On the relationship between stochastic Lagrangian models of turbulence and second-moment closures

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A detailed examination is performed of the relationship between stochastic Lagrangian models—used in PDF methods—and second-moment closures. To every stochastic Lagrangian model there is a unique corresponding second-moment closure. In terms of the second-order tensor that defines a stochastic Lagrangian model, corresponding models are obtained for the pressure-rate-of-strain and the triple-velocity correlations (that appear in the Reynolds-stress equation), and for the pressure-scrambling term in the scalar flux equation. There is an advantage in obtaining second-moment closures via this route, because the resulting models automatically guarantee realizability. Some new stochastic Lagrangian models are presented that correspond (either exactly or approximately) to popular Reynolds-stress models.

I. INTRODUCTION

Over the last 20 years, a standard approach to Reynolds-stress (or second-moment) turbulence closures has been established.[1–5] For the constant-property flows considered here, the starting point is the Navier–Stokes equations:

$$\frac{\partial U_i}{\partial x_i}=0 \tag{1}$$

and

$$\frac{DU_i}{Dt}=\frac{\partial U_i}{\partial t}+U_j\frac{\partial U_i}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\nu\frac{\partial^2 U_i}{\partial x_j\,\partial x_j}, \tag{2}$$

where $\mathbf{U}(\mathbf{x},t)$ is the velocity, $p(\mathbf{x},t)$ is the pressure (divided by density), and ν is the kinematic viscosity. The first step in the approach is to invoke the Reynolds decompositions

$$\mathbf{U}=\langle\mathbf{U}\rangle+\mathbf{u} \tag{3}$$

and

$$p=\langle p\rangle+p', \tag{4}$$

so that the Eulerian flow variables are written as the sums of their means (denoted by angled brackets) and their fluctuations (e.g., $\mathbf{u}$ and p'). Then the mean-momentum (or Reynolds) equations are obtained by taking the means of Eqs. (1) and (2). The Reynolds stresses $\langle u_iu_j\rangle$ appear as unknown in these equations.

The exact Reynolds stress equation [derived from Eqs. (1)–(4)] is

$$\frac{\partial}{\partial t}\langle u_iu_j\rangle+\langle U_l\rangle\frac{\partial\langle u_iu_j\rangle}{\partial x_l}=\mathscr{T}_{ij}+P_{ij}+\Pi_{ij}-\frac{2}{3}\epsilon\delta_{ij}. \tag{5}$$

The terms on the right-hand side represent, respectively: turbulent transport; production; redistribution; and dissipation. The redistribution term Π_{ij} is the focal point of Reynolds-stress modeling, and of this paper. If local isotropy exists, Π_{ij} is just the pressure rate of strain $\langle p'(\partial u_i/\partial x_j+\partial u_j/\partial x_i)\rangle$.

In the standard approach, Π_{ij} is approximated by a constitutive relation Π_{ij}^* of the form

$$\Pi_{ij}\approx\Pi_{ij}^*\left(\langle u_ku_l\rangle,\quad\frac{\partial\langle U_k\rangle}{\partial x_l},\epsilon\right). \tag{6}$$

The principal modeling task is to construct a specific expression for Π_{ij}^*. This is done partly mathematically—by requiring that Π_{ij}^* have the same known properties as Π_{ij} in particular circumstances—and partly empirically—by reference to experimental and simulation data, mainly for homogeneous turbulence.

The *modeled* Reynolds-stress equations are obtained by replacing Π_{ij} and $\mathscr{T}_{ij}$ in Eq. (5) by constitutive equations Π_{ij}^* and $\mathscr{T}_{ij}^*$, of the form of Eq. (6).

Thus, in the standard approach, a modeled Reynolds stress equation is obtained by constructing constitutive relations for one-point Eulerian statistics, such as the pressure rate of strain.

The same result (i.e., a modeled Reynolds-stress equation) can be obtained by a very different approach—from a *stochastic Lagrangian model.*[6–9]

In this second approach, the starting point is, again, the Navier–Stokes equations, but in Lagrangian form. Let $\mathbf{x}^+(t)$ and $\mathbf{U}^+(t)$ denote the position and velocity of a fluid particle. Then, by definition, $\mathbf{x}^+(t)$ evolves by

$$\frac{d}{dt}x_i^+(t)=U_i^+(t)\equiv U_i(\mathbf{x}^+[t],t). \tag{7}$$

The Navier–Stokes equations [Eq. (2)] can be written as

$$\begin{aligned}\frac{d}{dt}U_i^+(t)&=-\frac{\partial p}{\partial x_i}+\nu\frac{\partial^2 U_i}{\partial x_j\,\partial x_j}\\&=-\frac{\partial\langle p\rangle}{\partial x_i}+\nu\frac{\partial^2\langle U_i\rangle}{\partial x_j\,\partial x_j}-\frac{\partial p'}{\partial x_i}+\nu\frac{\partial^2 u_i}{\partial x_j\,\partial x_j},\end{aligned} \tag{8}$$

where it is understood that the Eulerian quantities on the right-hand side are evaluated at the particle location $\mathbf{x}^+(t)$. (The second line merely follows from a Reynolds decomposition, and is written for future reference.)

A stochastic Lagrangian model consists of stochastic processes $\mathbf{x}^*(t)$ and $\mathbf{U}^*(t)$ that model the fluid-particle properties $\mathbf{x}^+(t)$ and $\mathbf{U}^+(t)$. Here we consider models of the form[6]

$$\frac{dx_i^*}{dt}=U_i^* \tag{9}$$

and

$$\frac{dU_i^*}{dt}=-\frac{\partial\langle p\rangle}{\partial x_i}+\nu\frac{\partial^2\langle U_i\rangle}{\partial x_j\,\partial x_j}+G_{ij}(U_j^*-\langle U_j\rangle)+(C_0\epsilon)^{1/2}w_i. \tag{10}$$

In the final term, C_0 is a positive model constant, and $\mathbf{w}(t)$ is an isotropic white noise. [More properly, $\mathbf{W}(t)\equiv\int_0^t\mathbf{w}(s)ds$ is an isotropic Wiener process.[9]] The tensor $G_{ij}(\mathbf{x},t)$ is a specified function of the local values of $\langle u_iu_j\rangle$, $\partial\langle U_i\rangle/\partial x_j$ and ϵ, and again Eulerian quantities are evaluated at $\mathbf{x}^*(t)$. Comparing the model [Eq. (10)] with the Navier–Stokes equation [Eq. (8)], we can see that the terms in G_{ij} and C_0 together model the effects of the fluctuating pressure gradient and molecular viscosity.

Many other model equations can be derived[6–9] from the stochastic Lagrangian model, Eqs. (9) and (10). In particular, the "modeled" mean momentum equation is—by construction of the model—identical to the Reynolds equation, and the modeled Reynolds stress equation is

$$\frac{\partial}{\partial t}\langle u_iu_j\rangle+\langle U_l\rangle\frac{\partial\langle u_iu_j\rangle}{\partial x_l}=\mathscr{T}_{ij}+P_{ij}+G_{il}\langle u_ju_l\rangle+G_{jl}\langle u_iu_l\rangle+C_0\epsilon\delta_{ij}. \tag{11}$$

Thus, by a distinctly different route, this second approach yields a modeled Reynolds stress equation of an identical form to that obtained by the standard approach, Eq. (5): like Π_{ij}^*, the last three terms in Eq. (11) are functions of $\langle u_iu_j\rangle$, $\partial\langle U_i\rangle/\partial x_j$, and ϵ.

The stochastic process for $\mathbf{U}^*(t)$ is realizable [providing only that the coefficients in Eq. (10) are bounded]. Therefore, it follows,[7,9] that the Reynolds stresses implied by it are also realizable. In other words, Eq. (11) corresponds to a realizable Reynolds stress model.

The objective of this work is to explore the relationship between these two approaches: results are obtained that contribute to both. It is shown that it can be beneficial to derive second-moment closures via stochastic Lagrangian models, because realizability is simply assured, and because a scalar-flux model is obtained with few additional assumptions. Conversely, some new stochastic Lagrangian models (i.e. specifications of C_0 and G_{ij}) are obtained from existing Reynolds-stress closures. This is of value because the performance of Reynolds-stress closures (especially in inhomogeneous flows) has been more thoroughly investigated than that of stochastic Lagrangian models.

II. REYNOLDS-STRESS CLOSURES

In this section we summarize some existing models for the redistribution term Π_{ij}.

TABLE I. Definitions of the nondimensional, symmetric, deviatoric tensors $T_{ij}^{(n)}$.

$T_{ij}^{(1)}=b_{ij}$
$T_{ij}^{(2)}=b_{ij}^2-\frac{1}{3}b_{ll}^2\delta_{ij}$
$T_{ij}^{(3)}=S_{ij}$
$T_{ij}^{(4)}=S_{il}b_{lj}+S_{jl}b_{li}-\frac{2}{3}S_{lm}b_{ml}\delta_{ij}$
$T_{ij}^{(5)}=W_{il}b_{lj}+W_{jl}b_{li}$
$T_{ij}^{(6)}=S_{il}b_{lj}^2+S_{jl}b_{li}^2-\frac{2}{3}S_{lm}b_{ml}^2\delta_{ij}$
$T_{ij}^{(7)}=W_{il}b_{lj}^2+W_{jl}b_{li}^2$
$T_{ij}^{(8)}=b_{il}S_{lm}b_{mj}-\frac{1}{3}S_{lm}b_{ml}^2\delta_{ij}$

The exact term is defined by

$$\Pi_{ij}=\left\langle p'\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)\right\rangle-\left(\epsilon_{ij}-\frac{1}{3}\epsilon_{ll}\delta_{ij}\right), \tag{12}$$

where ϵ_{ij} is the dissipation tensor,

$$\epsilon_{ij}\equiv2\nu\left\langle\frac{\partial u_i}{\partial x_l}\frac{\partial u_j}{\partial x_l}\right\rangle. \tag{13}$$

It may be seen that Π_{ij} is a symmetric tensor with zero trace (since $\partial u_i/\partial x_i$ is zero). If local isotropy prevails, then the terms in ϵ_{ij} vanish in Eq. (12), and Π_{ij} is then the pressure rate of strain.

The class of model considered here can be written as

$$\Pi_{ij}^*=\epsilon\sum_{n=1}^{8}A^{(n)}T_{ij}^{(n)}, \tag{14}$$

where $A^{(n)}$ are scalar coefficients and $T_{ij}^{(n)}$ are the nondimensional, symmetric, deviatoric tensors given in Table I. They are defined in terms of the anisotropy tensor,

$$b_{ij}\equiv\langle u_iu_j\rangle/\langle u_lu_l\rangle-\tfrac{1}{3}\delta_{ij}, \tag{15}$$

and the normalized rate-of-strain and rotation tensors,

$$S_{ij}\equiv\frac{1}{2}\frac{k}{\epsilon}\left(\frac{\partial\langle U_i\rangle}{\partial x_j}+\frac{\partial\langle U_j\rangle}{\partial x_i}\right) \tag{16}$$

and

$$W_{ij}\equiv\frac{1}{2}\frac{k}{\epsilon}\left(\frac{\partial\langle U_i\rangle}{\partial x_j}-\frac{\partial\langle U_j\rangle}{\partial x_i}\right), \tag{17}$$

where $k\equiv\frac{1}{2}\langle u_iu_i\rangle$ is the turbulent kinetic energy. (An abbreviated notation is used in which b_{ij}^2 is written for $b_{il}b_{lj}$: thus b_{ij}^2 is the i-j component of $\mathbf{b}^2$, not the square of the component b_{ij}.)

The coefficients $A^{(n)}$ can depend on the scalar invariants of b_{ij}, S_{ij}, and W_{ij}: in particular, on

$$b'\equiv(b_{ii}^2)^{1/2} \tag{18}$$

and

$$P/\epsilon=-2b_{ij}S_{ji}, \tag{19}$$

where P is the production rate of k.

Equation (14) is not the most general possible model (in terms of ϵ, $\langle u_iu_j\rangle$, and $\partial\langle U_i\rangle/\partial x_j$) that is linear in $\partial\langle U_i\rangle/\partial x_j$. For example, the tensor

TABLE II. Coefficients $A^{(n)}$ for different Reynolds-stress models. (See the Appendix for details.)

Model	$A^{(1)}$	$A^{(2)}$	$A^{(3)}$	$A^{(4)}$	$A^{(5)}$	$A^{(6)}$	$A^{(7)}$	$A^{(8)}$	Model constants
Rotta	$-2C_1$	0	0	0	0	0	0	0	$C_1=4.15$
IPM	$-2C_1$	0	$\frac{4}{3}C_2$	$2C_2$	$2C_2$	0	0	0	$C_1=1.8,\ C_2=0.6$
LRR	$-2C_1$	0	$\frac{4}{5}$	$\frac{6}{11}(2+3C_2)$	$\frac{2}{11}(10-7C_2)$	0	0	0	$C_1=1.5,\ C_2=0.4$
SL	$-\beta+\frac{6}{5}(P/\epsilon)$	0	$\frac{4}{5}$	$12C_2$	$\frac{4}{3}(2-7C_2)$	$\frac{4}{5}$	$\frac{4}{5}$	$-\frac{8}{5}$	β see Ref. 13
									$C_2=\frac{1}{10}(1+\frac{4}{5}F^{1/2})$
SSG	$-2C_1-C_1^*(P/\epsilon)$	C_2	$C_3-C_3^*b'$	C_4	C_5	0	0	0	$C_1=1.7, C_1^*=1.8$
									$C_2=4.2,$
									$C_3=0.8, C_3^*=1.30$
									$C_4=1.25,\ C_5=0.40$

$$T_{ij}^{(9)}\equiv b_{ik}^2 W_{kl} b_{lj}+b_{jk}^2 W_{kl} b_{li}, \tag{20}$$

must be included to represent the model of Fu, Tselepidakis, and Launder.[10]

Table II shows the coefficients $A^{(n)}$ corresponding to five models: Rotta's model;[11] the isotropization of production model (IPM),[12,1] the Launder, Reece, and Rodi model (LRR);[1] the Shih–Lumley model (SL);[13] and the Speziale, Sarkar, and Gatski model (SSG).[14] Some notes on these models are provided in the Appendix.

Throughout this paper, a simple test case—derived from one of Abid and Speziale[17]—is used to contrast the performance of different Reynolds-stress models. This test case is of homogeneous, initially isotropic turbulence subjected to a constant shear, for which the only nonzero component of the mean velocity gradient is $\partial\langle U_1\rangle/\partial x_2=S_0$. In addition to the modeled Reynolds-stress equation, the following standard model equation is solved for the dissipation:

$$\frac{d\epsilon}{dt}=\frac{\epsilon^2}{k}\left(C_{\epsilon 1}\frac{P}{\epsilon}-C_{\epsilon 2}\right), \tag{21}$$

with $C_{\epsilon 2}=1.9$ and $C_{\epsilon 1}=1+(C_{\epsilon 2}-1)/1.6\approx 1.56$, so that the asymptotic value of P/ϵ is 1.6, in accord with experimental data.[21] [This expression for $C_{\epsilon 1}$ arises from the fact that $d(\epsilon/k)/dt$ tends to zero at large times.] For a given model, nondimensional quantities, as functions of the nondimensional time,

$$t'\equiv\int_0^t \frac{\epsilon(s)}{k(s)}\,ds, \tag{22}$$

depend solely on the normalized initial shear $S_0k(0)/\epsilon(0)$, which is taken to be unity.

Figure 1 shows the evolution of the anisotropy components b_{11} and b_{12} for four models (Rotta, IPM, LRR, and SSG).

Table III shows the asymptotic values ($t'\rightarrow\infty$) of the anisotropies and S_0k/ϵ for many models (with $P/\epsilon=1.6$ imposed), and from experimental data.[21] (The experimental values and those of the SL and FLT models are taken from Ref. 17. The values from LRR and SSG are calculated, and agree with those given by Abid and Speziale.)

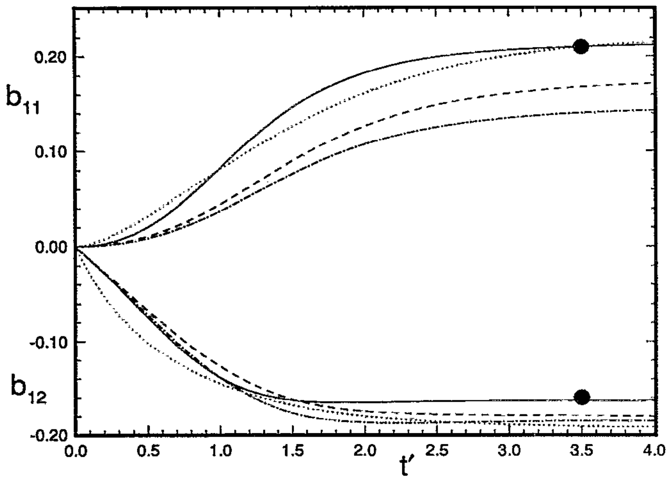

FIG. 1. Evolution of anisotropies in normalized time for homogeneous shear flow. Symbols, experimental data.[21] Lines, models: Rotta, dotted; IPM, dashed; LRR dot–dashed; SSG, solid.

TABLE III. Asymptotic values of anisotropy and S_0k/ϵ for different models. Here P/ϵ is specified to be 1.6.

	b_{11}	b_{12}	b_{22}	S_0k/ϵ
Experiment	0.21	−0.16	−0.13	5.0
Rotta	0.225	−0.193	−0.112	4.15
SLM	0.225	−0.193	−0.112	4.15
IPM	0.178	−0.181	−0.089	4.43
IPMa	0.113	−0.153	−0.056	5.23
LIPM	0.180	−0.181	−0.090	4.42
LRR	0.148	−0.185	−0.115	4.32
SL	0.110	−0.121	−0.112	6.61
FLT	0.183	−0.155	−0.127	5.16
SSG	0.215	−0.163	−0.142	4.90
SSGa	0.255	−0.205	−0.116	3.91
SSGb	0.241	−0.167	−0.125	4.80
LSSG	0.240	−0.166	−0.124	4.82
HP1	0.189	−0.138	−0.148	5.82
HP2	0.156	−0.187	−0.096	4.28

III. STOCHASTIC LAGRANGIAN MODEL

The general model considered is Eq. (10) with the tensor G_{ij}, given by

$$G_{ij}=\frac{\epsilon}{k}(\alpha_1\delta_{ij}+\alpha_2 b_{ij}+\alpha_3 b_{ij}^2)+H_{ijkl}\frac{\partial\langle U_k\rangle}{\partial x_l}, \qquad (23)$$

where

$$H_{ijkl}=\beta_1\delta_{ij}\delta_{kl}+\beta_2\delta_{ik}\delta_{jl}+\beta_3\delta_{il}\delta_{jk}+\gamma_1\delta_{ij}b_{kl}+\gamma_2\delta_{ik}b_{jl}+\gamma_3\delta_{il}b_{jk}+\gamma_4 b_{ij}\delta_{kl}+\gamma_5 b_{ik}\delta_{jl}+\gamma_6 b_{il}\delta_{jk}. \qquad (24)$$

Because of the inclusion of the term in α_3, Eq. (23) is a minor extension of the generalized Langevin model (GLM) proposed by Haworth and Pope.[19,20] There are 12 coefficients (α,β,γ), which can depend on the scalar invariants of b_{ij}, S_{ij}, and W_{ij}.

Some important observations concerning the coefficients are the following:

(1) The terms in β_1 and γ_4 multiply $\partial\langle U_l\rangle/\partial x_l$, which is zero for the incompressible flows considered. Therefore, their values are immaterial. We arbitrarily specify $\gamma_4=0$, while β_1 is specified below.

(2) The term in γ_1 is

$$\gamma_1\delta_{ij}b_{kl}\frac{\partial\langle U_k\rangle}{\partial x_l}.$$

Since the coefficients are allowed to depend on invariants (such as $b_{kl}\partial\langle U_k\rangle/\partial x_l$), this term is of the same form as that in α_1. Hence, without loss of generality we specify $\gamma_1=0$.

(3) As shown by Haworth and Pope,[19] in *isotropic turbulence*, exact kinematic relations are

$$\beta_1=\beta_3=-\tfrac{1}{5},\quad \beta_2=\tfrac{4}{5}. \qquad (25)$$

These relations are analogous to Crow's result[16] from RDT. Consequently, even though its value is immaterial, we specify $\beta_1=-\frac{1}{5}$.

(4) Speziale[22] has determined a transformation rule for the Reynolds stress equations in the extreme limit of *two-dimensional turbulence*. This rule is satisfied by the GLM if (in this limit) the coefficients satisfy

$$\beta_2-\beta_3+\tfrac{2}{3}(\gamma_2-\gamma_3)-\tfrac{1}{3}(\gamma_5-\gamma_6)=2. \qquad (26)$$

(5) The condition that the redistribution term does not affect the turbulent kinetic energy leads to the constraint

$$\tfrac{1}{2}+\tfrac{3}{4}C_0+\alpha_1+b_{ii}^2(\alpha_2+\tfrac{1}{3}\alpha_3)+b_{ii}^3\alpha_3+(\beta_2+\beta_3+\tfrac{1}{3}\gamma^*)I_1+\gamma^* I_2=0, \qquad (27)$$

where

$$\gamma^*\equiv\gamma_2+\gamma_3+\gamma_5+\gamma_6, \qquad (28)$$

$$I_1\equiv b_{ij}S_{ji}=-\frac{1}{2}\frac{P}{\epsilon} \qquad (29)$$

and

$$I_2\equiv b_{ij}^2 S_{ji}. \qquad (30)$$

A particular model within the class considered is defined by a specification of the coefficients C_0, α, β, and γ. We now define three models that have been used previously.

The simplified Langevin model (SLM)[6,20] is defined by $C_0=2.1$,

$$\alpha_1=-(\tfrac{1}{2}+\tfrac{3}{4}C_0), \qquad (31)$$

and all other coefficients zero. It is shown below—as has long been known[6]—that the SLM corresponds to Rotta's model.

Haworth and Pope[19,20] proposed two models, designated HP1 and HP2. The first, HP1, is defined by

$$C_0=2.1,\quad \alpha_2=3.7,\quad \alpha_3=0,$$
$$\beta_2=\tfrac{4}{5},\quad \beta_3=-\tfrac{1}{5},\quad \gamma_2=3.01,$$
$$\gamma_3=-2.18,\quad \gamma_5=4.29,\quad \gamma_6=-3.09.$$

This is the only model considered that satisfies Speziale's constraint. While this model gives satisfactory behavior for a wide range of homogeneous flows, it was found[20] to be unsatisfactory for free shear flows. The alternative, HP2, which gives satisfactory performance for free shear flows is defined by

$$C_0=2.1,\quad \alpha_2=3.78,\quad \alpha_3=0,$$
$$\beta_2=\tfrac{4}{5},\quad \beta_3=-\tfrac{1}{5},\quad \gamma_2=1.04,$$
$$\gamma_3=-0.34,\quad \gamma_5=1.99,\quad \gamma_6=-0.76.$$

IV. CORRESPONDING REYNOLDS-STRESS MODEL

As observed by Haworth and Pope,[19] to every stochastic Lagrangian model (of the form considered) there is a corresponding Reynolds-stress model. The corresponding redistribution term is obtained simply by equating the right-hand sides of the modeled Reynolds-stress equations obtained by the two approaches described in the Introduction, Eqs. (5) and (11). The result is

$$\Pi_{ij}^*=(\tfrac{2}{3}+C_0)\epsilon\delta_{ij}+G_{il}\langle u_l u_j\rangle+G_{jl}\langle u_l u_i\rangle. \qquad (32)$$

That is, a stochastic Lagrangian model [of the form of Eq. (10)] with specified C_0 and G_{ij} leads to a modeled Reynolds-stress equation with a redistribution term given by Eq. (32).

With the tensor G_{ij} being of the form considered in Sec. III [i.e., Eq. (23)], it follows that Π_{ij}^* [given by Eq. (32)] has a representation of the form considered in Sec. II [Eq. (14)].

It is just a matter of algebra, therefore, to determine the corresponding coefficients $A^{(n)}$. The result is that the GLM model given by Eqs. (23) and (24) corresponds to a Reynolds-stress model, with

$$A^{(1)}=4\alpha_1+\tfrac{4}{3}\alpha_2+2b_{ii}^2\alpha_3, \qquad (33)$$

$$A^{(2)}=4\alpha_2+\tfrac{4}{3}\alpha_3, \qquad (34)$$

$$A^{(3)}=\tfrac{4}{3}(\beta_2+\beta_3), \qquad (35)$$

$$A^{(4)}=2(\beta_2+\beta_3)+\tfrac{2}{3}(\gamma_2+\gamma_3+\gamma_5+\gamma_6), \qquad (36)$$

TABLE IV. RSM coefficients of different models (for isotropic turbulence).

	$A^{(1)}$	$A^{(2)}$	$A^{(3)}$	$A^{(4)}$	$A^{(5)}$	$A^{(6)}$	$A^{(7)}$	$A^{(8)}$
Rotta	−8.3	0	0	0	0	0	0	0
IPM	−3.6	0	0.8	1.2	1.2	0	0	0
LRR	−3.0	0	0.8	1.75	1.31	0	0	0
SL	−2.0	0	0.8	2.16	0.99	0.8	0.8	−1.6
SSG	−3.4	4.2	0.8	1.25	0.4	0	0	0
SLM	−8.3	0	0	0	0	0	0	0
HP1	−3.37	14.8	0.8	2.55	0.54	1.66	10.38	4.8
HP2	−3.26	15.12	0.8	2.49	1.09	1.4	2.76	4.92

$$A^{(5)}=2(\beta_2-\beta_3)+\tfrac{2}{3}(\gamma_2-\gamma_3-\gamma_5+\gamma_6), \tag{37}$$

$$A^{(6)}=2(\gamma_2+\gamma_3), \tag{38}$$

$$A^{(7)}=2(\gamma_2-\gamma_3), \tag{39}$$

and

$$A^{(8)}=4(\gamma_5+\gamma_6). \tag{40}$$

Table IV shows the numerical values of the coefficients $A^{(n)}$, both for Reynolds-stress models and for SLM, HP1, and HP2. (Coefficients depending on invariants are evaluated for $b'=0$ and infinite Reynolds number.) The following may be observed.

(1) Rotta and SLM have identical coefficients: this is discussed further in the next section.

(2) The values of $A^{(1)}$ for different models are comparable, except for Rotta and SLM, which have higher values to compensate for the lack of a rapid pressure model.

(3) Nonzero values of $A^{(2)}$ yield a nonlinear return to isotropy.[19,23] As observed by Sarkar and Speziale,[24] experimental data support the SSG value, rather than the much larger values of HP1 or HP2.

(4) Except for Rotta and SLM, all the models satisfy the RDT constraint $A^{(3)}=\tfrac{4}{5}$.

(5) HP1 and HP2 are distinguished by large values of $A^{(6)}$, $A^{(7)}$, and $A^{(8)}$, compared to the other models. For HP1, the very large value $A^{(7)}=10.38$ stems from the enforcement of Speziale's constraint [Eq. (26)].

Figure 2 compares the evolution of the anisotropies according to HP1, HP2, and SSG for the homogeneous-shear test case.

V. CORRESPONDING LAGRANGIAN MODELS

In the previous section, the Reynolds-stress model (RSM) coefficients $A^{(n)}$ are obtained explicitly in terms of the GLM coefficients α, β, and γ. In this section we consider the converse: namely, determining GLM coefficients α, β, and γ corresponding to RSM coefficients $A^{(n)}$. This is less straightforward.

Equations (35)–(40) form a set of six linear equations relating six RSM coefficients $A^{(3)}-A^{(8)}$ to six GLM coefficients: $\beta_2, \beta_3, \gamma_2, \gamma_3, \gamma_5$, and γ_6. However, the system has a rank deficiency of one. A solution for the GLM coefficients exists if, and only if, the coefficients $A^{(n)}$ satisfy

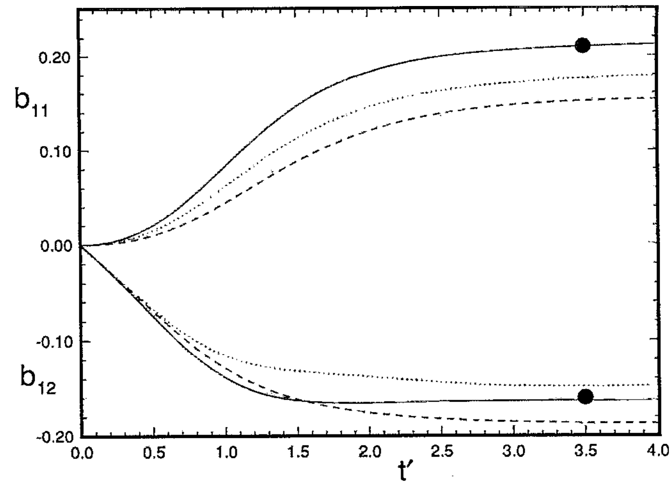

FIG. 2. Evolution of anisotropies in normalized time for homogeneous shear flow. Symbols, experimental data.[21] Lines, models: HP1, dotted; HP2, dashed; SSG, solid.

$$A^{*}=0, \tag{41}$$

where

$$A^{*}\equiv\tfrac{3}{2}A^{(3)}-A^{(4)}+\tfrac{1}{3}A^{(6)}+\tfrac{1}{6}A^{(8)}. \tag{42}$$

If the condition $A^{*}=0$ is satisfied, then there is a one-parameter family of solutions for $\beta_2, \beta_3, \gamma_2, \gamma_3, \gamma_5$, and γ_6.

We take γ_5 to be the free parameter, and then obtain

$$\beta_2=\tfrac{3}{8}A^{(3)}+\beta^{*}, \tag{43}$$

$$\beta_3=\tfrac{3}{8}A^{(3)}-\beta^{*}, \tag{44}$$

$$\gamma_2=\tfrac{1}{4}(A^{(6)}+A^{(7)}), \tag{45}$$

$$\gamma_3=\tfrac{1}{4}(A^{(6)}-A^{(7)}), \tag{46}$$

$$\gamma_6=\tfrac{1}{4}A^{(8)}-\gamma_5, \tag{47}$$

where

$$\beta^{*}=\tfrac{1}{4}A^{(5)}-\tfrac{1}{12}A^{(7)}-\tfrac{1}{24}A^{(8)}+\tfrac{1}{3}\gamma_5. \tag{48}$$

The three remaining coefficients, α_1, α_2, and α_3, are determined by the three equations, Eqs. (27), (33), and (34). The solution for α_2 is

$$\alpha_2=\frac{3}{F}\left[\frac{1}{2}+\frac{3}{4}C_0+s+\frac{1}{4}A^{(1)}-A^{(2)}\left(\frac{1}{8}b_{ii}^2-\frac{3}{4}b_{ii}^3\right)\right], \tag{49}$$

where F is the determinant of $\langle u_iu_j\rangle/(\tfrac{2}{3}k)$ [Eq. (107)], and s is defined by

$$s=(\tfrac{3}{4}A^{(3)}+\tfrac{1}{6}A^{(6)}+\tfrac{1}{12}A^{(8)})b_{ij}S_{ji}+(\tfrac{1}{2}A^{(6)}+\tfrac{1}{4}A^{(8)})b_{ij}^2S_{ji}. \tag{50}$$

With α_2 obtained from Eq. (49), the solutions for α_1 and α_3 are

$$\alpha_1=\tfrac{1}{4}A^{(1)}-\tfrac{3}{8}b_{ii}^2A^{(2)}-\alpha_2(\tfrac{1}{3}-\tfrac{3}{2}b_{ii}^2) \tag{51}$$

and

$$\alpha_3=\tfrac{3}{4}A^{(2)}-3\alpha_2. \tag{52}$$

The occurrence of $1/F$ in Eq. (49) raises questions concerning realizability that are now addressed. For a stochastic Lagrangian model, the modest realizability requirements are that the coefficients (α,β,γ) be bounded. Thus, for any such model, the corresponding Reynolds-stress model [with coefficients $A^{(n)}$ obtained from Eqs. (33)–(40)] is also realizable. It is evident from Eq. (49) that, as a two-component state (in which F is zero) is approached, the coefficient α_2 tends to infinity, unless the coefficients $A^{(n)}$ satisfy a special condition. Of the RSM models discussed above, only Rotta and SL satisfy this condition: the others imply infinite α in two-component turbulence. [It may be noted that if a more general model were considered (with b_{ij}^2 terms included in H_{ijkl}), then Eq. (49) would be unchanged, although s, Eq. (50), would contain additional terms.]

Both because of realizability, and because of the complexity of Eqs. (49) and (50), it is unappealing to consider stochastic Lagrangian models derived from Reynolds-stress models with α_2 determined from Eq. (49). Instead, in some of the models presented below, a simple expression for α_2 is used, which provides a good approximation to Eq. (49) (under normal circumstances).

Each of the Reynolds-stress closures discussed in Sec. II is now examined to determine a corresponding stochastic Lagrangian model—if one exists.

A. Rotta model

For Rotta's model, A^* [Eq. (42)] is zero, and hence corresponding stochastic Lagrangian models exist. The spirit of Rotta's model is simplicity, with no attempt to represent the rapid pressure terms. Consequently, an appropriate choice of the free parameter is $\gamma_5=0$, for then all the coefficients β and γ are zero. As a result, the tensor G_{ij} [Eq. (23)] does not depend on the mean velocity gradients, just as Π_{ij}^*, given by Rotta's model, does not.

For any specification of C_0 and of the Rotta constant C_1, the three remaining coefficients, α_1, α_2, and α_3, can be determined from Eqs. (49), (51), and (52). But a particularly simple model results if C_0 and C_1 are related in such a way that α_2 is zero. It is readily seen from Eq. (49) that this relation is

$$C_1=-\tfrac{1}{2}A^{(1)}=1+\tfrac{3}{2}C_0. \tag{53}$$

The resulting model is called the simplified Langevin model[19] (SLM), and is defined by

$$\alpha_1=-(\tfrac{1}{2}+\tfrac{3}{4}C_0), \tag{54}$$

with all other coefficients being zero. It has been used extensively in PDF methods (e.g., Refs. 25 and 26). The standard value $C_0=2.1$ leads to a Rotta constant of $C_1=4.15$, which is—not by coincidence—the value of C_1 specified here for the Rotta model.

B. IPM

For the IPM, the value of A^* is zero, and hence a family of corresponding stochastic Lagrangian models exists. A particular model corresponds to a particular specification of γ_5.

For isotropic turbulence, an exact result is

$$\beta_2-\beta_3=1 \tag{55}$$

[see Eq. (25)], while Eqs. (43) and (44) yield

$$\beta_2-\beta_3=2\beta^*. \tag{56}$$

A reasonable way to specify γ_5, therefore, is to require $\beta^*=\tfrac{1}{2}$. With this specification, from Eq. (48), we obtain

$$\gamma_5=\tfrac{3}{2}-\tfrac{3}{4}A^{(5)}+\tfrac{1}{4}A^{(7)}+\tfrac{1}{8}A^{(8)}. \tag{57}$$

This specification of γ_5 is used in all the models introduced below.

With γ_5 given by Eq. (57), for the IPM, Eqs. (43)–(47) yield

$$\begin{aligned}&\beta_2=\tfrac{1}{2}(1+C_2), \quad \beta_3=-\tfrac{1}{2}(1-C_2),\\ &\gamma_2=\gamma_3=0, \quad \gamma_5=-\gamma_6=\tfrac{3}{2}(1-C_2).\end{aligned} \tag{58}$$

The usual choice of $C_2=\tfrac{3}{5}$ gives $\beta_2=\tfrac{4}{5}$, $\beta_3=-\tfrac{1}{5}$, and $\gamma_5=\tfrac{3}{5}$.

The coefficients α_1, α_2, and α_3 for the IPM [obtained from Eqs. (49), (51), and (52)] are

$$\alpha_2=\frac{3}{F}\left[\frac{1}{2}+\frac{3}{4}C_0-\frac{1}{2}C_2\left(\frac{P}{\epsilon}\right)-\frac{1}{2}C_1\right], \tag{59}$$

$$\alpha_1=-\tfrac{1}{2}C_1-\alpha_2(\tfrac{1}{3}-\tfrac{3}{2}b_{ii}^2), \tag{60}$$

and

$$\alpha_3=-3\alpha_2. \tag{61}$$

We now consider three simple variants, denoted by IPMa, IPMb, and LIPM.

IPMa is defined by $\alpha_2=0$ (hence $\alpha_3=0$) and C_0 constant ($C_0=2.1$). Then, from Eq. (59), we obtain

$$C_1=1+\frac{3}{2}C_0-C_2\left(\frac{P}{\epsilon}\right). \tag{62}$$

This corresponds, then, to the IPM, but with the Rotta coefficient C_1 decreasing with P/ϵ. It appears that, in order to give a good performance, the Rotta coefficient should *increase* (or at least not decrease) with P/ϵ. The SSG model, for example, gives the coefficient increasing as 0.9 P/ϵ. Fu and Pope[27] used this model (IPMa) to calculate a two-dimensional recirculating flow with poor results, and hypothesized that the poor performance was due to the decrease of C_1 with P/ϵ. We have introduced IPMa here in order to make this point: it is most likely a poor model whose use is not advocated.

IPMb is defined by $\alpha_2=0$ (hence $\alpha_3=0$) and C_1 constant ($C_1=1.8$). Then, from Eq. (59), we obtain

$$C_0=\frac{2}{3}\left[C_1+\left(\frac{P}{\epsilon}\right)C_2-1\right]. \tag{63}$$

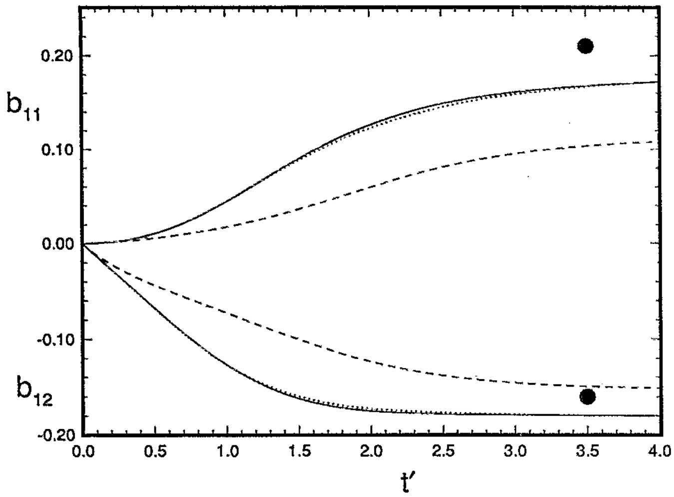

FIG. 3. Evolution of anisotropies in normalized time for homogeneous shear flow. Symbols, experimental data.[21] Lines, models: IPM, solid; IPMa, dashed; LIPM, dotted.

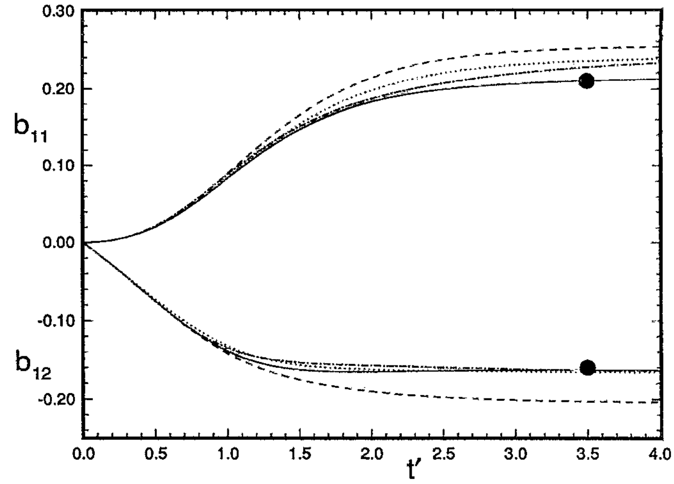

FIG. 4. Evolution of anisotropies in normalized time for homogeneous shear flow. Symbols, experimental data.[21] Lines, models: SSG, solid; SSGa, dashed; SSGb, dotted; LSSG, dot–dashed.

Thus, by making C_0 a coefficient that varies with P/ϵ, we obtain a relatively simple model that corresponds exactly to the IPM.

In early applications of the Langevin model (e.g., Refs. 3, 7, and 9), C_0 was identified as a Kolmogorov constant. Clearly, the dependence of C_0 on P/ϵ implied by Eq. (63) is at odds with this notion. However, more recently[8] it has become apparent that the value of the Kolmogorov constant is two to three times greater than the value $C_0=2.1$. If the connection between C_0 and the Kolmogorov constant is abandoned, the objection to Eq. (63) is removed, and IPMb may be a useful model.

The Lagrangian IP model (LIPM) is defined by constant values of α_2 and C_0 ($\alpha_2=3.5$ and $C_0=2.1$), with $\alpha_3=-3\alpha_2$ [Eq. (61)]. Then, Eq. (27) yields

$$\alpha_1=-\frac{1}{2}-\frac{3}{4}\,C_0+\frac{1}{2}\,C_2\,\frac{P}{\epsilon}+3\alpha_2 b_{ii}^3. \tag{64}$$

For the homogeneous shear test case, it is found that α_2, defined by Eq. (59), always lies between 3.4 and 3.7. Hence, it is reasonable to expect LIPM (with the simple specification $\alpha_2=3.5$) to yield results very close to those of IPM.

Figure 3 shows the evolution of anisotropy components for the models IPMa, IPMb, and LIPM. It may be seen that the latter two are barely distinguishable, while IPMa is significantly different. All three models have fixed (finite) values of α_2 and C_0 and are thus realizable.

As Reynolds-stress models, IPMb corresponds exactly to IPM; IPMa corresponds to IPM, with C_1 given by Eq. (62); and LIPM corresponds to IPM, with C_1 given by

$$C_1=1+\frac{3}{2}\,C_0-C_2\,\frac{P}{\epsilon}-\frac{2}{3}\,\alpha_2 F. \tag{65}$$

C. LRR and SL models

Neither LRR nor SL satisfy the condition $A^*=0$ [Eqs. (41) and (42)]. For LRR, the value of A^* is $\frac{6}{55}(1-15C_2)$, which equals -0.55 for $C_2=0.4$. For SL, the value of A^* is $-\frac{24}{25}F^{1/2}$ (with $F=1$ in isotropic turbulence).

There does not appear to be a profound physical significance to the fact that A^* is nonzero for these models. It implies that a corresponding stochastic Lagrangian model of the form of Eqs. (23) and (24) does not exist. But one would exist if higher-order terms (quadratic in **b**) were added to the representation of H_{ijkl}.

D. SSG model

For the SSG model, the value of A^* is $-(0.05+1.3b')$. Hence, the condition $A^*=0$ is not exactly satisfied, but it nearly is—at least for small b'. We are motivated, therefore, to develop a stochastic Lagrangian model that closely approximates SSG. The result is designated the Lagrangian SSG model (LSSG), with two intermediate steps being SSGa and SSGb.

The first step SSGa is defined to be the original model, but with $A^{(4)}=C_4$ changed to

$$A^{(4)}=\tfrac{3}{2}A^{(3)}=\tfrac{3}{2}(C_3-C_3^*b'), \tag{66}$$

so that A^* is zero. The performance of the model for the test problem is shown in Fig. 4. It may be seen that the change in $A^{(4)}$ results in a degradation in performance. However, as far as the shear-stress anisotropy is concerned, this defect is rectified by reducing C_3^* from 1.3 to 1.0—this defines SSGb.

With C_3 taken to be $\frac{4}{5}$, the stochastic model parameters β and γ for SSGb (and LSSG), obtained from Eqs. (43)–(48) and (66), are

$$\beta_2=\tfrac{4}{5}-\tfrac{3}{8}C_3^*b', \tag{67}$$

$$\beta_3=-\tfrac{1}{5}-\tfrac{3}{8}C_3^*b', \tag{68}$$

TABLE V. Stochastic Lagrangian model coefficients.

	α_1	α_2	α_3	β_2	β_3	γ_2	γ_3	γ_5	γ_6
SLM	$-(\frac{1}{2}+\frac{3}{4}C_0)$	0	0	0	0	0	0	0	0
LIPM	Eq. (64)	3.5	-10.5	0.8	-0.2	0	0	0.6	-0.6
LSSG	Eq. (72)	$4.0-1.7(P/\epsilon)$	$-8.85+5.1(P/\epsilon)$	$0.8-\frac{3}{8}b'$	$-0.2-\frac{3}{8}b'$	0	0	1.2	-1.2
HP1	Eq. (27)	3.7	0	0.8	-0.2	3.01	-2.18	4.29	-3.09
HP2	Eq. (27)	3.78	0	0.8	-0.2	1.04	0.34	1.99	-0.76

$$\gamma_2=\gamma_3=0, \tag{69}$$

and

$$\gamma_5=-\gamma_6=\tfrac{6}{5}, \tag{70}$$

with $C_3^*=1.0$.

The final model, LSSG, is an approximation to SSGb, in that [instead of using Eq. (49)] α_2 is more simply specified by

$$\alpha_2=4.0-1.7\frac{P}{\epsilon}. \tag{71}$$

Then α_3 is obtained from Eq. (52), and α_1, obtained from Eq. (27), is

$$\alpha_1=-\frac{1}{2}-\frac{3}{4}C_0+\frac{3}{8}(C_3-C_3^*b')\frac{P}{\epsilon}-\frac{1}{4}C_2b_{ii}^2 + \left(3\alpha_2-\frac{3}{4}C_2\right)b_{ii}^3. \tag{72}$$

Thus, as may be seen from Fig. 4, the relatively simple and realizable stochastic Langevin model LSSG provides a good correspondence to the SSG model.

As a Reynolds-stress model, LSSG has the same coefficients $A^{(n)}$ as SSG (see Table II), except that $A^{(4)}$ is given by Eq. (66) and $A^{(1)}$ is

$$A^{(1)}=-2-3C_0+\frac{4}{3}\alpha_2+\frac{3}{2}(C_3-C_3^*b')\frac{P}{\epsilon} + b_{ii}^2\left(\frac{1}{2}C_2-6\alpha_2\right)+b_{ii}^3(12\alpha_2-3C_2). \tag{73}$$

E. Summary

Table V summarizes the model coefficients α, β, and γ for the stochastic Lagrangian models considered here. The simplified Langevin model (SLM) corresponds precisely to Rotta's model, while LIPM and LSSG correspond (approximately) to IPM and SSG, respectively. The coefficients suggested by Haworth and Pope[19,20] are shown for comparison.

Asymptotic values of b_{ij} and S_0k/ϵ for all the models are shown in Table III.

VI. TRIPLE VELOCITY CORRELATION

Thus far, attention has been focused on the modeled Reynolds-stress equation, obtained by the two different approaches—the standard approach of directly modeling the redistribution term, or the alternative approach via stochastic Lagrangian models. The latter approach is more potent, however, in that stochastic Lagrangian models lead directly to models for other one-point statistics. This fact is demonstrated in this section by deriving a model for the triple velocity correlations, and in the next section by deriving a modeled scalar flux equation.

Let $g(\mathbf{v};\mathbf{x},t)$ denote the one-point Eulerian joint PDF of the fluctuating velocity $\mathbf{u}(\mathbf{x},t)$, where $\mathbf{v}=\{v_1,v_2,v_3\}$ are sample-space velocity variables. The stochastic Lagrangian model Eq. (10) implies a modeled evolution equation for $g(\mathbf{v};\mathbf{x},t)$, which can be derived by standard techniques.[9] The result is

$$\frac{\partial g}{\partial t}+\langle U_i\rangle\frac{\partial g}{\partial x_i}+v_i\frac{\partial g}{\partial x_i}+\frac{\partial\langle u_iu_j\rangle}{\partial x_j}\frac{\partial g}{\partial v_i} = -\frac{\partial}{\partial v_i}\left[\left(G_{ij}-\frac{\partial\langle U_i\rangle}{\partial x_j}\right)gv_j\right]+\frac{1}{2}C_0\epsilon\frac{\partial^2 g}{\partial v_i\,\partial v_i}. \tag{74}$$

A modeled evolution equation for the triple velocity correlation $\langle u_qu_ru_s\rangle$ is then obtained from Eq. (74) by multiplying by $v_qv_rv_s$ and integrating over all $\mathbf{v}$:

$$\begin{aligned}&\frac{\partial}{\partial t}\langle u_qu_ru_s\rangle+\langle U_i\rangle\frac{\partial}{\partial x_i}\langle u_qu_ru_s\rangle+\frac{\partial}{\partial x_i}\langle u_iu_qu_ru_s\rangle\\ &-\frac{\partial}{\partial x_j}\langle u_iu_j\rangle(\delta_{iq}\langle u_ru_s\rangle+\delta_{ir}\langle u_qu_s\rangle+\delta_{is}\langle u_qu_r\rangle)\\ &=\left(G_{ij}-\frac{\partial\langle U_i\rangle}{\partial x_j}\right)(\delta_{iq}\langle u_ju_ru_s\rangle+\delta_{ir}\langle u_ju_qu_s\rangle\\ &\quad+\delta_{is}\langle u_ju_qu_r\rangle).\end{aligned} \tag{75}$$

In order to obtain an algebraic model for $\langle u_qu_ru_s\rangle$, we neglect the first two terms in Eq. (75), and for the third use the Millionshchikov approximation,

$$\langle u_iu_qu_ru_s\rangle=\langle u_iu_q\rangle\langle u_ru_s\rangle+\langle u_iu_r\rangle\langle u_qu_s\rangle + \langle u_iu_s\rangle\langle u_qu_r\rangle. \tag{76}$$

For the simplest stochastic model (SLM) G_{ij} is simply $\alpha_1(\epsilon/k)\delta_{ij}$. In general, this term is isolated by introducing the tensor K_{ij}, defined to satisfy

$$G_{ij}-\frac{\partial\langle U_i\rangle}{\partial x_j}=\alpha_1\frac{\epsilon}{k}\delta_{ij}+K_{ij}. \tag{77}$$

With these definitions and approximations, after some algebra, Eq. (75) reduces to

$$\langle u_q u_r u_s\rangle = -C_s \frac{k}{\epsilon}\Big(\langle u_i u_q\rangle \frac{\partial\langle u_r u_s\rangle}{\partial x_i} + \langle u_i u_r\rangle \frac{\partial\langle u_q u_s\rangle}{\partial x_i} + \langle u_i u_s\rangle \frac{\partial\langle u_q u_r\rangle}{\partial x_i} - K_{qj}\langle u_j u_r u_s\rangle - K_{rj}\langle u_j u_q u_s\rangle - K_{sj}\langle u_j u_q u_r\rangle\Big), \quad (78)$$

where

$$C_s = -\frac{1}{3\alpha_1}. \quad (79)$$

The simplest case to consider is zero mean velocity gradients and G_{ij} given by the SLM. For then K_{ij} is zero, and Eq. (78) is identical to the model of Launder, Reece, and Rodi.[1] The value of $C_s=0.16$ given by Eq. (79) is comparable to that given in Ref. 1, $C_s=0.11$. But, in general, Eq. (78) accounts for the influence of mean velocity gradients and allows the use of a better model than SLM.

While the derivation of Eq. (78) is of theoretical interest, it is likely that the simpler models currently used in Reynolds-stress closures are adequate.

VII. SCALAR FLUX

The two approaches used to obtain modeled Reynolds-stress equations can, with some extensions, be used to obtain the modeled scalar flux equation.

Let $\phi(\mathbf{x},t)$ be a conserved passive scalar field, which evolves by

$$\frac{D\phi}{Dt} = \Gamma\nabla^2\phi, \quad (80)$$

where Γ is the molecular diffusivity. And let $\phi'(\mathbf{x},t)$ denote the fluctuating component, so that the Reynolds decomposition is

$$\phi = \langle\phi\rangle + \phi'. \quad (81)$$

In the first (standard) approach (see, e.g., Refs. 3 and 28), the above equations, together with the Navier–Stokes equation, are manipulated to yield the exact evolution equation for the scalar flux $\langle u_i\phi'\rangle$:

$$\frac{\partial}{\partial t}\langle u_i\phi'\rangle + \langle U_j\rangle \frac{\partial}{\partial x_j}\langle u_i\phi'\rangle = \mathscr{T}_i^\phi + P_i^\phi + \Pi_i^\phi - \epsilon_i^\phi. \quad (82)$$

The four terms on the right-hand side represent transport, production, pressure scrambling, and dissipation.

The production P_i^ϕ is in closed form in second-moment closures, and the dissipation ϵ_i^ϕ is zero if local isotropy prevails. Hence the central issue in modeling is the pressure-scrambling term

$$\Pi_i^\phi \equiv -\left\langle \phi' \frac{\partial p'}{\partial x_i}\right\rangle. \quad (83)$$

A standard model is

$$\Pi_i^\phi = -C_m \frac{\epsilon}{k}\langle u_i\phi'\rangle + \left(\frac{4}{5}\frac{\partial\langle U_i\rangle}{\partial x_j} - \frac{1}{5}\frac{\partial\langle U_j\rangle}{\partial x_i}\right)\langle u_j\phi'\rangle. \quad (84)$$

The first term is that of Monin,[29] with a standard value for the Monin constant C_m being 2.9.[5] The second term models the rapid-pressure contribution, and the specific form is known to be correct in isotropic turbulence.[3]

In the second (Lagrangian) approach, the value of the scalar following a fluid particle $\phi^+(t)$ is approximated by a model process $\phi^*(t)$. For the present purposes it suffices to use the simplest possible model, in spite of its known deficiencies. This is the IEM or LMSE[30,31] model,

$$\frac{d\phi^*}{dt} = -\frac{1}{2}\frac{\epsilon}{k} C_\phi(\phi^* - \langle\phi\rangle), \quad (85)$$

where the standard value of the model constant is $C_\phi=2.0$.[9]

From the Lagrangian models for U_i^* [Eq. (10)] and ϕ^* [Eq. (85)], the modeled equation for the scalar flux that is obtained is

$$\frac{\partial}{\partial t}\langle u_i\phi'\rangle + \langle U_j\rangle\frac{\partial}{\partial x_j}\langle u_i\phi'\rangle = \mathscr{T}_i^\phi + P_i^\phi + \left(G_{ij} - \frac{1}{2}C_\phi\frac{\epsilon}{k}\delta_{ij}\right)\langle u_j\phi'\rangle. \quad (86)$$

A comparison of this equation with its exact counterpart [Eq. (82)] shows that the final term in the above equation is the implied model for $\Pi_i^\phi - \epsilon_i^\phi$.

[It is arguable that in Eq. (86) the term in C_ϕ corresponds to dissipation, ϵ_i^ϕ, and hence is at odds with local isotropy. An alternative model that avoids this difficulty is obtained from Eq. (85) by replacing $\langle\phi\rangle$ by the conditional mean $\langle\phi|\mathbf{U}^*\rangle$.]

With G_{ij} given by Eq. (23), the implied model is

$$\Pi_i^\phi - \epsilon_i^\phi = -\left(\frac{1}{2}C_\phi - \alpha_1\right)\frac{\epsilon}{k}\langle u_i\phi'\rangle + (\alpha_2 b_{ij} + \alpha_3 b_{ij}^2) \times \frac{\epsilon}{k}\langle u_j\phi'\rangle + H_{ijkl}\frac{\partial\langle U_k\rangle}{\partial x_l}\langle u_j\phi'\rangle. \quad (87)$$

The first term is just the Monin model. It is interesting to observe that with the simplified Langevin model (SLM), the implied value of the Monin constant is

$$C_m = \tfrac{1}{2}(C_\phi + 1 + \tfrac{3}{2}C_0) = \tfrac{1}{2}(C_\phi + C_1) \approx 2.58. \quad (88)$$

The second term (in α_2 and α_3) represents a nonlinear relaxation of the scalar flux that vanishes in isotropic turbulence.

The final term in Eq. (87) (that involving H_{ijkl}) is the implied model for the rapid-pressure-scrambling term, denoted by Π_i^R. With p^R being the rapid pressure, the exact term is

$$\Pi_i^R = -\left\langle\phi'\frac{\partial p^R}{\partial x_i}\right\rangle, \quad (89)$$

while all models are of the form

$$\Pi_i^R = G_{ij}^R \langle u_j \phi' \rangle. \tag{90}$$

The standard model [Eq. (84)] corresponds to

$$G_{ij}^R = \frac{4}{5}\frac{\partial \langle U_i \rangle}{\partial x_j} - \frac{1}{5}\frac{\partial \langle U_j \rangle}{\partial x_i} = \frac{3}{5} S_{ij} + W_{ij}, \tag{91}$$

while the implied model from Eq. (87) is

$$G_{ij}^R = H_{ijkl} \frac{\partial \langle U_k \rangle}{\partial x_l}. \tag{92}$$

The most significant deduction from the present development is that G_{ij}^R (and hence Π_{ij}^R) is completely determined by the stochastic Lagrangian model for *velocity*. For Reynolds stress closures with an implied stochastic Lagrangian model (i.e., those for which $A^*=0$), the rapid-pressure-scrambling term is therefore completely determined by the pressure-rate-of-strain model coefficients $A^{(n)}$. Specifically (for RSMs satisfying $A^*=0$), we obtain, from Eqs. (24) and (43)–(48):

$$G_{ij}^R = \tfrac{3}{4} A^{(3)} S_{ij} + 2\beta^* W_{ij} + \tfrac{1}{2} A^{(6)} S_{il} b_{lj} + \tfrac{1}{4} A^{(8)} S_{jl} b_{li}$$
$$+ \tfrac{1}{2} A^{(7)} W_{il} b_{lj} + \tilde{A} W_{jl} b_{li}, \tag{93}$$

where $\tilde{A}$ is defined by

$$\tilde{A} = -3 + \tfrac{3}{2} A^{(5)} - \tfrac{1}{2} A^{(7)}. \tag{94}$$

Thus, a given RSM (with $A^*=0$) implies a model for Π_i^R.

For the models LIPM and LSSG, the implied models for Π_i^R are

$$G_{ij}^R = \tfrac{3}{5} S_{ij} + W_{ij} - \tfrac{6}{5} W_{jl} b_{li} \quad \text{(LIPM)}, \tag{95}$$

and

$$G_{ij}^R = (\tfrac{3}{5} - \tfrac{3}{4} C_3^* b') S_{ij} + W_{ij} - \tfrac{12}{5} W_{jl} b_{li} \quad \text{(LSSG)}. \tag{96}$$

For isotropic turbulence both revert to the standard model [Eq. (91)]. But both contain the additional term $\tilde{A} W_{jl} b_{li}$, with $\tilde{A} = -\frac{6}{5}$ and $\tilde{A} = -\frac{12}{5}$ for the two models.

Calculations are now presented to illustrate the performance of the different pressure scrambling models. The calculation are for the same case of homogeneous shear flow, as considered previously. There is also a constant mean scalar gradient in the x_2 direction ($\partial \langle \phi \rangle / \partial x_2 > 0$). Initially the scalar variance $\langle \phi'^2 \rangle$ is zero, and consequently so is the scalar flux. It is convenient to solve the ordinary differential equations for the normalized scalar variance,

$$\Phi \equiv \frac{\langle \phi'^2 \rangle \epsilon^2}{|\nabla \langle \phi \rangle|^2 k^3}, \tag{97}$$

and scalar flux

$$\theta_i \equiv \frac{\langle u_i \phi' \rangle \epsilon}{|\nabla \langle \phi \rangle| k^2}. \tag{98}$$

These equations [that ultimately stem from Eqs. (10), (21), and (85)] are

$$\frac{d\Phi}{dt} = -2\theta_j e_j - \Phi\left(2C_{\epsilon 2} + C_\phi - 3 + \frac{P}{\epsilon}(3 - 2C_\epsilon)\right), \tag{99}$$

and

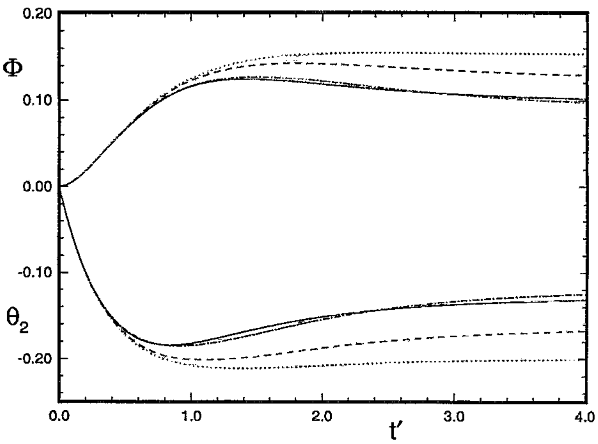

FIG. 5. Evolution of scalar variance and scalar flux in normalized time for homogeneous shear flow with $\partial\langle\phi\rangle/\partial x_2 > 0$. Models: SLM, dot-dashed; LIPM, dashed; LIPMA, dotted; LSSG, solid.

$$\frac{d\theta_i}{dt'} = -\theta_i\left(C_{\epsilon 2} + \frac{1}{2} C_\phi - 2 + \frac{P}{\epsilon}(2 - C_{\epsilon 1})\right) - \theta_j \frac{k}{\epsilon}\frac{\partial \langle U_i \rangle}{\partial x_j}$$
$$+ \frac{k}{\epsilon} G_{ij}\theta_j - \left(\frac{2}{3} + 2b_{ij}\right) e_j, \tag{100}$$

where t' is the normalized time [Eq. (22)], and $\mathbf{e}$ is the unit vector in the direction of $\nabla\langle\phi\rangle$ (i.e., $e_j = \delta_{2j}$).

In addition to Φ and θ_i, results are presented for the correlation coefficients,

$$\rho_1 = \langle u_1 \phi' \rangle / (\langle u_1^2 \rangle \langle \phi'^2 \rangle)^{1/2}, \tag{101}$$

and ρ_2 is similarly defined.

Calculations are presented for four models: SLM, LIPM, LSSG, and a model designated LIPMA. This last model is identical to LIPM, except that in the scalar flux equation the coefficient $\tilde{A}$ of $W_{jl} b_{li}$ is set to zero. Hence LIPMA corresponds to the standard rapid-pressure-scrambling model, and a comparison between LIPM and LIPMA reveals the importance of the term $\tilde{A} W_{jl} b_{li}$.

Figure 5 shows the evolution of the normalized variance Φ and scalar flux θ_2 for the different models. It may be observed that SLM—even though it lacks a rapid-pressure model—produces results very similar to LSSG. There is a 15%–20% difference between LIPM and LIPMA (at later times), which quantifies the significance of the term in $\tilde{A}$.

Figure 6 shows the correlation coefficients of $\langle u_i \phi' \rangle$, ρ_1, and ρ_2. In this case the models display very similar behavior, except that the deficiencies in SLM are revealed in ρ_2. Experimental values reported by Tavoularis and Corrsin[32] are shown for comparison.

VIII. IDENTIFICATION OF G_{ij}

The above developments show that the tensor G_{ij} is of fundamental significance: it leads to models for the pressure-rate-of-strain, pressure-scrambling, and triple-

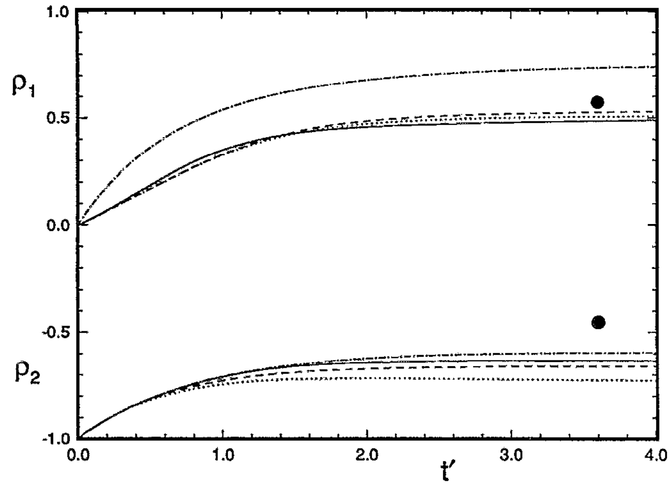

FIG. 6. Evolution of scalar flux correlation coefficients in normalized time for homogeneous shear flow with $\partial\langle\phi\rangle/\partial x_2>0$. Models: SLM, dot–dashed; LIPM, dashed; LIPMA, dotted; LSSG, solid. Symbols, experimental data.[32]

velocity correlation. It is natural to inquire, therefore: Can G_{ij} be measured? At least in part, it can, in direct numerical simulations (DNS).

By comparing the modeled evolution equation for the PDF of the fluctuating velocity $g(\mathbf{v};\mathbf{x},t)$ with the Navier–Stokes equations, Haworth and Pope[9] showed that the stochastic model [Eq. (10)] implies

$$G_{ij}v_j-\frac{1}{2}\,C_0\epsilon\,\frac{\partial \ln g}{\partial v_i}=\left\langle \nu\,\frac{\partial^2 u_i}{\partial x_j\,\partial x_j}-\frac{\partial p'}{\partial x_i}\middle|\mathbf{u}(\mathbf{x},t)=\mathbf{v}\right\rangle. \tag{102}$$

Since the term in C_0 is modeled, this equation cannot be used directly to measure G_{ij}. However, if G_{ij}^R is identified to be the contribution to G_{ij} from the rapid pressure p^R, then, from Eq. (102), we obtain

$$G_{ij}^R v_j=-\left\langle\frac{\partial p^R}{\partial x_i}\middle|\mathbf{u}=\mathbf{v}\right\rangle. \tag{103}$$

The conditional expectation of the rapid pressure gradient can be extracted from DNS. Hence the prediction of Eq. (103) that it is a linear function of $\mathbf{v}$ can be tested; and, if it is, G_{ij} can be measured. Alternatively—and more simply—a linear mean-square estimate of G_{ij} from Eq. (103) is

$$G_{ij}^R=R_{jk}^{-1}\left\langle u_k\,\frac{\partial p^R}{\partial x_i}\right\rangle, \tag{104}$$

where $\mathbf{R}^{-1}$ is the inverse of the Reynolds-stress tensor.

IX. CONCLUSION

It has been demonstrated that there is a close connection between stochastic Lagrangian models and second-moment closures. The main results are now itemized.

(1) To every stochastic Lagrangian model with coefficient tensor G_{ij} [Eq. (10)], there is a unique corresponding redistribution model Π_{ij}^* [Eq. (32)] that is realizable.

(2) For a stochastic Lagrangian model of the form considered [Eq. (23)], defined by coefficients α, β, and γ, the corresponding redistribution model is given by Eq. (14). The redistribution model coefficients $A^{(n)}$ are given in terms of α, β, and γ by Eqs. (33)–(40).

(3) The converses of 1 and 2 are more involved. For a given redistribution model Π_{ij}^*, there exist nonunique stochastic models G_{ij}, provided either that the Reynolds stress is nonsingular or that Π_{ij}^* is a realizable model. [That is, under these conditions Eq. (32) admits nonunique finite solutions for G_{ij}.]

(4) For redistribution models of the form considered [Eq. (14)], corresponding stochastic models of the form of Eqs. (23) and (24) exist if the coefficients $A^{(n)}$ satisfy a linear relation $A^*=0$ [Eq. (42)]. In that case, the corresponding coefficients α, β, γ are given by Eqs. (43)–(52), in which γ_5 is a free parameter.

(5) A redistribution model with simple coefficients $A^{(n)}$ (e.g., constants) can lead to a corresponding stochastic Lagrangian model with complicated coefficients, and vice versa. Two new stochastic Lagrangian models with simple coefficients LIPM and LSSG are presented, which to a good approximation correspond to the IPM and SSG models, respectively.

(6) A stochastic Lagrangian model is more potent than a redistribution model Π_{ij}^*, in that it can be used to obtain models for other one-point statistics.

(7) With additional (standard) approximations, a model is obtained for the triple velocity correlation $\langle u_q u_r u_s\rangle$, Eq. (78). In the simplest situations this reduces to the model of Lauder, Reece, and Rodi,[1] but, in general, contains additional terms.

(8) By adjoining a stochastic Lagrangian model for a conserved passive scalar ϕ, a model is obtained for the pressure-scrambling term in the equation for the scalar flux $\langle u_i\phi'\rangle$, Eq. (87). This suggests the addition of an extra term to existing models [Eqs. (95) and (96)].

(9) It is shown that the fundamental tensor G_{ij}^R can be measured using DNS [Eq. (104)].

From the viewpoint of second-moment closures, the principal outcome of this work is to suggest an alternative and advantageous modeling approach: starting from stochastic Lagrangian models, it is straightforward to derive second-moment closures that guarantee realizability.

From the viewpoint of stochastic Lagrangian models, the principal contribution of this work is to present the two new models, LIPM and LSSG. These models, used in the PDF framework,[9] can be expected to have similar performance to the well-established and tested IPM and SSG Reynolds-stress closures.

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APPENDIX: REYNOLDS-STRESS MODELS

Some information is provided here on the Reynolds-stress models defined in Table II.

1. Rotta's model

Rotta's model[11] is the simplest possible for the return to isotropy caused by the "slow" pressure fluctuations. It is usually used as one contribution in more complete models, in which the "rapid" pressure terms are also accounted for. Here, however, we use "Rotta model" to mean the turbulence model that results when only the Rotta term (i.e., $A^{(1)}T_{ij}^{(1)}$) is nonzero in the redistribution model.

A discussion on the value of the Rotta constant C_1 is provided by Launder.[15] The value $C_1=1$ corresponds to no return to isotropy, while values from 1.5 to 5.0 have been suggested by different authors. As discussed by Launder,[15] the higher values appear to be appropriate when the whole of the redistribution is modeled by the Rotta term. Here we take $C_1=4.15$.

2. Isotropization of production model (IPM)

The IPM, originally proposed by Naot *et al.*,[12] adds to the Rotta term, the following model for the rapid pressure terms:

$$-C_2(P_{ij}-\tfrac{1}{3}P_{ll}\delta_{ij}), \tag{A1}$$

where

$$P_{ij}=-\langle u_i u_l\rangle \frac{\partial\langle U_j\rangle}{\partial x_l}-\langle u_j u_l\rangle \frac{\partial\langle U_i\rangle}{\partial x_l}, \tag{A2}$$

is the production rate of the Reynolds stress $\langle u_i u_j\rangle$.

The "standard" values[5] for the constants are $C_1=1.8$ and $C_2=\frac{3}{5}$—and these are the values used here. This value of C_2 satisfies the RDT (rapid distortion theory) constraint of Crow.[16] However, Younis (see Ref. 15) suggests the lower value of 0.3.

3. Launder, Reece, and Rodi model (LRR)

The "standard" model constants (used here) are $C_1=1.5$ and $C_2=0.4$. This model has fallen into disfavor, due to its poor performance in shear flows.[5,17] However, recently, Shabbir and Shih[18] have suggested that its performance is at least as good as other current models if C_2 is changed to 0.55.

4. Shih and Lumley model (SL)

An important parameter in the SL model is

$$F=1-\tfrac{9}{2}b_{ii}^2+9b_{ii}^3, \tag{A3}$$

which is the determinant of $\langle u_i u_j\rangle/(\frac{1}{3}\langle u_l u_l\rangle)$. In isotropic turbulence F is unity: in one- or two-component turbulence it is zero. The coefficient C_2 is then specified as

$$C_2=\tfrac{1}{10}(1+\tfrac{4}{5}F^{1/2}). \tag{A4}$$

The Rotta coefficient β (see Table II) is an involved function of the invariants and the Reynolds number (see Ref. 13).

5. Speziale, Sarkar, and Gatski model (SSG)

The SSG model given in Table II is the original and standard version,[14] including the model coefficients.

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