J. Fluid Mech. (1994), *vol.* 280, *pp.* 395–407

Realizability of second-moment closure via stochastic analysis

By P. A. DURBIN[1] AND C. G. SPEZIALE[2]
[1]Center for Turbulence Research, Stanford University, Stanford, CA 94305-3030, USA
[2]Aerospace & Mechanical Engineering Department, Boston University, Boston, MA 02215, USA

(Received 8 November 1993 and in revised form 7 June 1994)

It is shown that realizability of second-moment turbulence closure models can be established by finding a Langevin equation for which they are exact. All closure models currently in use can be derived formally from the type of Langevin equation described herein. Under certain circumstances a coefficient in that formalism becomes imaginary. The regime in which models are realizable is, at least, that for which the coefficient is real. The present method does not imply unrealizable solutions when the coefficient is imaginary, but it does guarantee realizability when the coefficient is real; hence, this method provides sufficient, but not necessary, conditions for realizability. Illustrative computations of homogeneous shear flow are presented. It is explained how models can be modified to guarantee realizability in extreme non-equilibrium situations without altering their behaviour in the near-equilibrium regime for which they were formulated.

1. Introduction

The exact, unclosed Reynolds stress transport equation is usually the starting point for formulations of second-moment closure models. Modelling consists of replacing unclosed terms by semi-empirical formulae that express these terms as functions of the dependent variables. After introducing such models, quantities identified as '$\overline{u^2}$' or the like, no longer represent non-negative functions, obtained by squaring and averaging a random variable; rather, they are simply dependent variables of the model, obtained by solving a differential equation. However, it is desirable to formulate the equations of the model so that variables like $\overline{u^2}$ do maintain their non-negativity. The issue of realizability in turbulence modelling is whether solutions to the model are guaranteed to have non-negative variances and to satisfy other appropriate constraints, such as the Schwarz inequality between Reynolds stress components. Schumann (1977) and Lumley (1978) discuss these issues in the context of second-moment closure modelling. From a broader point of view, the adjective 'realizable' indicates that the solutions to the model equations could be second-order statistics of *some* stochastic process.

In Speziale, Abid & Durbin (1993) models based on the Schumann (1977)–Lumley (1978) methodology were re-examined and it was found that some such models did not guarantee realizability. That failure reflects certain major difficulties in applying this method. These difficulties motivated the present exploration of a simpler, alternative approach.

The obstacles in the Schumann (1977)–Lumley (1978) approach arise in the attempt to impose *strong* realizability, as discussed at length in Speziale *et al.* (1993). The *weak* form of realizability (Schumann, 1977, introduced this constraint but used the term 'over-realizability') is more tractable than the strong form. At the same time it safeguards against negative variances, thus achieving the objective of realizability constraints: namely, proscribing inadvertent, unphysical solutions to the model equations.

The present paper demonstrates how weak realizability can be analysed by a constructive method. This involves formulating a stochastic process for which the Reynolds stress model is the exact evolution equation of the second moments. The model then is guaranteed to be realizable because a correspondence to a well-defined stochastic process is established. In the present analysis, second-moment closure models of the type currently in use are shown to be exact for the statistics of a particular form of Langevin equation. Our analysis was heavily influenced by the papers of Haworth & Pope (1986) and Pope (1994). Those authors observed that the second-moment equation derived from the Langevin equation of a randomly evolving velocity vector constitutes a Reynolds stress closure model. In the present paper the analysis proceeds in the opposite direction: the second-moment closure is given and its realizability is analysed by finding a corresponding Langevin equation. We assume that the appropriate physics is accommodated by the second-moment closure; the stochastic analysis is purely a mathematical method for analysing such models.

The application of stochastic analysis to the realizability of turbulence models first arose in conjunction with spectral closures (Orszag 1977). Kraichnan (1961) advocated deriving statistical moment models from stochastic processes and proved realizability of the Direct Interaction Approximation (DIA) by showing that it produced the exact moment equation of a random coupling model. Langevin equations subsequently were used to prove realizability of the DIA and of Test-Field and EDQNM models (Orszag 1977).

Langevin equations are a special type of stochastic differential equation in which evolution is due to an imbalance between random forcing, deterministic forcing and deterministic damping. The presence of deterministic damping distinguishes Langevin equations from stochastic differential equations in general (Durbin 1983*a*). The Langevin equation can be regarded as a stochastic simulation of turbulent velocity fluctuations in a frame moving with the mean flow (Fung *et al.* 1992). The Langevin equation considered by Haworth & Pope (1986) and Pope (1994) is inadequate for the present task of analysing realizability of second-moment closure models; the Langevin equation that we will use is a special case of a more general form discussed in Durbin (1983*a*). The significant aspect of this general form is that anisotropic, white-noise forcing is included. Haworth & Pope (1986) argued on grounds of local isotropy that the forcing should be isotropic. Here we do not attribute any physical significance to the stochastic process. Anisotropic forcing is allowed simply to enable analysis of closure models that are not accessible from the Haworth & Pope (1986) formulation.

In this paper we will consider only models for homogeneous turbulence. These form a cornerstone of inhomogeneous turbulence modelling, so realizability in homogeneous turbulence is of primary importance.

2. Stochastic differential equations

This section provides some background for those unfamiliar with stochastic differential equations. It is highly non-rigorous; textbooks (e.g. Arnold 1974) can be consulted for a more complete development. Aspects relevant to turbulence modelling are discussed in Durbin (1983*b*) and in Pope (1985).

The simplest Langevin equation for an evolving random velocity vector is

$$\mathrm{d}u_i = -\frac{u_i}{T}\mathrm{d}t + (c_0\varepsilon)^{1/2}\,\mathrm{d}\mathscr{W}_i(t). \tag{2.1}$$

Here u_i is the dependent variable, t is the independent variable and $\mathscr{W}_i(t)$ is the Wiener stochastic process (Arnold 1974); u_i is a random function of t. The other quantities in (2.1) – T, c_0 and ε – are either constants or deterministic functions of t. The Wiener process can be thought of as a continuous random walk; its increments $\mathrm{d}\mathscr{W}_i(t)$ are the steps of the random walk – they provide Gaussian white-noise forcing in (2.1). The properties of these increments that will be used here are as follows:

$$\overline{\mathrm{d}\mathscr{W}_i} = 0, \quad \overline{\mathrm{d}\mathscr{W}_i\mathrm{d}\mathscr{W}_j} = \mathrm{d}t\,\delta_{ij}, \quad \overline{u_j\mathrm{d}\mathscr{W}_i} = 0. \tag{2.2}$$

The last of these is the non-anticipating property of Ito stochastic calculus; the second shows that $\mathrm{d}\mathscr{W}_i$ is an isotropic random process with magnitude of $O(\mathrm{d}t)^{1/2}$. When computing moment equations it is necessary to retain terms to $O(\mathrm{d}\mathscr{W}_i)^2$. It follows from $\mathrm{d}\mathscr{W} = O(\mathrm{d}t)^{1/2}$ that the stochastic process $u(t)$ defined by (2.1) is not differentiable with respect to t; $\mathrm{d}u/\mathrm{d}t$ is not defined as $\mathrm{d}t \to 0$. For present purposes, we wish to evaluate $\mathrm{d}\,\overline{u_iu_j}/\mathrm{d}t$ for the process (2.1). This is done as follows:

$$\begin{aligned}\mathrm{d}(u_iu_j) &= (u_i + \mathrm{d}u_i)(u_j + \mathrm{d}u_j) - u_iu_j \\ &= u_i\mathrm{d}u_j + u_j\mathrm{d}u_i + \mathrm{d}u_i\mathrm{d}u_j.\end{aligned} \tag{2.3}$$

Substituting (2.1) for the differentials in (2.3) and retaining terms to O(dt) gives

$$\mathrm{d}(u_iu_j) = -2\frac{u_iu_j}{T}\mathrm{d}t + c_0\varepsilon\mathrm{d}\mathscr{W}_i\mathrm{d}\mathscr{W}_j + (c_0\varepsilon)^{1/2}\,[\mathrm{d}\mathscr{W}_ju_i + \mathrm{d}\mathscr{W}_iu_j]. \tag{2.4}$$

Averaging this, using the rules (2.2), produces the second-moment equation

$$\frac{\mathrm{d}\,\overline{u_iu_j}}{\mathrm{d}t} = -2\frac{\overline{u_iu_j}}{T} + c_0\varepsilon\delta_{ij}. \tag{2.5}$$

Note that the isotropic term δ_{ij} in (2.5) is generated by the white-noise forcing in (2.1). *The results presented in this paper are a consequence entirely of this.*

Equation (2.5) can be regarded as a simple model for the evolution of anisotropic turbulence in the absence of mean velocity gradients. In that case the time-scale is set to $T = q^2/2\varepsilon$ where $q^2/2$ is the kinetic energy per unit mass and ε is the rate of its dissipation. The exact energy equation is

$$\frac{\mathrm{d}q^2}{\mathrm{d}t} = -2\varepsilon\,; \tag{2.6}$$

the trace of (2.5) is

$$\frac{\mathrm{d}q^2}{\mathrm{d}t} = (3c_0 - 4)\varepsilon. \tag{2.7}$$

Comparing these shows that if $c_0 = 2/3$ then (2.5) gives the correct energy equation. Equation (2.5) is the exact moment equation of the stochastic differential equation (2.1); hence, the solutions to this model are realizable as statistics of a stochastic process. Although (2.5) gives the correct energy equation, it is not a reasonable model for the individual components, $\overline{u_iu_j}$. It is used here solely to illustrate the mathematics.

The above shows how the second-moment equation of a given stochastic process (2.1) can be regarded as a closure model. The actual problem that we wish to address is the converse to this: we want to find a stochastic process that has a given second-moment equation. Consider the closure model

$$\frac{\mathrm{d}\,\overline{u_i u_j}}{\mathrm{d}t} = -\frac{c_1}{T}(\overline{u_i u_j} - \tfrac{1}{3}q^2\delta_{ij}) - \tfrac{2}{3}\varepsilon\delta_{ij} \tag{2.8}$$

for the above example of decaying anisotropic turbulence. It is easily verified, by applying the relations (2.2), that the second moments of

$$\mathrm{d}u_i = -\frac{c_1}{2T}u_i\mathrm{d}t + (c_0\varepsilon)^{1/2}\,\mathrm{d}\mathscr{W}_i(t) \tag{2.9}$$

are governed by equation (2.8), provided

$$c_0 = \frac{2}{3}\left(\frac{c_1 q^2}{2T\varepsilon} - 1\right).$$

It is essential to note that c_0 appears under a square root in (2.9): solutions to (2.8) are guaranteed to be realizable if (2.9) is a valid, real-valued stochastic process; this requires that c_0 be non-negative. Hence a *sufficient condition* for realizability of (2.8) is $c_0 \geqslant 0$. If $T = q^2/2\varepsilon$, then this condition is satisfied if $c_1 \geqslant 1$, which is the well-known condition of Rotta (Schumann 1977).

It should be noted that Langevin equations other than (2.9) have the second-moment equation (2.8): the second moment does not uniquely determine the stochastic process. Because of this, the association of realizability with $c_0 \geqslant 0$ provides a sufficient, but not necessary condition. Other Langevin equations with (2.8) as their second moment are easily obtained: simply add a deterministic force $F_i\mathrm{d}t$, or a random term $\overline{u_i u_k}\,\Omega_{kl}u_l\mathrm{d}t$, where Ω_{kl} is an antisymmetric non-random tensor, to the right-hand side of (2.9). Neither of these modifications alter the realizability condition $c_1 \geqslant 1$ because the isotropic terms in (2.8) are still generated by the white-noise forcing in (2.9). However, they do change the random process, demonstrating non-uniqueness of the correspondence between Langevin and Reynolds stress equations.

3. The IP model

A second-moment closure model is a set of evolution equations for the Reynolds stress tensor, $\overline{u_i u_j}$ and usually for the dissipation rate, ε. In homogeneous turbulence these consist of a system of ordinary differential equations. The exact equations contain terms that are not functions of the dependent variables, and hence are not a closed system. Modelling consists in replacing unclosed terms by functions of the dependent variables. Our concern in this paper is not with the process of formulating models, it is with analysing existing models. The original references describe the basis of the models.

One of the simplest models for homogeneous turbulence is the 'basic', or IP, model (Launder 1989). This is a sum of the Rotta return-to-isotropy and the Isotropization-of-Production formulae. Its evolution equation for the Reynolds stress is

$$\frac{\mathrm{d}\,\overline{u_i u_j}}{\mathrm{d}t} = -\frac{c_1}{T}(\overline{u_i u_j} - \tfrac{1}{3}q^2\delta_{ij}) - c_2(P_{ij} - \tfrac{2}{3}P\delta_{ij}) + P_{ij} - \tfrac{2}{3}\varepsilon\delta_{ij}. \tag{3.1}$$

The first two terms on the right-hand side are the Rotta and IP terms. The theoretical value of the IP constant c_2 is 3/5; the empirical, Rotta constant c_1 is taken to be 1.8. Here P_{ij} is the production tensor:

$$P_{ij} = -\overline{u_i u_k}\partial_k U_j - \overline{u_j u_k}\partial_k U_i, \tag{3.2}$$

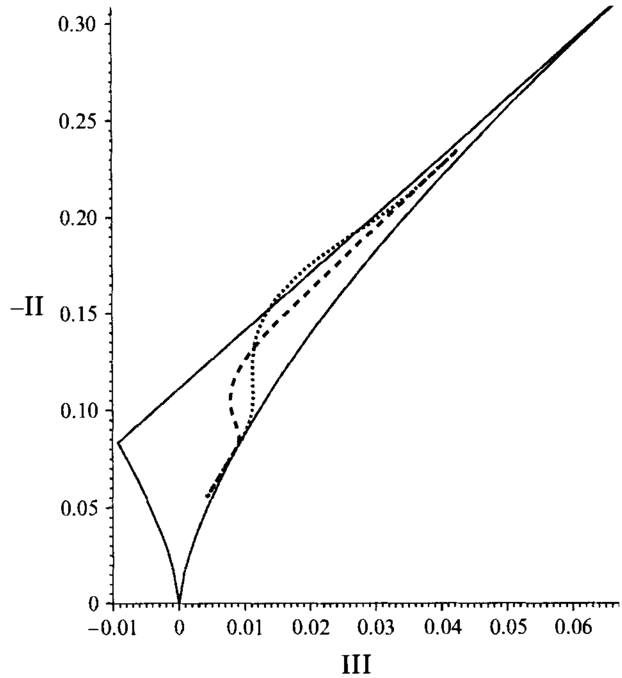

FIGURE 1. Solution trajectories in homogeneous shear flow projected onto the second-invariant/third-invariant plane. The interior of the curvilinear triangle is the realizable region. · · · ·, Original IP model; - - -, modified, realizable IP model.

where U_i is the mean velocity. $P = 1/2P_{kk}$ is the rate of turbulent energy production (per unit mass).

Equation (3.1) is the second moment of the Langevin equation

$$du_i = -\frac{c_1}{2T}u_i\mathrm{d}t + (c_2 - 1)u_k\partial_k U_i\mathrm{d}t + (c_0\varepsilon)^{1/2}\,\mathrm{d}\mathscr{W}_i(t) \tag{3.3}$$

provided that

$$c_0 = \frac{2}{3}\left(\frac{c_1 q^2}{2T\varepsilon} - 1 + c_2\frac{P}{\varepsilon}\right). \tag{3.4}$$

This was derived by inspection, essentially applying the method of the previous section in reverse; the formal verification of (3.2) and (3.3) follows by substituting into (2.3) and averaging using (2.2). Expression (3.4) for c_0 must be non-negative for (3.3) to be a valid Langevin equation because c_0 appears under a square-root. It follows from (3.4) that (3.1) will have realizable solutions if

$$\frac{P}{\varepsilon} \geqslant \frac{1 - c_1}{c_2} \tag{3.5}$$

where we have used $T \equiv q^2/2\varepsilon$ for the time-scale. For typical values of c_1 and c_2 the right-hand side of (3.5) is approximately -1. In most situations to which Reynolds stress models are applicable P/ε will be larger than -1, so that the IP model will have realizable solutions.

A succinct derivation of this result is as follows: the right-hand side of (3.4) is the coefficient of δ_{ij} in (3.1), non-dimensionalized by ε. This isotropic term is generated by squaring the white-noise forcing in (3.3). Hence, the sufficient condition (3.5) is simply that the coefficient of δ_{ij} in (3.1) has a real-valued square-root. The stochastic analysis explains why this assures realizability.

This proof of realizability is by construction: a stochastic process with statistics described by (3.1) can be realized by solving (3.3). The existence of such a process is *sufficient* for realizability, but the process is not unique; hence (3.5) is not a *necessary* condition. Nevertheless, we have found in numerical computations that unrealizable solutions to (3.1) can be found when P/ε is very near the bound given by (3.5). Figure 1 illustrates this via a computation of homogeneous shear flow turbulence. In homogeneous shear flow the mean velocity is in the x_1 direction and is given by $U_1 = Sx_2$, where S is the mean rate of shear. In the computation, $c_1 = 1.8$ and $c_2 = 0.6$: hence (3.5) guarantees realizable solutions when $P/\varepsilon \geqslant -4/3$, provided that the initial conditions are realizable. The initial conditions for this case are

$$Sq^2/\varepsilon = 3; \; b_{11} = b_{22} = 0.16; \; b_{33} = -0.32; \; b_{12} = 0.4; \; b_{13} = b_{23} = 0 \tag{3.6}$$

in which $b_{ij} = \overline{u_i u_j}/q^2 - \delta_{ij}/3$ is the anisotropy tensor. The initial location in figure 1 is $-\mathrm{II} = 0.237$; $\mathrm{III} = 0.043$, in which

$$\mathrm{II} = -\frac{b_{kl}b_{lk}}{2}; \; \mathrm{III} = \frac{b_{kl}b_{lm}b_{mk}}{3}.$$

The solid lines in figure 1 are boundaries of the Lumley (1978) triangle: realizable solutions must lie inside it. The dotted curve is a numerical solution to the IP model. Although the initial condition (3.6) makes $P/\varepsilon = -1.2$, which satisfies (3.5), as the solution evolves P/ε decreases below $-4/3$ and shortly thereafter exits the Lumley triangle. This is demonstrated in figure 2, which shows the evolution of P/ε and the function $F \equiv 1/9 + \mathrm{II} + 3\mathrm{III}$, defined in Lumley (1978). The latter is 0 on the upper boundary of the triangle in figure 1 and as the trajectory exits the triangle F crosses from positive to negative values. Before the trajectory re-enters the triangle P/ε has become greater than $-4/3$. This is why the caveat was made that (3.5) guarantees realizability *if* the initial conditions are realizable. The trajectory is ultimately attracted to the stable fixed point $-\mathrm{II} = 0.0563$; $\mathrm{III} = 0.0043$. In all computations the standard ε-equation,

$$\dot{\varepsilon} = \frac{2\varepsilon}{q^2}\left(c_{\varepsilon_1}P - c_{\varepsilon_2}\varepsilon\right), \tag{3.7}$$

with $c_{\varepsilon_1} = 1.5$ and $c_{\varepsilon_2} = 1.8$ was used. These constants give $P/\varepsilon = 1.6$ in equilibrium, which is the average of the experimental values measured for homogeneously sheared turbulence.

The solution to (3.3) is a Markovian stochastic process. It follows that (3.5) must be violated *at the instant* when a trajectory exits the Lumley triangle. The future state of a Markov process is statistically independent of its past; because (3.1) is exact for statistics of the Markov process (3.3), past transgressions of (3.5) are irrelevant to future behaviour. If a trajectory begins inside the triangle, P/ε drops below $-4/3$ but recovers before the trajectory reaches the boundary; the trajectory cannot then exit the triangle with $P/\varepsilon > -4/3$.

The Markov property and the non-anticipating property described in equation (2.2) make the dependence of coefficients in (3.3) on ensemble-averaged statistics easy to interpret. If the solution to (3.3) is advanced by finite difference integration, the coefficients used to step forward to $t + \Delta t$ must be evaluated at the present time, t.

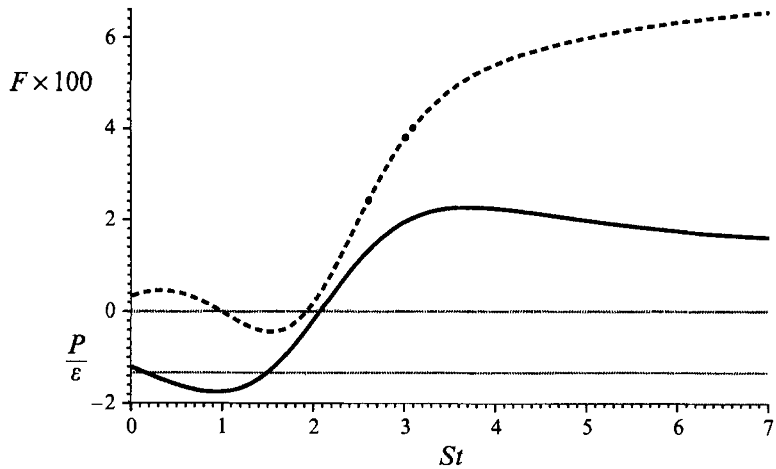

FIGURE 2. Time evolution of P/ε and $F \equiv 1/9 + \mathrm{II} + 3\mathrm{III}$ corresponding to the trajectory of the original IP model. As F becomes negative at $St \approx 1$ the solution exits the Lumley triangle. P/ε starts at -1.2 but soon decreases below $-4/3$, violating the *sufficient* condition for realizable trajectories. ——, P/ε; - - -, F.

Hence the information required to evaluate the coefficients is always available and does not affect the time advancement: the stochastic process is well defined.

Equation (3.4) suggests a method of guaranteeing that solutions are always realizable: one need only assure satisfaction of inequality (3.5). For example, if $c_1 = 1.8$ is replaced by

$$c_1 = \max[1.8, 1 - c_2 P/\varepsilon] \tag{3.8}$$

(assuming $T = q^2/2\varepsilon$) then $c_0 \geqslant 0$ unconditionally. Under most conditions this modification will reduce to $c_1 = 1.8$; under extreme conditions that would violate (3.5), the maximum in (3.8) will enforce realizability. This is illustrated by the dashed curve in figure 1: it remains inside the triangle. The effect of (3.8) is to enhance the return to isotropy when $P/\varepsilon < -4/3$. Obviously, a smooth function can be used instead of the *maximum*.

As a more extreme example, figure 3 shows trajectories for the initial condition $Sq^2/\varepsilon = 10$; $b_{11} = b_{22} = 0.15$; $b_{33} = -0.3$; $b_{12} = 0.3$; $b_{13} = b_{23} = 0$, for which $P/\varepsilon = -3.0$, $-\mathrm{II} = 0.158$ and $\mathrm{III} = 0.020$ initially. In this case the original IP model promptly exits the realizable region inside the triangle, while the model constrained by (3.8) stays well within it. It should be emphasized that (3.8) is an *ad hoc* mathematical device to enforce realizability in extreme situations. A model meant to predict the Reynolds stresses in such cases would have to incorporate empiricism into a function that enforced $c_0 \geqslant 0$ in a manner dictated by physical considerations.

4. The general linear model

Launder, Reece & Rodi (1975) derived the most general Reynolds stress closure that is linear in the anisotropy tensor. We will show that model to be the second

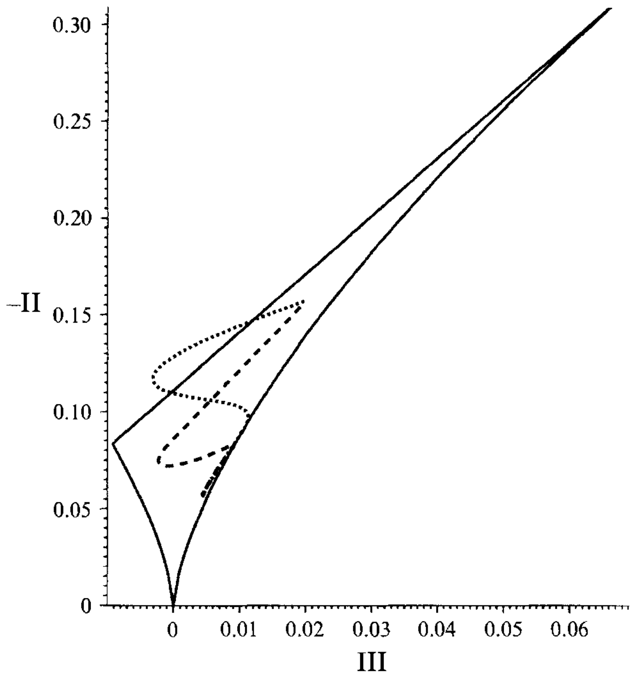

FIGURE 3. Solution trajectories as in figure 1 but with a different initial condition: $\cdots\cdot$, original IP model; - - -, modified, realizable IP model.

moment of the stochastic differential equation

$$du_i = -\frac{c_1}{2T}u_i dt + (c_2 - 1)u_k\partial_k U_i dt + c_3 u_k \partial_i U_k dt + (c_0\varepsilon)^{1/2}\, d\mathscr{W}_i(t) + (c_s\varepsilon)^{1/2}\, M_{ik} d\mathscr{W}'_k(t) \tag{4.1}$$

in which $\mathscr{W}$ and $\mathscr{W}'$ are independent Wiener processes ($\overline{d\mathscr{W}'_i d\mathscr{W}_j} = 0$). $\boldsymbol{M}$ is a symmetric matrix that is defined by

$$M_{ij}^2 - \frac{1}{3}M^2\delta_{ij} = -\frac{q^2}{2\varepsilon}S_{ij}, \tag{4.2}$$

where $M_{ij}^2 = M_{ik}M_{kj}$, $M^2 = M_{kk}^2$ and S_{ij} is the rate of strain tensor, defined as $(\partial_i U_j + \partial_j U_i)/2$. The matrix $\boldsymbol{M}$ can be described as a generalized square-root of $-q^2\boldsymbol{S}/2\varepsilon$. It can be constructed as follows: in incompressible flow, $\boldsymbol{S}$ is a symmetric matrix with eigenvalues that sum to zero; it can be diagonalized by the unitary matrix $\boldsymbol{U}$ of eigenvectors:

$$\frac{q^2}{2\varepsilon}\boldsymbol{S} = \boldsymbol{U}\cdot \mathrm{diag}[\lambda_1, \lambda_2, \lambda_3]\cdot {}^t\boldsymbol{U}, \tag{4.3}$$

where $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3$ are the eigenvalues in decreasing order. They satisfy the traceless condition

$$\lambda_1 + \lambda_2 + \lambda_3 = 0. \tag{4.4}$$

The generalized square-root matrix is given by

$$\boldsymbol{M} = \boldsymbol{U}\cdot \mathrm{diag}\left[0, (\lambda_1-\lambda_2)^{1/2}, (\lambda_1-\lambda_3)^{1/2}\right]\cdot {}^t\boldsymbol{U}. \tag{4.5}$$

By virtue of (4.4), $M^2 = 3\lambda_1$. It can be verified by substitution that $\boldsymbol{M}$ satisfies (4.2).

The Reynolds stress equation for (4.1) is derived by applying the rules (2.2):

$$\frac{\mathrm{d}\,\overline{u_i u_j}}{\mathrm{d}t} = -\frac{c_1}{T}\overline{u_i u_j} - c_2 P_{ij} - c_3 D_{ij} + c_s \varepsilon M_{ij}^2 + P_{ij} + c_0 \varepsilon \delta_{ij}. \tag{4.6}$$

$D_{ij} = -\overline{u_i u_k}\partial_j U_k - \overline{u_j u_k}\partial_i U_k$ is a tensor defined by Launder *et al.* (1975). Consistency with the energy equation

$$\frac{1}{2}\frac{\mathrm{d}q^2}{\mathrm{d}t} = P - \varepsilon \tag{4.7}$$

requires that

$$c_0 = \frac{2}{3}\left[c_1 - 1 + (c_2 + c_3)\frac{P}{\varepsilon}\right] - \frac{c_s}{3}M^2. \tag{4.8}$$

With this value, (4.6) becomes the General Linear Model

$$\frac{\mathrm{d}\,\overline{u_i u_j}}{\mathrm{d}t} = -\frac{c_1}{T}(\overline{u_i u_j} - \tfrac{1}{3}q^2\delta_{ij}) - c_2(P_{ij} - \tfrac{2}{3}P\,\delta_{ij}) - c_3(D_{ij} - \tfrac{2}{3}P\,\delta_{ij}) - c_s\frac{q^2}{2}S_{ij} + P_{ij} - \tfrac{2}{3}\varepsilon\delta_{ij}. \tag{4.9}$$

Realizability ($c_0 \geqslant 0$) is guaranteed if

$$c_1 \geqslant 1 - (c_2 + c_3)\frac{P}{\varepsilon} + \frac{c_s}{2}M^2 \tag{4.10}$$

(and if $c_s \geqslant 0$). For instance, if $c_1 = 1.8$ is usually a satisfactory value then

$$c_1 = \max\left[1.8,\ 1 - (c_2 + c_3)\frac{P}{\varepsilon} + \frac{3}{2}c_s\lambda_1\right] \tag{4.11}$$

will ensure realizability in extreme cases without altering the model in typical cases. $M^2 = 3\lambda_1$ has been substituted in (4.11); the rate of strain tensor enters the realizability condition via its most positive eigenvalue.

Again, a succinct derivation of (4.10) is to note that c_0 is the coefficient of δ_{ij} in the Reynolds stress model (4.9) after the representation (4.2) is substituted. A non-negative value of this coefficient assures realizable solutions. Launder *et al.* (1975) imposed certain symmetry and normalization constraints that led them to specialize (4.9) by setting

$$c_2 = \frac{c+8}{11};\ c_3 = \frac{8c-2}{11};\ c_s = \frac{60c-4}{55}, \tag{4.12}$$

where c is a constant they set to 0.4 – this is the LRR model. With (4.12), the condition (4.11) becomes

$$c_1 = \max\left[1.8,\ 1 - 0.873\frac{P}{\varepsilon} + 0.545\lambda_1\right]. \tag{4.13}$$

This modification to c_1 constrains the solutions of the LRR model to be realizable.

Figure 4 shows trajectories of the LRR model for homogeneously sheared turbulence, with initial conditions: $Sq^2/\varepsilon = 20$; $b_{11} = -0.27; b_{22} = -0.33$; $b_{33} = 0.6$; $b_{12} = b_{13} = b_{23} = 0$. These values give $P/\varepsilon = 0$, $-\mathrm{II} = 0.27$ and $\mathrm{III} = 0.053$. The initial value of $1 - 0.873P/\varepsilon + 0.545\lambda_1$ is 3.73 (note that $\lambda_1 = Sq^2/4\varepsilon$) so that (4.10) is violated when $c_1 = 1.8$. The dotted curve shows that the LRR model exits the realizable region for this initial condition. In this calculation, P/ε starts at 0 and subsequently becomes positive; it is equal to 0.78 at the time when the trajectory exits the Lumley

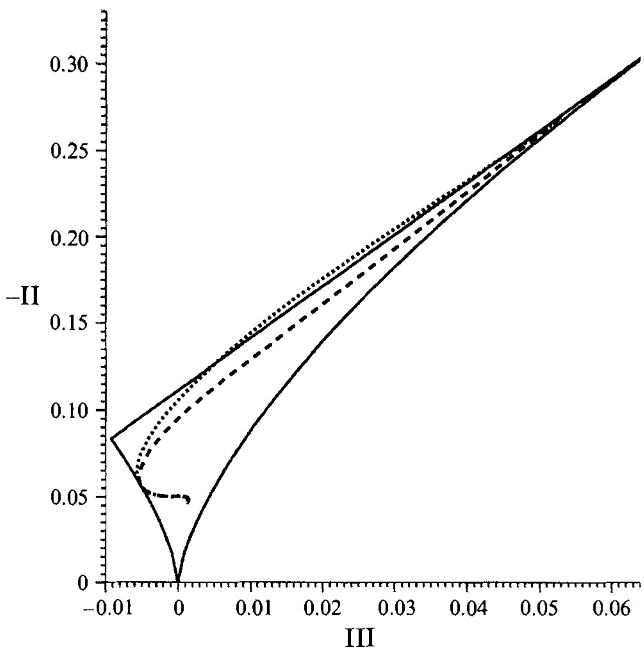

FIGURE 4. Solution trajectories of the LRR model projected onto the second-invariant/third-invariant plane. ····, original LRR model; - - -, modified, realizable LRR model.

triangle. Hence, the rate of strain can drive the LRR model unrealizable despite the rate of energy production being positive. This contrasts with the IP model, which can only become unrealizable if the production is negative. Thus, the sufficient conditions derived by the present method provide an insight into the existence of unrealizable trajectories. The solution trajectory remains inside the realizable region when the modification (4.13) is applied, as shown by the dashed curve in figure 4.

5. Non-linear models

The method of stochastic analysis outlined here is quite general and can be applied to Reynolds stress closures that are nonlinear in the anisotropy tensor as well. For instance, by adding the term

$$\frac{c_4}{2T} b_{ik} u_k \mathrm{d}t \tag{5.1}$$

to (4.1) and making the coefficients suitable functions of P/ε and II, a Langevin equation can be found for the SSG model (Speziale, Sarkar & Gatski 1991). To obtain this Langevin equation the coefficients in (4.1) and (5.1) are set to

$$\left.\begin{aligned} c_1 &= \tfrac{1}{2}\left[a_1 + a_1^* \frac{P}{\varepsilon} + \frac{a_2}{3}\right]; c_2 = \frac{a_4 + a_5}{4};\ c_3 = \frac{a_4 - a_5}{4}; \\ c_4 &= \frac{a_2}{2};\ c_s = \tfrac{2}{3}a_4 - a_3 + a_3^*(-2\mathrm{II})^{1/2}, \end{aligned}\right\} \tag{5.2}$$

where the constants of the SSG model are denoted by a_i (their numerical values are

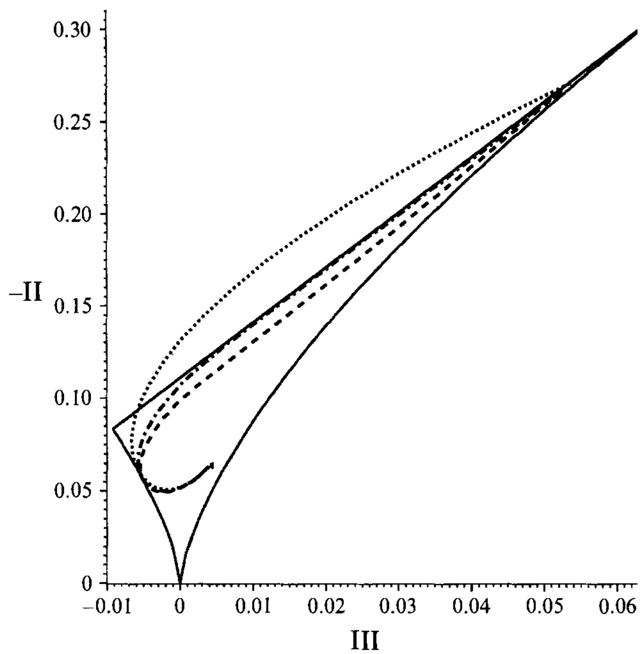

FIGURE 5. Solutions of the SSG model in the second-invariant/third-invariant plane. ····, Original SSG model; - - -, SSG model modified by (5.4); ——·——SSG model modified by (5.4) only when $F < 10^{-3}$.

$a_1 = 3.4$, $a_1^* = 1.8$, $a_2 = 4.2$, $a_3 = 4/5$, $a_3^* = 1.3$, $a_4 = 1.25$, $a_5 = 0.4$). In conjunction with (5.2)

$$c_0 = \frac{2}{3}\left[c_1 - 1 + (c_2 + c_3)\frac{P}{\varepsilon} + 2c_4 II\right] - c_s\lambda_1. \tag{5.3}$$

For the a_i given in Speziale *et al.* (1991), $c_s > 0$ so a sufficient condition for realizability is that the expression in (5.3) with (5.2) is non-negative. The sufficient condition (5.3) for realizability now depends upon the ratio of production to dissipation, the second invariant of the anisotropy tensor and the non-dimensional mean rate of strain. Realizability can be guaranteed by a method analogous to (3.8) or (4.11): constrain the model parameter a_1 by

$$\tfrac{1}{2}a_1 = \max\left[1.7,\ 1 - (c_1 - \tfrac{1}{2}a_1) - (c_2 + c_3)\frac{P}{\varepsilon} - 2c_4 II + \tfrac{3}{2}c_s\lambda_1\right]. \tag{5.4}$$

In the SSG model $a_1/2$ corresponds to the Rotta constant c_1 of the LRR and IP models; Speziale *et al.* selected the value 1.7 instead of the value 1.8 that was used in (3.8) and (4.11).

Figure 5 shows solutions to the original model and to the model modified by (5.4). The initial conditions are the same as in figure 4. Again P/ε is non-negative at all times. Initially $c_0 < 0$ and the original SSG model promptly exits the realizable region. The dashed curve imposes the constraint (5.4) to maintain a realizable trajectory.

Equation (5.4) prevents the solution from reaching the vicinity of the upper boundary of the Lumley triangle. This boundary is defined by $F \equiv 1/9 + \mathrm{II} + 3\mathrm{III} = 0$, $1/12 \leqslant -\mathrm{II} \leqslant 1/3$. The chain-dot curve is a computation in which (5.4) was imposed only when $F < 10^{-3}$. This illustrates the Markovian property that the solution cannot exit the Lumley triangle with $c_0 \geqslant 0$; thus, (5.4) need only be imposed near $F = 0$. It also serves to show that arbitrariness exists in the method of imposing realizability. This arbitrariness provides flexibility to incorporate empiricism into realizable models. Hence it is a virtue, not a fault, of the present method.

6. Discussion

The present analysis differs from those of Schumann (1977) and Lumley (1978). Theirs are local analyses in the neighbourhood of the two-component line of the Lumley triangle. The present approach is global and does not require detailed examination of the two-component limit.

The two-component state occurs when one component of the diagonalized Reynolds stress tensor – i.e. the tensor projected onto principal axes – vanishes. Call this component $\overline{u_\alpha u_\alpha}$ (with no implied summation on α). For functions differentiable with respect to time, the Schwarz inequality requires that when $\overline{u_\alpha u_\alpha} = 0$ then $\mathrm{d}\overline{u_\alpha u_\alpha}/\mathrm{d}t = 0$; an additional, positive second-derivative condition $\mathrm{d}^2\overline{u_\alpha u_\alpha}/\mathrm{d}t^2 > 0$ ensures that $\overline{u_\alpha u_\alpha} = 0$ is a local minimum. The imposition of these conditions, on a model for which the two-component state is attainable, is referred to as 'strong realizability'.

The 'weak realizability' constraint (Schumann 1977, Speziale *et al.* 1993) requires only $\mathrm{d}\overline{u_\alpha u_\alpha}/\mathrm{d}t > 0$ in a neighbourhood of $\overline{u_\alpha u_\alpha} = 0$. This makes the two-component state inaccessable, and hence obviates the need for a second-derivative condition. The second-derivative condition is the source of difficulty in applying the strong form of realizability.

Solutions to the Ito stochastic differential equations used in this paper are not differentiable with respect to time so $\mathrm{d}\overline{u_\alpha u_\alpha}/\mathrm{d}t$ need not vanish with $\overline{u_\alpha u_\alpha}$. However $\overline{u_\alpha u_\alpha}$ is a quantity squared so it will automatically be non-negative; a corollary is that if $\overline{u_\alpha u_\alpha}$ becomes zero at some instant, its derivative with respect to time at that instant must be non-negative. From equation (2.3)

$$\mathrm{d}\overline{u_\alpha u_\alpha} = 2\overline{u_\alpha \mathrm{d}u_\alpha} + \overline{(\mathrm{d}u_\alpha)^2}. \tag{6.1}$$

If $\overline{u_\alpha u_\alpha} = 0$ then $\overline{u_\alpha \mathrm{d}u_\alpha} = 0$ and (6.1) shows that $\mathrm{d}\overline{u_\alpha u_\alpha} = \overline{(\mathrm{d}u_\alpha)^2} \geqslant 0$. Thus the principal components of the Reynolds stress tensor cannot become negative because either the two-component state is repelling ($\mathrm{d}\overline{u_\alpha u_\alpha} > 0$ when $\overline{u_\alpha u_\alpha} = 0$) or, if the two-component line is reached, it cannot be crossed.

For each stochastic equation, $\overline{(\mathrm{d}u_\alpha)^2}$ in (6.1) is determined by the white-noise forcing. For equation (3.3), $\overline{(\mathrm{d}u_\alpha)^2} = c_0\varepsilon\mathrm{d}t$. If (3.8) is imposed then c_0 could become 0 near the two-component state. For the more general case (4.1), $\overline{(\mathrm{d}u_\alpha)^2} = c_0\varepsilon\mathrm{d}t + c_s\varepsilon M^2_{\alpha\alpha}$. In the presence of mean rate of strain this can be positive in the two-component state, even when (4.11) is imposed.

If a one-to-many correspondence of a second-moment closure to a family of uniformly valid Langevin equations can be found then the closure model is guaranteed to satisfy weak realizability, as defined in Schumann (1977) and Speziale *et al.* (1993).

REFERENCES

ARNOLD, L. 1974 *Stochastic Differential Equations.* John Wiley and Sons.

DURBIN, P. A. 1983*a* Asymptotic behavior of the Langevin equation in a non-homogeneous medium. Presented at 6*th* *Annual Meeting of the Canadian Applied Math. Soc., Toronto.*

DURBIN, P. A. 1983*b* Stochastic differential equations and turbulent dispersion. *NASA RP*-1103.

FUNG, J. C. H., HUNT, J. C. R., MALIK, N. A. & PERKINS, R. J. 1992 Kinematic simulation of homogeneous turbulence by unsteady random Fourier modes. *J. Fluid Mech.* **236**, 281.

HAWORTH, D. C. & POPE, S. B. 1986 A generalized Langevin model for turbulent flows. *Phys. Fluids* **30**, 1026.

KRAICHNAN, R. H. 1961 Dynamics of nonlinear stochastic systems. *J. Math. Phys.* **2**, 124.

LAUNDER, B. E. 1989 Second-moment closure: present...and future. *Intl J. Heat Fluid Flow* **10**, 282.

LAUNDER, B. E., REECE, G. J. & RODI, W. 1975 Progress in the development of a Reynolds stress turbulence closure. *J. Fluid Mech.* **68**, 537.

LUMLEY, J. L. 1978 Computational modeling of turbulent flows. *Adv. Appl. Mech.* **18**, 126.

ORSZAG, S. A. 1977 Statistical theories of turbulence. In *Fluid Dynamics, Les Houches.* Gordon and Breach.

POPE, S. B. 1985 PDF methods for turbulent reactive flows. *Prog. Energy Combust. Sci.* **11**, 119.

POPE, S. B. 1994 On the relationship between stochastic Lagrangian models of turbulence and second-moment closures. *Phys. Fluids* **6**, 973.

SCHUMANN, U. 1977 Realizability of Reynolds stress turbulence models. *Phys. Fluids* **20**, 721.

SPEZIALE, C. G., ABID, R. & DURBIN, P. A. 1993 New results on the realizability of Reynolds stress turbulence closures. *ICASE Rep. No. 93-76.*

SPEZIALE, C. G., SARKAR, S. & GATSKI, T. B. 1991 Modelling the pressure-strain correlation of turbulence: an invariant dynamical systems approach. *J. Fluid Mech.* **227**, 245.