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Explicit Algebraic Scalar Flux Approximation

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A new method is proposed to obtain explicit solutions of the algebraic approximation to second-moment closure models for the turbulent flux of passive scalars. Equivalently, the method gives exact equilibrium solutions to scalar flux transport models. An intermediate step relates scalar flux transport to the Lagrangian dispersion tensor in homogeneous turbulence. Solvability and stability properties of closure models are assessed by the solution. The exact solution serves as a closure model for the asymmetric eddy diffusion tensor.

I. Introduction

THE ability of turbulent motion to mix a passive scalar is a property of the flowfield, not of the scalar. A prediction method for scalar transport, then, might be regarded as a proposed relationship between the turbulent scalar flux and the Reynolds stresses responsible for that flux. The simplest model is Reynolds analogy or the turbulent Prandtl number. But this Prandtl number has been found to depend significantly on flow properties and geometry; more elaborate models will inevitably be needed for aerospace applications involving heat-transfer prediction. The present paper describes a mathematical analysis of equilibrium solutions to a commonly used closure of the scalar-flux transport equation. It develops a closed-form solution that explicitly relates scalar flux to Reynolds stress. The solution provided is for the case of a two-dimensional mean flow.

The algebraic stress approximation is a systematic method to derive non-Bousinesq constitutive relations for turbulent transport. It is formally equivalent to an equilibrium solution in homogeneous flow. So the present solution plays a dual role as an approximate constitutive relation and as an exact equilibrium solution. This connection between equilibrium states and algebraic approximation makes the present analysis relevant to the general subject of development and use of turbulence closure models.

The exact scalar-flux equation in homogeneous turbulence is[1]

$$\frac{\mathrm{d}\overline{\theta u_i}}{\mathrm{d}t} = -\overline{u_i u_j}\partial_j\Theta - \overline{\theta u_j}\partial_j U_i + \wp_{\theta_i} \tag{1}$$

The mean scalar concentration is Θ and $\overline{\theta u_i}$ is the turbulent Reynolds flux. The term $-\overline{\theta u_j}\partial_j U_i$ is the rate of turbulent flux production from mean flow gradients, and $-\overline{u_i u_j}\partial_j\Theta$ is production from mean scalar gradient. The definition

$$\wp_{\theta_i} = -(1/\rho)\overline{\theta\partial_i p} - (\kappa + \nu)\overline{\partial_j u_i \partial_j \theta} \tag{2}$$

incorporates all unclosed terms into a single expression. Closure requires that $\wp_{\theta_i}$ be replaced by a function of the dependent variable $\overline{\theta u_i}$. If the Reynolds stress $\overline{u_i u_j}$, mean velocity, and mean scalar concentration are given, the functional form

$$\wp_{\theta_i} = F_i(\overline{\theta u_\alpha}, \partial_\beta U_\alpha, \partial_\alpha\Theta, \overline{u_\alpha u_\beta}) \tag{3}$$

can be considered. The superposition principle for passive scalars allows only terms that are linear in concentration. The most general form of F_i, subject to this constraint, was discussed by Dakos and Gibson.[2] The following form has been used in several models[1,3]:

$$\wp_{\theta_i} = -(c_M\varepsilon/k)\overline{\theta u_i} + c_{\theta_1}\overline{u_i u_j}\partial_j\Theta + c_{\theta_2}\overline{\theta u_j}\partial_j U_i + c_{\theta_3}\overline{\theta u_j}\partial_i U_j \tag{4}$$

in which k is the turbulence kinetic energy and ε is the rate of its dissipation: $T \equiv k/\varepsilon$ provides a turbulent timescale. Substituting Eq. (4) into Eq. (1) gives the closed equation

$$\frac{\mathrm{d}\overline{\theta u_i}}{\mathrm{d}t} = (c_{\theta_1} - 1)\overline{u_i u_j}\partial_j\Theta + (c_{\theta_2} - 1)\overline{\theta u_j}\partial_j U_i - \frac{c_M\varepsilon}{k}\overline{\theta u_i} + c_{\theta_3}\overline{\theta u_j}\partial_i U_j \tag{5}$$

We wish to obtain the equilibrium solution to this equation.

II. Equilibrium Assumption

In homogeneous turbulence the mean temperature gradient is governed by

$$\frac{\mathrm{d}\partial_i\Theta}{\mathrm{d}t} = -\partial_i U_j \partial_j\Theta \tag{6}$$

so, in general, the mean gradient will be time dependent. As the first step toward obtaining a time-independent solution, we introduce the dispersion tensor D_{ij}, defined by

$$\overline{\theta u_i} = -D_{ij}\partial_j\Theta \tag{7}$$

Substituting this into Eq. (5), and using Eq. (6), gives the evolution equation

$$\frac{\mathrm{d}D_{ij}}{\mathrm{d}t} = D_{ik}\partial_k U_j + (1 - c_{\theta_1})\overline{u_i u_j} + (c_{\theta_2} - 1)\partial_k U_i D_{kj} - \frac{c_M\varepsilon}{k}D_{ij} + c_{\theta_3}D_{kj}\partial_i U_k \tag{8}$$

Note that D_{ij} is neither a symmetric nor a trace-free tensor.

The dispersion tensor is a property of the turbulence, not of the passive scalar; in Lagrangian theory $D_{ij} = \overline{u_i X_j}$, where $X_i(t)$ is the random position of a fluid element. Indeed, Durbin and Shabany[4] derive Eq. (8) from a Langevin equation for the fluid trajectories. Hence, the dispersion tensor should be normalized by turbulence statistics; the nondimensional form $K_{ij} = D_{ij}\varepsilon/k^2$ should become constant at equilibrium. Generally, k and ε themselves are not constant at equilibrium; for instance, in homogeneous straining flow, the $k - \varepsilon$ model predicts that both grow in time at the same exponential rate. The dispersion tensor (and eddy viscosity too) then grows in time like k^2/ε; similarly, $\overline{u_i u_j}$ grows like k, which is why the normalized quantity K_{ij} attains a constant equilibrium state.

Differentiating $K_{ij} = D_{ij}\varepsilon/k^2$ gives

$$\frac{\mathrm{d}K_{ij}}{\mathrm{d}t} = \frac{\varepsilon}{k^2}\frac{\mathrm{d}D_{ij}}{\mathrm{d}t} + \frac{D_{ij}}{k^2}\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} - \frac{2\varepsilon D_{ij}}{k^3}\frac{\mathrm{d}k}{\mathrm{d}t}$$

Using the standard k and ε equations

$$\frac{\mathrm{d}k}{\mathrm{d}t} = P - \varepsilon$$

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} = \frac{c_{\epsilon 1}P - c_{\epsilon 2}\varepsilon}{T}$$

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the transport equation for K_{ij} is obtained:

$$\frac{\mathrm{d}K_{ij}}{\mathrm{d}t} = K_{ik}\partial_k U_j + (1 - c_{\theta_1})\frac{\overline{u_i u_j}}{Tk} + (c_{\theta_2} - 1)\partial_k U_i K_{kj} - \frac{K_{ij}}{g_\theta T} + c_{\theta_3} K_{kj}\partial_i U_k \tag{9}$$

in which

$$g_\theta = [c_M + (2 - c_{\epsilon 1})\mathcal{P} + c_{\epsilon 2} - 2]^{-1}$$

and $\mathcal{P} = P/\varepsilon$.

III. Explicit Solution

The equilibrium condition is $\mathrm{d}K_{ij}/\mathrm{d}t = 0$. Introducing this into Eq. (9) and rewriting the velocity gradient in terms of the rate of strain and rate of rotation tensors results in the matrix equation

$$\boldsymbol{K} - \boldsymbol{K}\times\boldsymbol{S} + \boldsymbol{K}\times\boldsymbol{W} - a_1\boldsymbol{S}\times\boldsymbol{K} - a_2\boldsymbol{W}\times\boldsymbol{K} = \boldsymbol{\tau} \tag{10}$$

in which $a_1 = c_{\theta_2} + c_{\theta_3} - 1$, $a_2 = c_{\theta_2} - c_{\theta_3} - 1$, and

$$S_{ij} = \frac{g_\theta T(\partial_j U_i + \partial_i U_j)}{2}$$

$$W_{ij} = \frac{g_\theta T(\partial_j U_i - \partial_i U_j)}{2} \tag{11}$$

$$\tau_{ij} = (1 - c_{\theta_1})g_\theta \frac{\overline{u_i u_j}}{k}$$

Recall that $T = k/\varepsilon$. $\boldsymbol{\tau}$ is a scaled Reynolds stress tensor that acts as a source term in Eq. (10).

If expression (10) were used in a nonequilibrium, nonhomogeneous flow, it would be referred to as an algebraic flux model. As it stands, it is an implicit relation of the form

$$K_{ij} = F_{ij}(\boldsymbol{W}, \boldsymbol{S}, \boldsymbol{\tau}) \tag{12}$$

Pope[5] and Gatski and Speziale[6] explained how algebraic stress models (for $\overline{u_i u_j}/k$) can be solved explicitly by using tensor representation theorems. In that method, the solution is expanded in an integrity basis. The integrity basis provides the general tensorial form of the solution. The coefficients of the expansion are scalar functions of tensor invariants that must be found for the particular model. They are obtained through use of the Cayley–Hamilton theorem generalized to functions of two tensors. In the case of Eq. (12), the solution involves three tensors, $\boldsymbol{W}$, $\boldsymbol{S}$, and $\boldsymbol{\tau}$; although only terms linear in $\boldsymbol{\tau}$ arise, the lack of symmetry and trace-free constraints results in a seven-component integrity basis, even in two dimensions (in Pope's case,[5] the two-dimensional basis contained four elements). The lack of symmetry makes the analysis rather messy, and we were not able to obtain a solution by that method.

In the following, we describe a new method to obtain an explicit algebraic flux model by solving Eq. (10) in closed form. There is no need to expand the solution in the integrity basis, although the final formula can be put into that form. The approach uses properties of the direct product of two tensors (see Appendix A), combined with the generalized Cayley–Hamilton theorem.

First, Eq. (10) is written as

$$\boldsymbol{I}\times\boldsymbol{K}\times\boldsymbol{I} - \boldsymbol{I}\times\boldsymbol{K}\times\boldsymbol{S} + \boldsymbol{I}\times\boldsymbol{K}\times\boldsymbol{W} - a_1\boldsymbol{S}\times\boldsymbol{K}\times\boldsymbol{I} - a_2\boldsymbol{W}\times\boldsymbol{K}\times\boldsymbol{I} = \boldsymbol{\tau} \tag{13}$$

where $\boldsymbol{I}$ is the identity tensor. This is a matrix equation with a matrix unknown $\boldsymbol{K}$; it is of the form Eq. (A3). The method explained in Appendix A is used to rewrite this $n \times n$ matrix equation as an n^2-dimensional vector equation for $\boldsymbol{k}$ with a coefficient matrix similar to Eq. (A6):

$$(\boldsymbol{I}\otimes\boldsymbol{I}^T - \boldsymbol{I}\otimes\boldsymbol{S}^T + \boldsymbol{I}\otimes\boldsymbol{W}^T - a_1\boldsymbol{S}\otimes\boldsymbol{I}^T - a_2\boldsymbol{W}\otimes\boldsymbol{I}^T)\boldsymbol{k} = \boldsymbol{\tau} \tag{14}$$

In two dimensions

$$\boldsymbol{k} = (K_{11}, K_{12}, K_{21}, K_{22})^T \qquad \text{and} \qquad \boldsymbol{\tau} = (\tau_{11}, \tau_{12}, \tau_{21}, \tau_{22})^T$$

The direct product $\boldsymbol{A}\otimes\boldsymbol{B}$ of two $n \times n$ matrices is an $n^2 \times n^2$ matrix, as explained in Eq. (A1). Because $\boldsymbol{S}$ and $\boldsymbol{W}$ are symmetric and antisymmetric, respectively, Eq. (14) can be rewritten

$$(\boldsymbol{I}\otimes\boldsymbol{I} - \boldsymbol{I}\otimes\boldsymbol{S} - \boldsymbol{I}\otimes\boldsymbol{W} - a_1\boldsymbol{S}\otimes\boldsymbol{I} - a_2\boldsymbol{W}\otimes\boldsymbol{I})\boldsymbol{k} = \boldsymbol{\tau} \tag{15}$$

If we define the tensor $\boldsymbol{G}$ to be the matrix on the left,

$$\boldsymbol{G} = \boldsymbol{I}\otimes\boldsymbol{I} - \boldsymbol{I}\otimes\boldsymbol{S} - \boldsymbol{I}\otimes\boldsymbol{W} - a_1\boldsymbol{S}\otimes\boldsymbol{I} - a_2\boldsymbol{W}\otimes\boldsymbol{I} \tag{16}$$

then the solution to (15) is

$$\boldsymbol{k} = \boldsymbol{G}^{-1}\boldsymbol{\tau} \tag{17}$$

Consider the case of a two-dimensional mean flow. Then $\boldsymbol{G}$ is a 4×4 matrix. $\boldsymbol{G}^{-1}$ is given by the Cayley–Hamilton theorem[7]

$$\boldsymbol{G}^{-1} = (1/I_{G_4})\left[I_{G_3}\boldsymbol{I} - I_{G_2}\boldsymbol{G} + I_{G_1}\boldsymbol{G}^2 - \boldsymbol{G}^3\right] \tag{18}$$

where I_{G_1} to I_{G_4} are the four invariants of $\boldsymbol{G}$.

For a two-dimensional, incompressible mean flow,

$$\boldsymbol{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{12} & -S_{11} \end{pmatrix} \qquad \boldsymbol{W} = \begin{pmatrix} 0 & W_{12} \\ -W_{12} & 0 \end{pmatrix} \qquad \boldsymbol{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Then the explicit form of $\boldsymbol{G}$ is

$$\boldsymbol{G} = \begin{pmatrix} 1 - (1 + a_1)S_{11} & -S_{12} - W_{12} & -a_1 S_{12} - a_2 W_{12} & 0 \\ -S_{12} + W_{12} & 1 + (1 - a_1)S_{11} & 0 & -a_1 S_{12} - a_2 W_{12} \\ -a_1 S_{12} + a_2 W_{12} & 0 & 1 - (1 - a_1)S_{11} & -S_{12} - W_{12} \\ 0 & -a_1 S_{12} + a_2 W_{12} & -S_{12} + W_{12} & 1 + (1 + a_1)S_{11} \end{pmatrix} \tag{19}$$

It is shown in Appendix B that

$$\boldsymbol{G}^{-1} = (1/\beta_1)\{\beta_2\boldsymbol{I}\otimes\boldsymbol{I} + \beta_3\boldsymbol{I}\otimes(\boldsymbol{S} + \boldsymbol{W}) + \beta_4(a_1\boldsymbol{S} + a_2\boldsymbol{W})\otimes\boldsymbol{I} + 2(a_1\boldsymbol{S} + a_2\boldsymbol{W})\otimes(\boldsymbol{S} + \boldsymbol{W})\} \tag{20}$$

where

$$\beta_1 = 1 - (1 + a_1^2)S_{kk}^2 - (1 + a_2^2)W_{kk}^2 + \tfrac{1}{4}\left[(1 - a_1^2)S_{kk}^2 + (1 - a_2^2)W_{kk}^2\right]^2$$

$$\beta_2 = 1 - \tfrac{1}{2}(1 + a_1^2)S_{kk}^2 - \tfrac{1}{2}(1 + a_2^2)W_{kk}^2$$

$$\beta_3 = 1 - \tfrac{1}{2}(1 - a_1^2)S_{kk}^2 - \tfrac{1}{2}(1 - a_2^2)W_{kk}^2$$

$$\beta_4 = 1 + \tfrac{1}{2}(1 - a_1^2)S_{kk}^2 + \tfrac{1}{2}(1 - a_2^2)W_{kk}^2$$

The solution to Eq. (15) is then

$$\boldsymbol{k} = (1/\beta_1)[\beta_2\boldsymbol{I}\otimes\boldsymbol{I} + \beta_3\boldsymbol{I}\otimes(\boldsymbol{S} + \boldsymbol{W}) + \beta_4(a_1\boldsymbol{S} + a_2\boldsymbol{W})\otimes\boldsymbol{I} + 2(a_1\boldsymbol{S} + a_2\boldsymbol{W})\otimes(\boldsymbol{S} + \boldsymbol{W})]\boldsymbol{\tau} \tag{21}$$

and the solution to Eq. (10) is

$$\boldsymbol{K} = (1/\beta_1)[\beta_2\boldsymbol{\tau} + \beta_3\boldsymbol{\tau}\times(\boldsymbol{S} - \boldsymbol{W}) + \beta_4(a_1\boldsymbol{S} + a_2\boldsymbol{W})\times\boldsymbol{\tau} + 2(a_1\boldsymbol{S} + a_2\boldsymbol{W})\times\boldsymbol{\tau}\times(\boldsymbol{S} - \boldsymbol{W})] \tag{22}$$

The final solution (22) was obtained from Eq. (21) by following the steps (10) $\rightarrow$ (13) $\rightarrow$ (14) $\rightarrow$ (15) in reverse.

Equation (22) is an explicit algebraic expression for the nondimensional dispersion tensor $\boldsymbol{K}$ in equilibrium turbulence. Although the mean flow is two-dimensional, the turbulence field is three-dimensional. However, Eq. (10) shows that in a two-dimensional

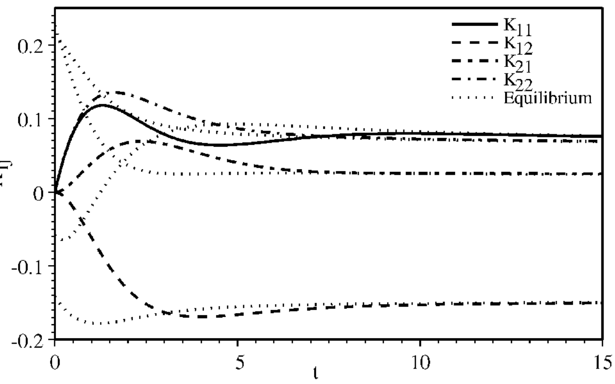

Fig. 1 Time-dependent solution for homogeneous shear flow.

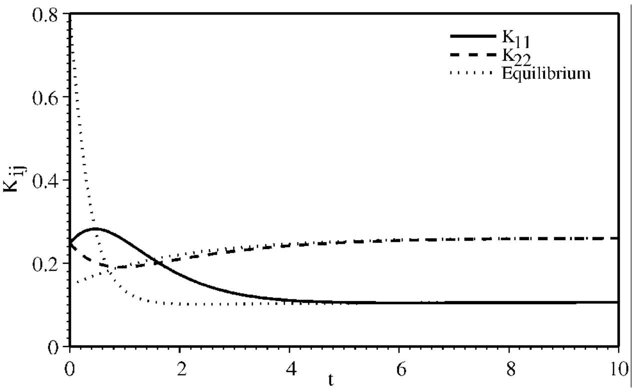

Fig. 2 Time-dependent solution for homogeneous plane straining flow.

mean flow $K_{33} = \tau_{33}$. Therefore, the coefficient of τ in Eq. (22) is simply altered [using Eq. (B1)] to obtain

$$\boldsymbol{K} = \boldsymbol{\tau} + (1/\beta_1)\big[2(\beta_2 - \beta_1)[(\boldsymbol{S}^2 \cdot \boldsymbol{\tau})/S^2_{kk}] + \beta_3 \boldsymbol{\tau} \cdot (\boldsymbol{S} - \boldsymbol{W})$$
$$+ \beta_4(a_1\boldsymbol{S} + a_2\boldsymbol{W}) \cdot \boldsymbol{\tau} + 2(a_1\boldsymbol{S} + a_2\boldsymbol{W}) \cdot \boldsymbol{\tau} \cdot (\boldsymbol{S} - \boldsymbol{W})\big] \tag{23}$$

which is valid for a two-dimensional mean flow and three-dimensional turbulence.

This provides a constitutive model for scalar transport. In the integrity basis method, the last term, involving the product of three matrices, would be expanded in terms of the relevant integrity basis ($\boldsymbol{\tau}$, $\boldsymbol{S}$, $\boldsymbol{W}$, $\boldsymbol{S}^2$, $\boldsymbol{W} \cdot \boldsymbol{S}$, $\boldsymbol{W} \cdot \boldsymbol{\tau}$, and $\boldsymbol{S} \cdot \boldsymbol{\tau}$); the resulting expression is rather more complicated.

The closed-form equilibrium solution is confirmed by Figs. 1 and 2. These contain time-dependent numerical solutions to Eq. (9) in conjunction with a solution to the corresponding $\overline{u_i u_j}$ equations of the SSG-model,[8] both obtained by a fourth-order Runge–Kutta method. Durbin and Shabany[4] report two sets of constants that produce results in close agreement with direct numerical simulation (DNS) data for the dispersion tensor of equilibrium homogeneous shear flow. We selected $c_{\theta_1} = 0$, $c_{\theta_2} = 0.41$, $c_{\theta_3} = 0.21$, and $c_M = 2.89$ from this paper to obtain the results shown in Figs. 1 and 2. The equilibrium ratios $K_{11}/K_{22} = 1.08$, $K_{12}/K_{22} = -2.22$, $K_{21}/K_{22} = 0.35$ attained in homogeneous shear flow are in rough agreement with DNS data; Rogers estimates $K_{11}/K_{22} \approx 1$, $K_{12}/K_{22} \approx -2$, $K_{21}/K_{22} \approx 0$ from his DNS data (private communication). At each time, the equilibrium solution (22) was evaluated and is plotted as a dotted line. This usage is the essence of the algebraic stress approximation; the equilibrium solution is used as an approximation in nonequilibrium states. Time is nondimensionalized by the rate of shear $\mathrm{d}U/\mathrm{d}y$ in Fig. 1 and by the rate of strain $\mathrm{d}U/\mathrm{d}x = -\mathrm{d}V/\mathrm{d}y$ in Fig. 2. The initial condition is that the turbulence is isotropic: $\overline{u_i u_j} = \frac{2}{3}\delta_{ij}k$. The initial condition $K_{ij} = 0$ was used in the shear-flow computation and the plane straining flow calculation was initialized by the equilibrium isotropic state $K_{ij} = \tau_{ij}$ [i.e., $\boldsymbol{S} = \boldsymbol{W} = 0$ in Eq. (23)]. Either of these two initial conditions produces similar qualitative behavior.

Figures 1 and 2 illustrate an initial rapid transient, during which the equilibrium approximation is invalid. By a nondimensional time of about 4, the quasiequilibrium solution is providing a good approximation to the time-dependent calculation.

IV. Solvability and Stability

The solution (22) gives a finite value for the components of the dispersion tensor unless $\beta_1 = 0$. Hence, $\beta_1 \neq 0$ is the solvability condition for Eq. (10). However, even when this condition is met, the solution might be an unstable equilibrium. To investigate this, we note that Eq. (22) is the steady solution to the differential equation (9), which can be written

$$\frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} + \frac{1}{g_\theta T}\boldsymbol{G} \cdot \boldsymbol{k} = \frac{1}{g_\theta T}\boldsymbol{\tau} \tag{24}$$

This has four independent homogeneous and one particular solution. The homogeneous solutions decay or grow with time, depending on whether the real part of the eigenvalues of $\boldsymbol{G}$ is positive or negative, respectively ($g_\theta > 0$ for parameters of interest). If all the homogeneous solutions decay with time, the particular solution (22) is a stable equilibrium. Thus, Eq. (22) is strictly valid only if all eigenvalues of $\boldsymbol{G}$ have positive real part. If we define

$$x \equiv \tfrac{1}{2}(1 + a_1^2)S^2_{kk} + \tfrac{1}{2}(1 + a_2^2)W^2_{kk}$$

and

$$y \equiv \tfrac{1}{4}(S^2_{kk} + W^2_{kk})(a_1^2 S^2_{kk} + a_2^2 W^2_{kk})$$

then the eigenvalues of $\boldsymbol{G}$ are

$$\lambda_i = 1 \pm \sqrt{x \pm 2\sqrt{y}} \tag{25}$$

for the four combinations of the $\pm$ values.

Figure 3 shows the regions in which the real part of the eigenvalues $\lambda_3 = 1 - \sqrt{x + 2\sqrt{y}}$ and $\lambda_4 = 1 - \sqrt{x - 2\sqrt{y}}$ is positive or negative. The SSG model[8] was used to obtain values of $a_1 = -0.38$, $a_2 = -0.8$, which were used to produce this figure. Other models give a similar stability diagram; in fact, it can be shown that the diagonal line in Fig. 3 is given by $S^2_{kk} = 2 - W^2_{kk}$ independently of the model constants a_1 and a_2. The eigenvalue that is most likely to have negative real part is $\lambda_3 = 1 - \sqrt{x + 2\sqrt{y}}$. Therefore, as soon as the real part of this eigenvalue becomes negative Eq. (24) will have an exponentially growing solution and there is no stable equilibrium. On the other hand, β_1 is the product of the eigenvalues of $\boldsymbol{G}$. Therefore, whenever $\beta_1 = 0$ at least one of the eigenvalues of $\boldsymbol{G}$ is zero; this shows that Eq. (22) is valid until the first zero of β_1 occurs. Note that homogeneous shear flow corresponds to the diagonal line $W^2_{kk} = -S^2_{kk}$ and lies in the stable region. It should be mentioned that when $W_{ij} = 0$ the stable equilibrium region is up to $\tilde{S}^2_{kk} \approx 55$ (using the same constants as used for Fig. 3), where $S_{ij} \equiv T(\partial_j U_i + \partial_i U_j)/2$. Hence, in most practical situations the model has stable equilibria.

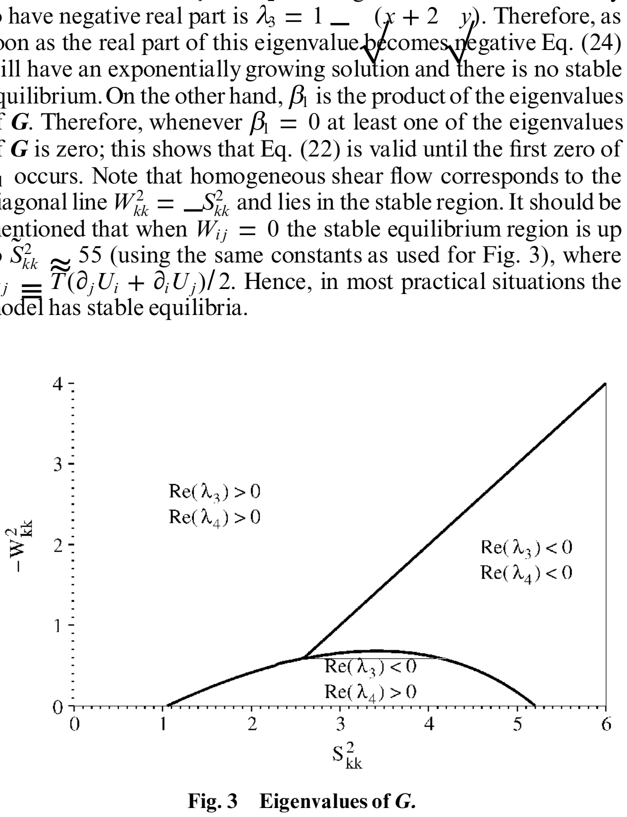

Fig. 3 Eigenvalues of *G*.

V. Correspondence to Reynolds Stress Model

Pope[9] and Durbin and Shabany[4] discuss the consistent formulation of scalar-flux and Reynolds-stress closures. In essence, they show that the model constants c_{θ_2} and c_{θ_3} are equal to corresponding coefficients in the rapid pressure-strain model. The eigenvalues of $\boldsymbol{G}$ depend on two independent variables, S^2_{kk} and W^2_{kk}, and g_θ depends on $\mathcal{P} \equiv P/\varepsilon$. S^2_{kk} is related to $\mathcal{P}$ through the equilibrium solution to the Reynolds stress closure

$$S^2_{kk} = (\mathcal{P} g^2_\theta / 2c_\mu) \tag{26}$$

where c_μ can be found for each particular model; the solvability condition for the Reynolds stress model is $1/c_\mu \neq 0$. It was shown implicitly by Pope[5] that, when the consistency condition (26) is imposed, the equilibrium approximation to the LRR model[10] is solvable for all $\boldsymbol{S}$ and $\boldsymbol{W}$ (Durbin and Shabany[4] note that the consistency condition generally imposes solvability).

The question arises whether this consistency condition will also prevent β_1 from vanishing when a self-consistent Reynolds-stress–scalar-flux closure is adopted. To avoid the possibility of the real part of λ_3 becoming negative, the limiting value of S^2_{kk} as $\mathcal{P} \to \infty$ would have to be less than the smallest value of S^2_{kk} at which the real part of this eigenvalue crosses zero. In what follows, it is shown that this condition is not generally met by second-order closure models.

For the SSG model, the expression for c_μ is[6]

$$c_\mu = \frac{(8/5 + 3c^*_s\sqrt{II})g}{2\left[3 - 2(g/g_\theta)^2 a_1^2 S^2_{kk} - 6(g/g_\theta)^2 a_2^2 W^2_{kk}\right]}$$

where $g = (c_1 + c^*_1\mathcal{P} + \mathcal{P} - 1)^{-1}$ in terms of the constants of the SSG model (recall that $\boldsymbol{S}$ contains a factor of g_θ in its definition). Substituting this into Eq. (26), the following expression for S^2_{kk} is obtained:

$$S^2_{kk} = \frac{\mathcal{P}g\left[3(g_\theta/g)^2 - 6a_2^2 W^2_{kk}\right]}{8/5 + 3c^*_s\sqrt{II} + 2a_1^2\mathcal{P}g} \tag{27}$$

where

$$\sqrt{II} = g\mathcal{P}|a_1|\left(\frac{1}{(g/g_\theta)^2 a_1^2 S^2_{kk}} - \frac{2a_2^2 W^2_{kk}}{a_1^2 S^2_{kk}} + \frac{2}{3}\right)^{\frac{1}{2}}$$

From the definitions of g and g_θ,

$$\lim_{\mathcal{P}\to\infty} g\mathcal{P} = \lim_{\mathcal{P}\to\infty} \frac{\mathcal{P}}{c_1 + c^*_1\mathcal{P} + \mathcal{P} - 1} = \frac{1}{c^*_1 + 1}$$

$$\lim_{\mathcal{P}\to\infty} \frac{g_\theta}{g} = \lim_{\mathcal{P}\to\infty} \frac{c_1 + c^*_1\mathcal{P} + \mathcal{P} - 1}{c_M + (2 - c_{\epsilon1})\mathcal{P} + c_{\epsilon2} - 2} = \frac{c^*_1 + 1}{2 - c_{\epsilon1}}$$

Therefore,

$$\sqrt{II_\infty} \equiv \lim_{\mathcal{P}\to\infty} \sqrt{II} = \frac{|a_1|}{c^*_1 + 1}\left(\frac{(c^*_1 + 1)^2}{(2 - c_{\epsilon2})^2 a_1^2 S^2_\infty} - \frac{2a_2^2 W^2_{kk}}{a_1^2 S^2_\infty} + \frac{2}{3}\right)^{\frac{1}{2}} \tag{28}$$

$$S^2_\infty \equiv \lim_{\mathcal{P}\to\infty} S^2_{kk} = \frac{3(c^*_1 + 1)^2 - 6a_2^2(2 - c_{\epsilon1})^2 W^2_{kk}}{\left[2a_1^2 + (8/5 + 3c^*_s\sqrt{II_\infty})(c^*_1 + 1)\right](2 - c_{\epsilon1})^2} \tag{29}$$

If c^*_s is not zero (SSG model), these equations have to be solved simultaneously for $\sqrt{II_\infty}$ and S^2_∞. On the other hand, for the IP (isotropization of production) or LRR model, $c^*_s = 0$ and Eq. (29) is independent of Eq. (28).

In Fig. 3 the smallest value of S^2_{kk} for which the real part of λ_3 is negative corresponds to pure straining flow $W_{ij} = 0$. In this case $\beta_1 = 0$ has two solutions:

$$S^2_{kk} = \frac{2}{(1 - a_1)^2} \qquad \text{and} \qquad \frac{2}{(1 + a_1)^2}$$

Hence, $\lambda_3 = 1 - \sqrt{(x + 2\sqrt{y})}$ becomes negative for $S^2_{kk} > 2/(1 - a_1)^2$ [or $S^2_{kk} > 2/(1 + a_1)^2$ if $a_1 > 0$]. Therefore, the equilibrium solution will be valid for all values of S_{ij} and W_{ij} if $S^2_\infty < 2/(1 - a_1)^2$. This condition is not satisfied by either the SSG or the LRR model; for example, in the LRR model, $a_1 = -0.125$, $c^*_1 = 0$, $c^*_s = 0$, and $c_{\epsilon1} = 1.44$, giving $S^2_\infty = 5.86$, while $2/(1 - a_1)^2 = 1.58$.

It seems quite likely that all existing models will have unphysical regions in which the equilibrium scalar-flux solution is unstable. The consistency condition (26) that prevents this for Reynolds stress closure has no analog for the scalar-flux model. However, it is rather straightforward to derive a condition on the model coefficient c_M so that $S^2_\infty < 2/(1 - a_1)^2$ is ensured. Because $S^2_{kk} = g^2_\theta \tilde{S}^2_{kk}$ with the definition $\tilde{S}_{ij} = \frac{1}{2}T(\partial_j U_i + \partial_i U_j)$, the condition $S^2_{kk} < 2/(1 - a_1)^2$ is satisfied if c_M is constrained by

$$c_M > 2 - c_{\epsilon2} - (2 - c_{\epsilon1})\mathcal{P} + \left\{\tfrac{1}{2}(1 - a_1)^2 \tilde{S}^2_{kk}\right\}^{\frac{1}{2}}$$

This constraint can be used to guide the development of models; for instance, a strain-dependent c_M can be formulated to ensure that stable equilibrium states always exist.

VI. Conclusions

The equilibrium solution of a transport equation for the normalized dispersion tensor was obtained for homogeneous turbulent flows, and the conditions in which the solution was a stable equilibrium were discussed. The solution was obtained by a new method that used the properties of a direct product of tensors to reduce a tensor equation to a vector equation. It was shown that, for homogeneous flows, the equilibrium solution was in good agreement with the time-dependent solution after a nondimensional time of about 4. This equilibrium solution provided an explicit algebraic flux model for nonequilibrium and nonhomogeneous flows.

Appendix A: Direct Product of Matrices

The direct product of the 2×2 matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ is a 4×4 matrix defined by

$$\boldsymbol{A} \otimes \boldsymbol{B} = \begin{pmatrix} a_{11}\boldsymbol{B} & a_{12}\boldsymbol{B} \\ a_{21}\boldsymbol{B} & a_{22}\boldsymbol{B} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix} \tag{A1}$$

The following properties of the direct product follow from its definition[11]:

1) If μ is a constant, $(\mu\boldsymbol{A}) \otimes \boldsymbol{B} = \boldsymbol{A} \otimes (\mu\boldsymbol{B}) = \mu(\boldsymbol{A} \otimes \boldsymbol{B})$.
2) $(\boldsymbol{A} + \boldsymbol{B}) \otimes \boldsymbol{C} = \boldsymbol{A} \otimes \boldsymbol{C} + \boldsymbol{B} \otimes \boldsymbol{C}$.
3) $\boldsymbol{A} \otimes (\boldsymbol{B} + \boldsymbol{C}) = \boldsymbol{A} \otimes \boldsymbol{B} + \boldsymbol{A} \otimes \boldsymbol{C}$.
4) $\boldsymbol{A} \otimes (\boldsymbol{B} \otimes \boldsymbol{C}) = (\boldsymbol{A} \otimes \boldsymbol{B}) \otimes \boldsymbol{C}$.
5) $(\boldsymbol{A} \otimes \boldsymbol{B})^T = \boldsymbol{A}^T \otimes \boldsymbol{B}^T$.

It can be proved that if $\boldsymbol{A}$ and $\boldsymbol{C}$ are $m \times m$ and $\boldsymbol{B}$ and $\boldsymbol{D}$ are $n \times n$ matrices, then $(\boldsymbol{A} \otimes \boldsymbol{B})(\boldsymbol{C} \otimes \boldsymbol{D}) = \boldsymbol{AC} \otimes \boldsymbol{BD}$ (Ref. 11). As a corollary of this, if $\boldsymbol{A}_1, \boldsymbol{A}_2, \ldots, \boldsymbol{A}_k$ are $m \times m$ matrices and $\boldsymbol{B}_1, \boldsymbol{B}_2, \ldots, \boldsymbol{B}_k$ are $n \times n$ matrices, then

$$\begin{aligned}&(\boldsymbol{A}_1 \otimes \boldsymbol{B}_1) \times (\boldsymbol{A}_2 \otimes \boldsymbol{B}_2) \cdots (\boldsymbol{A}_k \otimes \boldsymbol{B}_k) \\ &\quad = (\boldsymbol{A}_1 \times \boldsymbol{A}_2 \cdots \boldsymbol{A}_k) \otimes (\boldsymbol{B}_1 \times \boldsymbol{B}_2 \cdots \boldsymbol{B}_k)\end{aligned} \tag{A2}$$

The use of the direct product of matrices in solving linear matrix equations is of interest here. Consider the general matrix equation for the $n \times n$ unknown matrix $\boldsymbol{X}$:

$$\boldsymbol{A}_1 \times \boldsymbol{X} \times \boldsymbol{B}_1 + \boldsymbol{A}_2 \times \boldsymbol{X} \times \boldsymbol{B}_2 + \cdots + \boldsymbol{A}_k \times \boldsymbol{X} \times \boldsymbol{B}_k = \boldsymbol{C} \tag{A3}$$

where $\boldsymbol{A}_1, \ldots, \boldsymbol{A}_k, \boldsymbol{B}_1, \ldots, \boldsymbol{B}_k$, and $\boldsymbol{C}$ are $n \times n$ matrices. Note that this is n^2 scalar equations for the elements of $\boldsymbol{X}$. The r, s element of this equation can be written

$$\sum_{i,j}^{n} a_{ri} x_{ij} b_{js} = c_{rs} \tag{A4}$$

We define the n^2-dimensional vectors $\boldsymbol{x}$ and $\boldsymbol{c}$ by

$$\boldsymbol{x} = \sum_{i,j}^{n} x_{ij}\hat{e}_{(i-1)n+j} \qquad \boldsymbol{c} = \sum_{r,s}^{n} c_{rs}\hat{e}_{(r-1)n+s} \tag{A5}$$

where $\hat{e}_i$ are unit vectors. We want to find matrix $\boldsymbol{G}$ so that the matrix equation

$$\sum_{i}^{k} \boldsymbol{A}_i \times \boldsymbol{X} \times \boldsymbol{B}_i = \boldsymbol{C}$$

is equivalent to the vector equation $\boldsymbol{G} \times \boldsymbol{x} = \boldsymbol{c}$. Substituting Eq. (A5) into this equation and projecting onto the unit direction vectors gives

$$\sum_{i,j}^{n} g_{(r-1)n+s,(i-1)n+j}\, x_{ij} = c_{rs}$$

in index notation. Comparing the coefficient of x_{ij} to that in Eq. (A4) shows that

$$g_{(r-1)n+s,(i-1)n+j} = a_{ri} b_{js}$$

in other words, the matrix $\boldsymbol{G}$ has the element $a_{ri}b_{js}$ in row $(r-1)n+s$ and column $(i-1)n+j$. These are exactly the elements of matrix

$$\sum_{i}^{k} \boldsymbol{A}_i \otimes \boldsymbol{B}_i^T$$

Thus, the matrix equation (A3) is equivalent to $\boldsymbol{G}\boldsymbol{x} = \boldsymbol{c}$, where

$$\boldsymbol{G} = \boldsymbol{A}_1 \otimes \boldsymbol{B}_1^T + \boldsymbol{A}_2 \otimes \boldsymbol{B}_2^T + \ldots + \boldsymbol{A}_k \otimes \boldsymbol{B}_k^T \tag{A6}$$

The solution of the equation in this new form is equal to $\boldsymbol{x} = \boldsymbol{G}^{-1}\boldsymbol{c}$, where $\boldsymbol{G}^{-1}$ is the inverse of $\boldsymbol{G}$.

Appendix B: Derivation of G^{-1}

The inverse of 4×4 tensor $\boldsymbol{G}$ can be obtained by the Cayley–Hamilton theorem, Eq. (18). For the $\boldsymbol{G}$ given by Eq. (19),

$$I_{G_1} = 4 \qquad I_{G_2} = 6 - (1+a_1^2)S_{kk}^2 - (1+a_2^2)W_{kk}^2$$

$$I_{G_3} = 4 - 2(1+a_1^2)S_{kk}^2 - 2(1+a_2^2)W_{kk}^2$$

$$I_{G_4} = 1 - (1+a_1^2)S_{kk}^2 - (1+a_2^2)W_{kk}^2 + \tfrac{1}{4}\left[(1-a_1^2)S_{kk}^2 + (1-a_2^2)W_{kk}^2\right]^2$$

$\boldsymbol{G}^2$ is calculated by multiplying Eq. (16) by itself, and Eq. (A2) is used to obtain the product of two direct products:

$$\begin{aligned}
\boldsymbol{G}^2 &= (\boldsymbol{I}\otimes\boldsymbol{I} - \boldsymbol{I}\otimes\boldsymbol{S} - \boldsymbol{I}\otimes\boldsymbol{W} - a_1\boldsymbol{S}\otimes\boldsymbol{I} - a_2\boldsymbol{W}\otimes\boldsymbol{I})\\
&\quad \times(\boldsymbol{I}\otimes\boldsymbol{I} - \boldsymbol{I}\otimes\boldsymbol{S} - \boldsymbol{I}\otimes\boldsymbol{W} - a_1\boldsymbol{S}\otimes\boldsymbol{I} - a_2\boldsymbol{W}\otimes\boldsymbol{I})\\
&= \boldsymbol{I}\otimes\boldsymbol{I} - \boldsymbol{I}\otimes\boldsymbol{S} - \boldsymbol{I}\otimes\boldsymbol{W} - a_1\boldsymbol{S}\otimes\boldsymbol{I} - a_2\boldsymbol{W}\otimes\boldsymbol{I}\\
&\quad - \boldsymbol{I}\otimes\boldsymbol{S} + \boldsymbol{I}\otimes\boldsymbol{S}^2 + \boldsymbol{I}\otimes\boldsymbol{S}\times\boldsymbol{W} + a_1\boldsymbol{S}\otimes\boldsymbol{S} + a_2\boldsymbol{W}\otimes\boldsymbol{S}\\
&\quad - \boldsymbol{I}\otimes\boldsymbol{W} + \boldsymbol{I}\otimes\boldsymbol{W}\times\boldsymbol{S} + \boldsymbol{I}\otimes\boldsymbol{W}^2 + a_1\boldsymbol{S}\otimes\boldsymbol{W} + a_2\boldsymbol{W}\otimes\boldsymbol{W}\\
&\quad - a_1\boldsymbol{S}\otimes\boldsymbol{I} + a_1\boldsymbol{S}\otimes\boldsymbol{S} + a_1\boldsymbol{S}\otimes\boldsymbol{W} + a_1^2\boldsymbol{S}^2\otimes\boldsymbol{I}\\
&\quad + a_1a_2\boldsymbol{S}\times\boldsymbol{W}\otimes\boldsymbol{I} - a_2\boldsymbol{W}\otimes\boldsymbol{I} + a_2\boldsymbol{W}\otimes\boldsymbol{S} + a_2\boldsymbol{W}\otimes\boldsymbol{W}\\
&\quad + a_1a_2\boldsymbol{W}\times\boldsymbol{S}\otimes\boldsymbol{I} + a_2^2\boldsymbol{W}^2\otimes\boldsymbol{I}
\end{aligned}$$

From the generalized Cayley–Hamilton theorem in two dimensions,[7]

$$\boldsymbol{S}^2 = \tfrac{1}{2}S_{kk}^2\boldsymbol{I} \qquad \boldsymbol{W}^2 = \tfrac{1}{2}W_{kk}^2\boldsymbol{I} \qquad \boldsymbol{W}\boldsymbol{S} = -\boldsymbol{S}\boldsymbol{W} \tag{B1}$$

Using these and combining all like terms, the following expression for $\boldsymbol{G}^2$ is obtained:

$$\begin{aligned}
\boldsymbol{G}^2 &= \Delta_1\boldsymbol{I}\otimes\boldsymbol{I} - 2\boldsymbol{I}\otimes\boldsymbol{S} - 2\boldsymbol{I}\otimes\boldsymbol{W} - 2a_1\boldsymbol{S}\otimes\boldsymbol{I} - 2a_2\boldsymbol{W}\otimes\boldsymbol{I}\\
&\quad + 2a_1\boldsymbol{S}\otimes\boldsymbol{S} + 2a_2\boldsymbol{W}\otimes\boldsymbol{S} + 2a_1\boldsymbol{S}\otimes\boldsymbol{W} + 2a_2\boldsymbol{W}\otimes\boldsymbol{W}
\end{aligned} \tag{B2}$$

where

$$\Delta_1 = 1 + \tfrac{1}{2}S_{kk}^2(1+a_1^2) + \tfrac{1}{2}W_{kk}^2(1+a_2^2)$$

Similarly, the expression for $\boldsymbol{G}^3$ is obtained by multiplying Eq. (16) by Eq. (B2):

$$\begin{aligned}
\boldsymbol{G}^3 &= (3\Delta_1 - 2)\boldsymbol{I}\otimes\boldsymbol{I} - (3\Delta_1 - S_{kk}^2 - W_{kk}^2)(\boldsymbol{I}\otimes\boldsymbol{S} + \boldsymbol{I}\otimes\boldsymbol{W})\\
&\quad - (\Delta_1 + 2 + S_{kk}^2 + W_{kk}^2)(a_1\boldsymbol{S}\otimes\boldsymbol{I} + a_2\boldsymbol{W}\otimes\boldsymbol{I})\\
&\quad + 6a_1(\boldsymbol{S}\otimes\boldsymbol{S} + \boldsymbol{S}\otimes\boldsymbol{W}) + 6a_2(\boldsymbol{W}\otimes\boldsymbol{W} + \boldsymbol{W}\otimes\boldsymbol{S})
\end{aligned} \tag{B3}$$

Finally, substituting Eqs. (B2) and (B3) and the expressions for the invariants of $\boldsymbol{G}$ into Eq. (18), $\boldsymbol{G}^{-1}$ is obtained:

$$\begin{aligned}
\boldsymbol{G}^{-1} &= (1/\beta_1)[\beta_2\boldsymbol{I}\otimes\boldsymbol{I} + \beta_3(\boldsymbol{I}\otimes\boldsymbol{S} + \boldsymbol{I}\otimes\boldsymbol{W})\\
&\quad + \beta_4(a_1\boldsymbol{S}\otimes\boldsymbol{I} + a_2\boldsymbol{W}\otimes\boldsymbol{I}) + 2(a_1\boldsymbol{S}\otimes\boldsymbol{S} + a_2\boldsymbol{W}\otimes\boldsymbol{S}\\
&\quad + a_1\boldsymbol{S}\otimes\boldsymbol{W} + a_2\boldsymbol{W}\otimes\boldsymbol{W})]
\end{aligned} \tag{B4}$$

where β_1 to β_4 are given after Eq. (20). This expression can be simplified to Eq. (20) by using properties 2 and 3 of the direct product given in Appendix A.

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References

[1] Launder, B. E., "Heat and Mass Transport," *Turbulence*, edited by P. Bradshaw, Vol. 12, Topics in Applied Physics, Springer–Verlag, Berlin, 1978, pp. 231–287.

[2] Dakos, T., and Gibson, M. M., "On Modelling the Pressure Terms of the Scalar Flux Equations," *International Conference on Turbulent Shear Flows*, edited by F. Durst, B. E. Launder, J. L. Lumley, F. W. Schmidt, and J. H. Whitelaw, Vol. 5, Cornell Univ., Ithaca, NY, 1985, pp. 7–18.

[3] Durbin, P. A., "A Reynolds Stress Model for Near-Wall Turbulence," *Journal of Fluid Mechanics*, Vol. 249, April 1993, pp. 465–498.

[4] Durbin, P. A., and Shabany, Y., "Towards Consistent Formulation of Reynolds Stress and Scalar Flux Closures," *Proceedings of the International Symposium on Mathematical Modeling of Turbulent Flows* (Tokyo, Japan), Japan Society of Computational Fluid Dynamics, Tokyo, Japan, 1995, pp. 64–70.

[5] Pope, S. B., "A More General Effective-Viscosity Hypothesis," *Journal of Fluid Mechanics*, Vol. 72, Pt. 2, 1975, pp. 331–340.

[6] Gatski, T., and Speziale, C. G., "On Explicit Algebraic Stress Models for Complex Turbulent Flows," *Journal of Fluid Mechanics*, Vol. 254, Sept. 1994, pp. 59–78.

[7] Rivlin, R. S., "Further Remarks on the Stress-Deformation Relations for Isotropic Materials," *Journal of Rational Mechanics and Analysis*, Vol. 4, 1955, pp. 681–701.

[8] Speziale, C. G., Sarkar, S., and Gatski, T. B., "Modeling the Pressure-Strain Correlation of Turbulence: An Invariant Dynamical Systems Approach," *Journal of Fluid Mechanics*, Vol. 227, June 1991, pp. 245–272.

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

[10] Launder, B. E., Reece, G. J., and Rodi, W., "Progress in the Development of Reynolds Stress Turbulence Closure," *Journal of Fluid Mechanics*, Vol. 68, Pt. 3, 1975, pp. 537–566.

[11] Lancaster, P., *Theory of Matrices*, Academic, New York, 1969.

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