Professor Peters: If I remember right, in Batt's mixing layer the pdf's have intermittency spikes on both sides and a wide nearly Gaussian distribution in the middle. Can you show your calculation again? I remember the pdf's from Professor Bilger's paper. Maybe I am wrong, but I would extend the argument from Brown and Roshko's pdf. We know there that these are large structures. All the way across the mixing layer you have intermittency spikes on both sides and something in between. This doesn't appear to show up here. It seems it can't show up here because the physical mechanism is that the large structures bring those unmixed fuel pockets all the way across the mixing layer to the other side and into the center and both side to the middle. Since you have gradient transport, there is no mechanism to do that.

Professor Pope: If you look again at the calculated pdf's for Batt's mixing layer, you will see spikes at the extremes of the two end distributions. These, presumably, correspond to intermittency.

Professor Peters: But quantitatively Brown and Roshko's pdf's are very different. They have very high peak, on one side and way off on the other side they have something very well mixed. So actually, one could consider the fuel made of two parts, one with intermittency and another part being the turbulent part. It appears to me in general you took into account the turbulent part, but not the intermittent part.

Professor Pope: There are two possibilities. One is that Brown and Roshko's mixing layer and this one are different and the other possibility is that someone made a mistake. I performed the calculations with the boundary conditions appropriate to Batt's mixing layer. It appears that my calculations correspond fairly well with the experimental data. There is certainly the mechanism in the pdf equation to get two spikes. For Brown and Roshko's flow, I don't know whether I will get them or not. To find out, I would have to perform the calculations with the boundary conditions appropriate to that particular flow. You see, Batt's data is downstream in the mixing layer where the flow is fully developed, which may not be the case for Brown and Roshko's data.

Professor Peters: I would like to know where is this mechanism in your calculation which models the large transport across the layer which appears in the experimental data, and also appears in the vortex method where you have this transport.

Professor Pope: The pdf equation is a one-point equation. Therefore, there is no scale mentioned. If you measure a pdf, there is no scale, you don't know what is coming from a large structure or from a very fine structure. So I made no comment about the size of any structure or its coherence. I can't, it's a one-point closure. But it appears that, by disregarding any structure, the agreement is fairly good.

Professor Janicka: I have two questions. First, how do you handle the cross-correlation of the mixing term? You use the Curl model which is a very simple model for the description of this term. Do you neglect the cross correlation? If you have a two dimensional pdf, you get these derivatives in both directions.

Professor Pope: No, you don't neglect them. Curl's model is the only one which will work for any number of scalars.

Professor Janicka: It would be interesting to see the model for the multi-dimensional case for the description of the molecular mixing. Another question is: What about first-order reaction effects? You pointed out that you are able to describe the reaction rate very accurately. On the other hand, I have very little feeling about the molecular transport term. If I look at the equation for the second order moment, the molecular transport term is something like the dissipation rate. But if you have a strong reacting case, this dissipation rate is a function of the reaction rate again. Do you believe that this is an important effect? It is a first-order effect, not zero order effect.

Professor Pope: That is right. The point you make is: because we treat the term in which the reaction appears explicitly properly, doesn't mean we are treating reaction properly because it is implicitly in all the terms. Particularly, you mentioned the mixing term. I think you are right. I wouldn't want to try to justify that kind of modeling for the kind of flame Professor Williams was talking about. There, there is a very thin flame and then the details of the molecular processes are dominated by the reaction effects. I don't know what kind of combustion this kind of modeling is appropriate to. I think it is the kind in which the Kolmogorov scale is smaller than the laminar flame thickness. This is something that has been worrying me and I have been meaning to study more: under what combustion conditions, can you make the assumption that the details of molecular mixing do not really matter; that the macroscale determines the microscale and that the details do not matter. I don't know under what conditions this kind of assumption is valid. I certainly expect it to be valid for the CO-burnup and the NO production in the premixed flame.