Explicit Algebraic Scalar-Flux Models for Turbulent Reacting Flows

V. Adumitroaie, D. B. Taulbee, and P. Givi
Dept. of Mechanical and Aerospace Engineering, State University of New York at Buffalo, Buffalo, NY 14260

Explicit algebraic scalar-flux models that are valid for three-dimensional turbulent flows are derived from a hierarchy of second-order moment closures. The mathematical procedure is based on the Cayley–Hamilton theorem and is an extension of the scheme developed by Taulbee. Several closures for the pressure–scalar gradient correlations are considered and explicit algebraic relations are provided for the velocity–scalar correlations in both nonreacting and reacting flows. In the latter, the role of the Damköhler number is exhibited in isothermal turbulent flows with nonpremixed reactants. The relationship between these closures and traditional models based on the linear gradient-diffusion approximation is theoretically established. The results of model predictions are assessed by comparison with available laboratory data in turbulent jet flows.

Introduction

Despite extensive recent contributions in direct and large eddy simulations of turbulent reacting flows, the application of such simulations is limited to "simple flows" (Givi, 1994). Based on this fact, it is now widely recognized that the "statistical" approach is *still* the most practical means in computational turbulence, and future capabilities in predictions of engineering turbulent combustion systems depend on the extent of developments in statistical modeling.

The literature on computational prediction of nonreactive turbulent transport is rich with schemes based on single-point statistical closures for moments up to the second order (Taulbee, 1989). Referred to as Reynolds stress models (RSM), these schemes are based on transport equations for the second-order velocity correlations and lead to determination of "nonisotropic eddy-diffusivities." This methodology is more advantageous than the more conventional models based on the Boussinesq approximations with isotropic eddy diffusivities (such as the $k-\epsilon$ type of closures). However, the need for solving additional transport equations for the higher-order moments could potentially make RSM less attractive, especially for practical applications. For example, it has been recently demonstrated (Höfler, 1993) that the computational requirement associated with RSM for predictions of three-dimensional (3-D) engineering flows is significantly higher than that required to implement the $k-\epsilon$ model. The increase is naturally higher for second-order modeling of chemically reacting flows due to the additional length and time scales that have to be considered (Toor, 1991; Jones, 1994; Libby and Williams, 1994).

A modality to reduce the large number of equations associated with RSM is to utilize "algebraic" closures. Such closures are either derived directly from the RSM transport equations, or other types of representations (Speziale, 1991; Yoshizawa, 1988) that lead to anisotropic eddy diffusivities. One of the original contributions in the development of algebraic Reynolds stress models (ARSM) is due to Rodi (1976). In this work, all the stresses are determined from a set of "implicit" equations that must be solved in an iterative manner. A somewhat similar method was applied to the heat-flux equation by Gibson and Launder (1976). Pope (1975) offers an improvement of the procedure by providing an "explicit" solution for the Reynolds stresses. This solution is generated by the use of the Cayley–Hamilton theorem, but is only applicable for predictions of two-dimensional (2-D) mean flows. The extension of this formulation has been recently done by Taulbee (1992) and Gatski and Speziale (1993). In these efforts, the Cayley–Hamilton is used to generate explicit algebraic Reynolds stress models that are valid in both 2-D and 3-D flows.

The objective of this work is to expand upon the formulation developed by Taulbee (1992) (also see Taulbee et al., 1993) for predictions of turbulent flows involving scalar quantities (Brodkey, 1981). The specific objective is to provide explicit algebraic relations for the turbulent flux of scalar vari-

Current address of V. Adumitroaie: CFD Research Corp., Huntsville, AL 35805.

ables. Both nonreacting and reacting flows are considered. In the latter, a second-order, irreversible chemical reaction of the type $A + B \rightarrow P$ is considered in isothermal turbulent flows with initially segregated reactants (Brodkey, 1975; Toor, 1975). The closure explicitly accounts for the influence of the Damköhler number and includes the mixing solution in the limit of zero Damköhler number. Similar to previous contributions, the starting equations are the currently available differential equations for the second-order moments. Accordingly, several previously suggested closures for the pressure–scalar gradients correlations are considered. The final results are compared with available experimental data in turbulent jet flows.

Theoretical Background

With the convention that the angle brackets $\langle\,\rangle$ represent the ensemble mean value of a transport variable and the prime denotes its fluctuations from the mean, the nondimensionalized averaged equations in space (x_i, $i = 1, 2, 3$) and time (t) for incompressible, isothermal turbulent reacting flows are:

$$\frac{\partial\langle u_j\rangle}{\partial x_j} = 0, \tag{1}$$

$$\frac{\partial\langle u_i\rangle}{\partial t} + \frac{\partial\langle u_i\rangle\langle u_j\rangle}{\partial x_j} = -\frac{\partial\langle u_i'u_j'\rangle}{\partial x_j} - \frac{1}{\langle\rho\rangle}\frac{\partial\langle p\rangle}{\partial x_i} + \frac{1}{Re}\frac{\partial^2\langle u_i\rangle}{\partial x_j\partial x_j}, \quad i,j = 1,2,3 \tag{2}$$

$$\frac{\partial\langle Y_\alpha\rangle}{\partial t} + \frac{\partial\langle Y_\alpha\rangle\langle u_j\rangle}{\partial x_j} = -\frac{\partial\langle u_j'\rangle\langle Y_\alpha'\rangle}{\partial x_j} + \frac{1}{ScRe}\frac{\partial^2\langle Y_\alpha\rangle}{\partial x_j\partial x_j} + \langle\dot\omega_\alpha\rangle, \quad \alpha = A, B. \tag{3}$$

Here u_i, p, ρ, Y_α, Re, and Sc denote the ith component of the velocity vector, the pressure, fluid density, mass fraction of species α, the Reynolds number, and the Schmidt number, respectively, while $\langle\dot\omega_\alpha\rangle$ represents the rate of chemical reaction ($\langle\dot\omega_A\rangle = \langle\dot\omega_B\rangle$):

$$\langle\dot\omega_\alpha\rangle = -Da(\langle Y_A\rangle\langle Y_B\rangle + \langle Y_A'Y_B'\rangle), \tag{4}$$

where Da is the Damköhler number. The algebraic formulation entails a two-equation scheme in which the Reynolds stresses and the scalar fluxes are expressed by nonlinear functions of the mean gradients and the time scales of the flow (Wang and Tarbell, 1993). The mechanical time scale is determined by the solution of transport equations for the turbulent kinetic energy $\langle k\rangle = \langle u_i'u_i'\rangle/2$ and for the turbulent dissipation

$$\langle\epsilon\rangle = \frac{1}{Re}\left\langle\frac{\partial u_i'}{\partial x_j}\frac{\partial u_i'}{\partial x_j}\right\rangle.$$

For shear flows, these equations are (Pope, 1978):

$$\frac{\partial\langle k\rangle}{\partial t} + \frac{\partial\langle k\rangle\langle u_j\rangle}{\partial x_j} = -\frac{\partial}{\partial x_j}\left[\langle u_j'k\rangle + \frac{1}{\langle\rho\rangle}\langle p'u_j'\rangle\right] + \frac{1}{Re}\frac{\partial^2\langle k\rangle}{\partial x_j\partial x_j} - \langle u_i'u_j'\rangle\frac{\partial\langle u_i\rangle}{\partial x_j} - \frac{1}{Re}\left\langle\frac{\partial u_i'}{\partial x_j}\frac{\partial u_i'}{\partial x_j}\right\rangle, \tag{5}$$

$$\frac{\partial\langle\epsilon\rangle}{\partial t} + \frac{\partial\langle\epsilon\rangle\langle u_j\rangle}{\partial x_j} = -\frac{\partial}{\partial x_j}\left[\langle u_j'\epsilon\rangle + \frac{2}{Re}\left\langle\frac{\partial p'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}\right\rangle\right] + \frac{1}{Re}\frac{\partial^2\langle\epsilon\rangle}{\partial x_j\partial x_j} - C_{\epsilon_1}\frac{\langle\epsilon\rangle}{\langle k\rangle}\langle u_i'u_j'\rangle\frac{\partial\langle u_i\rangle}{\partial x_j} - C_{\epsilon_2}'\frac{\langle\epsilon\rangle^2}{\langle k\rangle}, \tag{6}$$

with $C_{\epsilon_1} = 1.44$ and $C_{\epsilon_2}' = 1.92 - C_{\epsilon_3}\chi$. The parameter χ represents the correction for the dissipation equation in round jets and is given by $\chi = (\langle k\rangle/\langle\epsilon\rangle)^3\{\mathbf{\Omega\Omega S}\}$, where {} denotes the trace, $\mathbf{S}$ represents the mean-flow strain-rate tensor, $S_{ij} = [\partial\langle u_i\rangle/\partial x_j + \partial\langle u_j\rangle/\partial x_i]/2$, and $\mathbf{\Omega}$ denotes the mean flow rotation-rate tensor, $\Omega_{ij} = [\partial\langle u_i\rangle/\partial x_j - \partial\langle u_j\rangle/\partial x_i]/2$. With $C_{\epsilon_3} = 0.89$, the spreading rate of jet flows is correctly predicted with the nonlinear stress–strain relation.

Treatment of the scalar variable requires the solution of additional transport equations (Chakrabarti et al., 1995) for the reactants' covariance $\langle Y_\alpha'Y_\beta'\rangle$, and dissipations

$$\langle\epsilon_{\alpha\beta}\rangle = \frac{1}{ScRe}\left\langle\frac{\partial Y_\alpha'}{\partial x_j}\frac{\partial Y_\beta'}{\partial x_j}\right\rangle.$$

For the former we have

$$\frac{\partial\langle Y_\alpha'Y_\beta'\rangle}{\partial t} + \frac{\partial\langle Y_\alpha'Y_\beta'\rangle\langle u_j\rangle}{\partial x_j} = -\frac{\partial\langle u_j'Y_\alpha'Y_\beta'\rangle}{\partial x_j} + \frac{1}{ScRe}\frac{\partial^2\langle Y_\alpha'Y_\beta'\rangle}{\partial x_j\partial x_j} - \langle u_j'Y_\alpha'\rangle\frac{\partial\langle Y_\beta\rangle}{\partial x_j} - \langle u_j'Y_\beta'\rangle\frac{\partial\langle Y_\alpha\rangle}{\partial x_j} - \frac{2}{ScRe}\left\langle\frac{\partial Y_\alpha'}{\partial x_j}\frac{\partial Y_\beta'}{\partial x_j}\right\rangle + \langle\dot\omega_\alpha Y_\beta'\rangle + \langle\dot\omega_\beta Y_\alpha'\rangle. \tag{7}$$

By neglecting the third-order mass-fraction correlations, the chemical-source terms in the expanded form read (no summation on Greek indexes in all subsequent equations) $\langle\dot\omega_\alpha Y_\beta'\rangle + \langle\dot\omega_\beta Y_\alpha'\rangle = -Da[(\langle Y_\alpha'Y_A'\rangle + \langle Y_\beta'Y_A'\rangle\langle Y_B\rangle + (\langle Y_\alpha'Y_B'\rangle + \langle Y_\beta'Y_B'\rangle)\langle Y_A\rangle]$. Full resolution of the nonlinear interactions in the chemical scalar fields requires significant computational effort in practical applications (Hill, 1976; Givi, 1989; Fox, 1996). The neglect of the higher-order scalar fluctuations for the configurations considered here is justified (Givi, 1989), but cannot be recommended for general applications (Wang and Tarbell, 1993). In such applications, the single-point probability density function (PDF) or the joint PDF of the scalar variable provides the required information (Toor, 1962; O'Brien, 1980; Dopazo, 1994; Fox, 1996). The inclusion of the PDF is not attempted here.

There are several methods for evaluating the scalar covariance dissipation (Jones, 1994; Newman et al., 1981; Jones and Musonge, 1988; Borghi, 1990). By using the first-order term in the two-scale direct-interaction approximation, Yoshizawa (1988) develops a generic model for the scalar dissipation. An equivalent functional expression is obtained from Yoshizawa's results by making use of the time-scales ratios $r_\alpha = 2\langle k\rangle\langle\epsilon_\alpha\rangle/(\langle\epsilon\rangle\langle Y_\alpha'^2\rangle)$ (hereinafter $\epsilon_\alpha \equiv \epsilon_{\alpha\alpha}$) and replacing the diffusion effect term by the inherent gradient of the turbulent flux. The equivalent form of this equation including the effects of chemical reaction is (Adumitroaie, 1997):

$$\frac{\partial\langle\epsilon_{\alpha\beta}\rangle}{\partial t} + \frac{\partial\langle\epsilon_{\alpha\beta}\rangle\langle u_j\rangle}{\partial x_j} = -\frac{\partial}{\partial x_j}\langle u_j'\epsilon_{\alpha\beta}\rangle + \frac{1}{ScRe}\frac{\partial^2\langle\epsilon_{\alpha\beta}\rangle}{\partial x_j\partial x_j}$$
$$- C_{y_1}\frac{\langle\epsilon\rangle}{\langle k\rangle}\frac{1}{2}\left(\langle u_j'Y_\alpha'\rangle\frac{\partial\langle Y_\beta\rangle}{\partial x_j} + \langle u_j'Y_\beta'\rangle\frac{\partial\langle Y_\alpha\rangle}{\partial x_j}\right)$$
$$- C_{y_2}\frac{\langle\epsilon_{\alpha\beta}\rangle}{\langle k\rangle}\langle u_i'u_j'\rangle\frac{\partial\langle u_i\rangle}{\partial x_j} - C_{y_3}\frac{\langle\epsilon_{\alpha\beta}\rangle^2}{\langle Y_\alpha'Y_\beta'\rangle}$$
$$- C_{y_4}\frac{\langle\epsilon\rangle\langle\epsilon_{\alpha\beta}\rangle}{\langle k\rangle} + \mathcal{S}_{\alpha\beta}, \quad (8)$$

in which the chemical-source term is of the form

$$\mathcal{S}_{\alpha\beta} = -Da[(\langle\epsilon_{A\alpha}\rangle + \langle\epsilon_{A\beta}\rangle)\langle Y_B\rangle + (\langle\epsilon_{B\beta}\rangle + \langle\epsilon_{\alpha B}\rangle)\langle Y_A\rangle]. \quad (9)$$

To determine the magnitudes of the model constants the transport equation for r_α as derived from Eqs. 5–8 can be used in the limiting case of mixing:

$$\frac{\langle k\rangle}{\langle\epsilon\rangle}\frac{1}{r_\alpha}\frac{dr_\alpha}{dt} = (C_{y_1} - r_\alpha)\frac{P_\alpha}{\epsilon_\alpha} + (1 - C_{\epsilon_1} + C_{y_2})\frac{P}{\epsilon}$$
$$+ \left(1 - \frac{C_{y_3}}{2}\right)r_\alpha + (C_{\epsilon_2}' - 1 - C_{y_4}) \quad (10)$$

where the production terms are $P = -\langle u_i'u_j'\rangle\partial\langle u_i\rangle/\partial x_j$ and $P_\alpha = -\langle u_j'Y_\alpha'\rangle\partial\langle Y_\alpha\rangle/\partial x_j$. In the experiments of Warhaft and Lumley (1978) on decaying heated-grid turbulent flows it has been observed that the magnitude of r_α is in the range $0.6 \le r_\alpha \le 2.4$. In the experiments of Beguier et al. (1978) on thermal turbulence in several thin shear flows it is indicated that $r_\alpha \approx 2$. Based on this information, using the procedure detailed by Jones and Musonge (1988) it is possible to estimate the magnitudes of the model constants: $C_{y_1} = r_\alpha = 2.0$, $C_{y_3} = 2.0$, $C_{y_4} = C_{\epsilon_2}' - 1 = 0.92 - C_{\epsilon_3}\chi$, $C_{y_2} = 0.5$.

To complete the closure formulation, all the third-order transport terms are described by the gradient diffusion hypothesis. Denoting by Ξ any of the fluctuation products on which the second-order correlations rest, we have:

$$\langle u_i'\Xi\rangle = -C_s\frac{\langle k\rangle}{\langle\epsilon\rangle}\langle u_i'u_j'\rangle\frac{\partial\langle\Xi\rangle}{\partial x_j}, \quad (11)$$

where C_s is taken to be equal to 0.22 for all nongradient correlations ($\Xi \equiv k$ and $\Xi \equiv Y_\alpha'^2$), whereas for the dissipations ($\Xi \equiv \epsilon$ and $\Xi \equiv \epsilon_\alpha$), $C_s = 0.18$. Also, the molecular transport terms are neglected under the assumption of high Reynolds–Peclet numbers flow.

Explicit Algebraic Models

An improved explicit ARSM for 3-D flow has been derived by Taulbee (1992) from the modeled transport equation for the Reynolds stresses. This model is based on the general linear pressure–strain closure given by Launder et al. (1975). The improvement is due to an extended range of validity; the model is valid in both small and large mean strain fields and time scales of turbulence. The nonlinear stress–strain relation for 3-D mean flows is of the form (Taulbee, 1992; Taulbee et al., 1993) $\mathbf{a} = \mathbf{a}(\mathbf{S}, \mathbf{\Omega})$, where $\mathbf{a}$ is the anisotropic stress tensor, $a_{ij} = [\langle u_i'u_j'\rangle/\langle k\rangle - 2\delta_{ij}/3]$. The ARSM depends on key turbulence parameters such as the turbulence time scale $\tau = \langle k\rangle/\langle\epsilon\rangle$; the production-to-dissipation ratio $P/\langle\epsilon\rangle$, where $P = -\langle k\rangle a_{ij}S_{ji}$ is the production of the turbulent kinetic energy; the invariants of the strain rate and rotation rate tensors $\sigma^2 = (S_{ij}S_{ji})$, $\omega^2 = (\Omega_{ij}\Omega_{ij})$; and the model coefficients of the pressure–strain correlation and the modeled dissipation equation.

A similar line of reasoning is followed to obtain a 3-D algebraic closure for the velocity–scalar correlations. The transport equations governing these correlations are transformed into algebraic expressions by making two assumptions: (1) existence of a "near-asymptotic" state, and (2) the difference in the transport terms is negligible. The starting equations for the convective scalar fluxes are described by

$$\frac{\partial\langle u_i'Y_\alpha'\rangle}{\partial t} + \frac{\partial\langle u_i'Y_\alpha'\rangle\langle u_j\rangle}{\partial x_j} = -\frac{\partial(\langle u_j'u_i'Y_\alpha'\rangle + \langle p'Y_\alpha'\rangle/\langle\rho\rangle\delta_{ij})}{\partial x_j}$$
$$+ \frac{1}{\langle\rho\rangle}\left\langle p'\frac{\partial Y_\alpha'}{\partial x_i}\right\rangle - \left(\langle u_j'u_i'\rangle\frac{\partial\langle Y_\alpha\rangle}{\partial x_j} + \langle u_j'Y_\alpha'\rangle\frac{\partial\langle u_i\rangle}{\partial x_j}\right)$$
$$- Da(\langle u_i'Y_\alpha'\rangle\langle Y_\beta\rangle + \langle u_i'Y_\beta'\rangle\langle Y_\alpha\rangle + \langle u_i'Y_\alpha'Y_\beta'\rangle)$$
$$+ \frac{1}{Re}\left[\frac{\partial}{\partial x_j}\left\langle Y_\alpha'\frac{\partial u_i'}{\partial x_j} + \frac{u_i'}{Sc}\frac{\partial Y_\alpha'}{\partial x_j}\right\rangle\right] - \frac{1+Sc}{ScRe}\left\langle\frac{\partial u_i'}{\partial x_j}\frac{\partial Y_\alpha'}{\partial x_j}\right\rangle. \quad (12)$$

On the RHS of this equation, the following terms are identified: turbulent transport, pressure–scalar gradient correlation, production by the mean velocity and the mean scalar gradients, chemical reaction effects, molecular transport (assumed negligible at high Peclet numbers), and viscous dissipation. Based on the Poisson equation satisfied by the pressure fluctuations one can arguably split the pressure-scalar gradient correlation into two parts corresponding to so-called rapid and slow terms (Lumley, 1978). The rapid term represents an inner product between the velocity gradient tensor and a third-order tensor, the last one subject to symmetry, continuity, and normalization constraints. As suggested by Lumley (1978), since the slow pressure–scalar gradient term and the viscous dissipation term are functions only of turbulent quantities, they can be incorporated into a single closure. The ensemble of the entire pressure-gradient term and viscous-dissipation term enjoys a general relation encompassing some of the formulations proposed in precedent contributions. Consequently, this is written

$$\Phi_{i\alpha} = \frac{1}{\langle\rho\rangle}\left\langle p'\frac{\partial Y'_\alpha}{\partial x_i}\right\rangle - \frac{1+Sc}{ScRe}\left\langle \frac{\partial u'_i}{\partial x_j}\frac{\partial Y'_\alpha}{\partial x_j}\right\rangle$$

$$= -\frac{\mathfrak{C}_{1\alpha}}{2}\frac{\langle\epsilon\rangle}{\langle k\rangle}\langle u'_i Y'_\alpha\rangle + \left[c_1\frac{\partial\langle u_i\rangle}{\partial x_j}\langle u'_j Y'_\alpha\rangle + c_2\frac{\partial\langle u_j\rangle}{\partial x_i}\langle u'_j Y'_\alpha\rangle\right.$$

$$+ c_3\frac{\partial\langle u_j\rangle}{\partial x_k}a_{ij}\langle u'_k Y'_\alpha\rangle + c_4\frac{\partial\langle u_k\rangle}{\partial x_j}(a_{ij}\langle u'_k Y'_\alpha\rangle + a_{jk}\langle u'_i Y'_\alpha\rangle)$$

$$\left. + c_5\frac{\partial\langle u_i\rangle}{\partial x_j}a_{jk}\langle u'_k Y'_\alpha\rangle + c_6\frac{\partial\langle Y_\alpha\rangle}{\partial x_j}a_{ij}\langle k\rangle\right]. \quad (13)$$

The model coefficients in this equation are taken from Launder (1975):

$$\mathfrak{C}_{1\alpha} = 6.4, \quad c_1 = 0.5, \quad c_i = 0; \quad i = 2,6, \quad (14)$$

Jones and Musonge (1988):

$$\mathfrak{C}_{1\alpha} = 6/\left[1 + 1.5(a_{jk}a_{jk})^{1/2}\right], \quad c_1 = 1.09, \quad c_2 = 0.51,$$

$$c_i = 0; \quad i = 3,5; \quad c_6 = 0.12, \quad (15)$$

Rogers et al. (1989):

$$\mathfrak{C}_{1\alpha} = 18\left(1 + \frac{130}{ScRe_t}\right)^{0.25}\left(1 + \frac{12.5}{Re_t^{0.48}}\right)^{-2.08} - \left(\frac{P}{\langle\epsilon\rangle} - 1\right)$$

$$- r_\alpha\left(\frac{P_\alpha}{\langle\epsilon_\alpha\rangle} - 1\right), \quad c_i = 0; \quad i = 1,6, \quad (16)$$

where $Re_t = 4\langle k\rangle^2/(\langle\epsilon\rangle\nu)$, and Shih et al. (1990):

$$\mathfrak{C}_{1\alpha} = \psi + r_\alpha - \frac{(\psi - 1)II_d}{\left(II_d + 3a_{jk}d_{jk}^2/2 - 3a_{jk}d_{jk}/2\right)} + HF_D^{1/2},$$

$$c_1 = 4/5, \quad c_2 = -1/5, \quad c_3 = 1/10,$$

$$c_4 = -3/10, \quad c_5 = 1/5, \quad c_6 = 0, \quad (17)$$

where $H = 1.1 + 0.55(2\psi - 1)\tanh[4(r_\alpha - 1)]$; $\psi = 1 + F/18\exp(-7.77/Re_l^{1/2})\{72/Re_l^{1/2} + 80.1\log[1 + 15.6(-II + 1.15III)]\}$, with $F = 1 + 27III/8 + 9II/4$, a parameter involving the second invariant $II = -1/2a_{ij}a_{ji}$ and the third invariant $III = -1/3a_{ij}a_{jk}a_{ki}$ of the Reynolds stress anisotropy tensor; $Re_l = 4\langle k\rangle^2/(9\langle\epsilon\rangle\nu)$ denotes the turbulence Reynolds number: $d_{jk} = (\langle u'_j Y'_\alpha\rangle\langle u'_k Y'_\alpha\rangle - \langle u'_j u'_k\rangle\langle Y'^2_\alpha\rangle)/(\langle u'_p Y'_\alpha\rangle\langle u'_p Y'_\alpha\rangle - 2\langle k\rangle\langle Y'^2_\alpha\rangle)$; $F_D = 9/2 - 27d_{jj}^2/2 + 9d_{jj}^3$; II_d is the second invariant of the tensor d_{jk}; $d_{jj}^2 = d_{jl}d_{lj}$; and $d_{jj}^3 = d_{jl}d_{lm}d_{mj}$.

To proceed, let us denote the mechanical–chemical correlation coefficient (normalized scalar flux) by:

$$\varphi_{i\alpha} = \frac{\langle u'_i Y'_\alpha\rangle}{(\langle k\rangle\langle Y'^2_\alpha\rangle)^{1/2}}. \quad (18)$$

The transport equation for the correlation coefficient $\varphi_{i\alpha}$ ($\alpha \neq \beta$) is of the form:

$$\frac{D\varphi_{i\alpha}}{Dt} = \frac{1}{(\langle k\rangle\langle Y'^2_\alpha\rangle)^{1/2}}$$

$$\times\left[\frac{\partial T^\alpha_{ij}}{\partial x_j} - \frac{\varphi_{i\alpha}}{2}\left(\frac{\langle k\rangle}{\langle Y'^2_\alpha\rangle}\right)^{1/2}\frac{\partial T^\alpha_j}{\partial x_j} - \frac{\varphi_{i\alpha}}{2}\left(\frac{\langle Y'^2_\alpha\rangle}{\langle k\rangle}\right)^{1/2}\frac{\partial T_j}{\partial x_j}\right]$$

$$-\left[\frac{\varphi_{i\alpha}\langle\epsilon_\alpha\rangle}{\langle Y'^2_\alpha\rangle}\left(\frac{P_\alpha}{\langle\epsilon_\alpha\rangle} - 1 + \frac{\mathfrak{S}_\alpha}{\langle\epsilon_\alpha\rangle}\right) + \frac{\varphi_{i\alpha}}{2\tau}\left(\frac{P}{\langle\epsilon\rangle} - 1\right)\right]$$

$$+ \bar{P}_{i\alpha} + \bar{\Phi}_{i\alpha} + \bar{\mathfrak{S}}_{i\alpha}, \quad (19)$$

where the notation D/Dt indicates the convective transport, and T^α_{ij}, T^α_j, and T_j denote turbulent transports of the scalar flux, the scalar variance, and the kinetic energy, respectively. Moreover $P_\alpha = -(\langle k\rangle\langle Y'^2_\alpha\rangle)^{1/2}\varphi_{j\alpha}\partial\langle Y_\alpha\rangle/\partial x_j$ is the production of scalar variance; $\mathfrak{S}_\alpha = \langle\dot{\omega}_\alpha Y'_\alpha\rangle$ is the chemical source term in the $\langle Y'^2_\alpha\rangle$ equation; and the remaining quantities are the normalized production, pressure-gradient, and the chemical-source term:

$$\bar{P}_{i\alpha} = -\left(\frac{\langle k\rangle}{\langle Y'^2_\alpha\rangle}\right)^{1/2}\left(a_{ij} + \frac{2}{3}\delta_{ij}\right)\frac{\partial\langle Y_\alpha\rangle}{\partial x_j} - \varphi_{j\alpha}(S_{ij} + \Omega_{ij}) \quad (20)$$

$$\bar{\Phi}_{i\alpha} = -\frac{\mathfrak{C}_{1\alpha}}{2\tau}\varphi_{i\alpha} + [(c_1 + c_2)S_{ij}\varphi_{j\alpha}$$

$$+ (c_1 - c_2)\Omega_{ij}\varphi_{j\alpha} + (c_3 + c_4)a_{ij}S_{jk}\varphi_{k\alpha} + c_5 a_{jk}S_{ij}\varphi_{k\alpha}$$

$$+ (c_3 - c_4)a_{ij}\Omega_{jk}\varphi_{k\alpha} + c_5 a_{jk}\Omega_{ij}\varphi_{k\alpha} + c_4 a_{jk}S_{jk}\varphi_{i\alpha}]$$

$$+ c_6\left(\frac{\langle k\rangle}{\langle Y'^2_\alpha\rangle}\right)^{1/2}a_{ij}\frac{\partial\langle Y_\alpha\rangle}{\partial x_j} \quad (21)$$

$$\bar{\mathfrak{S}}_{i\alpha} = -Da\left(\varphi_{i\alpha}\langle Y_\beta\rangle + \varphi_{i\beta}\langle Y_\alpha\rangle + \gamma_{i\alpha\beta}\langle Y'^2_\beta\rangle^{1/2}\right). \quad (22)$$

Here $\gamma_{i\alpha\beta} = \langle u'_i Y'_\alpha Y'_\beta\rangle/(\langle k\rangle\langle Y'^2_\alpha\rangle\langle Y'^2_\beta\rangle)^{1/2}$ is the normalized covariance flux vector.

The results of direct numerical simulations (DNS) of nonreacting passive scalar mixing in homogeneous turbulent shear flow (Rogers et al., 1989) suggest the existence of an asymptotic state for the normalized correlation coefficient $\varphi_{i\alpha}$, but not for the scalar flux itself. This observation justifies the first assumption, at least for reacting flows near the frozen limit. The second approximation is yet to be substantiated and its assessment requires future DNS or laboratory experiments. Under these assumptions the term representing the convective transport is set to zero and the difference in turbulence diffusion terms is discarded. This procedure leads to an algebraic system of equations for the two unknown vectors $\varphi_{i\alpha}$ and $\varphi_{i\beta}$:

$$\begin{cases}\boldsymbol{\varphi}_\alpha + D_\alpha\mathbf{A}\boldsymbol{\varphi}_\alpha + B_\alpha\boldsymbol{\varphi}_\beta + \mathbf{C}_\alpha = 0\\ \boldsymbol{\varphi}_\beta + D_\beta\mathbf{A}\boldsymbol{\varphi}_\beta + B_\beta\boldsymbol{\varphi}_\alpha + \mathbf{C}_\beta = 0,\end{cases} \quad (23)$$

where the coefficients are

$$D_\alpha = \frac{2\tau h_\alpha}{1+2Da\tau h_\alpha \langle Y_\beta \rangle}, \qquad D_\beta = \frac{2\tau h_\beta}{1+2Da\tau h_\beta \langle Y_\alpha \rangle}, \quad (24)$$

$$B_\alpha = Da\langle Y_\alpha \rangle D_\alpha, \qquad B_\beta = Da\langle Y_\beta \rangle D_\beta, \quad (25)$$

with

$$h_\alpha = \left[\mathcal{C}_{1\alpha} - 1 + (1+2c_4)\frac{P}{\langle \epsilon \rangle} + r_\alpha \left(\frac{P_\alpha}{\langle \epsilon_\alpha \rangle} - 1 + \frac{\mathcal{S}_\alpha}{\langle \epsilon_\alpha \rangle} \right) \right]^{-1}, \quad (26)$$

$$h_\beta = \left[\mathcal{C}_{1\beta} - 1 + (1-2c_4)\frac{P}{\langle \epsilon \rangle} + r_\beta \left(\frac{P_\beta}{\langle \epsilon_\beta \rangle} - 1 + \frac{\mathcal{S}_\beta}{\langle \epsilon_\beta \rangle} \right) \right]^{-1}, \quad (27)$$

and the vector terms read:

$$C_{i\alpha} = D_\alpha \left\{ \left(\frac{\langle k \rangle}{\langle Y_\alpha'^2 \rangle} \right)^{1/2} \left[(1-c_6)a_{ki} + \frac{2}{3}\delta_{ki} \right] \times \frac{\partial \langle Y_\alpha \rangle}{\partial x_k} + Da\langle Y_\beta'^2 \rangle^{1/2} \gamma_{i\alpha\beta} \right\}, \quad (28)$$

$$C_{i\beta} = D_\beta \left\{ \left(\frac{\langle k \rangle}{\langle Y_\beta'^2 \rangle} \right)^{1/2} \left[(1-c_6)a_{ki} + \frac{2}{3}\delta_{ki} \right] \times \frac{\partial \langle Y_\beta \rangle}{\partial x_k} + Da\langle Y_\alpha'^2 \rangle^{1/2} \gamma_{i\alpha\beta} \right\}. \quad (29)$$

Finally, the anisotropy of the turbulent diffusivity is ensured by the properties of the second-order tensor $\mathbf{A}$:

$$A_{ik} = [(1-c_1-c_2)S_{ik} + (1-c_1+c_2)\Omega_{ik} - (c_3+c_4)a_{ij}S_{jk} - c_5 a_{kj}S_{ji} - (c_3-c_4)a_{ij}\Omega_{jk} + c_5 a_{kj}\Omega_{ji}]. \quad (30)$$

This tensor turns out to be traceless ($A_{ii}=0$) as a consequence of incompressibility and of the particular values taken by the constants, c_i's. Now, the solution of the system of Eqs. 23 is conveniently represented in the form:

$$\begin{cases} \varphi_\alpha = -\mathbf{M}^{-1}[(\boldsymbol{\delta} + D_\beta \mathbf{A})\mathbf{C}_\alpha - B_\alpha \mathbf{C}_\beta] \\ \varphi_\beta = -\mathbf{M}^{-1}[(\boldsymbol{\delta} + D_\alpha \mathbf{A})\mathbf{C}_\beta - B_\beta \mathbf{C}_\alpha], \end{cases} \quad (31)$$

where $\mathbf{M}$ denotes the matrix $[(1-B_\alpha B_\beta)\boldsymbol{\delta} + (D_\alpha + D_\beta)\mathbf{A} + D_\alpha D_\beta \mathbf{A}^2]$. The expressions for the turbulent fluxes of reacting scalars exhibit the influence of the Damköhler number Da. Also, the coupling between the reactants is reflected by the nonlinear dependence on the mean scalars and the presence of the covariance flux.

To provide a computationally efficient algorithm, the matrix $\mathbf{M}$ is inverted analytically. This is achieved by the use of the Cayley–Hamilton theorem and yields an expansion defining a natural basis for this problem:

$$\varphi_\alpha = \sum_{n=0}^{2} a_n \mathbf{A}^n C_\alpha + \sum_{n=0}^{2} a_n' \mathbf{A}^n C_\beta. \quad (32)$$

In the Appendix the inversion procedure via the Cayley–Hamilton theorem is outlined and the coefficients a_n and a_n' are listed. The final results provide an explicit solution for the scalar fluxes. In the limit $Da \to \infty$, the use of the mixing solution ($Da = 0$) for the transport of a Shvab–Zel'dovich variable (Toor, 1962; Williams, 1985) is recommended.

Illustrative Examples

In this section, we present some sample results of numerical calculations based on the models given earlier. There are two primary reasons for conducting these simulations: (1) model assessments via comparisons with laboratory data, (2) demonstration of the model capabilities in comparison to traditional closures based on the linear gradient-diffusion approximation. The flow configurations considered consist of turbulent-plane and round-jet flows for which laboratory data are available. The mean flow motion in these shear flows is assumed 2-D or axisymmetric. The space coordinates are identified by $\mathbf{x} = [x, y]$, where x is the streamwise coordinate denoting the direction of the flow's principal evolution, and y represents the cross-stream direction. The velocity field is identified by $\mathbf{u} = [u, v]$. In nonreacting flow simulations the mass fraction of one conserved species, Y_A, is considered. In the jet configurations, $Y_A = 1$ is issued at the inlet into a surrounding of $Y_A = 0$. For the reactive case, $Y_A = 1$ is issued at the inlet into a surrounding of $Y_B = 1$. These species are assumed thermodynamically identical, and there is no trace of one of these species at the feed of the other one; that is, complete initial segregation. Also, the heat generated by the reaction is assumed negligible.

The transport equations governing the velocity and the scalar fields are of parabolic type with the thin-shear layer approximation. For 2-D mean flows, the ARSM (Taulbee, 1992) is of the form:

$$\mathbf{a} = -2C_\mu \tau \left[\mathbf{S} + b_1 g \tau \sigma^2 \left(\frac{2}{3}\boldsymbol{\delta} - \boldsymbol{\delta}^{(2)} \right) + b_2 g \tau (\mathbf{S}\boldsymbol{\Omega} - \boldsymbol{\Omega}\mathbf{S}) \right], \quad (33)$$

where $\boldsymbol{\delta}^{(2)} \equiv [\delta_{ij}^{(2)}] = 1$ for $i = j = 1, 2$ and 0 otherwise. The parameters C_μ and g are given by

$$C_\mu = \frac{4g/15}{1 - \frac{2}{3}(b_1 g\tau)^2 \sigma^2 + 2(b_2 g \tau)^2 \omega^2},$$

$$g = \left[C_1 + C_{\epsilon_2} - 2 + (2 - C_{\epsilon_1})P/\langle \epsilon \rangle + \frac{\tau}{\sigma}\frac{D\sigma}{Dt} \right]^{-1}, \quad (34)$$

where C_1, b_1, and b_2 are constants from the pressure–strain correlation model ($C_1 = 1.8$, $b_1 = (5 - 9C_2)/11$, $b_2 = (1 + 7C_2)/11$, $C_2 = 0.45$). In the self-preserving regions of turbulent shear flows, the convective term $D\sigma/Dt$ can be neglected. For 2-D mean flows, with zero rate of reaction the scalar-flux model is expressed as

$$\langle u_i' Y_\alpha' \rangle = -\frac{2\tau h_\alpha \langle k \rangle}{1 + II_G} \Delta_{ij} \frac{\partial \langle Y_\alpha \rangle}{\partial x_j}, \quad (35)$$

which has the gradient form, but with an anisotropic diffusivity. With the thin-shear layer approximation,

$$II_G = [(c_2 + c_4 a_{22})(1 - c_1 - c_3 a_{11} - c_5 a_{22}) - c_3^2 a_{12}^2] \times \left(2 h_\alpha \tau \frac{d\langle u \rangle}{dy}\right)^2 \quad (36)$$

and the nonzero components of the diffusivity tensor, Δ_{ij}, are

$$\Delta_{11} = \left(1 - 2c_3 \tau h_\alpha a_{12} \frac{d\langle u \rangle}{dy}\right)\left[(1 - c_6) a_{11} + \frac{2}{3}\right] - 2\tau h_\alpha (1 - c_6) a_{21} \frac{d\langle u \rangle}{dy} (1 - c_1 - c_3 a_{11} - c_5 a_{22}) \quad (37)$$

$$\Delta_{22} = \left(1 + 2c_3 \tau h_\alpha a_{12} \frac{d\langle u \rangle}{dy}\right)\left[(1 - c_6) a_{22} + \frac{2}{3}\right] + 2\tau h_\alpha (1 - c_6) a_{12} \frac{d\langle u \rangle}{dy} (c_2 + c_4 a_{22}) \quad (38)$$

$$\Delta_{33} = (1 + II_G)\left[(1 - c_6) a_{33} + \frac{2}{3}\right] \quad (39)$$

$$\Delta_{12} = \left(1 - 2c_3 \tau h_\alpha a_{12} \frac{d\langle u \rangle}{dy}\right)(1 - c_6) a_{12} - 2\tau h_\alpha \left[(1 - c_6) a_{22} + \frac{2}{3}\right] \frac{d\langle u \rangle}{dy} (1 - c_1 - c_3 a_{11} - c_5 a_{22}) \quad (40)$$

$$\Delta_{21} = \left(1 + 2c_3 \tau h_\alpha a_{12} \frac{d\langle u \rangle}{dy}\right)(1 - c_6) a_{21} + 2\tau h_\alpha \left[(1 - c_6) a_{11} + \frac{2}{3}\right] \frac{d\langle u \rangle}{dy} (c_2 + c_4 a_{22}). \quad (41)$$

These anisotropic diffusivities are determined directly from the velocity gradient, the components of anisotropic Reynolds stress tensor, and the model coefficients.

The numerical algorithm for the solution of the transport equations augmented by the algebraic closures is based on a first-order upwind differencing for the convection terms and a second-order central differencing scheme for all the other terms. Due to the anisotropic character of the algebraic closures, it is possible to evaluate all the components of the Reynolds stress tensor and the scalar-flux vectors. In this evaluation, the terms appearing as model coefficients (e.g., $P/\langle \epsilon \rangle$ in Eq. 26) are treated in an iterative procedure. The implementation of the boundary conditions is similar to that in many previous simulations of parabolic shear flows (e.g., Taulbee, 1989). In the results presented below, the spatial coordinates are presented by $\eta = y/(x - x_0)$ for hydrodynamic and

$$\eta^* = \frac{y}{y(\langle Y_A \rangle = 0.5 \langle Y_A \rangle_{CL})}$$

for the scalar variables. x_0 denotes the virtual origin of the jets. In the nonreacting jets, the subscript CL denotes values at the center line (i.e., $y = 0$). In the reacting jets, the corresponding profile of Y_A under no chemical reaction is employed in the normalization. In all the figures below, the transverse variations of the statistical variables are presented.

The experimental results pertaining to the velocity fields of planar jets as reported by Gutmark and Wygnanski (1976), Bradbury (1965), and Heskestad (1965) are compared with the model predictions in Figure 1. The agreement is reasonable for the mean streamwise velocity and also for the components of the Reynolds stress tensor. The predicted spreading rate ($dy_{\langle u \rangle / \langle u \rangle_{CL} = 0.5}/dx$) is 0.105, which is within the range suggested by experimental measurements. In Figure 2, the predicted results for the mean and the variance of the nonreacting scalar are compared with the experimental data reported by Browne et al. (1984), Bashir and Uberoi (1975), Uberoi and Singh (1975), Jenkins and Goldschmidt (1973), and Antonia et al. (1983). Figure 2 indicates that the models based on the coefficients proposed by Launder (1975), Jones and Musonge (1988), and Shih et al. (1990) predict the mean scalar values in these experiments reasonably well. These models also yield good predictions of the experimental data

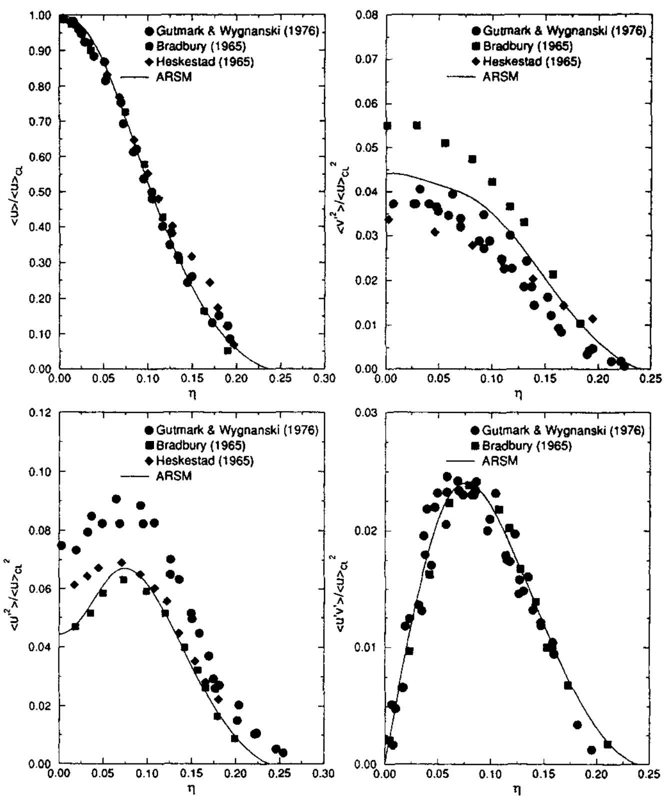

Figure 1. Cross-stream variation of $\langle u \rangle / \langle u \rangle_{CL}$, $\langle u'^2 \rangle / \langle u \rangle_{CL}^2$, $\langle v'^2 \rangle / \langle u \rangle_{CL}^2$, and $\langle u'v' \rangle / \langle u \rangle_{CL}^2$ for the planar jet.

of Uberoi and Singh (1975) for the scalar variance. All the other experimentally measured variance profiles are better predicted by the model with the coefficients of Rogers et al. (1989).

The procedure by which the Reynolds stress tensor and the scalar-flux vector are determined by our explicit solution allows a direct comparison of the calculated fluxes with data. This comparison is made in Figure 2 and indicates that the models with coefficients of Launder (1975), Jones and Musonge (1988), and Shih et al. (1990) yield results in reasonable agreements with the experimental data of Jenkins (1976), but overpredict the experimental data of Antonia (1985) and Browne et al. (1984). These data are in better agreement with the predicted fluxes based on the model of Rogers et al. (1989). The lower spreading rates predicted by the model of Rogers et al. (1989) are primarily due to the relatively large values adopted by the parameter $\mathcal{C}_{1\alpha}$. In this model, the proposed form of $\mathcal{C}_{1\alpha}$ and its correlation with the turbulence Reynolds number are determined with comparative assessments by DNS results of homogeneous turbulent shear flows. In the jet-flow experiments, as considered here, a direct application of the model yields relatively large values for $\mathcal{C}_{1\alpha}$, and thus small turbulent diffusivities. Consequently, the predicted scalar spreading rate is lower than that measured experimentally. Nevertheless, in the core region, the results predicted by this model are closer to the majority of available experimental data compared to predictions based on other models.

With these results it is possible to perform an *a posteriori* appraisal of the closures based on conventional linear gradient-diffusion hypotheses. For example, the parameters C_μ and Sc_t as given by

$$\langle u'v'\rangle = -\nu_t \frac{\partial \langle u\rangle}{\partial y}, \qquad \nu_t = C_\mu \frac{\langle k\rangle^2}{\langle \epsilon\rangle}, \tag{42}$$

$$\langle v'Y'_\alpha\rangle = -\frac{\nu_t}{Sc_t}\frac{\partial \langle Y_\alpha\rangle}{\partial y}, \tag{43}$$

can be directly evaluated. The explicit algebraic relation for C_μ is given by Eq. 34; the relation for the turbulent Schmidt number is

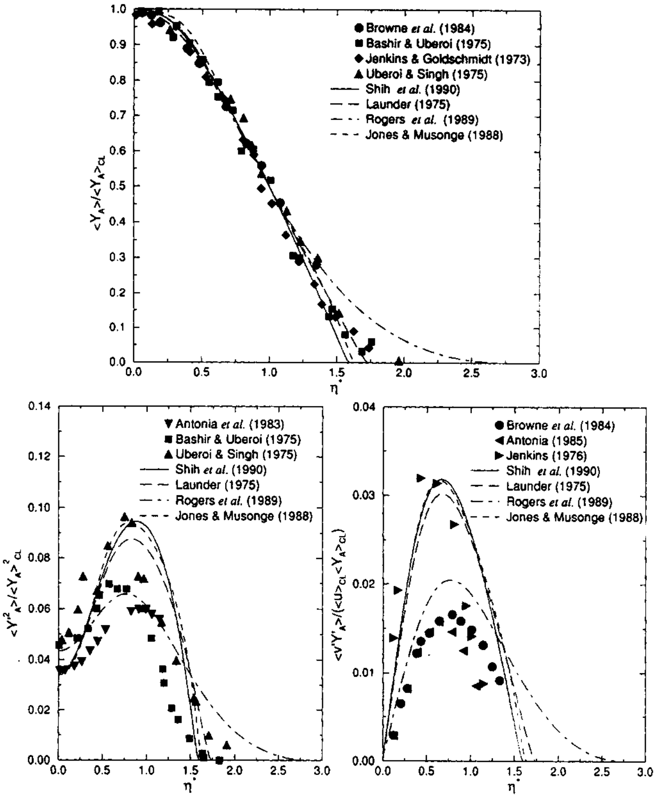

Figure 2. Cross-stream variation of $\langle Y_A\rangle/\langle Y_A\rangle_{CL}$, $\langle Y_A'^2\rangle/\langle Y_A\rangle_{CL}^2$, and $\langle v'Y_A'\rangle/(\langle u\rangle_{CL}\langle Y_A\rangle_{CL})$ for the planar jet.

$$Sc_t = \frac{1-4\left[c_3^2a_{12}^2-(c_2+c_4a_{22})(1-c_1-c_3a_{11}-c_5a_{22})\right]\left(h_\alpha\tau\frac{d\langle u\rangle}{dy}\right)^2}{h_\alpha\left\{\left(1+2c_3\tau h_\alpha a_{12}\frac{d\langle u\rangle}{dy}\right)\left[(1-c_6)a_{22}+\frac{2}{3}\right]+2\tau h_\alpha(1-c_6)a_{12}\frac{d\langle u\rangle}{dy}(c_2+c_4a_{22})\right\}}\times\frac{2g}{15\left[1+\left(b_2^2-\frac{b_1^2}{3}\right)\left(g\tau\frac{d\langle u\rangle}{dy}\right)^2\right]}. \tag{44}$$

Figure 3 shows the cross-stream variations of C_μ and of Sc_t and r_α based on the pressure–scalar gradient model in Shih et al. (1990). These results can be compared with $C_\mu = 0.09$ and $Sc_t = 0.7$, typically employed in the linear gradient-diffusion approximations. Also, the ratio of the velocity to scalar time scales (r_α) indicates that an approximate constant value can be used at the central region of the layer. This is in accord with the results of Beguier et al. (1978) and Tavoularis and Corrsin (1981). As expected, there are large variations for all these parameters near the free stream. The amplitude of the parameters at the free streams can be controlled by modifications of the boundary conditions. An extract specification of these conditions requires inputs from laboratory measurements.

Some of the influences of the chemical reaction on the scalar field in the turbulent plane jet are presented in Figures 4 and 5. In the calculations pertaining to these figures, the model coefficients of Launder (1975) are employed. The influence of reaction in modifying the amplitudes of the scalars' means (Figure 1), variances (not shown), and turbulent fluxes are captured by the model (Dutta and Tarbell, 1989; Gao and O'Brien, 1991). In accord with the physics of turbulent flows with segregated reactants, the unmixedness is negative throughout the layer (Shenoy and Toor, 1989; Leonard and Hill, 1991; Wang and Tarbell, 1993). The same is true in the limit of no chemistry; in that case, the amplitude is slightly larger (Leonard and Hill, 1988; Frankel et al., 1993, 1995).

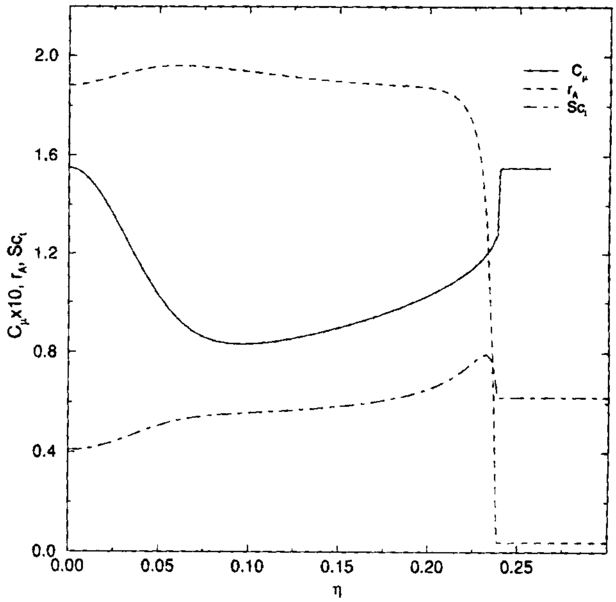

Figure 3. Cross-stream variation of C_μ, Sc_t, and r_A for the planar jet.

The comparison between the full second-order model (Eq. 12) and the algebraic closure in predicting the scalar fluxes is presented in Figure 5, and indicates that the transverse flux as predicted by the algebraic closure is in close agreement with that by the transport-equation model. However, there are differences between the two predictions of the streamwise flux near the jet center line. The zero value of this flux in the algebraic model is due to the thin-shear-layer approximation. The neglect of the axial diffusion in this approximation combined with the gradient diffusion nature of the algebraic model can only yield zero flux values at the axis of symmetry. While the thin-shear-layer approximation is also invoked in the transport equation model, the inclusion of the streamwise convective effects in the transport equations can, and does, yield nonzero flux values. If the thin-layer assumption is relaxed in the algebraic model, the inclusion of axial scalar gradients would generate nonzero scalar-flux values at the center line, thus reducing the disagreement. It must be noted that for this class of flows the cross-stream scalar flux is more dominant than the streamwise flux in influencing the mean scalar distribution and the production terms. Thus, the agreement observed in Figure 5 is encouraging in support of the algebraic approximation. Nevertheless, this is demonstrated here only for a "simple" flow configuration. The im-

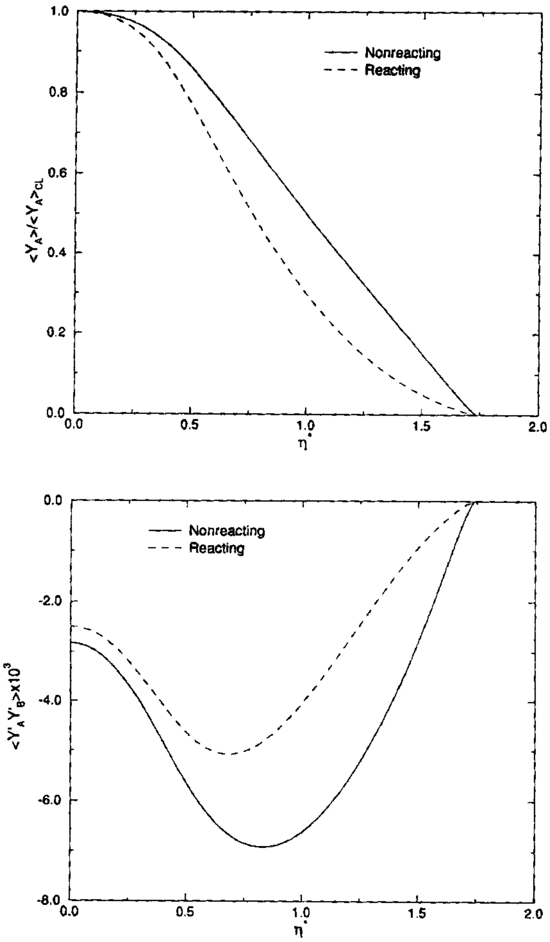

Figure 4. Cross-stream variation of $\langle Y_A\rangle/\langle Y_A\rangle_{CL}$ and $\langle Y_A' Y_B'\rangle$ for the nonreacting and reacting planar jets.

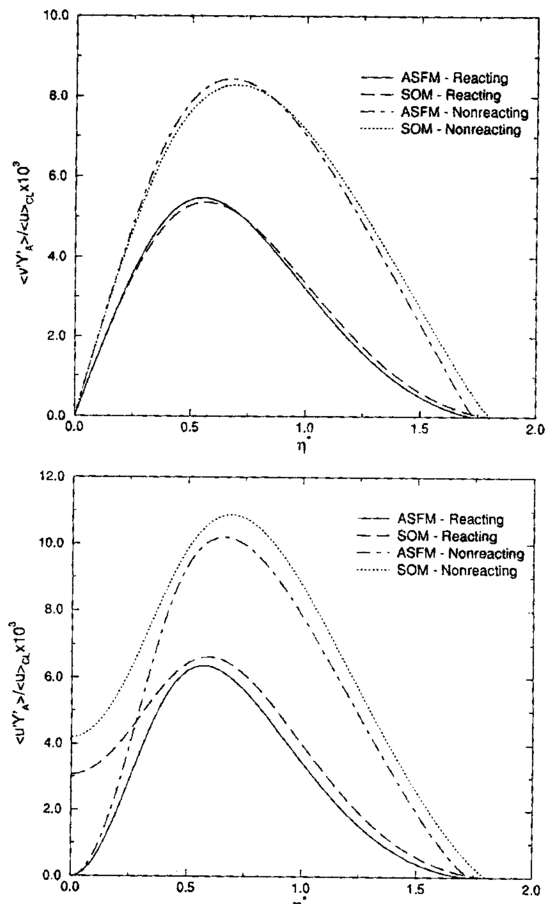

Figure 5. Cross-stream variation of $\langle v'Y_A'\rangle/\langle u\rangle_{CL}$ and $\langle u'Y_A'\rangle/\langle u\rangle_{CL}$ for the nonreacting and reacting planar jets.

It was computed via the algebraic scalar-flux model (ASFM) and the full second-order transport-equation model (SOM).

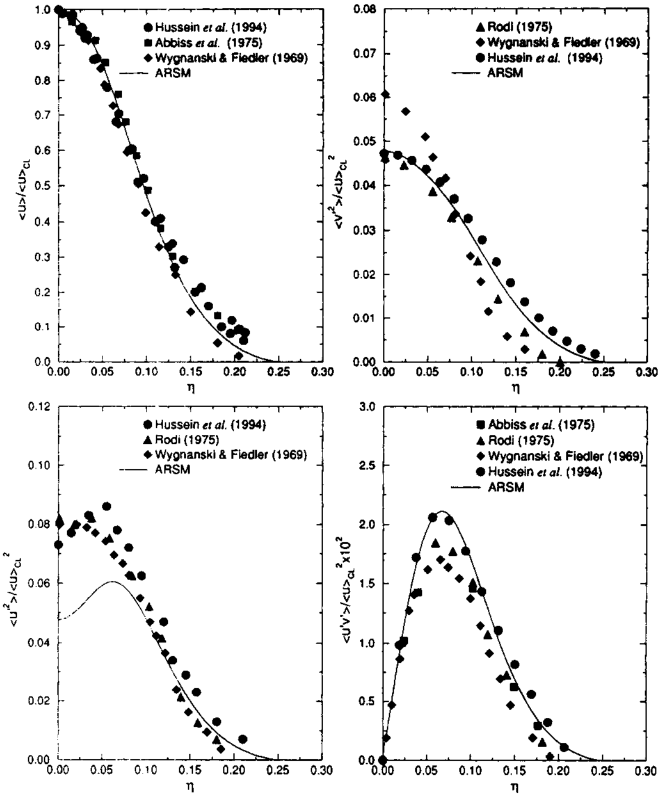

Figure 6. Cross-stream variation of $\langle u \rangle / \langle u \rangle_{CL}$, $\langle u'^2 \rangle / \langle u \rangle_{CL}^2$, $\langle v'^2 \rangle / \langle u \rangle_{CL}^2$, and $\langle u'v' \rangle / \langle u \rangle_{CL}^2$ for the round jet.

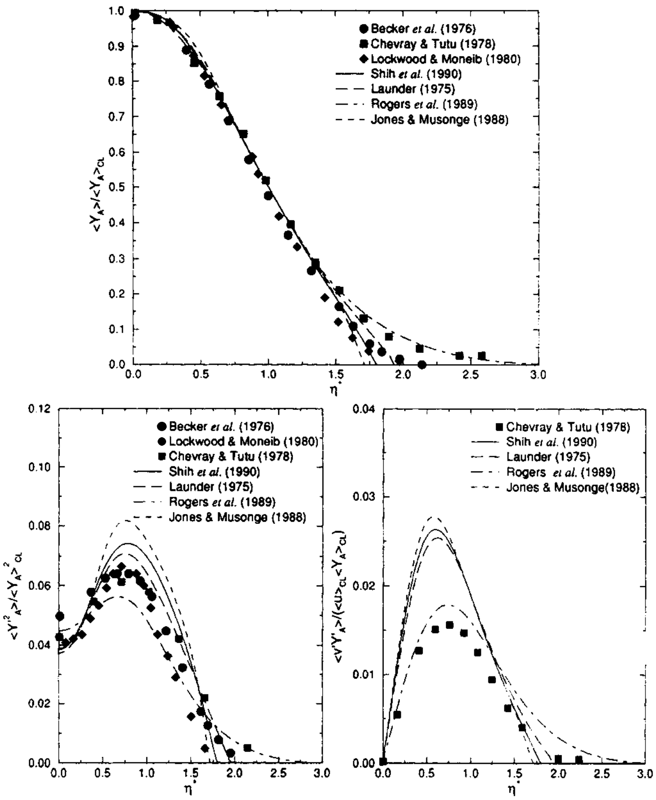

Figure 7. Cross-stream variation of $\langle Y_A \rangle / \langle Y_A \rangle_{CL}$, $\langle Y_A'^2 \rangle / \langle Y_A \rangle_{CL}^2$, and $\langle v'Y_A' \rangle / (\langle u \rangle_{CL} \langle Y_A \rangle_{CL})$ for the round jet.

plementation of the model for complex flows would be very useful in further assessment of the algebraic approximation.

The performance of the models for prediction of axisymmetric jet flows is assessed in Figures 6 and 7 where the experimental data of Hussein et al. (1994), Abbiss et al. (1975), Wygnanski and Fiedler (1969), and Rodi (1975) are used for hydrodynamics variables, and those of Chevray and Tutu (1978), Becker et al. (1976), and Lockwood and Moneib (1980) for the scalar variables. The predicted hydrodynamic spreading rate with the axisymmetric correction is 0.094, and is in agreement with the experimental results of Hussein et al. (1994). Again, all the mean values are reasonably well predicted. The same is true for the Reynolds stresses, except for the streamwise normal stress in the central region for which an improvement of about 30% can be obtained if all the components of the rate of deformation tensor are considered. Consistent with the planar-jet results, the model with coefficients of Rogers et al. (1989) results in lower scalar diffusivities. This model also yields lower values for the second-order moments in the core. The model predictions based on the coefficients of Launder (1975), Jones and Musonge (1988), and Shih et al. (1990) overpredict the experimentally measured scalar's covariance and turbulent fluxes. The predictions based on the model of Rogers et al. (1989) again yield better agreement for the scalar fluxes. It is important, however, to indicate that the experiments of Chevray and Tutu (1978) are not conducted in the self-preserving regions of the jet. Therefore a definite assessment cannot be made without comparisons with further data.

From the preceding comparisons, it can be concluded that the algebraic model developed here provides an effective means of predicting the second-order moments in reacting turbulent flows. Because of their anisotropic feature, these algebraic schemes are more general than the conventional linear gradient-diffusion schemes (Toor, 1991). The explicit nature of the relations is particularly convenient for applications in practical flows of the type considered by Höfler (1993). With the reasonable agreement of the model results with experimental data in simple configurations, the methodology is recommended for predictions of more complex flows. Even so, the restrictions stemming from the assumptions involved in the development of the models have to be clearly underscored. The results shown here indicate the need for refinement of current pressure-gradient correlation closures. Moreover, the modeled transport equations for the passive scalar dissipations have known inconsistencies (Pope, 1983). These and the nature of the pressure-correlation models might raise realizability concerns, which can be considerably alleviated by implementing some of the techniques developed by Shih and Shabbir (1994). The present models are devised for high Reynolds–Peclet number flows; therefore some corrections might be required for modeling of the near-wall regions. In flows with important nonlocal effects such as the action of diffusion over long distances, rapidly varying flows, or other kind of flows far from equilibrium, the results by algebraic models are expected to have a larger departure from those by the full second-order moment formulation. In flows with very large strain fields there is a potential for singular behavior of the scalar-flux models. This issue requires further investigations of complex flows. Further improvements are recommended by considering low Reynolds–Peclet number effects, the higher-order moments of the scalar–scalar fluctuations in reacting flows, and the effects of exothermicity in nonequilibrium chemically reacting systems.

Acknowledgment

This work is part of a research program sponsored by the NASA Langley Research Center under Grant NAG-1-1122. Dr. J. Philip Drummond is the Technical Monitor. Computational resources are provided by the SEAS Computing Center at SUNY-Buffalo.

Literature Cited

Abbiss, J. B., L. J. S. Bradbury, and M. P. Wright, "Measurements in an Axisymmetric Jet Using a Photon Correlator," *Proc. LDA Symp.*, Copenhagen, Denmark (1975).

Adumitroaie, V., PhD Thesis, Dept. of Mechanical and Aerospace Engineering, State Univ. of New York at Buffalo, Buffalo (1997).

Antonia, R. A., L. W. Browne, A. J. Chambers, and S. Rajagopalan, "Budget of Temperature Variance in a Turbulent Plane Jet," *Int. J. Heat Mass Transfer*, **26**, 41 (1983).

Antonia, R. A., "On a Heat Transfer Model for a Turbulent Plane Jet," *Int. J. Heat Mass Transfer*, **28**, 1805 (1985).

Bashir, J., and M. S. Uberoi, "Experiments on Turbulent Structure and Heat Transfer in a Two Dimensional Jet," *Phys. Fluids*, **18**, 405 (1975).

Becker, H. A., H. C. Hottel, and G. C. Williams, "The Nozzle Fluid Concentration Field of the Round Turbulent Free Jet," *J. Fluid Mech.*, **30**, 285 (1976).

Beguier, C., I. Dekeyser, and B. E. Launder, "Ratio of Scalar and Velocity Dissipation Time Scales in Shear Flow Turbulence," *Phys. Fluids*, **21**, 307 (1978).

Borghi, R., "Turbulent Premixed Combustion: Further Discussions on the Scales of Fluctuations," *Combust. Flame*, **80**, 304 (1990).

Bradbury, L. J. S., "The Structure of Self-Preserving Turbulent Plane Jet," *J. Fluid Mech.*, **23**, 31 (1965).

Brodkey, R. S., ed., *Turbulence in Mixing Operation*, Academic Press, New York (1975).

Brodkey, R. S., "Fundamental of Turbulent Motion," *Chem. Eng. Commun.*, **8**, 1 (1981).

Browne, L. W. B., A. R. Antonia, and A. J. Chambers, "The Interaction Region of a Turbulent Plane Jet," *J. Fluid Mech.*, **149**, 355 (1984).

Chakrabarti, M., R. M. Kerr, and J. C. Hill, "Direct Numerical Simulation of Chemical Selectivity in Homogeneous Turbulence," *AIChE J.*, **41**, 2356 (1995).

Chevray, R., and N. K. Tutu, "Intermittency and Preferential Transport of Heat in a Round Jet," *J. Fluid Mech.*, **88**, 133 (1978).

Dopazo, C., "Recent Developments in PDF Methods," *Turbulent Reacting Flows*, Chap. 7, P. A. Libby and F. A. Williams, eds., Academic Press, New York, p. 375 (1994).

Dutta, A., and J. M. Tarbell, "Closure Models for Turbulent Reacting Flows," *AIChE J.*, **35**, 2013 (1989).

Fox, R. O., "Computational Methods for Turbulent Reacting Flows in Chemical Process Industry," *Rev. Inst. Fr. Pet.*, **51**, 215 (1996).

Frankel, S. H., C. K. Madnia, and P. Givi, "Comparative Assessment of Closures for Turbulent Reacting Flows," *AIChE J.*, **39**, 899 (1993).

Frankel, S. H., P. A. McMurtry, and P. Givi, "Linear Eddy Modeling of Reactant Conversion and Selectivity in Homogeneous Turbulence," *AIChE J.*, **41**, 258 (1995).

Gao, F., and E. E. O'Brien, "Direct Numerical Simulations of Reacting Flows in Homogeneous Turbulence," *AIChE J.*, **37**, 1459 (1991).

Gatski, T. B., and C. G. Speziale, "On Explicit Algebraic Stress Models for Complex Turbulent Flows," *J. Fluid Mech.*, **254**, 59 (1993).

Gibson, M. M., and B. E. Launder, "On the Calculation of Horizontal, Turbulent, Free Shear Flows under Gravitational Influence," *ASME J. Heat Transfer*, **98C**, 81 (1976).

Givi, P., "Model Free Simulations of Turbulent Reactive Flows," *Prog. Energy Combust. Sci.*, **15**, 1 (1989).

Givi, P., "Spectral and Random Vortex Methods in Turbulent Reacting Flows," *Turbulent Reacting Flows*, Chap. 8, P. A. Libby and F. A. Williams, eds., Academic Press, London, p. 475 (1994).

Gutmark, E., and I. Wygnanski, "The Planar Turbulent Jet," *J. Fluid Mech.*, **73**, 465 (1976).

Heskestad, G., "Hot Wire Measurements in a Plane Turbulent Jet," *J. Appl. Mech.*, **32**, 721 (1965).

Hill, J. C., "Homogeneous Turbulent Mixing with Chemical Reaction," *Ann. Rev. Fluid Mech.*, **8**, 135 (1976).

Höfler, T., "Reynolds Stress Model (RSM) in FIRE," *FIRE Newsl.*, **5**, 1 (1993).

Hussein, H. J., S. P. Capp, and W. K. George, "Velocity Measurements in a High-Reynolds-number, Momentum-Conserving, Axisymmetric, Turbulent Jet," *J. Fluid Mech.*, **258**, 31 (1994).

Jenkins, P. E., and V. W. Goldschmidt, "Mean Temperature and Velocity in a Plane Turbulent Jet," *ASME J. Fluids Eng.*, **95**, 581 (1973).

Jenkins, P. E., "Some Measured Temperature Characteristics in a Two Dimensional Heated Jet of Air," *AMS J. Eng. Power*, **98**, 501 (1976).

Jones, W. P., and P. Musonge, "Closure of the Reynolds Stress and Scalar Flux Equations," *Phys. Fluids*, **31**, 3589 (1988).

Jones, W. P., "Turbulence Modelling and Numerical Solution Methods for Variable Density and Combusting Flows," *Turbulent Reacting Flows*, Chap. 6, P. A. Libby and F. A. Williams, eds., Academic Press, London, p. 309 (1994).

Launder, B. E., G. J. Reece, and W. Rodi, "Progress in the Development of a Reynolds-Stress Turbulence Closure," *J. Fluid Mech.*, **68**, 537 (1975).

Launder, B. E., "On the Effects of a Gravitational Field on the Turbulent Transport of Heat and Momentum," *J. Fluid Mech.*, **67**, 569 (1975).

Leonard, A. D., and J. C. Hill, "Direct Numerical Simulation of Turbulent Flows with Chemical Reaction," *J. Sci. Comput.*, **3**, 25 (1988).

Leonard, A. D., and J. C. Hill, "Scalar Dissipation and Mixing in Turbulent Reacting Flows," *Phys. Fluids A.*, **3**, 1286 (1991).

Libby, P. A., and F. A. Williams, eds., *Turbulent Reacting Flows*, Academic Press, London (1994).

Lockwood, F. C., and H. A. Moneib, "Fluctuating Temperature Measurement in a Heated Round Free Jet," *Combust. Sci. Technol.*, **22**, 63 (1980).

Lumley, J. L., "Computational Modeling of Turbulent Flows," *Adv. Appl. Mech.*, **18**, 123 (1978).

Newman, G. R., B. E. Launder, and J. L. Lumley, "Modelling the Behaviour of Homogeneous Scalar Turbulence," *J. Fluid Mech.*, **111**, 217 (1981).

O'Brien, E. E., "The Probability Density Function (PDF) Approach to Reacting Turbulent Flows," *Turbulent Reacting Flows*, Chap. 5, P. A. Libby and F. A. Williams, eds., Springer-Verlag, Heidelberg, p. 185 (1980).

Pope, S. B., "A More General Effective-Viscosity Hypothesis," *J. Fluid Mech.*, **72**, 331 (1975).

Pope, S. B., "An Explanation of the Turbulent Round-jet/Plane-jet Anomaly," *AIAA J.*, **16**, 279 (1978).

Pope, S. B., "Consistent Modeling of Scalars in Turbulent Flows," *Phys. Fluids*, **26**, 404 (1983).

Rodi, W., "A New Method of Analyzing Hot-wire Signals in Highly Turbulent Flow and Its Evaluation in Round Jet," Disa Information 17 (1975).

Rodi, W., "A New Algebraic Relation for Calculating the Reynolds Stresses," *ZAMM*, **56**, T219 (1976).

Rogers, M. M., N. N. Mansour, and W. C. Reynolds, "An Algebraic Model for the Turbulent Flux of a Passive Scalar," *J. Fluid Mech.*, **203**, 77 (1989).

Shenoy, U. V., and H. L. Toor, "Turbulent Micromixing Parameters from Reactive Mixing Measurements," *AIChE J.*, **35**, 1692 (1989).

Shih, T.-H., and A. Shabbir, "Methods of Ensuring Realizability for Non-realizable Second Order Closures," ICOMP 94-14, NASA Lewis Research Center, Cleveland, OH (1994) (also available as *NASA TM 106681*).

Shih, T.-H., J. L. Lumley, and J.-Y. Chen, "Second-Order Modeling of Passive Scalar in a Turbulent Shear Flow," *AIAA J.*, **28**, 610 (1990).

Speziale, C. G., "Analytical Methods for the Development of Reynolds Stress Closures in Turbulence," *Ann. Rev. Fluid Mech.*, **23**, 107 (1991).
Taulbee, D. B., J. R. Sonnenmeier, and K. W. Wall, "Stress Relation for Three-Dimensional Turbulent Flows," *Phys. Fluids*, **6**, 1399 (1993).
Taulbee, D. B., "Engineering Turbulence Models," *Advances in Turbulence*, W. K. George and R. Arndt, eds., Hemisphere, New York, p. 75 (1989).
Taulbee, D. B., "An Improved Algebraic Reynolds Stress Model and Corresponding Nonlinear Stress Model," *Phys. Fluid A*, **4**, 2555 (1992).
Tavoularis, S., and S. Corrsin, "Experiments in Nearly Homogeneous Turbulent Shear Flow with a Uniform Mean Temperature Gradient. Part 1," *J. Fluid Mech.*, **104**, 311 (1981).
Toor, H. L., "Mass Transfer in Dilute Turbulent and Nonturbulent Systems with Rapid Irreversible Reactions and Equal Diffusivities," *AIChE J.*, **8**, 70 (1962).
Toor, H. L., "The Non-premixed Reaction: $A+B \rightarrow$ Products," *Turbulence in Mixing Operation*, R. S. Brodkey, ed., Academic Press, New York, p. 123 (1975).
Toor, H. L., "Turbulent Diffusivities in Reacting Systems," *AIChE J.*, **37**, 1737 (1991).
Uberoi, M. S., and P. I. Singh, "Turbulent Mixing in a Two Dimensional Jet," *Phys. Fluids*, **18**, 764 (1975).
Wang, D. M., and J. M. Tarbell, "Closure Models for Turbulent Reacting Flows with a Non-homogeneous Concentration Field," *Chem. Eng. Sci.*, **48**, 3907 (1993).
Warhaft, Z., and J. L. Lumley, "An Experimental Study of the Decay of Temperature Fluctuations in Grid-Generated Turbulence," *J. Fluid Mech.*, **88**, 659 (1978).
Williams, F. A., *Combustion Theory*, 2nd ed., Benjamin/Cummings, Menlo Park, CA (1985).
Wygnanski, I., and H. Fiedler, "Some Measurements in the Self-Preserving Jet," *J. Fluid Mech.*, **38**, 577 (1969).
Yoshizawa, A., "Statistical Modelling of Passive-Scalar Diffusion in Turbulent Shear Flows," *J. Fluid Mech.*, **195**, 541 (1988).

Appendix

The procedure leading to explicit solutions for the scalar-flux vector, as governed by Eq. 23 is described here.

Consider an arbitrary 3-D second-order tensor $\boldsymbol{Q} \equiv [Q_{ij}]$, and the corresponding Kronecker tensor $\boldsymbol{\delta} \equiv [\delta_{ij}]$. According to the Cayley–Hamilton theorem, this matrix satisfies its own characteristic polynomial:

$$\boldsymbol{Q}^3 - I_Q \boldsymbol{Q}^2 + II_Q \boldsymbol{Q} - III_Q \boldsymbol{\delta} = \boldsymbol{0}, \tag{A1}$$

where $I_Q = \{\boldsymbol{Q}\} = Q_{ii}$, $II_Q = 1/2[\{\boldsymbol{Q}\}^2 - \{\boldsymbol{Q}^2\}] = 1/2[Q_{ii}Q_{jj} - Q_{ij}Q_{ji}]$, $III_Q = 1/6[\{\boldsymbol{Q}\}^3 - 3\{\boldsymbol{Q}\}\{\boldsymbol{Q}^2\} + 2\{\boldsymbol{Q}^3\}] = 1/6[Q_{ii}Q_{jj}Q_{kk} - 3Q_{ii}Q_{jk}Q_{kj} + 2Q_{ij}Q_{jk}Q_{ki}]$ are the three tensorial invariants. Multiplying the characteristic polynomial with $\boldsymbol{Q}^{-1}$ and solving for the inverse, we obtain

$$\boldsymbol{Q}^{-1} = \frac{1}{III_Q}\left(\boldsymbol{Q}^2 - I_Q \boldsymbol{Q} + II_Q \boldsymbol{\delta}\right). \tag{A2}$$

This relation can be used now to find explicit solutions to the problem considered here. For example, for the case with $Da = 0$ (pure mixing), we can write

$$\boldsymbol{\varphi}_\alpha = -(\boldsymbol{\delta} + \boldsymbol{G})^{-1}\boldsymbol{C}, \tag{A3}$$

where $\boldsymbol{G} = D_\alpha \boldsymbol{A}$. Hence

$$(\boldsymbol{\delta}+\boldsymbol{G})^{-1} = \frac{1}{III_{\delta+G}}[\boldsymbol{G}^2 + (2 - I_{\delta+G})\boldsymbol{G} + (1 - I_{\delta+G} + II_{\delta+G})\boldsymbol{\delta}]. \tag{A4}$$

It is easy to show that $I_{\delta+G} = I_G + \{\boldsymbol{\delta}\}$, $II_{\delta+G} = 2I_G + II_G + \{\boldsymbol{\delta}\}$, $III_{\delta+G} = I_G + II_G + III_G + (\{\boldsymbol{\delta}\}/3)$. Therefore the normalized scalar flux vector takes the form:

$$\boldsymbol{\varphi}_\alpha = a_0 \boldsymbol{C} + a_1 \boldsymbol{G}\boldsymbol{C} + a_2 \boldsymbol{G}^2 \boldsymbol{C} \tag{A5}$$

with the coefficients:

$$a_0 = -\frac{1 + I_G + II_G}{1 + I_G + II_G + III_G} \tag{A6}$$

$$a_1 = \frac{1 + I_G}{1 + I_G + II_G + III_G} \tag{A7}$$

$$a_2 = -\frac{1}{1 + I_G + II_G + III_G}. \tag{A8}$$

In a solenoidal velocity field the pressure–scalar gradient correlation includes a rapid term that satisfies the zero-divergence constraint. This further translates into $\{\boldsymbol{A}\} = 0$; thus,

$$a_0 = -\frac{1 - \frac{1}{2}\{\boldsymbol{G}^2\}}{1 - \frac{1}{2}\{\boldsymbol{G}^2\} + \frac{1}{3}\{\boldsymbol{G}^3\}} \tag{A9}$$

$$a_1 = \frac{1}{1 - \frac{1}{2}\{\boldsymbol{G}^2\} + \frac{1}{3}\{\boldsymbol{G}^3\}} \tag{A10}$$

$$a_2 = -\frac{1}{1 - \frac{1}{2}\{\boldsymbol{G}^2\} + \frac{1}{3}\{\boldsymbol{G}^3\}} \tag{A11}$$

The reacting case is somewhat more complex. Nonetheless, by following the same procedure explicit solutions are obtained:

$$\boldsymbol{\varphi}_\alpha = a_0 \boldsymbol{C}_\alpha + a_0' \boldsymbol{C}_\beta + a_1 \boldsymbol{A}\boldsymbol{C}_\alpha + a_1' \boldsymbol{A}\boldsymbol{C}_\beta + a_2 \boldsymbol{A}^2 \boldsymbol{C}_\alpha + a_2' \boldsymbol{A}^2 \boldsymbol{C}_\beta \tag{A12}$$

$$\boldsymbol{\varphi}_\beta = b_0 \boldsymbol{C}_\alpha + b_0' \boldsymbol{C}_\beta + b_1 \boldsymbol{A}\boldsymbol{C}_\alpha + b_1' \boldsymbol{A}\boldsymbol{C}_\beta + b_2 \boldsymbol{A}^2 \boldsymbol{C}_\alpha + b_2' \boldsymbol{A}^2 \boldsymbol{C}_\beta, \tag{A13}$$

with the coefficients:

$$a_0 = -\frac{F_\beta\left(F_\alpha + D_\alpha^2\frac{\{A^3\}}{3}\right) + B_\alpha B_\beta\left[\frac{\{A^3\}}{3}(D_\beta F_\alpha - ED_\alpha)D_\beta - E\left(E + \frac{\{A^3\}}{3}D_\alpha D_\beta\right)\right]}{(1-B_\alpha B_\beta)\left(F_\alpha F_\beta - E^2 B_\alpha B_\beta\right)}, \quad \text{(A14)}$$

$$a'_0 = B_\alpha \frac{F_\alpha\left(F_\beta + D_\beta^2\frac{\{A^3\}}{3}\right) + D_\alpha\frac{\{A^3\}}{3}(D_\alpha F_\beta - ED_\beta) - EB_\alpha B_\beta\left(E + \frac{\{A^3\}}{3}D_\alpha D_\beta\right)}{(1-B_\alpha B_\beta)\left(F_\alpha F_\beta - E^2 B_\alpha B_\beta\right)}, \quad \text{(A15)}$$

$$a_1 = \frac{B_\alpha B_\beta[E(D_\beta - D_\alpha) + F_\alpha D_\beta] - D_\alpha F_\beta}{D_\alpha\left(F_\alpha F_\beta - E^2 B_\alpha B_\beta\right)} \quad \text{(A16)}$$

$$a'_1 = \frac{B_\alpha}{D_\alpha}\frac{D_\alpha F_\beta - D_\beta F_\alpha - E(D_\beta - D_\alpha B_\alpha B_\beta)}{F_\alpha F_\beta - E^2 B_\alpha B_\beta} \quad \text{(A17)}$$

$$a_2 = \frac{D_\alpha F_\beta - ED_\beta B_\alpha B_\beta}{F_\alpha F_\beta - E^2 B_\alpha B_\beta} \quad \text{(A18)}$$

$$a'_2 = -B_\alpha \frac{D_\alpha F_\beta - ED_\beta}{F_\alpha F_\beta - E^2 B_\alpha B_\beta}, \quad \text{(A19)}$$

with the shorthand notations:

$$F_\alpha = (1-B_\alpha B_\beta)\left(D_\alpha\frac{\{A^2\}}{2} - \frac{1}{D_\alpha} - \frac{B_\alpha B_\beta}{D_\beta}\right) - D_\alpha^2\frac{\{A^3\}}{3} \quad \text{(A20)}$$

$$F_\beta = (1-B_\alpha B_\beta)\left(D_\beta\frac{\{A^2\}}{2} - \frac{1}{D_\beta} - \frac{B_\alpha B_\beta}{D_\alpha}\right) - D_\beta^2\frac{\{A^3\}}{3} \quad \text{(A21)}$$

$$E = \left(\frac{1}{D_\alpha} + \frac{1}{D_\beta}\right)(1 - B_\alpha B_\beta) - D_\alpha D_\beta\frac{\{A^3\}}{3}. \quad \text{(A22)}$$

The coefficients b_i are obtained from the a_i's through the permutations $\alpha \to \theta$, $\beta \to \alpha$, $\theta \to \beta$, $a_0 \to b'_0$, $a'_0 \to b_0$, $a_1 \to b'_1$, $a'_1 \to b_1$, $a_2 \to b'_2$, and $a'_2 \to b_2$.

Manuscript received Dec. 16, 1996, and revision received Mar. 14, 1997.