Transport equation for the joint probability density function of velocity and scalars in turbulent flow

S. B. Pope

Mechanical Engineering Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 20 August 1980; accepted 21 January 1981)

The transport equation for the joint probability density function of velocity and scalars is shown to provide a good basis for modeling turbulent reactive flows. As in the equation for the probability density function of the scalars alone, nonlinear reaction schemes can be treated without approximation. The advantage of considering the joint probability density function equation is that convection (by both the mean and fluctuating velocities) appears in closed form. Consequently, the gradient-diffusion assumption for turbulent transport is avoided. 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 modeled transport equation for the joint probability density function can be solved by the Monte-Carlo method for inhomogeneous flows with complex reactions.

I. INTRODUCTION

Many models of turbulent reactive flow involve the probability density function of one or more scalars. For turbulent diffusion flames (where mixing is the rate-controlling process), the instantaneous fluid composition can be determined from the mixture fraction $f(\mathbf{x}, t)$. Consequently, mean properties can be determined from $p(\hat{f}; \mathbf{x}, t)$, the probability density function of f[1]; if $Q(f)$ is any function of f, its mean $\langle Q(f)\rangle$ is given by

$$\langle Q(f)\rangle = \int p(\hat{f})Q(\hat{f})d\hat{f}. \tag{1}$$

Similarly for an idealized premixed turbulent flame, all mean properties can be determined from $p(\hat{c}; \mathbf{x}, t)$, the probability density function of the progress variable $c(\mathbf{x}, t)$[2]. In general,[3] the instantaneous composition of a reacting mixture of gases can be determined from the set of σ scalars comprising mass fractions and enthalpy $\boldsymbol{\phi}(\mathbf{x}, t) = \phi_1, \phi_2 \cdots \phi_\sigma$. With $\psi = \psi_1, \psi_2 \cdots \psi_\sigma$ being the composition space corresponding to $\boldsymbol{\phi}$, the mean of any quantity $\langle Q(\boldsymbol{\phi})\rangle$ can be determined from the joint probability density function $p(\boldsymbol{\psi}; \mathbf{x}, t)$ by

$$\langle Q(\boldsymbol{\phi})\rangle = \int p(\psi)Q(\psi)d\psi\ . \tag{2}$$

This fundamental property of probability density functions [Eq. (2)] is useful in modeling reactive flows since it provides a way of determining the means of highly nonlinear quantities, specifically, reaction rates. Before Eq. (2) can be used, however, the probability density function must be determined. The most common approach,[2-6] is to assume a parametric form for the probability density function in terms of its first and second moments, for which modeled transport equations are solved. Recently, several workers[7-9] have used the direct approach of modeling and solving a transport equation for the probability density function itself. In the probability density function transport equation, models of turbulent mixing and transport are required, but the effects of reaction appear in closed form, however complicated the reaction scheme.

The direct approach of solving a modeled transport equation for the joint probability density function was restricted to simple cases because, by finite-difference means, the equation is difficult to solve. This is mainly because the dimensionality of $p(\psi_1, \psi_2 \cdots \psi_\sigma; \mathbf{x}, t)$ can be large. However, a Monte-Carlo method has been devised[10] to solve the joint probability density function equation for the general case. The method has been used[11] to calculate the joint probability density function of three species (C_3H_8, CO, and NO) in a premixed propane/air flame. An essential feature of the Monte-Carlo method is that, at any location, the joint probability density function is represented by an ensemble Φ composed of N elements: the nth element has properties $\boldsymbol{\phi}^{(n)} = \phi_1^{(n)}, \phi_2^{(n)} \cdots \phi_\sigma^{(n)}$. The ensemble average of an arbitrary function $Q(\boldsymbol{\phi})$ is defined by

$$\hat{Q}(\boldsymbol{\phi}) = \frac{1}{N}\sum_{n=1}^{N} Q(\boldsymbol{\phi}^{(n)})\ . \tag{3}$$

The Monte-Carlo method provides a true simulation of the probability density function equation since, as N tends to infinity, the ensemble average converges to the mean; that is,

$$\lim_{N\to\infty}\hat{Q}(\boldsymbol{\phi}) = \langle Q(\boldsymbol{\phi})\rangle\ . \tag{4}$$

The great advantage of basing a closure scheme on the transport equation for $p(\boldsymbol{\psi}; \mathbf{x}, t)$ is that nonlinear reactions can be handled without approximation. 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 $k-\epsilon$ model[12]) is needed to determine the velocity and turbulence fields. In the present paper, the probability approach is extended to the joint probability density function equation of the velocity $\mathbf{U} = U_1, U_2, U_3$ and the scalars $\boldsymbol{\phi}$. This equation, which can be solved by the Monte-Carlo method, does not suffer from the weaknesses of the equation for $p(\boldsymbol{\psi}; \mathbf{x}, t)$.

 0031-9171/81/040588-09$00.90

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

In the next section, the transport equation for $f(\mathbf{V}, \psi; \mathbf{x}, t)$ is derived for a general turbulent reactive flow. This equation is examined to determine the effect that each term has on $f(\mathbf{V}, \boldsymbol{\psi})$. In the following section, the equation is considered in more detail for constant-density flows, and a model is provided for each of the unclosed terms. The modeling can be expected to be reliable since it is compatible with accurate and proven Reynolds-stress closures.

Previous work on modeling the equation for $p(\boldsymbol{\psi}; \mathbf{x}, t)$ has already been mentioned.[7-9] Lundgren[13] has considered the transport equation for the probability density function of velocity $f(\mathbf{V}; \mathbf{x}, t)$ and proposed simple relaxation models for the unclosed terms. Ievlev[14] derived a general transport equation for the n-point joint probability density function of velocity and enthalpy. A closure was proposed in which the $n+1$ point distribution is approximated in terms of n point distributions. The present modeling (which exploits recent advances in Reynolds-stress closures) can be expected to be more accurate than relaxation modeling and is more tractable than Ievlev's closure.

II. THE JOINT PROBABILITY DENSITY FUNCTION EQUATION

At any point in a turbulent reactive mixture of gases, the state of the fluid can be characterized 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 $\boldsymbol{\phi} = \phi_1, \phi_2 \cdots \phi_\sigma$ as

$$\phi_\alpha = m_\alpha \ , \quad \alpha = 1, 2 \cdots \sigma - 1 , \tag{5}$$

$$\phi_\sigma = h . \tag{6}$$

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

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho U_i) = 0 , \tag{7}$$

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial p}{\partial x_j} + \rho g_j , \tag{8}$$

and

$$\frac{\partial}{\partial t}(\rho \phi_\alpha) + \frac{\partial}{\partial x_i}(\rho U_i \phi_\alpha) = -\frac{\partial J_i^\alpha}{\partial x_i} + \rho S_\alpha , \tag{9}$$

where $\mathbf{g}$ is the gravitational acceleration, τ_{ij} is the viscous stress tensor, and $\mathbf{J}^\alpha$ 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 $\boldsymbol{\phi}$,

$$\rho = \rho(\boldsymbol{\phi}), \ S_\alpha = S_\alpha(\boldsymbol{\phi}) . \tag{10}$$

The dependence of the density on pressure fluctuations has been removed by virtue of the assumption of low Mach number.

The joint probability density function of the velocities and scalars is defined in terms of Dirac delta functions by

$$f(\mathbf{V}, \psi; \mathbf{x}, t) \equiv \langle f'(\mathbf{V}, \psi; \mathbf{x}, t) \rangle , \tag{11}$$

where the angular brackets indicate an ensemble mean and

$$f'(\mathbf{V}, \psi; \mathbf{x}, t) \equiv \prod_{j=1}^{3} \delta(U_j(\mathbf{x}, t) - V_j) \times \prod_{\alpha=1}^{\sigma} \delta(\phi_\alpha(\mathbf{x}, t) - \psi_\alpha) . \tag{12}$$

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

$$d\mathbf{V} = dV_1 dV_2 dV_3 , \tag{13}$$

and

$$d\boldsymbol{\psi} = d\psi_1 d\psi_2 \cdots d\psi_\sigma . \tag{14}$$

From these definitions, the following basic properties of the joint probability density function can be deduced:

$$f(\mathbf{V}) = \int f(\mathbf{V}, \boldsymbol{\psi}) d\boldsymbol{\psi} , \tag{15}$$

$$f(\boldsymbol{\psi}) = \int f(\mathbf{V}, \boldsymbol{\psi}) d\mathbf{V} , \tag{16}$$

$$1 = \int\int f(\mathbf{V}, \boldsymbol{\psi}) d\mathbf{V}\, d\boldsymbol{\psi} , \tag{17}$$

and for any function $Q(\mathbf{U}, \boldsymbol{\phi})$,

$$\langle Q(\mathbf{U}, \boldsymbol{\phi}) \rangle = \int\int f(\mathbf{V}, \boldsymbol{\psi}) Q(\mathbf{V}, \boldsymbol{\psi}) d\mathbf{V}\, d\boldsymbol{\psi} . \tag{18}$$

$f(\mathbf{V})$ and $f(\boldsymbol{\psi})$ are the separate probability density functions of velocity and scalars, and the integrations are performed over the whole of the spaces.

The transport equation for $f(\mathbf{V}, \boldsymbol{\psi})$ is obtained from the definition of f and from the transport equations for $\mathbf{U}$ and $\boldsymbol{\phi}$. Differentiating Eq. (12), we obtain

$$\frac{\partial f'}{\partial t} = -\frac{\partial f'}{\partial V_j}\frac{\partial U_j}{\partial t} - \frac{\partial f'}{\partial \psi_\alpha}\frac{\partial \phi_\alpha}{\partial t} , \tag{19}$$

where summation is implied over repeated suffices (j and α). With a similar expression for the spatial derivative, substituting for $\partial U_j / \partial t$ and $\partial \phi_\alpha / \partial t$ from Eqs. (8) and (9) and averaging, we obtain the equation for f:

$$\rho(\psi)\left(\frac{\partial}{\partial t}+V_i\frac{\partial}{\partial x_i}\right)f$$
$$=\frac{\partial}{\partial V_j}\left(\left\langle f'\frac{\partial p}{\partial x_j}\right\rangle-f\rho(\psi)g_j+\left\langle f'\frac{\partial \tau_{ij}}{\partial x_i}\right\rangle\right)$$
$$+\frac{\partial}{\partial \psi_\alpha}\left(-f\rho(\psi)S_\alpha+\left\langle f'\frac{\partial J_i^\alpha}{\partial x_i}\right\rangle\right). \tag{20}$$

Before examining Eq. (20) term by term, several general comments can be made. First, it should be remembered that f is a function of the independent variables $\mathbf{V}, \psi, \mathbf{x}$, and t: thus, $\rho(\psi)$ is the local density; local, that is, in ψ space. Similarly, $\mathbf{V}$ is the local velocity in $\mathbf{V}$ space. The derivative with respect to V_j of the first terms on the right-hand side of Eq. (20) indicates that the terms represent transport of f in $\mathbf{V}$ space; the terms disappear when the equation is integrated over the whole of $\mathbf{V}$ space to form the equation for $f(\psi)$. Similarly, because of the derivative with respect to ψ_α, the last terms represent transport of f in ψ space. It will be seen that some of these terms represent transport in more than one space. Before Eq. (20) can be solved, the three terms involving correlations with f' need to be modeled. Each of these terms can be re-expressed as a conditionally expected value; for example,

$$\left\langle f'\frac{\partial p}{\partial x_j}\right\rangle=fE\left(\frac{\partial p}{\partial x_j}\middle|\mathbf{U}=\mathbf{V},\phi=\psi\right). \tag{21}$$

The first term in Eq. (20) is the local density times the rate of change of f along a local particle path; that is,

$$\left(\frac{\partial}{\partial t}+V_i\frac{\partial}{\partial x_i}\right)f(\mathbf{V},\psi;\mathbf{x},t)=\frac{\partial}{\partial t}f[\mathbf{V},\psi;\mathbf{y}(t),t]\ , \tag{22}$$

where

$$\frac{d\mathbf{y}}{dt}=\mathbf{V}. \tag{23}$$

This term accounts for convection by both the mean and fluctuating velocities. In moment formulations, convection by the fluctuating velocity appears an an unknown correlation that is usually modeled 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 probability density function 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 $f(\mathbf{V},\psi)$ rather than $f(\psi)$.

The usefulness of the equation for $f(\psi)$ 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 $f(\mathbf{V},\psi)$: the term containing S_α in Eq. (20) shows that the effect of reaction (which appears in closed form) is to transport f in composition space.

The final term in Eq. (20) 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 ϕ, we assume simple gradient diffusion

$$J_i=-\Gamma\frac{\partial\phi}{\partial x_i}\ , \tag{24}$$

where Γ is the diffusive coefficient. Then, the term can be decomposed as

$$\frac{\partial}{\partial\psi}\left\langle f'\frac{\partial J_i}{\partial x_i}\right\rangle=\frac{\partial}{\partial x_i}\Gamma\frac{\partial f}{\partial x_i}-\frac{\partial^2}{\partial\psi^2}\left\langle f'\Gamma\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_i}\right\rangle. \tag{25}$$

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[8] 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 (the term containing τ_{ij}) 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. The effects of diffusion and viscosity are discussed further in the next section where models for the processes are presented.

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

$$\frac{\partial}{\partial V_j}\left\langle f'\frac{\partial p}{\partial x_j}\right\rangle=\frac{\partial f}{\partial V_j}\frac{\partial\langle p\rangle}{\partial x_j}+\frac{\partial^2}{\partial x_j\partial V_j}\langle f'p'\rangle$$
$$+\frac{1}{2}\frac{\partial^2}{\partial V_j\partial V_k}\left\langle f'p'\left(\frac{\partial U_k}{\partial x_j}+\frac{\partial U_j}{\partial x_k}\right)\right\rangle, \tag{26}$$

where p' is the fluctuating pressure

$$p'=p-\langle p\rangle\ . \tag{27}$$

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. Libby and Bray[15] have attributed the cause of counter-gradient diffusion to the mean pressure gradient affecting different density fluids differently. In this formulation the effect appears in closed form. Transport of f due to the fluctuating pressure gradient is discussed in the next section where a model for the correlation $\langle f'p'\rangle$ is provided.

The final term 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 modelers. 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. Again, the

term is discussed at length in the next section where a model is provided.

In summary, a transport equation for $f(\mathbf{V}, \psi; \mathbf{x}, t)$ has been derived, Eq. (20). Each term in the equation represents transport of f in $\mathbf{x}$, $\mathbf{V}$, or ψ space. The terms representing convection, the effect of gravity, the mean pressure gradient and reaction appear in closed form. In the next section, models are provided for the unclosed terms which account for the fluctuating pressure gradient and for molecular viscosity and diffusivity.

III. MODELING

The joint probability density function equation for a constant-property flow is considered in more detail in this section and models for the unknown terms are provided. The constant density is set to unity ($\rho = 1$) and Newtonian viscosity and Fickian diffusion are assumed:

$$\tau_{ij} = -\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right), \tag{28}$$

$$J_i^\alpha = -\Gamma \frac{\partial \phi_\alpha}{\partial x_i}, \tag{29}$$

where μ and Γ are the viscosity and diffusivity. Since there is no buoyancy effect in constant-density flow, gravity is ignored ($\mathbf{g} = 0$).

It is convenient to decompose the velocity into its mean and fluctuating components

$$\mathbf{U} = \langle \mathbf{U} \rangle + \mathbf{u}, \tag{30}$$

and to consider the joint probability density function of $\mathbf{u}$ and ϕ, $g(\mathbf{v}, \psi; \mathbf{x}, t)$. This joint probability density function is defined by

$$g(\mathbf{v}, \psi; \mathbf{x}, t) \equiv \langle g'(\mathbf{v}, \psi; \mathbf{x}, t) \rangle, \tag{31}$$

where

$$g'(\mathbf{v}, \psi; \mathbf{x}, t) \equiv \prod_{j=1}^{3} \delta[u_j(\mathbf{x}, t) - v_j] \times \prod_{\alpha=1}^{\sigma} \delta[\phi_\alpha(\mathbf{x}, t) - \psi_\alpha]. \tag{32}$$

The joint probability density functions $f(\mathbf{V}, \psi; \mathbf{x}, t)$ and $g(\mathbf{v}, \psi; \mathbf{x}, t)$ are simply related by

$$\mathbf{v} = \mathbf{V} - \langle \mathbf{U} \rangle. \tag{33}$$

There are three reasons for preferring to model the equation for g: correlations such as $\langle g'(\mathbf{v}, \psi; \mathbf{x}, t) u_i(\mathbf{x} + \mathbf{r}, t) \rangle$ tend to zero as $\mathbf{r}$ tends to infinity; g is invariant under Gallilean transformations; and Reynolds stresses and scalar fluxes are readily obtained from g by

$$\langle u_i u_j \rangle = \int\int g(\mathbf{v}, \psi; \mathbf{x}, t) v_i v_j \, d\mathbf{v} \, d\psi, \tag{34}$$

and

$$\langle u_i \phi_\alpha \rangle = \int\int g(\mathbf{v}, \psi; \mathbf{x}, t) v_i \psi_\alpha \, d\mathbf{v} \, d\psi. \tag{35}$$

After a modeled equation for $g(\mathbf{v}, \psi; \mathbf{x}, t)$ has been obtained, the equivalent equation for $f(\mathbf{V}, \psi; \mathbf{x}, t)$ can readily be recovered.

A transport equation for g can be obtained either by transforming the equation for f or directly from the equations for $\mathbf{u}$ and ϕ. In either case, the result is

$$\left(\frac{\partial}{\partial t} + \langle U_i \rangle \frac{\partial}{\partial x_i}\right) g + v_i \frac{\partial g}{\partial x_i} = \frac{\partial g}{\partial v_j}\left(v_i \frac{\partial}{\partial x_i}\langle U_j \rangle - \frac{\partial}{\partial x_i}\langle u_i u_j \rangle\right) + \frac{\partial^2}{\partial x_j \partial v_j}\langle g' p' \rangle + \frac{\partial^2}{\partial v_j \partial v_k}\left\langle g' p' \frac{\partial u_k}{\partial x_j}\right\rangle + \frac{\partial}{\partial v_j}\left\langle g' \frac{\partial \tau'_{ij}}{\partial x_i}\right\rangle - \frac{\partial}{\partial \psi_\alpha}[g S_\alpha(\psi)] + \frac{\partial}{\partial \psi_\alpha}\left\langle g' \frac{\partial J_i^\alpha}{\partial x_i}\right\rangle. \tag{36}$$

The main difference between this equation for g and that for f [Eq. (20)] is the inclusion of the first term on the right-hand side which represents transport of g in $\mathbf{v}$ space due to mean-velocity and Reynolds-stress gradients. The terms on the left-hand side taken together represent the rate of change of g along a local particle path; or, taken separately, they represent the rate of change of g along a mean streamline, and transport in $\mathbf{x}$ space by velocity fluctuations. The four terms containing correlations with g' require modeling.

The transport equation for the Reynolds-stresses $\langle u_j u_k \rangle$ can be obtained by multiplying Eq. (36) by $v_j v_k$ and integrating over $\mathbf{v}$ and ψ:

$$\left(\frac{\partial}{\partial t} + \langle U_i \rangle \frac{\partial}{\partial x_i}\right)\langle u_j u_k \rangle + \frac{\partial}{\partial x_i}\langle u_i u_j u_k \rangle = -\langle u_i u_j \rangle \frac{\partial}{\partial x_i}\langle U_k \rangle - \langle u_i u_k \rangle \frac{\partial}{\partial x_i}\langle U_j \rangle - \frac{\partial}{\partial x_i}\langle p'(u_j \delta_{ik} + u_k \delta_{ij}) \rangle + \left\langle p'\left(\frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j}\right)\right\rangle - 2\mu\left\langle \frac{\partial u_j}{\partial x_i}\frac{\partial u_k}{\partial x_i}\right\rangle + \frac{\partial}{\partial x_i}\mu\frac{\partial}{\partial x_i}\langle u_j u_k \rangle. \tag{37}$$

Since this equation has been studied extensively and models for the unknown terms are available,[17,18] it provides useful guidance in the modeling of the equation for g. Consequently, we give here a brief description of the terms in the equation and how they can be modeled, following for the most part, the work of Launder, Reece, and Rodi.[17]

The first term is the rate of change of $\langle u_j u_k \rangle$ along a mean streamline and the second represents transport by the triple correlations. In a Reynolds-stress closure, a model for the triple correlations is required but, in the probability density function equation, the corresponding term appears in closed form. Production of the Reynolds stresses by mean velocity gradients appears in closed form in both the Reynolds-stress and probability density function equations. The final term in the equation represents the transport of the Reynolds stresses by viscosity and is negligible at high Reynolds number.

In both the Reynolds-stress and probability density function equations, models for the remaining terms are required. The viscous dissipation is presumed to be isotropic

$$\epsilon_{jk}=2\mu\left\langle\frac{\partial u_j}{\partial x_i}\frac{\partial u_k}{\partial x_i}\right\rangle=\frac{2}{3}\epsilon\delta_{jk}, \tag{38}$$

where ϵ, the rate of dissipation of turbulent kinetic energy, is given by

$$\epsilon=\mu\left\langle\frac{\partial u_j}{\partial x_i}\frac{\partial u_j}{\partial x_i}\right\rangle. \tag{39}$$

Throughout, it is assumed that ϵ is known, either from the solution of another transport equation or from a length-scale specification.

The two remaining terms involve correlations with the fluctuating pressure p'. The divergence of the equation for u is

$$\nabla^2 p'=-2\frac{\partial u_j}{\partial x_i}\frac{\partial}{\partial x_j}\langle U_i\rangle-\frac{\partial^2 u_i u_j}{\partial x_i\partial x_j}, \tag{40}$$

which shows that there are two sources of pressure fluctuations; one due to the interaction of turbulence with the mean velocity gradients and the other solely due to turbulence. These two contributions to p' are denoted by $p^{(1)}$ and $p^{(2)}$, respectively. The pressure rate-of-strain correlation can therefore be considered in two parts. The first part $R_{jk}^{(1)}$ is generally modeled by

$$R_{jk}^{(1)}\equiv\left\langle p^{(1)}\left(\frac{\partial u_j}{\partial x_k}+\frac{\partial u_k}{\partial x_j}\right)\right\rangle=(A_{jklm}+A_{kjlm})k\frac{\partial}{\partial x_m}\langle U_l\rangle, \tag{41}$$

where k is the turbulent kinetic energy

$$k=1/2\langle u_i u_i\rangle, \tag{42}$$

and A is a nondimensional tensor function of the Reynolds stresses. There have been several suggestions for the tensor A.[17-19] The second part of the pressure rate-of-strain correlation $R_{jk}^{(2)}$ is usually modeled as a linear return to isotropy[20]

$$R_{jk}^{(2)}\equiv\left\langle p^{(2)}\left(\frac{\partial u_j}{\partial x_k}+\frac{\partial u_k}{\partial x_j}\right)\right\rangle=-C_2\frac{\epsilon}{k}\left(\langle u_j u_k\rangle-\frac{2}{3}k\delta_{jk}\right). \tag{43}$$

Launder *et al.* suggest a value of 1.5 for the constant C_2.

The remaining term represents transport due to the pressure-velocity correlation and is generally ignored. Lumley,[21] however, has suggested the following model to account for the correlation of u_j with $p^{(2)}$:

$$\langle p'u_j\rangle=C_1\langle u_j u_k u_k\rangle, \tag{44}$$

where the constant C_1 takes the value $-1/5$.

We now return to the transport equation for $g(\mathbf{v},\psi;\mathbf{x},t)$ and start by modeling the pressure transport term. The correlation $\langle g'p'\rangle$ can be re-expressed as an expected value

$$\langle g'p'\rangle=gE(p'|\mathbf{u}=\mathbf{v},\ \phi=\psi). \tag{45}$$

Since the density is constant, the scalar field $\phi(\mathbf{x},t)$ has no effect upon the velocity field and hence no effect upon the pressure field: thus,

$$E(p'|\mathbf{u}=\mathbf{v},\phi=\psi)=E(p'|\mathbf{u}=\mathbf{v}). \tag{46}$$

That p' is a scalar and that $\langle p'\rangle$ is zero requires that $E(p'|\mathbf{u}=\mathbf{v})$ be a scalar function in v space and that

$$\int gE(\mathbf{p}'|\mathbf{u}=\mathbf{v})d\mathbf{v}=0. \tag{47}$$

Subject to these conditions, the simplest possible model is

$$E(p'|\mathbf{u}=\mathbf{v})=C_1(v_i v_i-2k). \tag{48}$$

When Eq. (48) is multiplied by $v_j g$ and integrated to form a model for $\langle p'u_j\rangle$, Lumley's model [Eq. (44)] is obtained.

The pressure-velocity correlation $\langle p'u_j\rangle$ has not been measured directly nor are such measurements likely to be forthcoming. The correlation can be determined by difference from measurements of the remaining terms in the turbulent kinetic energy equation. By this method, which clearly makes high demands on experimental accuracy, Wygnanski and Fiedler[22,23] have determined $\langle p'u_j\rangle$ is a round jet and a plane mixing layer. For the round jet, the pressure transport generally augments the transport by the triple correlations suggesting a positive value of C_1. For the mixing layer, the converse is the case. This is clearly a subject for further investigation. But for the moment, we just note that a simple model for $E(p'|\mathbf{u}=\mathbf{v})$, Eq. (48), is consistent with Lumley's proposal for $\langle p'u_j\rangle$, Eq. (44),

Next, we consider the first part of the redistributive term

$$Q^{(1)}(\mathbf{v};\mathbf{x},t)\equiv\frac{\partial^2}{\partial v_j\partial v_k}\left\langle g'p^{(1)}\frac{\partial u_k}{\partial x_j}\right\rangle, \tag{49}$$

where the dependence upon ψ has been removed by arguments similar to those used here. We now develop a model for $Q^{(1)}$ for the case of homogeneous turbulence, expecting that this contains the major contribution even in the inhomogeneous case. For the homogeneous case, $Q^{(1)}$ can be re-expressed as

$$Q^{(1)}(\mathbf{v};\mathbf{x},t)=\frac{\partial}{\partial v_j}\left\langle g'\frac{\partial p^{(1)}}{\partial x_j}\right\rangle, \tag{50}$$

and from Eq. (40),

$$\nabla^2\frac{\partial p^{(1)}}{\partial x_j}=-2\frac{\partial^2 u_m}{\partial x_i\partial x_j}\frac{\partial\langle U_i\rangle}{\partial x_m}. \tag{51}$$

Thus, $Q^{(1)}$ can be determined from $\langle g'(\partial p^{(1)}/\partial x_j)\rangle$, which can be expressed as

$$\left\langle g'\frac{\partial p^{(1)}}{\partial x_j}\right\rangle=-2\frac{\partial\langle U_l\rangle}{\partial x_m}gB_{mlj}, \tag{52}$$

where

$$gB_{mlj}(\mathbf{v};\mathbf{x},t)=\left\langle g'\nabla^{-2}\frac{\partial^2 u_m}{\partial x_i\partial x_j}\right\rangle, \tag{53}$$

and ∇^{-2} is the inverse of the Laplacian. Alternatively, by using Green's theorem, we can express B in terms of the conditionally expected value of $\mathbf{u}(\mathbf{x}+\mathbf{r})$

$$B_{mlj}(\mathbf{v};\mathbf{x},t)=\frac{1}{4\pi}\int\frac{\partial^2}{\partial r_i\partial r_j}\times E(u_m(\mathbf{x}+\mathbf{r})|\mathbf{u}(\mathbf{x})=\mathbf{v})|\mathbf{r}|^{-1}d\mathbf{r}. \tag{54}$$

Since B has dimensions of velocity, it can be expected to be independent of the length scale of turbulence. This

expectation is confirmed by Eq. (54) from which it can be shown that B is unchanged by an arbitrary normalization of the separation vector r. This being the case, it appears reasonable to model B as a function of v and the Reynolds-stress tensor. It is expedient to assume further that B is a linear function of v, since this leads to a model that is compatible with Reynolds-stress closures. Some support for these assumptions is provided by the observation that setting $l=j$ in Eq. (53) yields

$$B_{mll}=v_m. \tag{55}$$

The general form of the proposed model is

$$B_{mij}=v_q C_{qmij}. \tag{56}$$

The nondimensional tensor C (which may be a function of the Reynolds stresses) can be determined from the tensor A that appears in the modeling of the pressure rate-of-strain correlation, Eq. (41). That modeling gives

$$\left\langle p^{(1)}\frac{\partial u_k}{\partial x_j}\right\rangle=\frac{\partial\langle U_l\rangle}{\partial x_m}\,kA_{jklm}, \tag{57}$$

while, in terms of C, Eqs. (52) and (56) give

$$\left\langle p^{(1)}\frac{\partial u_k}{\partial x_j}\right\rangle=2\,\frac{\partial\langle U_l\rangle}{\partial x_m}\langle u_k u_q\rangle\langle C_{qmij}\rangle. \tag{58}$$

A comparison of these two equations shows that C and A are related by

$$A_{jklm}=(2/k)\langle u_k u_q\rangle C_{qmij}, \tag{59}$$

or

$$C_{qmij}=1/2k\langle u_k u_q\rangle^{-1}A_{jklm}. \tag{60}$$

Thus, for a given pressure rate-of-strain model (given A) there is an equivalent model for C and hence $Q^{(1)}$ can be deduced.

Launder *et al.* give a model for A which can be written in terms of the normalized Reynolds-stress tensor

$$b_{ij}=\langle u_i u_j\rangle/\langle u_l u_l\rangle-1/3\delta_{ij},$$

and a single constant C_3 for which the value 0.4 is suggested. After much algebra, the corresponding tensor C is found to be

$$\begin{aligned}C_{qmij}=&(2/5+6\beta\gamma)\delta_{qm}\delta_{ij}-(1/10+9\alpha\gamma)\\&\times(\delta_{qi}\delta_{mj}+\delta_{qj}\delta_{im})+[1/5-12\alpha\nu\\&+(6\nu+2/3)\beta]b_{qm}\delta_{ij}-\alpha(b_{qi}\delta_{mj}+b_{qj}\delta_{im})\\&+[1/10-9\gamma(9\alpha+\beta)-33\alpha\nu]\delta_{qm}b_{ij}\\&+[-3/10+9\alpha\nu-27\gamma(\alpha-\beta)](\delta_{qi}b_{mj}+\delta_{qj}b_{im})\\&-(9\alpha+\beta)b_{qm}b_{ij}+3(\beta-\alpha)(b_{qi}b_{mj}+b_{qj}b_{im})\\&-2\beta b^2_{qm}\delta_{ij}+3\alpha(b^2_{qi}\delta_{mj}+b^2_{qj}\delta_{im})\\&+(27\alpha+3\beta)b^2_{qm}b_{ij}+9(\alpha-\beta)(b^2_{qi}b_{mj}+b^2_{qj}b_{im}),\end{aligned} \tag{61}$$

where

$$\alpha=(1-15C_3)/(330\nu), \tag{62}$$

$$\beta=-(3+10C_3)/(110\nu), \tag{63}$$

$$\gamma=1/3b^3_{ii}, \tag{64}$$

and

$$\nu=1/2b^2_{ii}-3\gamma-1/9. \tag{65}$$

Although C can be deduced from a model of A, there are two reasons to prefer modeling C directly. First, a simpler expression than Eqs. (61)–(65) is likely to result. Second, and more important, Eq. (59) shows that A can always be determined from C, but Eq. (60) shows that C can be determined from A only when the inverse of the Reynolds-stress tensor exists. Physically, the Reynolds-stress tensor becomes singular when the turbulence becomes two-dimensional. Then, it is known[21] that current models for A do not guarantee realizability; that is, they do not guarantee that the normal stresses remain non-negative. In the model by Launder *et al.*, as the turbulence becomes two-dimensional, ν [Eq. (65)] tends to zero, and so α and β [Eqs. (62) and (63)] tend to infinity. The model for C then becomes infinite.

The direct modeling of C is left to a future study. We note, however, that from such a model, the corresponding tensor A can be determined [from Eq. (59)], which leads to a pressure rate-of-strain model that guarantees realizability.

Whether the tensor C is obtained from Eqs. (61)–(65) or by other means, the model for $Q^{(1)}$ is

$$Q^{(1)}(\mathbf{v};\mathbf{x},t)=-2C_{qmij}\,\frac{\partial\langle U_l\rangle}{\partial x_m}\,\frac{\partial}{\partial v_j}(gv_q). \tag{66}$$

The second part of the redistribution term is

$$Q^{(2)}(\mathbf{v};\mathbf{x},t)=\frac{\partial^2}{\partial v_j\partial v_k}\left\langle g'p^{(2)}\frac{\partial u_k}{\partial x_j}\right\rangle. \tag{67}$$

A model for this term has been constructed which is best understood in terms of the Monte-Carlo method used to solve the joint probability density function equation. The simulation corresponds to a random reorientation of $g(\mathbf{v},\psi;\mathbf{x},t)$ in v space. In the Monte-Carlo method, at given $(\mathbf{x},t)$, the joint probability density function $g(\mathbf{v},\boldsymbol{\psi})$ is represented by an ensemble of N elements the nth of which has velocity and composition $\mathbf{u}^{(n)},\boldsymbol{\phi}^{(n)}$. The simulation of $Q^{(2)}$ is as follows; at a rate $C_2N\epsilon/k$, pairs of elements (denoted by n and m) are selected at random from the ensemble. The velocities of the two elements are then replaced with the values

$$\mathbf{u}^{(n)}=\mathbf{v}^*(\mathbf{u}_0^{(n)},\mathbf{u}_0^{(m)},\xi), \tag{68}$$

and

$$\mathbf{u}^{(m)}=\mathbf{v}^*(\mathbf{u}_0^{(n)},\mathbf{u}_0^{(m)},-\xi), \tag{69}$$

where

$$\begin{aligned}\mathbf{v}^*(\mathbf{u}^{(n)},\mathbf{u}^{(m)},\xi)=&1/2(\mathbf{u}^{(n)}+\mathbf{u}^{(m)})\\&+1/2\,\xi\,|\mathbf{u}^{(n)}-\mathbf{u}^{(m)}|,\end{aligned} \tag{70}$$

$\mathbf{u}_0^{(n)}$ is the initial value of $\mathbf{u}^{(n)}$, and ξ is a random vector of unit length, uniformly distributed on the unit sphere. (The same value of ξ is used for both elements of the pair, but different values are used for different pairs.) This transformation of $\mathbf{u}_0^{(n)},\mathbf{u}_0^{(m)}$ to $\mathbf{u}^{(n)},\mathbf{u}^{(m)}$ corresponds to a random rotation of the elements in v space around

their mean position. Since neither their mean position nor their separation is altered, the transformation conserves both energy and momentum; the effect of the random reorientation is to decrease the anisotropy.

An analysis of this simulation shows that, as N tends to infinity, the corresponding model for $Q^{(2)}$ is

$$Q^{(2)}(\mathbf{v},\psi;\mathbf{x},t) = 2C_2\frac{\epsilon}{k}\left(\int\int g(\mathbf{v}',\psi)\int g(\mathbf{v}'',\psi'')d\psi'' \times\frac{1}{4\pi}\int_S \delta[\mathbf{v}-\mathbf{v}^*(\mathbf{v}',\mathbf{v}'',\boldsymbol{\zeta})]\,d\boldsymbol{\zeta}\,d\mathbf{v}'\,d\mathbf{v}'' - g(\mathbf{v},\psi)\right), \quad (71)$$

where $\int_S d\boldsymbol{\zeta}$ represents the integration over the surface of the unit sphere. This expression is not as intractable as it appears; and, by multiplying by $v_j v_k$ and integrating, the corresponding pressure rate-of-strain model can be determined. The result is

$$R_{jk}^{(2)} = -C_2(\epsilon/k)(\langle u_j u_k\rangle - 2/3k\delta_{jk}), \quad (72)$$

which is just the same linear return to isotropy as Rotta's model, Eq. (43). In addition, computer experiments show that the simulated probability density function tends, correctly, to a Gaussian.

In the viscous mixing term of Eq. (36), the correlation can be re-expressed as the expected value

$$\left\langle g'\frac{\partial\tau_{ij}'}{\partial x_i}\right\rangle = gE\left(\frac{\partial\tau_{ij}'}{\partial x_i}\middle|\mathbf{u}=\mathbf{v},\ \phi=\psi\right) = gE\left(\frac{\partial\tau_{ij}'}{\partial x_i}\middle|\mathbf{u}=\mathbf{v}\right). \quad (73)$$

Again, the dependence upon ψ can be removed because the velocity field is independent of the scalar field. At present, there is no completely satisfactory model for this term. In spite of its known imperfections,[24,3] Curl's model[25] is most likely the best available and is certainly the simplest. His model, also known as the coalescence/dispersal model, is best described in terms of the ensemble representation of the probability density function. At location $\mathbf{x}$, pairs of elements (denoted by n and m) are selected at random from the ensemble at a rate $N\epsilon/k$. With the same notation as before, mixing proceeds by

$$\mathbf{u}^{(n)} = \mathbf{u}^{(m)} = \tfrac{1}{2}(\mathbf{u}_0^{(n)} + \mathbf{u}_0^{(m)}); \quad (74)$$

that is, each element mixes by adopting the average velocity of the pair. In terms of the probability density function, this model is

$$\frac{\partial}{\partial v_j}\left\langle g'\frac{\partial\tau_{ij}'}{\partial x_j}\right\rangle = 2\frac{\epsilon}{k}\left(8\int g(\mathbf{v}+\mathbf{v}',\psi)\int g(\mathbf{v}-\mathbf{v}',\psi')d\psi'd\mathbf{v}' - g(\mathbf{v},\psi)\right). \quad (75)$$

An expression for the corresponding model for ϵ_{jk} is obtained by multiplying Eq. (75) by $-v_j v_k$ and integrating; the result is

$$\epsilon_{jk} = \frac{\epsilon\langle u_j u_k\rangle}{k} = \frac{2}{3}\epsilon\delta_{jk} - \frac{\epsilon}{k}\left(\langle u_j u_k\rangle - \frac{2}{3}k\delta_{jk}\right). \quad (76)$$

It may be seen that as well as producing isotropic dissipation, $2/3\epsilon\delta_{jk}$, Curl's model also produces some Rotta redistribution. Thus, in order that the modeling as a whole produce the desired result, the constant $C_2 = 1.5$ in the model for redistribution is changed to $C_2' = C_2 - 1 = 0.5$. Then, Curl's model produces the isotropic dissipation plus two thirds of the redistribution, and the remaining third of the redistribution is provided by the random reorientation simulation.

The final term in Eq. (36) to be modeled is the diffusive mixing term that produces a transport of g in ψ space. It is analogous to the viscous mixing term that has just been considered. The correlation can be re-expressed as the expected value

$$\left\langle g'\frac{\partial J_i^\alpha}{\partial x_i}\right\rangle = gE\left(\frac{\partial J_i^\alpha}{\partial x_i}\middle|\mathbf{u}=\mathbf{v},\phi=\psi\right). \quad (77)$$

In a turbulent reactive flow, the steep gradients of ϕ_α that make significant contributions to this expected value can be caused by two agencies; turbulent velocity fluctuations, and reaction. This term has previously[10] been approximated by Curl's model[25]; and, in proposing its use, we must recognize that this model is appropriate only when the effect of reaction on the microscale is small. To deal properly with flows with very fast reactions (such as premixed flames), an improved model is required.

In the Monte-Carlo method, the implementation of Curl's model for diffusive mixing is precisely analogous to its implementation for viscous mixing. At location $\mathbf{x}$, pairs of elements (denoted by n and m) are selected at random from the ensemble at a rate $C_4 N\epsilon/k$. Then, mixing proceeds by the elements adopting their average values of ϕ;

$$\phi^{(n)} = \phi^{(m)} = \tfrac{1}{2}(\phi_0^{(n)} + \phi_0^{(m)}). \quad (78)$$

An analytic expression for this simulation of mixing is

$$\frac{\partial}{\partial\psi_\alpha}\left\langle g'\frac{\partial J_i^\alpha}{\partial x_i}\right\rangle = C_4\frac{\epsilon}{k}\left(2^\sigma\int g(\mathbf{v},\psi+\psi')\int g(\mathbf{v}',\psi-\psi')d\mathbf{v}'d\psi' - g(\mathbf{v},\psi)\right). \quad (79)$$

From this expression, the effect of mixing on the variance of the single scalar ϕ can be shown to be

$$\frac{\partial}{\partial t}\langle\phi'^2\rangle = -C_4\frac{\epsilon}{k}\langle\phi'^2\rangle. \quad (80)$$

Thus, C_4 is identified as a standard turbulence-model constant for which Spalding[26] suggests the value $C_4 = 2.0$.

All the unknown terms in the transport equation for $g(\mathbf{v},\psi;\mathbf{x},t)$ in a constant-property flow have now been modeled. Viscous and diffusive mixing are modeled by Curl's coalescence/dispersal model which also accounts for two thirds of the Rotta redistribution. The remaining third is simulated by a random reorientation of g in v space. The first part of the redistribution is modeled as a flux of g in v space that is linear in g, v and the mean-velocity gradient, and a tensor function of the Reynolds stresses. This tensor function can be determined from the equivalent tensor in Reynolds-stress closures [see Eqs. (60) and (61)]. A new model, Eq. (48), has been proposed for the pressure transport. A major advantage of the transport equation for $g(\mathbf{v},\psi;\mathbf{x},t)$ is that no closure approximations are re-

quired for the terms pertaining to convective transport and chemical reaction.

The transport equation for $f(\mathbf{V}, \psi; \mathbf{x}, t)$ corresponding to the modeled equation for $g(\mathbf{v}, \psi; \mathbf{x}, t)$ is

$$\frac{\partial f}{\partial t} + V_i \frac{\partial f}{\partial x_i} + \frac{\partial}{\partial \psi_\alpha}[f S_\alpha(\psi)] + \frac{\partial f}{\partial V_j}\frac{\partial \langle p \rangle}{\partial x_j} = C_1 \frac{\partial^2}{\partial x_i \partial V_i}[f(V_i V_i - \langle U_i U_i \rangle)] - 2C_{\alpha m l j}\frac{\partial \langle U_l \rangle}{\partial x_m}\frac{\partial}{\partial V_j}[f(V_\alpha - \langle U_\alpha \rangle)]$$
$$+ 2C_2'\frac{\epsilon}{k}\left(\int\int f(\mathbf{V}', \psi)\int f(\mathbf{V}', \psi'')d\psi''\frac{1}{4\pi}\int_S \delta[\mathbf{V} - \mathbf{v}^*(\mathbf{V}', \mathbf{V}'', \xi)]\,d\xi\, d\mathbf{V}'\, d\mathbf{V}'' - f\right)$$
$$+ 2\frac{\epsilon}{k}\left(8\int f(\mathbf{V}+\mathbf{V}', \psi)\int f(\mathbf{V}-\mathbf{V}', \psi')d\psi' d\mathbf{V}' - f\right) + C_4\frac{\epsilon}{k}\left(2^\sigma \int f(\mathbf{V}, \psi+\psi')\int f(\mathbf{V}', \psi-\psi')d\mathbf{V}'d\psi' - f\right). \quad (81)$$

The terms on the left-hand side of the equation are exact, while those on the right-hand side are modeled. It is interesting to note that if equations for the means $\langle U_j \rangle$ and $\langle \phi_\alpha \rangle$ are derived from Eq. (81), the right-hand side, modeled terms make no contribution: their effect is on the second and higher moments. The first two modeled terms are functions of f only while the last three terms also depend on the turbulent frequency ϵ/k. These three integral terms appear to be complicated, but they represent very simple processes in the Monte-Carlo simulation.

IV. DISCUSSION AND CONCLUSION

The transport equation for the joint probability density function of velocity and scalars has been shown to provide an advantageous basis for modeling turbulent reactive flows. The effects of reaction and convective transport appear in closed form; and, because $f(\mathbf{V}, \psi)$ contains simultaneous information of both velocity and scalar fields, proper account can be taken of the two-way interaction between turbulence and reaction. The Monte-Carlo method can be used to solve the joint probability density function for inhomogeneous flows with complex reactions.

In order to close the transport equation for the joint probability density function, models are required for the terms involving the fluctuating pressure and viscous and diffusive mixing. Such models have been provided for constant-density flows. 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 probability density function 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 modeling. Curl's coalescence/dispersal model is suggested.

The modeling of the pressure terms can be expected to be satisfactory. The terms pertain to the energy containing motions which are well characterized by the joint probability density function; the pressure transport and the first part of the redistribution can be modeled without a knowledge of the scale of turbulence. Indeed, it appears that modeling the first part of the redistribution for the probability density function equation leads to an improved model for the Reynolds-stress equation, one that guarantees realizability. The modeling of the mixing terms is less satisfactory. Mixing occurs on the microscale. The rate of mixing is deduced from the dissipation rate ϵ, and the modeled transport equation for ϵ is a major source of uncertainty. In addition, experimental evidence[27,28] shows that, in general, the rate of diffusive mixing cannot be uniquely related to ϵ. The effects of reaction on the microscale have also been ignored. (These criticisms, it should be remembered, apply to all one-point closures, not just to the joint probability density function equation.) The specific form of Curl's model can also be criticized,[24] since it can produce unrealistic shapes for the probability density function and it does not lead to a Gaussian as the limit of decaying fluctuations.

It would be premature to consider in detail the modeling of the joint probability density function equation for variable-density flows. It can be noted, however, that the effects of reaction, convective transport and buoyancy still appear in closed form. In addition, because the joint probability density function provides simultaneous information about the velocity and scalar fields, it can be expected that the effects of density fluctuations can be satisfactorily incorporated into the modeled terms.

[1] W. R. Hawthorne, D. S. Weddell, and H. C. Hottel, in *Third Symposium on Combustion, Flame and Explosive Phenomena* (Williams and Wilkins, Baltimore, 1949), p. 266.
[2] K. N. C. Bray and J. B. Moss, University of Southampton, England, Report AASU 335 (1974).
[3] S. B. Pope, Philos. Trans. R. Soc. London Ser. A **291**, 529 (1979).
[4] F. C. Lockwood and A. S. Naguib, Combust. Flame **24**, 109 (1975).
[5] S. B. Pope, Combust. Flame **29**, 235 (1977).
[6] C. duP. Donaldson and A. K. Varma, Combust. Sci. Technol. **13**, 55 (1976).
[7] C. Dopazo and E. E. O'Brien, Acta Astronaut. **1**, 1239 (1974).
[8] S. B. Pope, Combust. Flame **27**, 299 (1976).
[9] J. Janicka, W. Kolbe, and W. Kollmann, in *Proceedings of the Heat Transfer and Fluid Mechanics Institute* (Stanford University Press, Stanford, 1978), p. 296.
[10] S. B. Pope, Combust. Sci. Technol. (to be published).
[11] S. B. Pope, in *Eighteenth Symposium on Combustion* (Combustion Institute) (to be published).

[12]B. E. Launder and D. B. Spalding, *Mathematical Models of Turbulence* (Academic, London, 1972).
[13]T. S. Lundgren, Phys. Fluids **12**, 485 (1969).
[14]V. M. Ievlev, Dokl. Akad. Nauk **208**, 1044 (1973).
[15]P. A. Libby and K. N. C. Bray, Combust. Flame **39**, 33 (1980).
[16]J. B. Moss, Combust. Sci. Tech. **22**, 119 (1980).
[17]B. E. Launder, G. J. Reece, and W. Rodi, J. Fluid Mech. **68**, 537 (1975).
[18]J. L. Lumley and B. Khajeh-Nouri, Adv. Geophys. **18A**, 169 (1974).
[19]A. Lin and M. Wolfshtein, in *First Symposium on Turbulent Shear Flows* (Pennsylvania State University, University Park, Pennsylvania, 1977), p. 437.
[20]J. C. Rotta, Z. Phys. **129**, 547 (1951).
[21]J. L. Lumley, in *Prediction Methods for Turbulent Flows*, edited by W. Kollmann (Hemisphere, Washington, D.C., 1980), p. 1.
[22]I. Wygnanski and H. E. Fiedler, J. Fluid Mech. **38**, 577 (1969).
[23]I. Wygnanski and H. E. Fiedler, J. Fluid Mech. **41**, 327 (1970).
[24]C. Dopazo, Phys. Fluids **22**, 20 (1979).
[25]R. L. Curl, AIChE J. **9**, 175 (1963).
[26]D. B. Spalding, Chem. Eng. Sci. **26**, 95 (1971).
[27]C. Béguier, I. Dekeyser, and B. E. Launder, Phys. Fluids **21**, 307 (1978).
[28]Z. Warhaft and J. L. Lumley, J. Fluid Mech. **88**, 659 (1978).