Equation for the Probability Density Function of Velocity and Scalar for Turbulent Shear Flows

W. Kollmann* and A. Wu†
University of California at Davis, Davis, California

The transport equation for the probability density function (pdf) of velocity and scalars is analyzed in the Lagrangian and Eulerian frames. A closed form for the two-time pdf is developed. The time scale for the turbulent velocity fluctuations is determined as an integral of the autocorrelation, thus avoiding a transport equation for the dissipation rate. The model is applied to a plane mixing layer and evaluated by comparison of moments up to third order with experiments.

Introduction

THE probability density function (pdf) transport equation for velocity and scalar variables at a single point is considered in Lagrangian and Eulerian frames. It contains two term groups that cannot be expressed in terms of single-point pdf only, but require two-point pdf or simultaneous pdf of velocity and deformation rate. The first group involves pressure gradient fluctuations, and the second group contains molecular transport terms (viscous stress and diffusive flux). Closure is constructed for the pressure group as a return to isotropy[1] and for the molecular transport group as an integral expression,[2] which can be viewed as a Poisson process reducing variances while leaving mean values unaffected. Both closure expressions require a turbulent time scale. This time scale is determined from the autocorrelations in time as proportional to the (Lagrangian) macrotime scale.[3] Thus, no equation for the dissipation rate or another quantity for the calculation of time scale has to be solved with the pdf equation. This method for the determination of the turbulent time scale is the main contribution of the present paper.

The method of numerical solution of the closed version of the pdf equation is a stochastic simulation technique similar to the method developed by Pope.[1] This solution method allows calculation of autocorrelation in time, thus providing the time scale. The flow in a turbulent mixing layer is calculated, and the performance of the closure model is evaluated by comparison to measured moments of velocity up to third order.

Pdf-Transport Equations

The description of turbulent flows in terms of pdf offers two unique advantages compared to methods based on statistical moments:

1) Turbulent diffusion can be treated in closed form if the values of all three velocity components are independent variables of the pdf.

2) Chemical source terms can be treated in closed form if all the thermochemical variables are included as independent variables of the pdf.

The pdf of velocity and scalar variables at a single point in time and space provides, however, no information on time and length scales. The pdf for velocity and scalars at two points in space and time would contain the desired scale information, but the number of independent variables would be unacceptably large. However, if the pdf at two points in time only is considered, it becomes apparent that turbulent time scales can be determined with acceptable numerical effort for the solution of the pdf equation. This approach will now be developed in detail for incompressible flows.

The flow of a Newtonian fluid with constant density is governed by the balances for mass and momentum. They can be given in the Lagrangian frame as follows[5]:

$$1/6\ \epsilon_{\alpha\beta\gamma}\ \epsilon_{\partial\eta\omega} \frac{\partial X_\alpha}{\partial a_\partial} \frac{\partial X_\beta}{\partial a_\eta} \frac{\partial X_\gamma}{\partial a_\omega} = 1 \tag{1}$$

$$\frac{\partial V_\alpha}{\partial t} = -\frac{1}{2\rho} \epsilon_{\alpha\beta\gamma}\ \epsilon_{\omega_1\omega_2\omega_3} \frac{\partial X_\beta}{\partial a_{\omega_2}} \frac{\partial X_\gamma}{\partial a_{\omega_3}} \frac{\partial P}{\partial a_{\omega_1}} + G_\alpha$$
$$+ \frac{\nu}{2} \epsilon_{\beta_1\beta_2\beta_3}\ \epsilon_{\omega_1\omega_2\omega_3} \frac{\partial X_\partial}{\partial a_{\omega_2}} \frac{\partial X_\eta}{\partial a_{\omega_3}} \frac{\partial}{\partial a_{\omega_1}} \left(\frac{\partial X_\partial}{\partial a_{\beta_2}} \frac{\partial X_\eta}{\partial a_{\beta_3}} \frac{\partial V_\alpha}{\partial a_{\beta_1}} \right) \tag{2}$$

Displacement $X(t,a)$ and velocity are related by

$$\frac{\partial X_\alpha}{\partial t} = V_\alpha \tag{3}$$

and the independent variables are the time t and the identifying variable a defined by

$$a_\alpha = X_\alpha(0,a) \tag{4}$$

Finally, denote $P(t,a)$ the pressure and $G_\alpha(t,a)$ the external force per unit mass. Since the balance equations in the Lagrangian frame are rather awkward, we shall also use the mixed Eulerian/Lagrangian formulation of Eqs. (1) and (2). The transformation between the frames is given by

$$x = X(t,a), \qquad a = X^{-1}(t,x)$$

where X^{-1} denotes the inverse mapping of $X(t,a)$. Variables in the Lagrangian frame are denoted by capital letters and in the Eulerian frame by lowercase letters. Hence, relations such as

$$v(t,x) = V[t, X^{-1}(t,x)]$$

hold for all dependent variables. Mass conservation appears

Presented as Paper 87-1348 at the AIAA 19th Fluid Dynamics, Plasma Dynamics, and Lasers Conference, Honolulu, HI, June 8–10, 1987; received July 1, 1987; revision received April 5, 1988.

*Professor, Department of Mechanical Engineering.
†Graduate Student, Department of Mechanical Engineering.

now as differential equation for velocity

$$\frac{\partial v_\alpha}{\partial x_\alpha} = 0 \tag{5}$$

and momentum balance as

$$\frac{dv_\alpha}{dt} = -\frac{1}{\rho}\frac{\partial p}{\partial x_\alpha} + g_\alpha + \nu \Delta v_\alpha \tag{6}$$

where

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} + v_\alpha \frac{\partial}{\partial x_\alpha} \tag{7}$$

denotes the Eulerian form of the partial time derivative in the Lagrangian frame.

Consider now a material point **a** at times t_0, t_1, and t_2 and define the fine-grained pdf[1] by

$$\hat{f} = \prod_{i=0}^{2} \delta(X^i - x^i)\delta(V^i - v^i) \tag{8}$$

where $X^i \equiv X(t^i, a)$, $V^i \equiv V(t^i, a)$ are position and velocity at times t^0, t^1, and t^2 of the material point identified by $X^0 = a$. The expectation of $\hat{f}$ allows the definition of the Lagrangian two-time pdf $\mathfrak{F}_2$:

$$\mathfrak{F}_2(x^1, v^1, x^2, v^2; t^1, t^2) = \int dx^0 \int dv^0 \langle \hat{f} \rangle \tag{9}$$

The quantity

$$\mathfrak{F}_2(x^1, v^1, x^2, v^2; t^1, t^2) dx^1 dv^1 dx^2 dv^2$$

is the probability to find a material point at x^1 with velocity v^1 at time t^1 and at x^2 with v^2 at time t^2. The properties of $\mathfrak{F}_2$ and its relation to conditional and single-point pdf will be discussed first. The Eulerian two-point and two-time pdf F_2 defined by

$$F_2(v^1, v^2; x^1, x^2, t^1, t^2) \equiv \langle \prod_{i=1}^{2} \delta[v(x^i, t^i) - v^i] \rangle$$

is a function of the same set of independent variables. The Eulerian pdf F_2 is, however, not equal to the Lagrangian pdf $\mathfrak{F}_2$. This can be seen from the evaluation of the limit t^2 approaching t^1. Assuming at least continuous velocity fields, we get for the Lagrangian case

$$\lim_{t^2 \to t^1} \mathfrak{F}_2(x^1, v^1, x^2, v^2; t^1, t^2) = \mathfrak{F}_1(x^1, v^1; t^1)\delta(v^1 - v^2)\delta(x^1 - x^2)$$

and for the Eulerian case

$$\lim_{t^2 \to t^1} F_2(v^1, v^2, x^1, x^2, t^1, t^2) = F_2(v^1, v^2; x^1, x^2, t^1, t^1)$$

and $F_2(v^1, v^2; x^1, x^2, t^1, t^1)$ does not contain atomic contributions as long as $x^1 \neq x^2$. Hence, $\mathfrak{F}_2$ and F_2 are not identical. Integration of the Lagrangian pdf $\mathfrak{F}_2$ over the properties at time t^1

$$\mathfrak{F}_1(v, x; t) = \int dx^1 \int dv^1 \, \mathfrak{F}_2(x^1, v^1, x, v; t^1, t) \tag{10}$$

leads to the single-point pdf $\mathfrak{F}_1$ of velocity and position. The Eulerian single point pdf $F_1(v; x, t)$ and the Lagrangian pdf $\mathfrak{F}_1(v, x; t)$ depend on the same set of independent variables but they are not equal. First, we note that F_1 is pdf with respect to v; hence,

$$\int dv F_1(v; x, t) = 1$$

holds, but $\mathfrak{F}_1$ is pdf with respect to v and x; hence,

$$\int dv \int dx \, \mathfrak{F}_1(v, x; t) = 1$$

holds. The relation between $F_1(v; x, t)$ and $\mathfrak{F}_1(v, x; t)$ can be established by considering the sets S_E and S_L defined by

$$F_1(v; x, t) dv \equiv \text{prob}\{S_E\}$$

$$\mathfrak{F}_1(v, x; t) dv dx \equiv \text{prob}\{S_L\}$$

The set S_E consists of all velocities $v(x, t)$ measured at (x, t) such that

$$v \le v(x, t) \le v + dv$$

Since x is for each sample the location of a material point that started at a at time $t = 0$, it follows that S_E is also the set of all material points, such that $x = X(a, t)$ and $v \le V(a, t) \le v + dv$. The set S_L is, according to Eqs. (9) and (10), the set of all material points a such that $x \le X(a, t) \le x + dx$ and $v \le V(a, t) \le v + dv$ hold. It follows that $S_E \subset S_L$ and that S_E can be viewed in the Lagrangian frame as the set of all material points such that $v \le V(a, t) \le v + dv$ conditioned with $x = X(a, t)$. Hence,

$$F_1(v; x, t) = \mathfrak{F}_1^c(v \mid x; t)$$

where $\mathfrak{F}_1^c$ denotes the conditional pdf:

$$\mathfrak{F}_1^c(v \mid x; t) \equiv \frac{\mathfrak{F}_1(v, x; t)}{\mathfrak{F}(x; t)}$$

The Lagrangian pdf of position $\mathfrak{F}(x, t)$ can be assumed to be constant at $t = 0$ (without restricting generality, because it is the pdf for sampling material points):

$$\mathfrak{F}(x; 0) = 1/m[D(0)], \qquad 0 < m[D(0)] < \infty$$

where $m[D(0)]$ denotes the volume of the flow domain D at $t = 0$. Since $x(a, t)$ is a differentiable and volume-preserving mapping of the initial flow domain onto the domain at later times, it follows that

$$\mathfrak{F}(x; t) = \mathfrak{F}(x; 0) = 1/m[D(0)]$$

and therefore

$$F_1(v; x, t) = m[D(0)]\mathfrak{F}_1(v, x; t)$$

hold.

The Lagrangian two-time pdf $\mathfrak{F}_2$ can be expressed in terms of the conditional pdf $\mathfrak{F}_c$:

$$\mathfrak{F}_2(x^1, v^1, x^2, v^2; t^1, t^2) = \mathfrak{F}_c(x^2, v^2; t^2 \mid x^1, v^1; t^1)\mathfrak{F}_1(x^1, v^1; t^1)$$

The expression

$$\mathfrak{F}_c(x^2, v^2; t^2 \mid x^1, v^1; t^1) dx^2 dv^2$$

is now the probability that a material point is at x^2 with velocity v^2 at time t^2, provided that it was at x^1 with v^1 at time t^1. Hence, it follows that

$$F_1(v; x, t) = \int dx^1 \int dv^1 F_1(v^1; x^1, t^1)\mathfrak{F}_c(x, v; t \mid x^1, v^1; t^1)$$

holds. The conditional pdf $\mathfrak{F}_c$ is thus recognized as the probability density for the transition from (x^1, v^1) at time t^1 to (x, v) at time t. Another pdf, which will be required later for the determination of time scales, can be established by integration over all locations x^1 corresponding to t^1, which is assumed to be before t^2:

$$\mathfrak{F}_2^*(v^1,x^2,v^2;t^1,t^2) = \int dx^1 \mathfrak{F}_2(x^1,v^1,x^2,v^2;t^1,t^2)$$

Associated with $\mathfrak{F}_2^*$ is the conditional pdf $\mathfrak{F}_c^*$, defined by

$$\mathfrak{F}_c^*(x^2,v^2;t^2 \mid v^1;t^1) \equiv \frac{\mathfrak{F}_2^*(v^1,x^2,v^2;t^1,t^2)}{\mathfrak{F}_1(v^1;t^1)} \tag{11}$$

$\mathfrak{F}_c^*$ is now the pdf of velocity and location of material points at time t^2 conditioned with the velocity v^1 at the earlier time t^1, irrespective of the earlier location x^1.

The transport equation for the Lagrangian two-time pdf $\mathfrak{F}_2$ can be derived from

$$\frac{\partial \hat{f}}{\partial t^i} = -\frac{\partial X_\alpha^i}{\partial t^i}\frac{\partial \hat{f}}{\partial x_\alpha^i} - \frac{\partial V_\alpha^i}{\partial t^i}\frac{\partial \hat{f}}{\partial v_\alpha^i}, \qquad i = 1,2$$

Averaging leads to the preliminary form of the pdf transport equation

$$\frac{\partial \mathfrak{F}_2}{\partial t^i} + v_\alpha^i \frac{\partial \mathfrak{F}_2}{\partial x_\alpha^i} = -\frac{\partial}{\partial v_\alpha^i}\left\langle \frac{\partial V_\alpha^i}{\partial t^i}\hat{f}\right\rangle, \qquad i = 1,2$$

Integration over x^1 leads to

$$\frac{\partial \mathfrak{F}_2^*}{\partial t} + v_\alpha \frac{\partial \mathfrak{F}_2^*}{\partial x_\alpha} = -\frac{\partial}{\partial v_\alpha}\left\langle \frac{\partial V_\alpha}{\partial t}\hat{f}^*\right\rangle \tag{12}$$

where $\mathfrak{F}_2^*\ (v^1,x,v;t^1,t)$, and

$$\hat{f}^* \equiv \partial(V^1 - v^1)\partial(X - x)\partial(V - v)$$

The right-hand side of Eq. (12) can be evaluated using the mixed formulation [Eqs. (5-7)]. The transport equation for the pdf $\mathfrak{F}_2^*$ appears, then, in the following form:

$$\frac{\partial \mathfrak{F}_2^*}{\partial t} + v_\alpha \frac{\partial \mathfrak{F}_2^*}{\partial x_\alpha} = -\frac{\partial}{\partial v_\alpha}\left(\left\langle \nu \frac{\partial^2 V_\alpha}{\partial X_\beta \partial X_\beta}\ \middle|\ C\right\rangle \mathfrak{F}_2^*\right) + \frac{\partial}{\partial v_\alpha}\left(\left\langle \frac{1}{\rho}\frac{\partial P}{\partial X_\alpha}\ \middle|\ C\right\rangle \mathfrak{F}_2^*\right) + \frac{\partial}{\partial v_\alpha}\left(\left\langle G_\alpha \mid C\right\rangle \mathfrak{F}_2^*\right) \tag{13}$$

where C denotes the condition

$$C \equiv (V^1 = v^1, X = x, V = v)$$

appearing in the conditional fluxes. It follows from Eq. (11) that the conditional pdf $\mathfrak{F}_c^*$ satisfies the same transport equation (13). Furthermore, it satisfies the single-point Eulerian/Lagrangian pdf $\mathfrak{F}_1(x,v;t)$,

$$\mathfrak{F}_1(x,v;t) = \int dx^1 \int dv^1 \mathfrak{F}_2(x^1,v^1,x,v;t^1,t)$$

a transport equation having the same structure as Eq. (13). This equation can be derived from Eq. (13) by integration or directly from the basic laws:

$$\frac{\partial \mathfrak{F}_1}{\partial t} + v_\alpha \frac{\partial \mathfrak{F}_1}{\partial x_\alpha} = -\frac{\partial}{\partial v_\alpha}\left(\left\langle \nu \frac{\partial^2 V_\alpha}{\partial X_\beta \partial X_\beta}\ \middle|\ C\right\rangle \mathfrak{F}_1\right) + \frac{\partial}{\partial v_\alpha}\left(\left\langle \frac{1}{\rho}\frac{\partial P}{\partial X_\alpha}\ \middle|\ C\right\rangle \mathfrak{F}_1\right) + \frac{\partial}{\partial v_\alpha}\left(\left\langle G_\alpha \mid C\right\rangle \mathfrak{F}_1\right) \tag{14}$$

The condition C is now given by

$$C \equiv (X = x, V = v)$$

The structural similarity of Eqs. (13) and (14) indicates that the numerical effort for the solution of the two-time pdf equation should not be significantly larger than the effort for the single-point pdf $\mathfrak{F}_1$.

The pdf $\mathfrak{F}_2$, $\mathfrak{F}_2^*$, and $\mathfrak{F}_1$ can be extended to include scalar variables in addition to velocity and location without difficulty. Consider the passive scalar variables $\phi_i(t,a)$, $i = 1(1)n$, which are governed in the Lagrangian frame by transport equations,

$$\frac{\partial \phi_i}{\partial t} = S_i(\phi_1 \ldots \phi_n) + \frac{\Gamma}{2}\epsilon_{\beta_1\beta_2\beta_3}\epsilon_{\omega_1\omega_2\omega_3}\frac{\partial X_{\alpha 2}}{\partial a_{\omega_2}}\frac{\partial X_{\alpha 3}}{\partial a_{\omega_3}}\frac{\partial}{\partial a_{\omega_1}} \times \left(\frac{\partial X_{\alpha 2}}{\partial a_{\beta_2}}\frac{\partial X_{\alpha 3}}{\partial a_{\beta_3}}\frac{\partial \phi_i}{\partial a_{\beta_1}}\right), \qquad i = 1(1)n \tag{15}$$

or, in mixed Eulerian/Lagrangian formulation,

$$\frac{d\phi_i}{dt} = \Gamma \Delta \phi_i + S_i(\phi_1 \ldots \phi_n) \tag{16}$$

where S_i denotes the source term, which may be a nonlinear function of the ϕ_i at the same point (x,t) as the other terms in Eq. (16). The definition (8) of f is now extended to

$$\hat{f} = \prod_{i=1}^{2} \partial(X^i - x^i)\partial(V^i - v^i) \prod_{j=1}^{n} \partial(\phi_j^i - \Psi_j^i) \tag{17}$$

and the two-time pdf $\mathfrak{F}_2$ is now given by

$$\mathfrak{F}_2(x^1,v^1,\Psi_1^1 \ldots \Psi_n^1,x^2,v^2,\Psi_1^2 \ldots \Psi_n^2;t^1,t^2) \equiv \langle \hat{f} \rangle$$

and $\mathfrak{F}_2^*$ by

$$\mathfrak{F}_2^*(v^1,\Psi_1^1 \ldots \Psi_n^1,x^2,v^2,\Psi_1^2 \ldots \Psi_n^2;t^1,t^2) = \int dx^1 \mathfrak{F}_2$$

and $\mathfrak{F}_c^*$ by the relation analogous to Eq. (11). All transport equations carry over to the extended pdf. We note the equation for $\mathfrak{F}_2^*$,

$$\frac{\partial \mathfrak{F}_2^*}{\partial t} + v_\alpha \frac{\partial \mathfrak{F}_2^*}{\partial x_\alpha} = -\frac{\partial}{\partial v_\alpha}\left(\left\langle \nu \frac{\partial^2 V_\alpha}{\partial X_\beta \partial X_\beta}\ \middle|\ C^*\right\rangle \mathfrak{F}_2^*\right) + \frac{\partial}{\partial v_\alpha}\left(\left\langle \frac{1}{\rho}\frac{\partial P}{\partial x_\alpha}\ \middle|\ C^*\right\rangle \mathfrak{F}_2^*\right) + \frac{\partial}{\partial v_\alpha}\left(\left\langle G_\alpha\ \middle|\ C^*\right\rangle \mathfrak{F}_2^*\right) - \sum_{j=1}^{n}\frac{\partial}{\partial \Psi_j}\left\{\left[\left\langle \Gamma \frac{\partial^2 \phi_j}{\partial X_\beta \partial X_\beta}\ \middle|\ C^*\right\rangle + S_j(\Psi_1 \ldots \Psi_n)\right]\mathfrak{F}_2^*\right\} \tag{18}$$

where the condition C^* is now given by

$$C^* \equiv [X = x, V = v, \phi_j = \Psi_j,\ j = 1(1)n$$
$$V^1 = v^1,\ \phi_j^1 = \Psi_j^1,\ j = 1(1)n]$$

The extension to nonpassive scalars (variable density flows) is straightforward but cumbersome, because the energy equation and state relations must be added to the Navier-Stokes system. It will not be considered here.

Time Scales

Turbulent flows are characterized by a continuous spectrum of excited scales in time and space. If the turbulent flow is described in terms of the pdf of velocity and scalars at a single point in space and time, then it is not possible to infer any information on length or time scales from it, and equations for quantities determining scales must be solved in conjunction with the pdf equation. The pdf of velocity and scalars at two points in time allows direct calculation of time scales from the pdf, whereas the pdf at two points in space and time allows direct evaluation of length and time scales. The former case will be considered in detail.

Let $\mathfrak{F}_2(x^1,v^1,x^2,v^2;t^1,t^2)$ be the solution (integrated over the scalar space) of the transport equation for the two-time Lagrangian pdf, and let $t^1 < t^2$. Thus the correlation of the velocity V_α of a material point, which is at x^1 at time t^1, with the velocity V_β of the same point at x^2 and t^2 is given by

$$\langle V_\alpha V_\beta \rangle = \int dv^1 \int dv^2 v_\alpha^1 v_\beta^2 \mathfrak{F}_2(x^1,v^1,x^2,v^2;t^1,t^2) \qquad (19)$$

Further integration over the flow domain $D(t^1)$ leads to the correlation of $V_\beta[t^2,X^{-1}(t^2,x^2)]$ with V_α at t^1, irrespective of the location x^1,

$$R_{\alpha\beta}(x^2,t^1t^2) = \int_{D(t_1)} dx^1 \int dv^1 \int dv^2 v_\alpha^1 v_\alpha^2 \mathfrak{F}_2$$
$$= \int dv^1 \int dv^2 v_\alpha^1 v_\beta^2 \mathfrak{F}_2^* (v^1,x^2,v^2;t^1,t^2) \qquad (20)$$

and division by $R_{\alpha\beta}(x^2,t^2,t^2)$ results in the temporal correlation coefficient (no sum over α or β, notation changed to $x = x^2, t^1 = t, t^2 = t + \tau$),

$$\rho_{\alpha\beta}(x,t,\tau) \equiv \frac{R_{\alpha\beta}(x,t,t+\tau)}{R_{\alpha\beta}(x,t,t)} \qquad (21)$$

provided that the denominator is nonzero. The correlation coefficient for $\alpha = \beta$ defines the Lagrangian macroscale in time by

$$\tau_{\alpha\beta}(x,t) \equiv \int_0^\infty d\tau \rho_{\alpha\beta}(x,t,\tau) \qquad (22)$$

Dimensional arguments show that

$$\tau \equiv \frac{1}{3}\sum_{\alpha=1}^{3} \tau_{\alpha\alpha}$$

and kinetic energy

$$k(x,t) \equiv \tfrac{1}{2} R_{\alpha\alpha}(x,t,t) \qquad (23)$$

define a quantity $\tilde{\epsilon}$ with the dimension of the dissipation rate:

$$\tilde{\epsilon} \equiv \frac{k}{\tau}$$

If the Lagrangian time scale is equal to the Eulerian scale, then $\tilde{\epsilon}$ is indeed the (Eulerian) rate of dissipation of kinetic energy. Corrsin[6] carried out an investigation of the relation between Eulerian and Lagrangian scales and found that they are roughly equal for high Reynolds number turbulence. Hence, we determine the dissipation rate

$$\epsilon \equiv \nu \left\langle \frac{\partial v_\beta}{\partial x_\alpha} \frac{\partial v_\beta}{\partial x_\alpha} \right\rangle \qquad (24)$$

in the Eulerian frame from

$$\epsilon \cong C_e \frac{k}{\tau} \qquad (25)$$

where C_e is a constant of order unity. ($C_e = 1.0$ was used in the present model.)

Closure Problems

The transport equation (18) for the two-time pdf $\mathfrak{F}_2^*$ contains three conditional expectations that must be regarded as new unknown variables if the external force G_α is not fluctuating. ($G_\alpha = 0$ will be assumed in the following.) It is convenient for the discussion of the closure problems and for the solution method to consider the basic laws [Eqs. (3, 6, and 14)] as stochastic differential equations for the dynamics of a fluid material point[1,7]:

$$dX_\alpha = v_\alpha(t,X)dt \qquad (26)$$

$$dV_\alpha = \left[\nu\Delta\langle v_\alpha\rangle - \frac{1}{\rho}\frac{\partial\langle p\rangle}{\partial x_\alpha}\right]dt + \left[\nu\Delta v_\alpha' - \frac{1}{\rho}\frac{\partial p'}{\partial x_\alpha}\right]dt \qquad (27)$$

$$d\phi_i = \Gamma\Delta\langle\phi_i\rangle dt + S_i(\phi_1 \ldots \phi_n)dt + \Gamma\Delta\phi_i' \, dt, \qquad i = 1(1)n \qquad (28)$$

Note that the left-hand sides are the change of position, velocity, and scalars in the Lagrangian frame, whereas the right-hand side is written in the Eulerian frame. Eulerian variables are split into mean and fluctuation:

$$v_\alpha = \langle v_\alpha\rangle + v_\alpha', \qquad p = \langle p\rangle + p', \qquad \phi_i = \langle\phi_i\rangle + \phi_i'$$

Equations (24-26) are complemented with the mass conservation equation (1) or (5).

The group of terms representing the effect of molecular transport on the pdf will be considered first. It is denoted by

$$D_2 \equiv -\frac{\partial}{\partial v_\alpha}\left(\left\langle \nu \frac{\partial^2 V_\alpha}{\partial X_\beta \partial X_\beta} \middle| C^* \right\rangle_2^*\right) - \sum_{j=1}^{n} \frac{\partial}{\partial \Psi_j}\left(\left\langle \Gamma \frac{\partial^2 \phi_i}{\partial X_\beta \partial X_\beta} \middle| C^* \right\rangle_2^*\right) \qquad (29)$$

The properties of this group are well known,[1,2] and they imply, in particular, that mean values are unaffected by D_2, whereas second-order (centered) moments are reduced by D_2. The closure model developed in Ref. 2 satisfies those conditions. It can be generalized to any number of variables[8] and is, in terms of the pdf $\mathfrak{F}_2^*$, given by

$$D_2 \cong 3\frac{C_E}{\tau}\left[\int\cdots\int d\tilde{\omega}\int\cdots\int d\tilde{\tilde{\omega}}\, \mathfrak{F}_2^*(\omega^1,x^2,\tilde{\omega}) \times \mathfrak{F}_2^*(\omega^1,x^2,\tilde{\tilde{\omega}})T(\tilde{\omega},\tilde{\tilde{\omega}} \mid \omega^2) - \mathfrak{F}_2^*(\omega^1,x^2,\omega^2)\right] \qquad (30)$$

where ω denotes the set of variables $(v, \Psi_1 \ldots \Psi_n)$. The function T plays the role of a transition probability for the interaction of fluid elements and is subject to the following conditions according to Ref. 8:

$$T(\tilde{\omega},\tilde{\tilde{\omega}} \mid \omega^2) = 0 \qquad (31)$$

if one or more than one of the variables ω^2 is not in the interval $[\tilde{\omega},\tilde{\tilde{\omega}}]$,

$$T(\tilde{\omega},\tilde{\tilde{\omega}} \mid \omega^2) = T(\tilde{\omega},\tilde{\tilde{\omega}} \mid \tilde{\omega} + \tilde{\tilde{\omega}} - \omega^2) \qquad (32)$$

and finally

$$\int d\omega^2 T(\tilde{\omega},\tilde{\tilde{\omega}} \mid \omega^2) = 1/N \qquad (33)$$

where

$$N \equiv \int d\tilde{\omega}\mathfrak{F}_2^*(\omega^1,x^2,\tilde{\omega}) \qquad (34)$$

The transition probability T for the present closure is based on the assumption that the values of velocity and scalars of the interfacing fluid element approach each other with uniform probability. Hence T is given by

$$T(\tilde{\omega},\tilde{\tilde{\omega}} \mid \omega^2) = \prod_{i=1}^{n} |\tilde{\tilde{\Psi}}_i - \tilde{\Psi}_i|^{-1} \, |\tilde{\tilde{v}} - \tilde{v}|^{-1} \qquad (35)$$

and $C_F = 0.2$ is the constant in Eq. (30). The variance equation corresponding to Eq. (3) can be established by straightforward integration

$$\left(\frac{\partial\langle\phi_i'^2\rangle}{\partial t}\right)_{D_2} = -\frac{C_F}{\tau}\langle\phi_i'^2\rangle$$

for T given by Eq. (35). This result can be used to estimate C_F from experiments, if the time scale τ is known. The model of Eq. (30) implies that two fluid elements (material volume small compared to the volume of flow domain) must interact in such a way that the mean values of velocity and scalars remain unchanged and variances are decreased. Hence, it follows that for each realization more than one element must be present at a given time. Equations (27) and (28) must, therefore, be regarded as stochastic partial differential equations with this closure for the fluctuating viscous/diffusive terms.

The influence of the fluctuating pressure gradient on the dynamics of the pdf $\mathfrak{F}_2^*$ is represented by the stochastic reorientation model put forward by Pope.[1] Pairwise interaction of fluid elements is carried out, such that the velocities are randomized without affecting the mean velocity or the kinetic energy of the fluctuations. The effect of the stochastic reorientation model in the Reynolds-stress tensor is equivalent to Rotta's "return to isotropy" closure. Several closure models for the rapid part of the fluctuating pressure gradient have been developed.[1,7] For the present case, only the stochastic reorientation model was included with an adjusted model constant ($C_1 = 0.6$) to take into account the new definition of the time scale and to represent the effect of the whole pressure term. Closure models for the rapid part are currently being developed.

Solution Method

The numberical solution of the pdf equation (18) is carried out with a stochastic simulation technique.[1,7] The pdf $\mathfrak{F}_2^*$ is represented by M stochastic particles with equal mass. Each particle is identified by the set $(x, v, \Psi_1 \ldots \Psi_n)_i$ of values for the independent variables at the current time t. In addition to the current state, the values of $v, \Psi_1 \ldots \Psi_n$ at earlier times $t^1 < t$ are stored for the evaluatiaon of temporal correlations. The movement of the particles in physical space and the velocity-scalar space is governed by the stochastic differential equations (26–28), where the fluctuating contributions on the right-hand side of Eqs. (27) and (28) are represented by the stochastic mixing model [Eq. (30)] and the reorientation model for the pressure fluctuations. The solution procedure is set up according to a fractional step method where, in each fractional step, a single operation acts on the ensemble of particles for the entire time interval. These operations represent convection, dissipation, pressure fluctuations, and mean pressure gradient. For a given time interval Δt, the steps are carried out as follows:

1) Convection/diffusion: The particles are moved in physical space according to their individual velocity.

2) Dissipation: Two particles are selected with probability $(3/2)C_E(\Delta t/\tau)$ from a small quasihomogenous neighborhood (grid cell), and the values of velocity and scalars change then according to (given here for velocity, asterisk denotes intermediate solution)

$$V_i^*(t + \Delta t) = V_i^*(t) + {\textstyle\frac{1}{2}}\,\eta_{ij}\left[V_j^*(t) - V_i^*(t)\right]$$

$$V_j^*(t + \Delta t) = V_j^*(t) + {\textstyle\frac{1}{2}}\,\eta_{ij}\left[V_i^*(t) - V_j^*(t)\right]$$

where η_{ij} is a random variable with uniform probability over the unit interval. This model leaves mean values unchanged and reduces the variances.

3) Fluctuating pressure gradient: Particles are selected with probability $C_1(\Delta t/\tau)$, and the fluctuating velocity vector is reorientated without change in length. The mean velocity hence remains unchanged, and the kinetic energy is redistributed among the Reynolds-stress components such that isotropy is approached.

Mean pressure gradient: Mass conservation in the mean[1] requires the change of the particle velocity due to the mean pressure gradient. The particle position after convection (step 1) is

$$X^* = X(t) + V(t)\Delta t$$

The mean pressure gradient at this position changes V to

$$V_N = V(t) - (\Delta t/\rho)\nabla\langle p\rangle$$

and the corrected particle position is then

$$X(t + \Delta t) = X^* + (\Delta t/2)[V(t) + V_N]$$

Mass conservation is then satisfied in the statistical mean.[1] The convergence question for this method of simulation is discussed in detail by Pope.[1] It follows essentially from the central limit theorem that the expectation of well-behaved functions of the random variables converges with $1/\sqrt{N}$, where N is the number of samples.

The determination of the mean pressure gradient requires careful smoothing of the mean velocity field, which is performed using cross-validated least squares cubic splines.[10] The same method of smoothing was applied for the presentation of the results in Figs. 1–11. The turbulent shear flow considered here requires boundary conditions on free boundaries to be satisfied. The mean velocity and mean scalars are prescribed, and the fluctuations are small compared to the values in the high shear region. These conditions are met if particles with the velocity and scalar values of the freestreams are entrained, if particles leave the computational domain, or if the domain is extended according to the growth of the shear layer. In the initial phase of the integration, one modification of the scale calculation was introduced, since time histories are not yet established. The length scale was determined as $l \cong 0.35\delta$, where $\delta \cong |y_{0.9} - y_{0.1}|$ is the thickness of the shear layer. As soon as two-time correlations were available, the scale calculation was switched to Eq. (22).

Results and Discussion

The closure model for pdf equation (18) described in the previous section was tested in a plane mixing layer. Recent experiments by Mehta and Westphal[4] were used for the evaluation of the numerical results. The numerical simulation of the

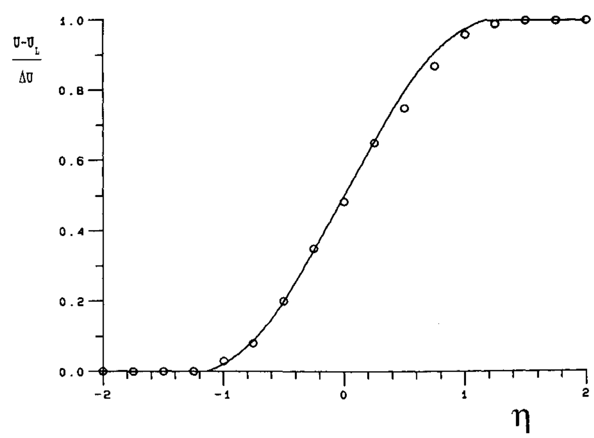

Fig. 1 Mean velocity for the plane mixing layer compared with experiment.[4]

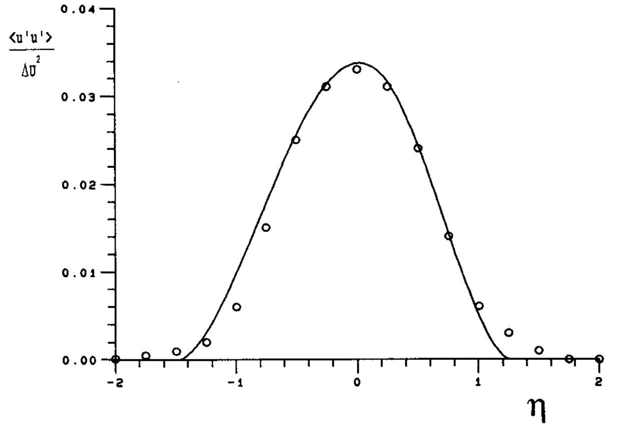

Fig. 2 Streamwise component of normal stresses compared with experiment.[4]

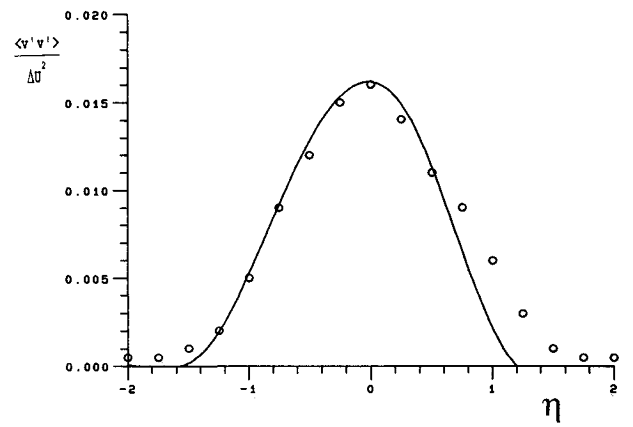

Fig. 3 Cross-stream component of normal stresses compared with experiment.[4]

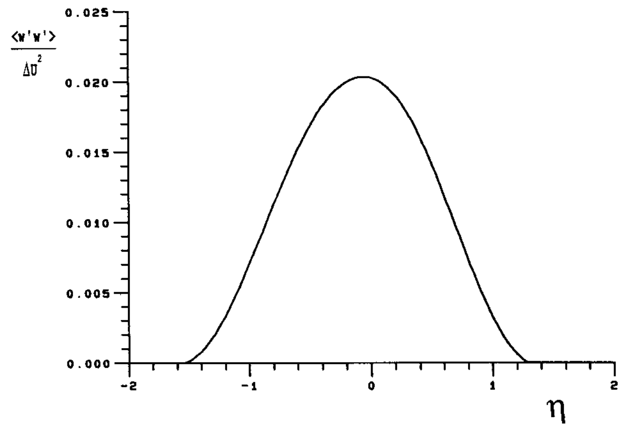

Fig. 4 Transverse component of normal stresses for plane mixing layer.

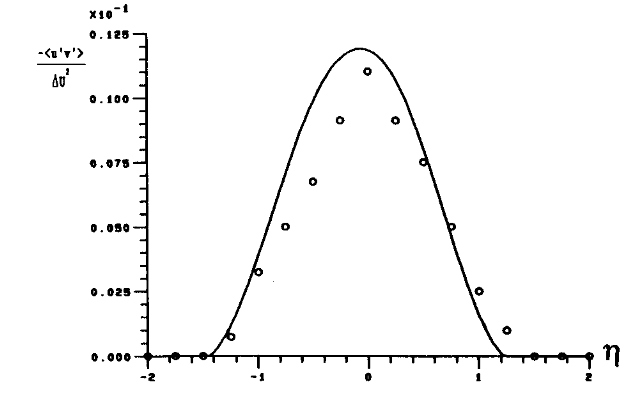

Fig. 5 Shear stress for the plane mixing layer compared with experiment. [4]

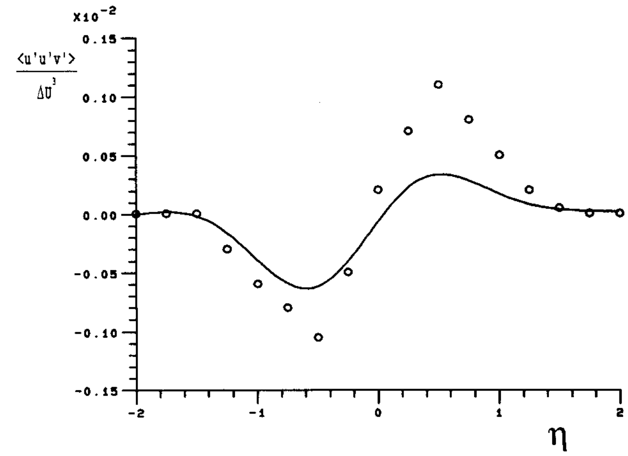

Fig. 6 Triple correlation $\langle u'u'v'\rangle$ for the plane mixing layer compared with experiment.[4]

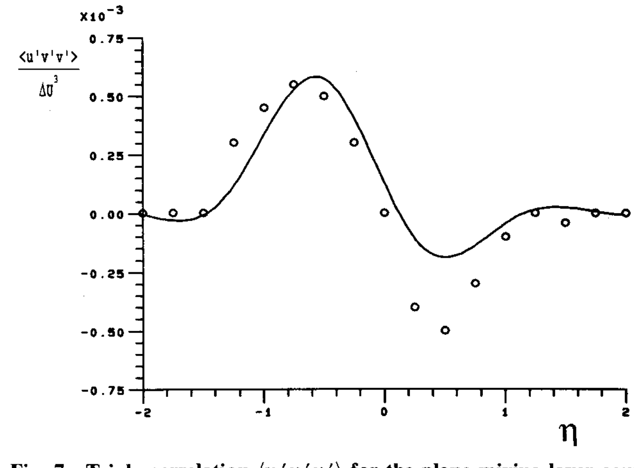

Fig. 7 Triple correlation $\langle u'v'v'\rangle$ for the plane mixing layer compared with experiment.[4]

mixing layer was carried out with $N = 16{,}000$ particles up to the longitudinal location corresponding to the measurement station. The mean velocity profile in Fig. 1 shows the agreement between the prediction (full line, smoothed with cubic splines[10]) and the experiment (symbols[4]) which can be expected for current methods of prediction. The normalized components of the Reynolds-stress tensor

$$\frac{\langle v_\infty' v_\beta'\rangle}{\Delta u^2}(\eta), \qquad \eta \equiv \frac{y - y_{0.5}}{\delta}, \qquad \delta \equiv |y_{0.1} - y_{0.9}|$$

where $\Delta u \equiv |u_E - u_I|$ is the difference of the freestream velocities, are compared to the experiment in Figs. 2–5. The velocity pdf allows direct calculation of $\langle v_\alpha' v_\beta'\rangle$:

$$\langle v_\alpha' v_\beta'\rangle = \int \mathrm{d}\boldsymbol{v}\, (v_\alpha - \langle v_\alpha\rangle)(v_\beta - \langle v_\beta\rangle)\mathfrak{F}_1(\boldsymbol{v},\boldsymbol{x},t)$$

which is shown as solid lines in Figs. 2–5, where the symbols denote the experimental values. The agreement is again reasonable. A more sensitive measure of agreement between calculation and experiment is provided by the triple correlations in Figs. 6 and 7. It is noteworthy that the predictions for both triple correlations are qualitatively correct, but the calculated $\langle u'^2 v'\rangle/\Delta u^3$ is too low, wheras $\langle v'v'^2\rangle/\Delta u^3$ in Fig. 7 agrees well with the experiment on the low-speed side of the mixing

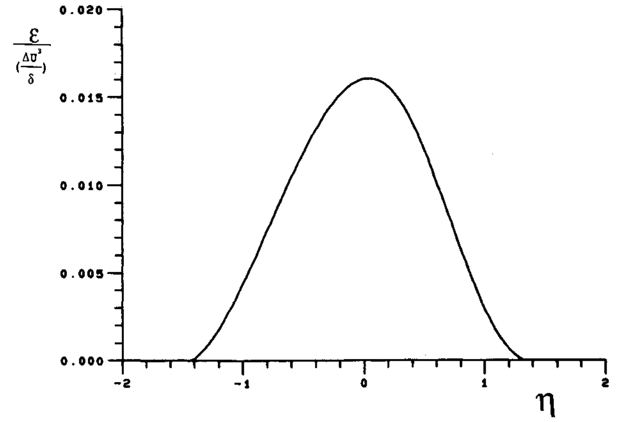

Fig. 8 Turbulent dissipation rate ϵ for plane mixing layer ($\delta \cong y_{0.9} - y_{0.1}$).

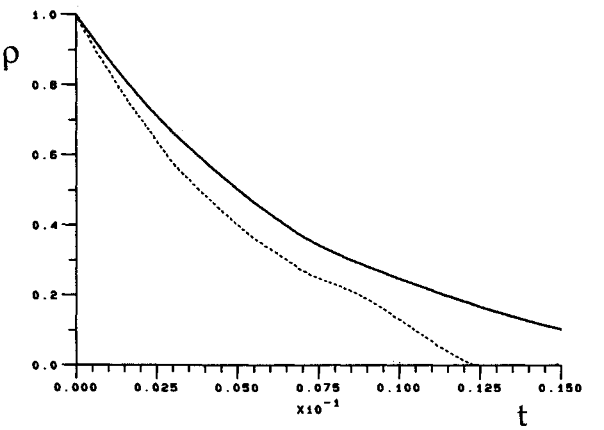

Fig. 9 Two-point correlation with time (in seconds) for the plane mixing layer at $\eta = -0.52$ (solid line) and $\eta = 0.29$ (dotted line).

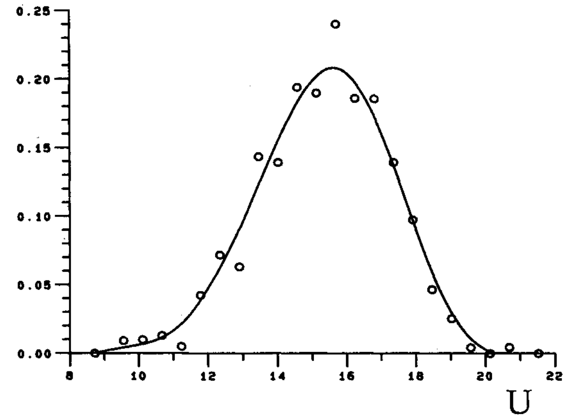

Fig. 10 One-point velocity pdf at $\eta = 0$ (U in m/s).

layer. The present closure of the pdf equation does not yet contain the rapid part of the pressure term. Consequently, the stochastic reorientation model for the slow part of the pressure term is stronger than it would be with a model for the rapid part, and thus the triple correlations are damped more than necessary. Figure 8 contains the dissipation rate $\epsilon\delta/\Delta u^3$ deduced from the Lagrangian integral time scale τ according to Eq. (25). It is about twice as large as the dissipation rate predicted by a second-order closure model, and the model constants C_E and C_1 for the dissipation and pressure terms in the pdf equation were modified accordingly. Two-time correlation coefficients at $\eta = 0.287$ and 0.518 are shown in Fig. 9

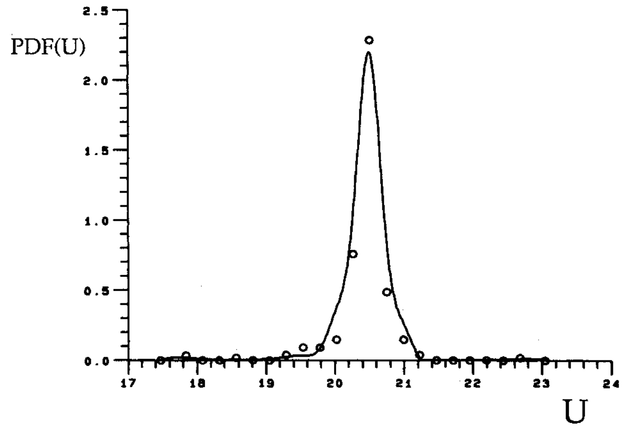

Fig. 11 One-point velocity pdf at $\eta = 1$ (U in m/s).

as function of the delay time τ. Finally, two examples of the marginal pdf $\mathfrak{F}_1(u)$ are shown in Figs. 10 and 11. The symbols in both figures are the calculated raw (unsmoothed) pdf, whereas the lines are the smoothed (cubic splines) pdf. Both pdf have significant skewness, and the pdf in Fig. 11 exhibits considerable flatness.

Conclusions

The two-time pdf equation was shown to be amenable to numerical solution using stochastic simulation techniques. The autocorrelation coefficient in time allows direct calculation of the macrotime scale, thus dispensing with the transport equation for the dissipation rate, which is the weakest part in single-point closure schemes. The proposed pdf model was applied to the prediction of a plane mixing layer and showed good agreement of moments up to order three with the experiment.

Acknowledgment

This work was supported by the Air Force Office of Scientific Research, Grant No. AFOSR-84-0219.

References

[1]Pope, S. B., "Pdf Methods for Tubulent Reactive Flows," *Energy and Combustion Science,* Vol. 11, No. 2, 1985, pp. 119–192.

[2]Kollmann, W. and Janicka, J., "The Probability Density Function of a Passive Scalar in Turbulent Shear Flows," *Physics of Fluids*, Vol. 25, Oct. 1982, pp. 1755–1769.

[3]Pope, S. B., "Consistent Modeling of Scalars in Turbulent Flows," *Physics of Fluids,* Vol. 26, Feb. 1983, pp. 404–408.

[4]Mehta, R. D. and Westphal, R. V., "An Experimental Study of a Plane Mixing Layer Development," NASA TM-86698, 1985.

[5]Corrsin, S., "Theories of Turbulent Dispersion," *Mecanique de la Turbulence,* edited by A. Farve, Centre National de la Recherche Scientifique, Publ. 108, Paris, 1962, pp. 27–52.

[6]Corrsin, S., "Estimates of the Relations Between Eulerian and Lagrangian Scales in Large Reynolds Number Turbulence," *Journal of the Atmospheric Sciences,* Vol. 20, March 1963, pp. 115–119.

[7]Haworth, D. C. and Pope, S. B., "A Generalized Langevin Model for Turbulent Flows," *Physics of Fluids,* Vol. 29, Feb. 1986, pp. 387–405.

[8]Kollmann, W. and Jones, W. P., "Multi-Scalar pdf Transport Equations for Turbulent Diffusion Flames," *Turbulent Shear Flows* 5, edited by L. J. S. Bradbury, F. Durst, B. E. Launder, F. W. Schmidt, and J. H. Whitelaw, Springer-Verlag, Berlin, FRG, 1987, pp. 296–309.

[9]Rotta, J. C., "Statistische Theorie Nichthomogener Turbulenz," *Zeitschrift fuer Physik,* Vol. 129, Sept. 1951, pp. 547–572.

[10]Craven, R. and Wahba, G., "Smoothing Noisy Data with Spline Functions," *Numerical Mathematics,* Vol. 31, No. 4, 1979, pp. 377–403.