Figure 11. Computed model predictions for the time evolution of the ratio of production to dissipation ($\mathcal{P}/\varepsilon$) in homogeneous shear flow corresponding to the initial conditions $(b_{11})_0 = -0.32$, $(b_{22})_0 = -0.32$, $SK_0/\varepsilon_0 = 50$: (a) IP Model, (b) Shih-Lumley Model and (c) the FLT Model.

Figure 12. Time evolution of the normal Reynolds stress $\tau_{22}/(\tau_{22})_0$ in homogeneous shear flow: Comparison of computed results for the FLT Model (corresponding to $(b_{11})_0 = (b_{22})_0 = -0.0833$, $SK_0/\varepsilon_0 = 50$) with the Rapid Distortion Theory (RDT) solution.æ

LIST OF FIGURES

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$$C_{\varepsilon 1} = 1.44,\ C_{\varepsilon 2} = 1.90 \tag{B10}$$

$$C_1 = -120II\sqrt{F} - 2\sqrt{F} + 2, \quad C_2 = 144II\sqrt{F} \tag{B11}$$

IP Model

$$\Pi_{ij} = -C_1 \varepsilon b_{ij} - C_2(\mathcal{P}_{ij} - \frac{2}{3}\mathcal{P}\delta_{ij}) \tag{B12}$$

$$C_{\varepsilon 1} = 1.44, \quad C_{\varepsilon 2} = 1.90 \tag{B13}$$

where

$$C_1 = 3.6,\ C_2 = 0.6 \tag{B14}$$

$$\mathcal{P}_{ij} = -\tau_{ik}\frac{\partial \overline{v}_j}{\partial x_k} - \tau_{jk}\frac{\partial \overline{v}_i}{\partial x_k} \tag{B15}$$

$$\mathcal{P} = -\tau_{ij}\frac{\partial \overline{v}_i}{\partial x_j}. \tag{B16}$$

APPENDIX B

The detailed form of the turbulence models considered in the paper are as follows:

Shih & Lumley Model

$$\begin{aligned}\Pi_{ij} \;=\;& -C_1\varepsilon b_{ij} + \frac{4}{5}K\overline{S}_{ij} + 12\alpha_5 K\Big(b_{ik}\overline{S}_{jk} + b_{jk}\overline{S}_{ik} \\ & -\frac{2}{3}b_{kl}\overline{S}_{kl}\delta_{ij}\Big) + \frac{4}{3}(2-7\alpha_5)K(b_{ik}\overline{\omega}_{jk} + b_{jk}\overline{\omega}_{ik}) \\ & +\frac{4}{5}K(b_{il}b_{lm}\overline{S}_{jm} + b_{jl}b_{lm}\overline{S}_{im} - 2b_{ik}\overline{S}_{kl}b_{lj} \\ & -3b_{kl}\overline{S}_{kl}b_{ij}) + \frac{4}{5}K(b_{il}b_{lm}\overline{\omega}_{jm} + b_{jl}b_{lm}\overline{\omega}_{im})\end{aligned} \tag{B1}$$

$$C_{\varepsilon 1} = 1.20, \quad C_{\varepsilon 2} = \frac{7}{5} + 0.49\exp(-2.83/\sqrt{Re_t})[1-0.33ln(1-55II)] \tag{B2}$$

$$\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{v}_i}{\partial x_j} + \frac{\partial \overline{v}_j}{\partial x_i}\right),\ \overline{\omega}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{v}_i}{\partial x_j} - \frac{\partial \overline{v}_j}{\partial x_i}\right) \tag{B3}$$

$$C_1 = 2 + \frac{F}{9}\exp(-7.77/\sqrt{Re_t})\{72/\sqrt{Re_t} + 80.1\ ln[1+62.4(-II+2.3III)]\} \tag{B4}$$

$$F = 1 + 9II + 27III \tag{B5}$$

$$II = -\frac{1}{2}b_{ij}b_{ij}, \quad III = \frac{1}{3}b_{ij}b_{jk}b_{ki} \tag{B6}$$

$$Re_t = \frac{4}{9}\frac{K^2}{\nu\varepsilon} \tag{B7}$$

$$\alpha_5 = \frac{1}{10}\left(1 + \frac{4}{5}F^{\frac{1}{2}}\right) \tag{B8}$$

Fu, Launder & Tselepidakis Model

$$\begin{aligned}\Pi_{ij} \;=\;& -C_1\varepsilon b_{ij} + C_2\varepsilon\left(b_{ik}b_{kj} - \frac{1}{3}b_{kl}b_{kl}\delta_{ij}\right) \\ & +\frac{4}{5}K\overline{S}_{ij} + 1.2K\left(b_{ik}\overline{S}_{jk} + b_{jk}\overline{S}_{ik} - \frac{2}{3}b_{kl}\overline{S}_{kl}\delta_{ij}\right) \\ & +\frac{26}{15}K(b_{ik}\overline{\omega}_{jk} + b_{jk}\overline{\omega}_{ik}) + \frac{4}{5}K(b_{ik}b_{kl}\overline{S}_{jl} \\ & +b_{jk}b_{kl}\overline{S}_{il} - 2b_{ik}\overline{S}_{kl}b_{lj} - 3b_{kl}\overline{S}_{kl}b_{ij}) \\ & +\frac{4}{5}K\left(b_{ik}b_{kl}\overline{\omega}_{jl} + b_{jk}b_{kl}\overline{\omega}_{il}\right) - \frac{14}{5}K\left[8II(b_{ik}\overline{\omega}_{jk}\right. \\ & \left.+b_{jk}\overline{\omega}_{ik}) + 12\left(b_{ik}b_{kl}\overline{\omega}_{lm}b_{mj} + b_{jk}b_{kl}\overline{\omega}_{lm}b_{mi}\right)\right]\end{aligned} \tag{B9}$$

Capelli's identity, given by the determinant

$$e_{\alpha\gamma\lambda}e_{\beta\nu\sigma} = \begin{vmatrix} \delta_{\alpha\beta} & \delta_{\alpha\nu} & \delta_{\alpha\sigma} \\ \delta_{\gamma\beta} & \delta_{\gamma\nu} & \delta_{\gamma\sigma} \\ \delta_{\lambda\beta} & \delta_{\lambda\nu} & \delta_{\lambda\sigma} \end{vmatrix} \tag{A9}$$

can be applied to the fourth term on the right-hand-side of (A8). After simplifying, we arrive at the final result:

$$\begin{aligned} (\ddot{T})_{\alpha\beta} \quad = \quad & \ddot{T}_{\alpha\beta} + 2e_{\alpha\gamma\delta}\Omega_\gamma \dot{T}_{\delta\beta} + 2e_{\beta\gamma\delta}\Omega_\gamma \dot{T}_{\delta\alpha} + e_{\alpha\gamma\delta}\dot{\Omega}_\gamma T_{\delta\beta} \\ & + e_{\beta\gamma\delta}\dot{\Omega}_\gamma T_{\delta\alpha} + 3\Omega_\alpha\Omega_\sigma T_{\sigma\beta} + 3\Omega_\beta\Omega_\sigma T_{\sigma\alpha} \\ & - 4\Omega^2 T_{\alpha\beta} - 2T_{\sigma\sigma}\Omega_\alpha\Omega_\beta + 2(\Omega^2 T_{\sigma\sigma} - \Omega_\gamma\Omega_\sigma T_{\gamma\sigma})\delta_{\alpha\beta}. \end{aligned} \tag{A10}$$

APPENDIX A

Relative to a coordinate system with unit vectors $\boldsymbol{\lambda}_\alpha$ that is undergoing a time-dependent rotation, any symmetric tensor $\boldsymbol{T}$ takes the form:

$$\boldsymbol{T} = T_{\alpha\beta}\boldsymbol{\lambda}_\alpha\boldsymbol{\lambda}_\beta. \tag{A1}$$

Hence, the first time derivative is given by

$$\dot{\boldsymbol{T}} = \dot{T}_{\alpha\beta}\boldsymbol{\lambda}_\alpha\boldsymbol{\lambda}_\beta + T_{\alpha\beta}\dot{\boldsymbol{\lambda}}_\alpha\boldsymbol{\lambda}_\beta + T_{\alpha\beta}\boldsymbol{\lambda}_\alpha\dot{\boldsymbol{\lambda}}_\beta \tag{A2}$$

since $\boldsymbol{\lambda}_\alpha = \boldsymbol{\lambda}_\alpha(t)$. It is well known that for any unit vector $\boldsymbol{\lambda}_\alpha$ rotating with angular velocity $\boldsymbol{\Omega}$ we have (cf. Goldstein 1980)

$$\begin{aligned} \dot{\boldsymbol{\lambda}}_\alpha &= \boldsymbol{\Omega}\times\boldsymbol{\lambda}_\alpha \\ &= e_{\delta\gamma\alpha}\Omega_\gamma\boldsymbol{\lambda}_\delta. \end{aligned} \tag{A3}$$

Hence,

$$\dot{\boldsymbol{T}} = (\dot{T}_{\alpha\beta} + e_{\alpha\gamma\delta}\Omega_\gamma T_{\delta\beta} + e_{\beta\gamma\delta}\Omega_\gamma T_{\delta\alpha})\boldsymbol{\lambda}_\alpha\boldsymbol{\lambda}_\beta \tag{A4}$$

or equivalently

$$(\dot{\boldsymbol{T}})_{\alpha\beta} = \dot{T}_{\alpha\beta} + e_{\alpha\gamma\delta}\Omega_\gamma T_{\delta\beta} + e_{\beta\gamma\delta}\Omega_\gamma T_{\delta\alpha}. \tag{A5}$$

The second time derivative is given by

$$\ddot{\boldsymbol{T}} = \ddot{T}_{\alpha\beta}\boldsymbol{\lambda}_\alpha\boldsymbol{\lambda}_\beta + 2\dot{T}_{\alpha\beta}\dot{\boldsymbol{\lambda}}_\alpha\boldsymbol{\lambda}_\beta + 2\dot{T}_{\alpha\beta}\boldsymbol{\lambda}_\alpha\dot{\boldsymbol{\lambda}}_\beta + 2T_{\alpha\beta}\dot{\boldsymbol{\lambda}}_\alpha\dot{\boldsymbol{\lambda}}_\beta + T_{\alpha\beta}\ddot{\boldsymbol{\lambda}}_\alpha\boldsymbol{\lambda}_\beta + T_{\alpha\beta}\boldsymbol{\lambda}_\alpha\ddot{\boldsymbol{\lambda}}_\beta. \tag{A6}$$

Since,

$$\begin{aligned} \ddot{\boldsymbol{\lambda}}_\alpha &= \dot{\boldsymbol{\Omega}}\times\boldsymbol{\lambda}_\alpha + \boldsymbol{\Omega}\times\dot{\boldsymbol{\lambda}}_\alpha \\ &= \dot{\boldsymbol{\Omega}}\times\boldsymbol{\lambda}_\alpha + \boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{\lambda}_\alpha) \\ &= e_{\delta\gamma\alpha}\dot{\Omega}_\gamma\boldsymbol{\lambda}_\delta + \Omega_\alpha\Omega_\delta\boldsymbol{\lambda}_\delta - \Omega^2\boldsymbol{\lambda}_\alpha \end{aligned} \tag{A7}$$

we have

$$\begin{aligned} \ddot{\boldsymbol{T}} = &(\ddot{T}_{\alpha\beta} + 2e_{\alpha\gamma\delta}\Omega_\gamma\dot{T}_{\delta\beta} + 2e_{\beta\gamma\delta}\Omega_\gamma\dot{T}_{\delta\alpha} \\ &+2e_{\alpha\gamma\delta}e_{\beta\nu\sigma}\Omega_\gamma\Omega_\nu T_{\delta\sigma} + e_{\alpha\gamma\delta}\dot{\Omega}_\delta T_{\delta\beta} \\ &e_{\beta\gamma\delta}\dot{\Omega}_\gamma T_{\delta\alpha} + \Omega_\alpha\Omega_\delta T_{\delta\beta} + \Omega_\beta\Omega_\delta T_{\delta\alpha} \\ &-2\Omega^2 T_{\alpha\beta})\boldsymbol{\lambda}_\alpha\boldsymbol{\lambda}_\beta \end{aligned} \tag{A8}$$

where $\Omega^2 \equiv \Omega_\sigma\Omega_\sigma$.

Finally, some comments are warranted concerning the important implications that these results have for turbulence modeling. The notion that realizability constraints can be used to calibrate a second-order closure model appears now to be fundamentally unsound. The process of ensuring realizability is decidedly *non-unique*. There is no apparent way to satisfy the strong form of realizability in the existing hierarchy of second-order closures and there are an infinity of ways in which the weak form of realizability can be implemented.

This brings us to the more fundamental question: Why is there such an obsession with realizability constraints in second-order closure modeling? It is a well established result that the standard form of the modeled dissipation rate equation (12) guarantees limited realizability – namely, non-negative values for the turbulent kinetic energy and dissipation rate in homogeneous turbulence (see Speziale 1990). Furthermore, so long as the fixed points of the model are realizable and sufficiently strong attractors, at worst there will be a *short transient* where one or two components of the turbulent kinetic energy become negative. This, in general, does not have to be computationally fatal, particularly if, for inhomogeneous flows, the turbulent diffusion terms are modeled with isotropic gradient transport models such as those introduced by Mellor and Herring (1973) (numerical instabilities generally arise from negative diffusivities). Typically the short transients where realizability violations occur are in turbulent flows that are so far from equilibrium that simple one-point closures cannot be expected to apply in the first place. In an effort to avoid short lived regimes where the solution can become unrealizable, models developed based on realizability constraints have been complicated substantially, leading to highly ill-behaved solutions that have no greater predictive capabilities than those of the simpler models near the limits of realizable turbulence. In fact, the higher-degree nonlinearities introduced to satisfy realizability often render a model ill-behaved to the point where the solution is contaminated by large amplitude oscillations for long durations of time. This is extremely unwise. It would be far preferable to introduce mathematical devices to avoid computationally dangerous unrealizable behavior in turbulent flows that are far from equilibrium without compromising the near-equilibrium predictions of a model. A simple mathematical means for making any existing second-order closure model realizable in this fashion, based on a stochastic analysis, is the subject of a companion paper (Durbin and Speziale 1993).

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their model containing $F^{1/2}$ are made single-valued in a physically consistent fashion – a simplification which invariably leads to a violation of the crucial positive second derivative constraint which requires that $0 < \ddot{\tau}_{(\alpha\alpha)} < \infty$ when $\tau_{(\alpha\alpha)}$ vanishes. Since the Shih-Lumley model was calibrated largely based on what now appear to be questionable realizability considerations, it becomes more understandable why the model does not perform well in basic benchmark turbulent flows as recently shown by Speziale, Gatski and Sarkar (1992) and Abid and Speziale (1993).

(2) The centrifugal acceleration generated by rotations of the principal axes of the Reynolds stress tensor can render $\ddot{\tau}_{(\alpha\alpha)}$ singular at the limits of one component turbulence and axisymmetric two component turbulence (the endpoints A and B of the two-component line of the Lumley anisotropy invariant map shown in Figure 4(a)). This makes it impossible to guarantee the satisfaction of the positive second derivative constraint (27) in existing second-order closure models – a deficiency that can lead to realizability violations. It thus appears to be impossible to *identically* satisfy the strong form of realizability in the current generation of second-order closures.

(3) The only way to unequivocally guarantee realizability in the current generation of second order closures is via the weak form of realizability where access to one or two component states of turbulence is avoided. The weak form of realizability as first proposed by Pope (1985) does indeed guarantee non-negative component energies in arbitrary homogeneous turbulent flows. However, there is an associated Schwarz inequality inconsistency with this form of weak realizability that led us to propose an alternative form which allows model predictions to come arbitrarily close to one and two component states. Interestingly enough, the Fu, Launder and Tselepidakis (FLT) model satisfies this alternative form of weak realizability and thus, unlike the Shih-Lumley model, it guarantees positive component energies in general homogeneous turbulent flows.

(4) In an attempt to satisfy the strong form of realizability, both the Shih-Lumley and FLT models introduce higher degree nonlinearities in the modeling of the rapid pressure-strain correlation. It was demonstrated in computations of homogeneous shear flow that these higher-order terms cause the models to become highly ill-behaved near one or two component states of turbulence where they generate large amplitude oscillations that are unphysical. Older models such as the Launder, Reece and Rodi and IP models that are linear do not have this problem. It must be remembered that the rapid pressure-strain correlation is, by its definition, linear in the energy spectrum tensor – a property that such nonlinear models do not possess.

IP, FLT and Shih-Lumley models (see Figures 11(a)-(c)). The IP model predicts a $\mathcal{P}/\varepsilon$ that peaks at $St \approx 10$ and then monotonically approaches its equilibrium value of $\mathcal{P}/\varepsilon \approx 2$ (see Figure 11(a)). While we have no confidence in the quantitative accuracy of these results, the crucial point is that the IP model predicts a strictly *non-negative* turbulence production. On the other hand, the Shih-Lumley and FLT models predict that $\mathcal{P}/\varepsilon$ undergoes large amplitude oscillations between positive and negative values (see Figures 11(b) - 11(c)). We believe that these results are highly unphysical; there is no apparent physical mechanism by which a homogeneous shear flow can produce a negative turbulence production, given that it is initially non-negative. Further evidence concerning the unphysical nature of large amplitude oscillations in homogeneous shear flow can be obtained from Rapid Distortion Theory (RDT) which we would expect to be an excellent approximation to the Navier-Stokes equations for homogeneous shear flow when $SK_0/\varepsilon_0 = 50$ (see Lee, Kim and Moin 1990). In Figure 12, the prediction of the FLT model for the time evolution of $\tau_{22}/(\tau_{22})_0$ is compared with the RDT solution for the initial conditions:

$$(b_{11})_0 = -0.0833, \quad (b_{22})_0 = -0.0833, \quad \frac{SK_0}{\varepsilon_0} = 50 \tag{68}$$

where $(b_{ij})_0 = 0$ for $i \neq j$. These initial conditions correspond to an axisymmetric homogeneous turbulence for which we were able to compute an energy spectrum tensor – an input that is needed as an initial condition for RDT. It is clear from the results in Figure 12 that the FLT model is predicting spurious oscillations (the same is true of the Shih-Lumley model which is not shown). These spurious oscillations appear to arise from the introduction of higher-degree nonlinearities in b_{ij} within the rapid pressure-strain models (see Appendix B). It must be remembered that the rapid pressure-strain correlation, from its definition, is a *linear* functional of the energy spectrum tensor. The IP model – which unlike the Shih-Lumley and FLT models is consistent with this linear property – does not experience unphysical oscillations. Evidence is beginning to accumulate concerning the counter-productive effect that higher degree nonlinearities have on the performance of pressure-strain models.

5. Conclusions

The results of a detailed study on the realizability of second-order closure models has been presented within the framework of homogeneous turbulence. Several interesting and surprising conclusions were arrived at which can be summarized as follows:

(1) The Shih-Lumley model is *not* a realizable model and, in many instances, suffers more realizability violations than the older and more widely used IP model of Launder and co-workers. This lack of realizability becomes apparent when the non-analytic terms in

the Shih-Lumley model are shown for the initial conditions

$$(b_{11})_0 = -0.32, \quad (b_{22})_0 = -0.12, \quad \frac{SK_0}{\varepsilon_0} = 50 \tag{65}$$

in homogeneous shear flow (again, $(b_{ij})_0 = 0$ for $i \neq j$). The Shih-Lumley model becomes unrealizable whereas for these same initial conditions, the IP model again yields realizable results as shown in Figure 7(b). Other computations indicated that the Shih-Lumley model can be driven unrealizable for virtually any initial conditions that are near a two-component state of turbulence – results that are consistent with the analysis presented in the previous section.

As mentioned earlier, the IP model is not a fully realizable second-order closure. However, the only way that the IP model can be made to yield unrealizable results in homogeneous shear flow is for the initial production to be *negative* and of a sufficient magnitude. This is easy to see once we recognize that when a principal Reynolds stress $\tau_{(\alpha\alpha)}$ vanishes the IP model yields (see Appendix B)

$$\Pi_{(\alpha\alpha)} - \frac{2}{3}\varepsilon = \frac{1}{3}C_1\varepsilon - \frac{2}{3}\varepsilon + \frac{2}{3}\mathcal{P} \tag{66}$$

which become negative only if $\mathcal{P} < \left(1 - \frac{1}{2}C_1\right)\varepsilon$ (this then yields $\dot{\tau}_{(\alpha\alpha)} < 0$ which leads to realizability violations). In Figure 8(a) the trajectories in the phase space $(-II, III)$ obtained from the IP model are shown for the initial conditions:

$$(b_{11})_0 = -0.24, \quad (b_{22})_0 = 0.17, \quad (b_{12})_0 = 0.2, \quad \frac{SK_0}{\varepsilon_0} = 50. \tag{67}$$

Since $(b_{12})_0$ is positive, the initial production is negative and the IP model becomes unrealizable. On the other hand, the FLT model – which is a nonlinear extension of the IP model that was formulated to satisfy realizability constraints – yields realizable results for these initial conditions as shown in Figure 8(b). Although it is realizable, the FLT model has problems with large amplitude oscillations like those of the Shih-Lumley model. This is illustrated in Figures 9(a)-9(b) where the predictions of the FLT model for F and b_{12} are compared with results obtained from the IP model. The IP model is only unrealizable for a relatively short transient (i.e., for $0 < St < 2$). Although the FLT model is realizable, its solution is contaminated by large amplitude oscillations until $St \approx 15$.

In order to further illustrate the problem that nonlinear models such as the Shih-Lumley and FLT models have with large amplitude oscillations, we return to the near one-component initial conditions (63). For this case, the FLT model is realizable as demonstrated by the phase space trajectories shown in Figure 10. However, some interesting conclusions can be drawn from a comparison of the ratio of production to dissipation $(\mathcal{P}/\varepsilon)$ predicted by the

The Lumley anisotropy invariant map is superimposed on this figure; realizable turbulence lies within this curvilinear triangle where the origin corresponds to isotropic turbulence, point A corresponds to two-component axisymmetric turbulence, and point B corresponds to one-component turbulence (see Lumley 1978). It is clear from Figure 4(a) that the Shih-Lumley model becomes unrealizable since its solution exits the triangle. The computations were conducted by setting $F^{1/2} = \sqrt{|F|}$ in the rapid model; this is the only way that their model is both single-valued and computable to an equilibrium state. As alluded to earlier, if we set $F^{1/2} = \sqrt{F}$, their model has no solution after F passes through zero (when solved numerically with any finite time step, a negative value of F is eventually computed before the critical time where F vanishes is arrived at – an occurrence that causes the program to terminate in an error). The computed results were validated numerically by an exhaustive grid refinement study.

In contrast to these results, the IP model of Launder and co-workers is fully realizable for this set of initial conditions as shown in Figure 4(b). The time evolution of F predicted by the Shih-Lumley and IP models is compared in Figure 5(a) where, henceforth, the dimensionless time $t^* \equiv St$. Two noteworthy conclusions can be drawn from these results: (a) The Shih-Lumley model is unrealizable ($F < 0$) for the large elapsed time of $0 < St < 15$, and (b) the Shih-Lumley model undergoes large amplitude oscillations until $St \approx 120$ – a result that will be shown later to be unphysical. Similar conclusions can be drawn from Figure 5(b) for the time evolution of the shear anisotropy b_{12}. The Shih-Lumley model oscillates between positive and negative values which appears to be highly unphysical (positive values of b_{12} correspond to *negative* turbulence production).

One might be tempted to argue that the initial conditions (63) are extreme and, therefore, constitute an overly stringent test of the Shih-Lumley model. However, it should be said at the outset that a model which claims to satisfy the strong form of realizability must withstand such a test – particularly, since the older IP model, which makes no claim of being generally realizable, is able to do so. Furthermore, even if we relax the initial conditions (63) somewhat to the alternative values:

$$(b_{11})_0 = -0.3, \quad (b_{22})_0 = -0.3, \quad \frac{SK_0}{\varepsilon_0} = 10 \tag{64}$$

the Shih-Lumley model still predicts unrealizable results as shown in Figure 6(a). The model remains ill-behaved, yielding large amplitude oscillations for the time evolutions of F and b_{12}, as shown in Figures 6(b) - 6(c). We also conducted a variety of calculations for initial conditions that were near the center of the two-component line of the Lumley anisotropy invariant map. In Figure 7(a), the trajectories in the phase space $(-II, III)$ predicted by

Corrsin 1981, Tavoularis and Karnik 1989, and Rogers, Moin and Reynolds 1986). In these experiments, an initially isotropic turbulence evolves after it is subjected to a uniform shear rate S. However, in order to provide a stringent test of realizability, we will consider initial conditions that are anisotropic and close to a one or two component state of turbulence where $F \approx 0$ (the existing physical and numerical experiments as mentioned above have concentrated on isotropic initial conditions where $F = 1$). Furthermore, we will consider large initial values of the shear parameter SK/ε which can make a model more prone to experience realizability violations.

The computations of homogeneous shear flow to be presented consist of numerical solutions of the nonlinear ordinary differential equations (6) and (12) subject to the constant mean velocity gradient tensor

$$\frac{\partial \overline{v}_i}{\partial x_j} = S\delta_{i1}\delta_{j2} \tag{61}$$

and the initial conditions

$$b_{ij} = (b_{ij})_0, \quad \frac{SK}{\varepsilon} = \frac{SK_0}{\varepsilon_0} \tag{62}$$

at time $t = 0$. Three models will be considered for Π_{ij}, $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ in Eqs. (6) and (12): the Shih-Lumley (SL) model; the Fu, Launder and Tselepidakis (FLT) model; and the IP model which is a simplified form of the Launder, Reece and Rodi (1975) model that has been used in a variety of applications starting with Gibson and Launder (1978). The detailed form of these models is provided in Appendix B. Time accurate solutions were computed using a fourth-order accurate Runge-Kutta numerical integration scheme. As in all existing second-order closures, the models predict that b_{ij} and SK/ε eventually achieve equilibrium values that are independent of the initial conditions (these constitute the fixed points of the nonlinear differential equations (6) and (12)). Each of the models yield realizable fixed points for homogeneous shear flow. A comparison of the equilibrium predictions of each of these three models with physical and numerical experiments can be found in Speziale, Gatski and Mac Giolla Mhuiris (1990) and Speziale, Gatski and Sarkar (1992).

First, we will present computed results for the initial conditions

$$(b_{11})_0 = (b_{22})_0 = -0.32, \qquad \frac{SK_0}{\varepsilon_0} = 50 \tag{63}$$

given that $(b_{ij})_0 = 0$ for $i \neq j$ (here, and in the other computations to follow, the corresponding initial condition for b_{33} can be obtained from the traceless constraint $b_{ii} = 0$). This corresponds to a strong uniform shear applied to an initially anisotropic turbulence that is close to a one-component state (the reader should remember that if $b_{11} = b_{22} = -1/3$, then $\tau_{11} = \tau_{22} = 0$). Figure 4(a) shows the computed trajectories of the Shih-Lumley model in the phase space $(-II, III)$ corresponding to these initial conditions for homogeneous shear flow.

be compelling. Weak realizability only precludes an initially three-component homogeneous turbulence from achieving a one or two component state in *finite time*; it renders no constraint on inhomogeneous turbulent flows such as those which occur near a solid boundary. The more serious criticism of weak realizability is that (51) is inconsistent with the Navier-Stokes equations. As proven by Schumann (1977), when a principal Reynolds stress component $\tau_{(\alpha\alpha)}$ vanishes, we must have $\dot{\tau}_{(\alpha\alpha)} = 0$. This can be easily seen from the associated Schwarz inequality:

$$\dot{\tau}_{(\alpha\alpha)} \equiv 2\overline{u_{(\alpha)}\dot{u}_{(\alpha)}} \leq 2\tau_{(\alpha\alpha)}^{1/2}\overline{(\dot{u}_{(\alpha)}\dot{u}_{(\alpha)})}^{1/2}. \tag{56}$$

¿From (56) it is clear that $\dot{\tau}_{(\alpha\alpha)}$ vanishes when $\tau_{(\alpha\alpha)}$ vanishes. Hence, we propose an alternative form of weak realizability: When a principal Reynolds stress $\tau_{(\alpha\alpha)}$ vanishes, we require that $\dot{\tau}_{(\alpha\alpha)} = 0$; however, when $\tau_{(\alpha\alpha)}$ is in a neighborhood of zero, we then enforce the constraint that $\dot{\tau}_{(\alpha\alpha)} > 0$. The latter condition guarantees that an initially three-component turbulence never achieves a one or two component state; however, it allows model predictions to come arbitrarily close to the boundaries of realizable turbulence unlike the formulation of Pope (1985). This alternative form of weak realizability might be satisfied as follows: when $\tau_{(\alpha\alpha)}$ is arbitrarily close to zero, enforce the constraints

$$\Phi^{(S)}_{(\alpha\alpha)} = \frac{2}{3}\varepsilon + CF^a \tag{57}$$

$$\Phi^{(R)}_{(\alpha\alpha)} = O(F^b) \tag{58}$$

with $b > a$ and $C > 0$. In traditional slow pressure-strain models, (57) corresponds to the conditions

$$C_1 = 2 + O(F^a) > 2 \tag{59}$$

$$C_2 \leq 3(C_1 - 2). \tag{60}$$

Here, the exponents a and b are completely arbitrary (for simplicity, we have absorbed ${}_D\varepsilon_{ij}$ into $\Phi^{(S)}_{ij}$). Interestingly enough, the model of Fu, Launder, and Tselepidakis (1987) (see Appendix B) satisfies this alternative form of weak realizability with the exponent $a = \frac{1}{2}$ and $b = 1$. In the next section, we will demonstrate computationally that this model is realizable, i.e., it never yields negative component energies.

4. Illustrative Computations

The theoretical points discussed in the previous section will now be demonstrated computationally for homogeneous shear flow. The test case of homogeneous shear flow is selected since it constitutes one of the simplest and most important benchmark turbulent flows that has been documented extensively by physical and numerical experiments (Tavoularis and

We thus conclude that *it appears to be impossible to identically satisfy the strong form of realizability in the current generation of second-order closure models.* The only way to unequivocally guarantee realizability in the current version of second-order closures is to avoid access to one or two component states of turbulence in the homogeneous limit.

3.2. The Weak Form of Realizability

We will now consider the weak form of realizability where one or two component states are inaccessible in finite time. As first presented by Pope (1985), weak realizability is satisfied if, when a principal Reynolds stress $\tau_{(\alpha\alpha)}$ vanishes,

$$\dot{\tau}_{(\alpha\alpha)} > 0. \tag{51}$$

This condition ensures that an initially three-component turbulence never achieves a two-component state. Realizability is guaranteed without the need to impose a second derivative constraint. Haworth and Pope (1986) derived a second-order closure based on a Langevin equation. Weak realizability is satisfied therein as follows: When a principal Reynolds stress $\tau_{(\alpha\alpha)}$ vanishes,

$$\Phi^{(R)}_{(\alpha\alpha)} = 0 \tag{52}$$

$$\Phi^{(S)}_{(\alpha\alpha)} - \frac{2}{3}\varepsilon > 0. \tag{53}$$

In the Haworth and Pope (1986) model, ${}_D\varepsilon_{ij} = 0$, so it follows that (52)–(53) ensures the satisfaction of the weak realizability constraint (51). In that model – as in virtually every version of the current generation of second-order closures – the slow pressure strain correlation is modeled as

$$\Phi^{(S)}_{ij} = -C_1\varepsilon b_{ij} + C_2\varepsilon(b_{ik}b_{kj} - \frac{1}{3}b_{k\ell}b_{k\ell}\delta_{ij}) \tag{54}$$

where the coefficients C_1 and C_2 can be functions of the invariants II and III as well as the turbulence Reynolds number. Since $b_{(\alpha\alpha)} = -\frac{1}{3}$ when $\tau_{(\alpha\alpha)} = 0$, the constraint (53) can be satisfied when a principal Reynolds stress component vanishes provided that (see Sarkar and Speziale 1990)

$$C_1 > 2, \quad C_2 \leq 3(C_1 - 2). \tag{55}$$

Hence, any slow pressure-strain model of form (54)–(55), when combined with a rapid pressure-strain model that vanishes in the two component limit, will be realizable.

Lumley and co-workers have criticized weak realizability on the grounds that one and two component states are made inaccessible; they often cite the two-component turbulence that occurs near a solid boundary as a counter-example. We do not consider this criticism to

$\dot{\tau}_{\alpha\beta} = \dot{\tau}_{(\alpha\alpha)}\delta_{\alpha\beta}$, it follows that

$$\begin{aligned}
\ddot{\tau}_{(\alpha\alpha)} &= -6\Omega^2_{(\alpha)}\tau_{(\alpha\alpha)} + 4\Omega^2\tau_{(\alpha\alpha)} + 2(tr\boldsymbol{\tau})\Omega^2_{(\alpha)} \\
&\quad +2\left[\sum_{\alpha=1}^{3}\tau_{(\alpha\alpha)}\Omega^2_{(\alpha)} - \Omega^2(tr\boldsymbol{\tau})\right] + g_{(\alpha\alpha)}
\end{aligned} \tag{46}$$

where $\Omega^2 \equiv \Omega^2_{(1)} + \Omega^2_{(2)} + \Omega^2_{(3)}$ and $tr\boldsymbol{\tau} \equiv \tau_{(11)} + \tau_{(22)} + \tau_{(33)}$. In all existing second-order closure models, f_{ij} is taken to be of the form:

$$f_{ij} = \tilde{f}_{ij}(\boldsymbol{\tau}, \overline{\boldsymbol{S}}, \overline{\boldsymbol{\omega}}, \varepsilon) \tag{47}$$

where, relative to the fixed coordinate system x_i, the components of $\overline{\boldsymbol{S}}$ and $\overline{\boldsymbol{\omega}}$ are given by

$$\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{v}_i}{\partial x_j} + \frac{\partial \overline{v}_j}{\partial x_i}\right), \quad \overline{\omega}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{v}_i}{\partial x_j} - \frac{\partial \overline{v}_j}{\partial x_i}\right). \tag{48}$$

Here, we are considering homogeneous turbulent flows where $\overline{S}_{ij}$ and $\overline{\omega}_{ij}$ are constant tensors. However, while $\dot{\overline{S}}_{ij}$ and $\dot{\overline{\omega}}_{ij}$ are zero, the same is not true for $\dot{\overline{S}}_{\alpha\beta}$ and $\dot{\overline{\omega}}_{\alpha\beta}$ which are non-zero and depend on $\boldsymbol{\Omega}$ due to the rotation of the principal axes. Hence, $\dot{\tilde{f}}_{\alpha\beta}$ depends explicitly on $\boldsymbol{\Omega}$ with a functional form determined by (47) and the homogeneous turbulence under consideration. In order to isolate the terms arising from the rotation of the principal axes, we wrote (45) in terms of $g_{\alpha\beta}$ since:

$$\begin{aligned}
g_{\alpha\beta} \equiv (\dot{\boldsymbol{f}})_{\alpha\beta} &= \left(\frac{\partial \tilde{\boldsymbol{f}}}{\partial \boldsymbol{\tau}} \cdot \dot{\boldsymbol{\tau}} + \frac{\partial \tilde{\boldsymbol{f}}}{\partial \varepsilon}\dot{\varepsilon}\right) : \ \boldsymbol{\lambda}_\alpha \boldsymbol{\lambda}_\beta \\
&= \left(\frac{\partial \tilde{\boldsymbol{f}}}{\partial \boldsymbol{\tau}} \cdot \tilde{\boldsymbol{f}} + \frac{\partial \tilde{\boldsymbol{f}}}{\partial \varepsilon}\dot{\varepsilon}\right) : \ \boldsymbol{\lambda}_\alpha \boldsymbol{\lambda}_\beta
\end{aligned} \tag{49}$$

after (44) and (47) are implemented. It is clear from (49) that $g_{(\alpha\alpha)}$ does not depend explicitly on $\boldsymbol{\Omega}$ (this stands in contrast to $\dot{\tilde{f}}_{(\alpha\alpha)}$ which depends on $\dot{\overline{S}}_{\alpha\beta}$, $\dot{\overline{\omega}}_{\alpha\beta}$ and, hence, on $\boldsymbol{\Omega}$ as a result of (16)). The off diagonal components of (19) give

$$\Omega_{(1)} = \frac{\tilde{f}_{(23)}}{\tau_{(22)} - \tau_{(33)}}, \quad \Omega_{(2)} = \frac{\tilde{f}_{(13)}}{\tau_{(33)} - \tau_{(11)}}, \quad \Omega_{(3)} = \frac{\tilde{f}_{(12)}}{\tau_{(11)} - \tau_{(22)}}. \tag{50}$$

Hence, $\boldsymbol{\Omega}$ can become singular when a principal component of the Reynolds stress tensor, say $\tau_{(11)}$, vanishes; this will happen when $\tau_{(22)}$ or $\tau_{(33)}$ also vanishes (the one-component limit) and when $\tau_{(22)} = \tau_{(33)}$ (the axisymmetric two-component limit). At these two critical points – which constitute the end points of the two component line of the Lumley anisotropy invariant map – the second derivative $\ddot{\tau}_{(\alpha\alpha)}$ can become singular according to (46) and (50). This makes it impossible to satisfy the crucial constraint (27).

made single-valued, as required on physical grounds, it fails to satisfy the crucial positive second derivative condition – a fatal flaw that can lead to realizability violations. In the next section, illustrative computations of homogeneous shear flow will be presented which definitively demonstrate that the Shih-Lumley model is not realizable.

Rotations of the Principal Axes

The use of the non-analytic term $F^{1/2}$ is not a viable means for ensuring realizability as shown above. The question remains as to whether there exist alternative mathematical forms that can identically satisfy the strong form of realizability. It will now be shown that the centrifugal acceleration generated by rotations of the principal axes of the Reynolds stress tensor can make $\ddot{\tau}_{(\alpha\alpha)}$ singular at two of the most extreme limits of realizable turbulence in any version of the present generation of second-order closures. If $\ddot{\tau}_{(\alpha\alpha)}$ is singular, realizability cannot be guaranteed. For example, consider the differential equation

$$\dot{F} = -F^{2/5}. \tag{42}$$

Eq. (42) has the exact solution

$$F = \left[F_0^{3/5} - \frac{3}{5}t^*\right]^{5/3} \tag{43}$$

which becomes negative and violates realizability. It is a simple matter with Eq. (42) to show that when $F = 0$: $\dot{F} = 0$ and $\ddot{F} = +\infty$. Hence, a singular second derivative, even if it is positive, can be fatal with respect to realizability.

By differentiating (14), we obtain the equation

$$\ddot{\boldsymbol{\tau}} = \dot{\boldsymbol{f}}. \tag{44}$$

¿From Appendix A, it follows that the component form of (44) relative to the principal axes is given by:

$$\begin{aligned} \ddot{\tau}_{\alpha\beta} = & -2e_{\alpha\gamma\delta}\Omega_\gamma\dot{\tau}_{\delta\beta} - 2e_{\beta\gamma\delta}\Omega_\gamma\dot{\tau}_{\delta\alpha} \\ & -e_{\alpha\gamma\delta}\dot{\Omega}_\gamma\tau_{\delta\beta} - e_{\beta\gamma\delta}\dot{\Omega}_\gamma\tau_{\delta\alpha} - 3\Omega_\alpha\Omega_\sigma\tau_{\sigma\beta} \\ & -3\Omega_\beta\Omega_\sigma\tau_{\sigma\alpha} + 4\Omega^2\tau_{\alpha\beta} + 2\tau_{\sigma\sigma}\Omega_\alpha\Omega_\beta \\ & +2(\Omega_\gamma\Omega_\sigma\tau_{\gamma\sigma} - \Omega^2\tau_{\sigma\sigma})\delta_{\alpha\beta} + g_{\alpha\beta} \end{aligned} \tag{45}$$

where $g_{\alpha\beta} \equiv (\dot{\boldsymbol{f}})_{\alpha\beta}$ (we write this equation in terms of $g_{\alpha\beta}$ since, unlike $\dot{f}_{\alpha\beta}$, it is free of any explicit dependence on $\boldsymbol{\Omega}$). Since, relative to the principal axes, we have $\tau_{\alpha\beta} = \tau_{(\alpha\alpha)}\delta_{\alpha\beta}$ and

(37). However, there is a problem: for $0 \le t^* \le 2$, we have $F^{1/2} \ge 0$ whereas for $t^* \ge 2$ we have $F^{1/2} \le 0$ as a result of (35). Hence, it is clear that the solutions of (33) are remaining realizable by virtue of $F^{1/2}$ shifting branches between $\sqrt{F}$ and $-\sqrt{F}$. It is unacceptable for a turbulence model to have multiple valued functions; when calculating a complex turbulent flow, how do we know when to take $F^{1/2}$ equal to $\sqrt{F}$ or $-\sqrt{F}$? There is no physically based selection rule. The differential equations corresponding to the two branches of $F^{1/2}$ are

$$\dot{F} = \sqrt{F} \tag{38}$$

and

$$\dot{F} = -\sqrt{F} \tag{39}$$

Eq. (39) has no solution for $t^* > 2$ (the solutions to (38) and (39) for $0 \le t^* \le 2$ are illustrated with the solid lines in Figure 2). Shih and Lumley tacitly take $F^{1/2} = \sqrt{F}$ (if they were to take $F^{1/2} = -\sqrt{F}$, then two component states would not be accessible when $C > 0$; furthermore, their model then predicts equilibrium values of the normal Reynolds stress anisotropies that are of the wrong sign). Hence, the Shih-Lumley model actually behaves like the generic differential equation (39) in the vicinity of $F = 0$ (for $C > 0$) which has no solution when $t^* > 2$. A differential equation like (39) that yields an undefined F is technically *unrealizable* since we must have $0 \le F \le 1$ in a realizable turbulence.

The fact that there is a realizability problem with (39) can more easily be seen in an alternative way. If (39) had realizable solutions for all times where $F \ge 0$, then we should be able to replace $\sqrt{F}$ in (39) with the $\sqrt{|F|}$. The stable solution to the differential equation

$$\dot{F} = -\sqrt{|F|} \tag{40}$$

is illustrated in Figure 3 and it is decidedly unrealizable: $F \to -\infty$ as $t^* \to \infty$ (although (40) formally has the fixed point $F = 0$, it is unstable). The results displayed in Figure 3 were obtained by a Runge-Kutta numerical integration. It can be shown that the analytical form of the stable solution to (40) is given by

$$F = \left(\sqrt{F_0} - \frac{1}{2}t^*\right)^2 [1 - 2H(t^* - 2)] \tag{41}$$

where $H(\cdot)$ is the Heaviside function. From (41) it follows that $\ddot{F}$ is discontinuous at the critical time $t^* = 2$ when F vanishes; the one-sided second derivatives are $\ddot{F}^- = \frac{1}{2}$ and $\ddot{F}^+ = -\frac{1}{2}$ when $F = 0$. For the nonlinear differential equation (39), $\ddot{F}^- = \frac{1}{2}$ whereas $\ddot{F}^+$ does not exist at $t^* = 2$ where $F = 0$. In either case, $\ddot{F}$ is undefined when $F = 0$ and, hence, the crucial second derivative constraint (27) is not satisfied. This leads us to the following important conclusion: *When the non-analytic terms in the Shih-Lumley model are* true for $F \geq 0$ (see Figure 1). A turbulence that becomes unrealizable by passing through a one-component state can correspond to $F \geq 0$. For example, consider a first order Taylor expansion for b_{ij} in the neighborhood of a one component turbulence where $\tau_{11} = \tau_{22} = 0$:

$$b_{ij} = \begin{pmatrix} -\frac{1}{3} - \alpha t & 0 & 0 \\ 0 & -\frac{1}{3} - \beta t & 0 \\ 0 & 0 & \frac{2}{3} + (\alpha + \beta)t \end{pmatrix}. \tag{34}$$

Here α and β are constants and t is a short elapsed time after a one-component state is achieved. When either α or β is greater than zero, the turbulence becomes unrealizable since $-\frac{1}{3} \leq b_{(ii)} \leq \frac{2}{3}$ for realizable turbulence. It is a simple matter to show from Eq. (30) that if $\alpha > 0$ and $\beta = 0$, then $F = 0$; furthermore, when $\alpha > 0$ and $\beta > 0$, then $F > 0$. In either case, the turbulence becomes unrealizable with $F \geq 0$. This leads us to our first pertinent conclusion: *The methodology of Shih and Lumley is fundamentally incapable of guaranteeing realizability for turbulent flows that are near a one-component state.* While this is not the major deficiency with the Shih-Lumley approach, it is still of consequence since turbulence that is near a one-component state is asymptotically approached in certain geophysical flows with strong stratification (see Zeman and Lumley 1976). A model that claims to be fully realizable must accommodate such a limit.

The Central Problem of Non-Analyticity

The major deficiency with the Shih-Lumley model lies in its use of the non-analytic function $F^{1/2}$ as a means to satisfy realizability. If the dimensionless time $t^* = \int C dt$ is introduced into (33), it follows that its exact solution can be written in the form

$$F^{1/2} = F_0^{1/2} - \frac{1}{2} t^*. \tag{35}$$

Since $F^{1/2} = \pm\sqrt{F}$ (where $\sqrt{F}$ denotes the positive value of the square root, i.e. $\sqrt{F} \equiv |F^{1/2}|$), it follows that there are two principal branches to the solution:

$$F = (\sqrt{F_0} + \frac{1}{2} t^*)^2 \tag{36}$$

and

$$F = (\sqrt{F_0} - \frac{1}{2} t^*)^2 \tag{37}$$

which are illustrated graphically in Figure 2 for an initial condition of $F_0 = 1$. If, starting from any $F_0 > 0$, we want to pass through a two-component state of turbulence (where $F = 0$) and then turn back up, we must pick the second branch of this solution given by

Tensorially invariant forms that behave like (28) near $\tau_{(\alpha\alpha)} \approx 0$ (where $\alpha = 1, 2$ or 3) were obtained by Shih and Lumley by the introduction of the invariant function

$$F = 1 + 9II + 27III \tag{29}$$

where II and III are, respectively, the second and third invariants of the anisotropy tensor b_{ij} (see Appendix B and Lumley 1978). It is a simple matter to show that

$$F = \frac{27}{8}\frac{\tau_{(11)}\tau_{(22)}\tau_{(33)}}{K^3} \tag{30}$$

in terms of the principal Reynolds stresses. For any realizable turbulence, we must have $0 \leq F \leq 1$ (see Lumley 1978). This prompted Shih and Lumley (1985) to suggest the tensorially invariant form

$$\dot{\tau}_{(\alpha\alpha)} \propto F^{1/2} \tag{31}$$

in the limit as $\tau_{(\alpha\alpha)}$, and hence F, goes to zero. The full tensorial asymptotic form of the Shih-Lumley model near $\tau_{(\alpha\alpha)} = 0$ is given by

$$\dot{\tau}_{(\alpha\alpha)} = -\alpha_1 K \left(\frac{\partial \overline{v}_{(\alpha)}}{\partial x_{(\alpha)}} - \alpha_2 \mathcal{P}\right) F^{1/2} \tag{32}$$

where $\mathcal{P} = -\tau_{ij}\partial\overline{v}_i/\partial x_j$ is the turbulence production and α_1 and α_2 are model constants that are positive. Since the coefficient that multiplies $F^{1/2}$ in (32) can be negative, the Shih-Lumley model allows access to one and two-component states of turbulence.

The One-Component Limit

The logic used by Shih and Lumley appears on the surface to be sound. They argued that (28) guarantees that when $\tau_{(\alpha\alpha)}$ vanishes, it follows that $\dot{\tau}_{(\alpha\alpha)}$ vanishes with $\ddot{\tau}_{(\alpha\alpha)} > 0$ – a set of conditions which should ensure that $\tau_{(\alpha\alpha)}$ never becomes negative as discussed in the previous section. While this line of reasoning appears to be correct at first glance, a deeper analysis uncovers a fundamental problem. By making use of (30), it is clear that for $\tau_{(\alpha\alpha)}$ and F close to zero, (32) can be rewritten in the form

$$\dot{F} = -CF^{1/2} \tag{33}$$

where in the neighborhood of $\tau_{(\alpha\alpha)} = 0$ we can treat the coefficient C as a constant. On the basis of (33) it follows that when $F = 0$: $\dot{F} = 0$ and $\ddot{F} = \frac{1}{2}C^2$ which is positive. However, as we will soon see, it would be a mistake to conclude that (33) guarantees realizability due to a variety of difficulties. Even though (33) can yield solutions where $F \geq 0$ for all times, there is a subtle problem. While $F < 0$ corresponds to unrealizable turbulence, the converse is not (see Schumann 1977 and Lumley 1978). This constraint is typically satisfied by guaranteeing that when $\tau_{(\alpha\alpha)}$ vanishes:

$$\Phi^{(S)}_{(\alpha\alpha)} - {}_D\varepsilon_{(\alpha\alpha)} = \frac{2}{3}\varepsilon \tag{25}$$

$$\Phi^{(R)}_{(\alpha\alpha)} = 0 \tag{26}$$

where $\boldsymbol{\Phi}^{(S)}$ and $\boldsymbol{\Phi}^{(R)}$ are, respectively, the slow and rapid parts of the pressure-strain correlation (here, $\boldsymbol{\Phi} = \boldsymbol{\Phi}^{(S)} + \boldsymbol{\Phi}^{(R)}$; cf. Lumley 1978). While the realizability constraints (25)–(26) are a rigorous consequence of the Navier-Stokes equations, in and of themselves, they are neither necessary nor sufficient to guarantee realizability. As shown by Pope (1985), realizability can be satisfied if (24) is replaced with the weaker constraint $\dot{\tau}_{(\alpha\alpha)} \geq 0$. Furthermore, even if the constraint $\dot{\tau}_{(\alpha\alpha)} = 0$ is satisfied when $\tau_{(\alpha\alpha)}$ vanishes, an added second derivative condition must be met for full realizability; namely, we *must* have

$$0 \leq \ddot{\tau}_{(\alpha\alpha)} < \infty. \tag{27}$$

If $\ddot{\tau}_{(\alpha\alpha)} = 0$, then the first non-vanishing derivative of $\ddot{\tau}_{(\alpha\alpha)}$ must be positive and bounded. It is crucial that the non-negative second derivative constraint (27) be properly satisfied to guarantee the realizability of second-order closures that allow one or two component states of turbulence to be accessible in finite time (i.e., (27) is a critical constraint for the satisfaction of the *strong form of realizability*). This constraint has not been properly analyzed in previous applications of realizability to second-order closure modeling, as we will show in the next section.

3. Analysis of Existing Second-Order Closures

In this section, the strong form of realizability will be critically assessed based on an analysis of the model proposed by Shih and Lumley. A new statement of the weak form of realizability will also be provided along with an example of a model (the Fu, Launder and Tselepedakis model) that satisfies this constraint and is realizable.

3.1. The Strong Form of Realizability

In the Shih-Lumley model (see Appendix B), an attempt is made to satisfy the second derivative constraint (27) by the construction of a rapid pressure-strain model that behaves asymptotically as

$$\dot{\tau}_{(\alpha\alpha)} \propto \tau^{1/2}_{(\alpha\alpha)} \tag{28}$$

near two-component states of turbulence where $\tau_{(\alpha\alpha)} \approx 0$. Here, it is understood that the proportionality factor must be *negative* in order to allow access to two-component states.

vectors $\boldsymbol{e}_i \equiv (\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$, the components of (14) are given by (6). However, relative to the principal axes – which have the base vectors $\boldsymbol{\lambda}_\alpha \equiv (\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \boldsymbol{\lambda}_3)$ – the component form of (14) is more complex since the basis is rotating in time. For any symmetric second rank tensor $\boldsymbol{T}$, it can be shown that (see Appendix A)

$$(\dot{\boldsymbol{T}})_{\alpha\beta} = \dot{T}_{\alpha\beta} + e_{\alpha\gamma\delta}\Omega_\gamma T_{\delta\beta} + e_{\beta\gamma\delta}\Omega_\gamma T_{\delta\alpha} \tag{16}$$

where $e_{\alpha\beta\gamma}$ is the permutation tensor and $\Omega_\alpha = \Omega_\alpha(t)$ is the angular velocity at which the principal axes are rotating. Relative to the principal axes, (14) takes the form

$$\dot{\tau}_{\alpha\beta} = f_{\alpha\beta} - e_{\alpha\gamma\delta}\Omega_\gamma \tau_{\delta\beta} - e_{\beta\gamma\delta}\Omega_\gamma \tau_{\delta\alpha}. \tag{17}$$

However, the Reynolds stress tensor is diagonal relative to the principal axes:

$$\tau_{\alpha\beta} = \tau_{(\alpha\alpha)}\delta_{\alpha\beta} \tag{18}$$

where $\tau_{(\alpha\alpha)}$ (for $\alpha = 1, 2, 3$) are the principal Reynolds stresses and the Einstein summation convention is suspended for indices that lie within parentheses. From (17) it is now clear that

$$\dot{\tau}_{(\alpha\alpha)}\delta_{\alpha\beta} = f_{\alpha\beta} - e_{\alpha\gamma\beta}\Omega_\gamma \tau_{(\beta\beta)} - e_{\beta\gamma\alpha}\Omega_\gamma \tau_{(\alpha\alpha)} \tag{19}$$

and, thus, we have

$$\dot{\tau}_{(\alpha\alpha)} = f_{(\alpha\alpha)} \tag{20}$$

by setting $\alpha = \beta$ since $e_{\alpha\gamma\alpha} = 0$ from the definition of the permutation tensor. It has thus been shown that, consistent with the earlier proof presented by Lumley (1978), rotations of the principal axes of the Reynolds stress tensor have no effect on the formulation of the first derivative constraint. As we will demonstrate later, such rotations have an important effect on the formulation of the second derivative constraint.

Schumann (1977) showed that when $\tau_{(\alpha\alpha)} = 0$, it follows that the correlations

$$P_{(\alpha\alpha)} = 0, \quad \Phi_{(\alpha\alpha)} = 0, \quad \varepsilon_{(\alpha\alpha)} = 0 \tag{21}$$

as a rigorous consequence of their definitions and the Schwarz inequality. Since

$$f_{(\alpha\alpha)} = P_{(\alpha\alpha)} + \Phi_{(\alpha\alpha)} - \varepsilon_{(\alpha\alpha)} \tag{22}$$

it follows that $f_{(\alpha\alpha)}$ vanishes when $\tau_{(\alpha\alpha)} = 0$. This leads us to the long established realizability constraint: *When*

$$\tau_{(\alpha\alpha)} = 0 \tag{23}$$

it follows that

$$\dot{\tau}_{(\alpha\alpha)} = 0 \tag{24}$$

are, respectively, the pressure-strain correlation and the dissipation rate tensor. The dissipation rate tensor can be split into isotropic and deviatoric parts, respectively, as follows:

$$\varepsilon_{ij} = \frac{2}{3}\varepsilon\delta_{ij} + {}_D\varepsilon_{ij} \tag{8}$$

where

$$\varepsilon \equiv \nu\overline{\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}} \tag{9}$$

is the scalar dissipation rate. Writing

$$\Phi_{ij} - \varepsilon_{ij} = \Pi_{ij} - \frac{2}{3}\varepsilon\delta_{ij} \tag{10}$$

with $\Pi_{ij} \equiv \Phi_{ij} - {}_D\varepsilon_{ij}$, it follows from (6) that closure is achieved once models for Π_{ij} and ε are provided. The current generation of second-order closures are based on models for Π_{ij} and ε that reduce to the general form (cf. Reynolds 1987 and Speziale 1991)

$$\Pi_{ij} = \varepsilon\mathcal{A}_{ij}(\boldsymbol{b}) + K\mathcal{M}_{ijk\ell}(\boldsymbol{b})\frac{\partial\overline{v}_k}{\partial x_\ell} \tag{11}$$

$$\dot{\varepsilon} = -C_{\varepsilon 1}\frac{\varepsilon}{K}\tau_{ij}\frac{\partial\overline{v}_i}{\partial x_j} - C_{\varepsilon 2}\frac{\varepsilon^2}{K} \tag{12}$$

for homogeneous turbulent flows. In (11)–(12),

$$K = \frac{1}{2}\tau_{ii}, \quad b_{ij} = \frac{\tau_{ij} - \frac{2}{3}K\delta_{ij}}{2K} \tag{13}$$

are, respectively, the turbulent kinetic energy and anisotropy tensor; the coefficients $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ are typically taken to be either constants or functions of the turbulence Reynolds number $Re_t \equiv K^2/\nu\varepsilon$ and, possibly, the dimensionless invariants of $\partial\overline{v}_i/\partial x_j$.

As first pointed out by Schumann (1977) and Lumley (1978), it is easier to examine the question of realizability in a coordinate system aligned with the principal axes of the Reynolds stress tensor. However, considerable care must be taken in such an analysis since the principal axes of the Reynolds stress tensor can rotate in a time-dependent manner for temporally evolving homogeneous turbulent flows. In coordinate free notation, (6) can be written as a dynamical system:

$$\dot{\boldsymbol{\tau}} = \boldsymbol{f} \tag{14}$$

where

$$\boldsymbol{f} = \boldsymbol{P} + \boldsymbol{\Pi} - \frac{2}{3}\varepsilon\boldsymbol{I} \tag{15}$$

given that $\boldsymbol{I}$ is the unit tensor and $\boldsymbol{P}$ is the production tensor whose components are provided by the first two terms on the right-hand-side of (6). In a fixed coordinate system with base via a stochastic analysis to guarantee realizability in such extreme cases with better behaved predictions. These issues will be discussed in detail in the sections to follow and illustrative calculations of homogeneous shear flow will be provided.

2. Realizability Constraints for Second-Order Closures

We will consider incompressible turbulent flows governed by the Navier-Stokes and continuity equations

$$\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \nu \nabla^2 v_i \tag{1}$$

$$\frac{\partial v_i}{\partial x_i} = 0 \tag{2}$$

where v_i is the velocity vector, P is the kinematic pressure, and ν is the kinematic viscosity of the fluid. As in all studies of Reynolds stress modeling, the velocity and pressure are decomposed into mean and fluctuating parts as follows:

$$v_i = \overline{v}_i + u_i, \quad P = \overline{P} + p \tag{3}$$

where an overbar represents an ensemble mean. The Reynolds-averaged Navier-Stokes and continuity equations take the form

$$\frac{\partial \overline{v}_i}{\partial t} + \overline{v}_j \frac{\partial \overline{v}_i}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} + \nu \nabla^2 \overline{v}_i - \frac{\partial \tau_{ij}}{\partial x_j} \tag{4}$$

$$\frac{\partial \overline{v}_i}{\partial x_i} = 0 \tag{5}$$

where $\tau_{ij} \equiv \overline{u_i u_j}$ is the Reynolds stress tensor. From its definition, it is clear that τ_{ij} has non-negative eigenvalues – a property that realizability constraints seek to preserve in Reynolds stress models.

In order to achieve closure, (4)–(5) must be supplemented with a Reynolds stress model that ties τ_{ij} to the global history of the mean velocity field in a physically reasonable fashion. We will analyze second-order closure models that are based on the Reynolds stress transport equation which, for homogeneous turbulence, simplifies to the form (cf. Hinze 1975)

$$\dot{\tau}_{ij} = -\tau_{ik} \frac{\partial \overline{v}_j}{\partial x_k} - \tau_{jk} \frac{\partial \overline{v}_i}{\partial x_k} + \Phi_{ij} - \varepsilon_{ij} \tag{6}$$

where

$$\Phi_{ij} = \overline{p \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)}, \quad \varepsilon_{ij} = 2\nu \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k}} \tag{7}$$

known as the *weak form of realizability.* Pope only required that when a principal Reynolds stress component vanishes, its time derivative be positive. This does guarantee realizability in that non-negative energy components cannot occur when this constraint is satisfied. It also has the advantage of eliminating the need to enforce the positive second time derivative constraint, since a model that properly satisfies the weak form of realizability can never access one or two component states of turbulence in finite time. Lumley and co-workers criticized the weak form of realizability on the grounds that states of two-component turbulence – which can occur in practical turbulent flows near a solid boundary – were inaccessible. Nevertheless, Haworth and Pope (1986) and Pope (1993) derived second-order closures for homogeneous turbulence from a Langevin equation that satisfied this weak form of realizability and, hence, guaranteed positive component energies. While Langevin equations had been used to prove realizability of the DIA and EDQNM two-point closures (see Kraichnan 1961 and Orszag 1970, 1977), Pope was the first to bring this stochastic analysis into the realm of second-order closure modeling.

The purpose of the present paper is to clarify the issue of realizability in second-order closure modeling and to discuss alternative means of ensuring realizable solutions. In regard to the former point, there are a variety of confusing and conflicting claims in the literature that need to be clarified – a task that can be accomplished within the context of homogeneous turbulence. It will be proven mathematically and demonstrated computationally that the Shih-Lumley model yields unrealizable solutions. The lack of realizability arises from the failure to satisfy the necessary positive second time derivative constraint when a principal Reynolds stress vanishes – a crucial condition that must be satisfied by models that allow access to one or two component states of turbulence. This problem only becomes apparent when the non-analytic terms in the Shih-Lumley model are made single-valued as required for physical consistency (a turbulence model cannot contain functions that are multiple-valued and give rise to non-unique solutions). It will furthermore be shown that the centrifugal acceleration generated by rotations of the principal axes of the Reynolds stress tensor can make second and higher-order time derivatives singular at the most extreme limits of two component turbulence. This is a heretofore neglected effect that appears to make any version of the present generation of second-order closures incapable of identically satisfying the strong form of realizability. Formulations of the weak form of realizability – which do give rise to realizable models – are examined critically and a more physically consistent statement of this constraint is provided. However, models that satisfy the weak, as well as the strong, form of realizability can be ill-behaved near one and two component states of turbulence due to the unnecessary introduction of higher-degree nonlinearities to satisfy realizability. In a related paper (Durbin and Speziale 1993), it is shown how linear models can be modified

1. Introduction

Second-order closure models have been an active area of research in turbulence modeling for the past few decades. Since second-order closures are based on the Reynolds stress transport equation – which accounts for both history and nonlocal effects – these models, in principle, allow for the description of more turbulence physics than lower level closures. Schumann (1977) was the first to systematically address the issue of realizability in second-order closure modeling. The constraint of realizability requires that a Reynolds stress model yield non-negative component energies in all turbulent flows, with the Schwarz inequality satisfied for each off-diagonal component of the Reynolds stress tensor. Schumann showed that realizability is satisfied identically by a model if, starting from any realizable initial conditions, it predicts a Reynolds stress tensor with non-negative eigenvalues for all later times. He also provided a variety of necessary conditions for the satisfaction of realizability and briefly outlined a proposed method for making unrealizable second-order closures realizable. This issue was of interest since it had long been known that unrealizable second-order closure models can lead to numerical instabilities. The *ad hoc* numerical technique of clipping – whereby when a negative component energy is computed it is arbitrarily set to zero – was introduced to alleviate just such a problem (see Deardorff 1973).

Lumley (1978, 1983) was the first to advocate the systematic use of realizability constraints in the formulation and calibration of second-order closure models. He clarified the constraints that a second-order closure should satisfy in order to be consistent with the *strong form of realizability*: When a principal Reynolds stress component vanishes, its time rate must also vanish and its second derivative must be positive. However, Lumley made a significant departure from Schumann (1977) in so far as he suggested that realizability could serve as a powerful new constraint in determining the allowable mathematical form of Reynolds stress models. Lumley (1978) also introduced the constraint of joint realizability into second-order closure modeling whereby the Schwarz inequality is imposed on scalar fluxes. A few years later, Shih and Lumley (1985) developed a rapid pressure-strain model based on the implementation of invariant tensor theory and realizability constraints alone. They combined this new rapid model (after some subsequent modifications were made) with the slow pressure-strain and isotropic dissipation rate models that Lumley (1978) had developed earlier. The resulting second-order closure has been commonly referred to as the Shih-Lumley model in the literature. Shih and Lumley – who claimed that their model was the first generally realizable second-order closure – subsequently reported a few applications to turbulent shear flows (see Shih and Lumley 1992, 1993). However, they did not report any tests of their model demonstrating whether it did indeed guarantee realizable solutions.

Pope (1985) departed from the approach of Lumley in proposing what has come to be

NEW RESULTS ON THE REALIZABILITY OF REYNOLDS STRESS TURBULENCE CLOSURES

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ABSTRACT

The realizability of Reynolds stress models in homogeneous turbulence is critically assessed from a theoretical standpoint. It is proven that a well known second-order closure formulated by Shih and Lumley using the strong realizability constraints of Schumann is, in fact, not a realizable model. The problem arises from the failure to properly satisfy the necessary positive second time derivative constraint when a principal Reynolds stress vanishes – a fatal flaw that becomes apparent when the non-analytic terms in their model are made single-valued as required on physical grounds. It is furthermore shown that the centrifugal acceleration generated by rotations of the principal axes of the Reynolds stress tensor can make the second derivative singular at the most extreme limits of realizable turbulence. This previously overlooked effect appears to make it impossible to identically satisfy the strong form of realizability in any version of the present generation of second-order closures. On the other hand, models properly formulated to satisfy the weak form of realizability – wherein states of one or two component turbulence are not accessible in finite time – are found to be realizable. However, unlike the simpler and more commonly used second-order closures, these models can be ill-behaved near the extreme limits of realizable turbulence due to the way that higher-degree nonlinearities are often unnecessarily introduced to satisfy realizability. Illustrative computations of homogeneous shear flows are presented to demonstrate these points which can have important implications for turbulence modeling.

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