Consistency conditions for random-walk models of turbulent dispersion

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Random-walk models have long been used to calculate the dispersion of passive contaminants in turbulence. When applied to nonstationary and inhomogeneous turbulence, the model coefficients are functions of the Eulerian turbulence statistics. More recently the same random-walk models have been used as turbulence closures in the evolution equation for the Eulerian joint probability density function (pdf) of velocity. There are, therefore, consistency conditions relating the coefficients specified in a random-walk model of dispersion and the Eulerian pdf calculated using the same random-walk model. It is shown that even if these conditions are not satisfied, the dispersion model does not violate the second law of thermodynamics: all that is required to avoid a second-law violation is that the mean pressure gradient be properly incorporated. It is also shown that for homogeneous turbulence the consistency conditions are satisfied by a linear Gaussian model; and that for inhomogeneous turbulence they are satisfied by a nonlinear Gaussian model.

I. INTRODUCTION

The Langevin equation has long been used to model the dispersion of passive contaminants in homogeneous turbulence (see Refs. 1–5, for example). The equation is a stochastic model for the position $\hat{\mathbf{x}}(t)$ and velocity $\hat{\mathbf{U}}(t)$ of a fluid particle

$$d\hat{\mathbf{x}} = \hat{\mathbf{U}}\, dt, \tag{1}$$

$$d\hat{\mathbf{U}} = -\hat{\mathbf{U}}\, dt/T_{\mathrm{L}} + D^{1/2}\, d\mathbf{W}. \tag{2}$$

Here T_{L} is the Lagrangian integral time scale, D is a positive constant, and $\mathbf{W}$ is an isotropic Wiener process, with the basic properties

$$\langle \mathbf{W} \rangle = 0, \quad \langle dW_i\, dW_j \rangle = dt\, \delta_{ij}, \tag{3}$$

where angled brackets denote means.

Since the beginning of this decade, extensions of the simple Langevin equation have been used in two different contexts. First, in pdf methods,[6–9] from a generalization of Eq. (2), a model equation is deduced for the one-point Eulerian joint probability density function of velocity $f(\mathbf{V};\mathbf{x},t)$. We denote by $f_c(\mathbf{V};\mathbf{x},t)$ the solution of this equation, where the subscript c indicates that the pdf is *calculated* from a generalized Langevin equation. The first two moments of f_c are the calculated mean Eulerian velocity

$$\langle U_i(\mathbf{x},t) \rangle_c = \int V_i f_c(\mathbf{V};\mathbf{x},t) d\mathbf{V}, \tag{4}$$

and the calculated Reynolds stresses

$$\langle u_i u_j \rangle_c = \int (V_i - \langle U_i \rangle_c)(V_j - \langle U_j \rangle_c) f_c(\mathbf{V}) d\mathbf{V}, \tag{5}$$

where $\int d\mathbf{V}$ indicates integration over all velocities. In pdf methods the essential extension to the simple Langevin equation is to make the deterministic term [the first term on the right-hand side of Eq. (2)] a general linear function of $\hat{\mathbf{U}}$. We refer to this as the generalized Langevin equation, or as the linear Gaussian model.

The second application of extended Langevin equations is to dispersion in inhomogeneous turbulence. The aim of a dispersion calculation is to calculate the mean concentration field $\langle C(\mathbf{x},t) \rangle$ of a passive contaminant originating from a given source distribution. In this context modifications to the Langevin equation have been made both to the deterministic term,[10,11] and to the form of the random term.[12–14] The coefficients in the modified Langevin equation depend upon Eulerian statistics of the velocity field. In dispersion calculations, rather than being calculated, these statistics are specified, possibly from measurements. We denote by $f_s(\mathbf{V};\mathbf{x},t)$ the *specified* Eulerian joint pdf of velocity, although in practice only some moments (e.g., $\langle U_i \rangle_s$ and $\langle u_i u_j \rangle_s$) are needed.

This paper is concerned with the "thermodynamic constraint" and with the consistency of dispersion models. Sawford[14] introduced the thermodynamic constraint that an "initially uniform distribution of material be maintained." That is, if $\langle C(\mathbf{x},t) \rangle$ is initially uniform, it remains so. We introduce the following consistency condition for stochastic models [e.g., Eq. (2)] used in dispersion calculations: a dispersion model is completely consistent if the calculated pdf $f_c(\mathbf{V};\mathbf{x},t)$ is equal to that specified $f_s(\mathbf{V};\mathbf{x},t)$. Usually, however, only a few moments of f_s are specified. Thus we define a dispersion model to be consistent to order n if the moments of f_c, up to order n, are equal to those of f_s.

The principal contributions of this paper are to show the following.

(i) A necessary and sufficient condition for the satisfaction of the thermodynamic constraint is that the calculated mean velocity field $\langle \mathbf{U} \rangle_c$ satisfy the continuity equation. This, in turn, requires that the mean pressure gradient be properly incorporated in the random-walk model.

(ii) The additional constraints deduced by Sawford[14] can be interpreted as consistency conditions. They are not necessary to the satisfaction of the thermodynamic constraint.

(iii) In modifying the Langevin equation [Eq. (2)], physical arguments favor leaving the random term unal-

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tered, and modifying the deterministic term.

(iv) A nonlinear Gaussian model can be completely consistent.

(v) A linear Gaussian model (i.e., the generalized Langevin equation) is consistent to second order if the model coefficients satisfy an algebraic relation [Eq. (26)]. For homogeneous turbulence this relation can always be satisfied and then, if the turbulence is Gaussian, the model is completely consistent.

(vi) A model should not be regarded as being defective if it is inconsistent when applied to an unphysical specified turbulence field—for example, inhomogeneous Gaussian turbulence.

II. NONLINEAR GAUSSIAN MODEL

For definiteness we consider the turbulent flow of a constant-property Newtonian fluid. The continuity and momentum equations are

$$\frac{\partial U_i}{\partial x_i} = 0, \tag{6}$$

and

$$\frac{\partial U_j}{\partial t} + U_i \frac{\partial U_j}{\partial x_i} = \nu \nabla^2 U_j - \frac{1}{\rho}\frac{\partial p}{\partial x_j}, \tag{7}$$

where $\mathbf{U}(\mathbf{x},t)$ is the Eulerian velocity, $p(\mathbf{x},t)$ the pressure, and ρ and ν are the constant density and kinematic viscosity, respectively.

We consider the generalization of Eq. (2) to the nonlinear Gaussian model

$$d\hat{U}_i = M_i\, dt + H_i(\hat{\mathbf{U}})dt + D^{1/2}\, dW_i. \tag{8}$$

The coefficients $\mathbf{M}$ and D may depend on position and time, but are independent of $\hat{\mathbf{U}}$. Since $\mathbf{M}$ represents a mean drift, without loss of generality, we specify that the model function $\mathbf{H}(\hat{\mathbf{U}})$ has zero mean: to be precise, we specify

$$\int \mathbf{H}(\mathbf{V},\mathbf{x},t) f_c(\mathbf{V};\mathbf{x},t) d\mathbf{V} = 0. \tag{9}$$

For the linear Gaussian model, or the generalized Langevin equation,[6–9] the function $\mathbf{H}(\hat{\mathbf{U}})$ is specified to be

$$H_i(\hat{\mathbf{U}}) = G_{ij}(\hat{U}_j - \langle U_j \rangle_c), \tag{10}$$

where the tensor coefficient G may depend on $(\mathbf{x},t)$ but is independent of $\hat{\mathbf{U}}$.

From Eq. (8) it is possible[9] to derive an evolution equation for the Eulerian pdf of velocity $f_c(\mathbf{V};\mathbf{x},t)$

$$\frac{\partial f_c}{\partial t} + V_i \frac{\partial f_c}{\partial x_i} = -M_i \frac{\partial f_c}{\partial V_i} - \frac{\partial}{\partial V_i}[f_c H_i(\mathbf{V})] + \frac{1}{2} D \frac{\partial^2 f_c}{\partial V_i\, \partial V_i}. \tag{11}$$

From the solution to this equation $\langle \mathbf{U}\rangle_c$, $\langle u_i u_j \rangle_c$, and other calculated moments can be determined. Because of the imperfection of the model, these calculated moments may differ to some extent from the true values $\langle \mathbf{U}\rangle$ and $\langle u_i u_j \rangle$.

A. The random term

We first discuss the physical justification for the form of the random term in Eq. (8). This justification is based on Kolmogorov's hypotheses of self-similarity and local isotropy in the inertial subrange. Let $D^{\mathrm{L}}_{ij}(s,\mathbf{x},t)$ be the Lagrangian structure function defined by

$$D^{\mathrm{L}}_{ij}(s,\mathbf{x},t) \equiv \langle (\hat{U}_i(t+s) - \hat{U}_i(t)) \times (\hat{U}_j(t+s) - \hat{U}_j(t)) | \hat{\mathbf{x}}(t) = \mathbf{x}\rangle. \tag{12}$$

This is the covariance of the velocity increment $\hat{\mathbf{U}}(t+s) - \hat{\mathbf{U}}(t)$ of fluid particles passing through $\mathbf{x}$ at time t. According to Kolmogorov's hypotheses,[15] for times s that are much larger than the Kolmogorov time scale, but much smaller than the integral scale, to first order in s we have[15]

$$D^{\mathrm{L}}_{ij}(s,\mathbf{x},t) = C_0 \epsilon(\mathbf{x},t) s \delta_{ij}, \tag{13}$$

where $\epsilon(\mathbf{x},t)$ is the mean dissipation rate and C_0 is a universal constant. As first observed by Obukhov,[16] the random term in the Langevin equation is consistent with Eq. (13), provided the coefficient D is chosen to be

$$D = C_0 \epsilon. \tag{14}$$

Anand and Pope[3] have estimated C_0 to be 2.1.

There may be many stochastic models for $\hat{\mathbf{U}}(t)$ that are consistent with Eq. (13) for intervals s corresponding to inertial scales. But, to be consistent with the Kolmogorov hypotheses (even the refined hypotheses[17]), such models must (for these time intervals) depend on the large scale motions solely through the dissipation. The models of van Dop *et al.*[13] and Sawford[14] do not conform to this requirement.

B. Thermodynamic constraint

Using the simple Langevin equation [Eq. (2)] in inhomogeneous turbulence, Wilson *et al.*[18] observed that marked fluid particles tended to become congregated in regions of low turbulence intensity rather than becoming uniformly distributed. Legg and Raupach[10] correctly diagnosed that the problem lay in the omission of the mean drift $\mathbf{M}$ due to the mean pressure gradient. Subsequently the problem has been studied by Thomson,[12] van Dop *et al.*,[13] and Sawford.[14]

To address the problem Sawford,[14] following Thomson, introduced the "thermodynamic constraint" that an initially uniform distribution of material be maintained. The same principle can be phrased differently in terms of marked fluid particles. Let $q(\mathbf{x},t)$ be the number density of marked fluid particles. Then if, initially, $q(\mathbf{x},t)$ is uniform, then it remains uniform (in an unbounded flow, or with appropriate boundary conditions on q).

This condition and its satisfaction are analyzed and discussed in detail in Sec. 4.7 of Ref. 9 (the analysis and discussion are not repeated here). For a random-walk model, such as Eq. (8), to satisfy this condition, it is necessary and sufficient that the calculated mean velocity satisfy the continuity equation

$$\frac{\partial}{\partial x_i}\langle U_i \rangle_c = 0. \tag{15}$$

Whether a random walk satisfies Eq. (15) depends on the specification of $\mathbf{M}$ in Eq. (8). For consistency with the mean of the Navier–Stokes equation [Eq. (7)], $\mathbf{M}$ should be

$$\mathbf{M} = \nu \nabla^2 \langle \mathbf{U}\rangle_c - (1/\rho)\nabla \langle p \rangle_c. \tag{16}$$

Pope[9] has shown that a necessary and sufficient condition for Eq. (15) to be satisfied is that $\langle p\rangle_c$ be consistently determined from the Poisson equation

$$\nabla^2\langle p\rangle_c = -\rho\frac{\partial^2}{\partial x_i\,\partial x_j}(\langle U_i\rangle_c\langle U_j\rangle_c + \langle u_iu_j\rangle_c). \quad (17)$$

It is important to note that the source in this Poisson equation is based on calculated moments ($\langle \mathbf{U}\rangle_c$ and $\langle u_iu_j\rangle_c$). If, instead, the specified moments are used, and if the consistency condition to second order is not satisfied, then the incorrect pressure gradient is obtained. As a consequence the thermodynamic constraint may be violated. Conversely, if the consistency condition is satisfied to second order, then the specified pressure gradient can be used without the thermodynamic constraint being violated.

In summary, the satisfaction of Eq. (17) is a necessary and sufficient condition for the satisfaction of Eq. (15) that, in turn, is a necessary and sufficient condition for the satisfaction of the thermodynamic constraint.

Sawford[14] obtains conditions additional to those found by Pope[9] and stated above to be sufficient. In fact, the additional conditions can be viewed as consistency conditions and are not necessary for the satisfaction of the thermodynamic constraint.

III. CONSISTENCY CONDITIONS

A. Significance

The condition for complete consistency is that the calculated pdf, $f_c(\mathbf{V};\mathbf{x},t)$, be the same as the specified pdf, $f_s(\mathbf{V};\mathbf{x},t)$. A third pdf we need to consider is $f(\mathbf{V};\mathbf{x},t)$—the true pdf for the flow in question. This pdf can, in principle, be obtained by error-free measurement, or from the exact solution of the Navier–Stokes equation.

If the true pdf is specified (i.e., $f_s = f$) then clearly it is desirable to satisfy the consistency condition (i.e., $f_c = f_s$). The more closely the consistency condition is satisfied, the closer the calculated pdf (f_c) is to the true pdf (f). Hence the more accurate is the dispersion calculation.

On the other hand, if the specified pdf f_s is not the true pdf, then there is no good reason to satisfy the consistency condition. (Recall that satisfaction of the consistency condition is not necessary to the satisfaction of the thermodynamic constraint.)

An example of an untrue pdf being specified is the test case of inhomogeneous Gaussian turbulence.[12,14] In this case, f_s is specified to be joint normal everywhere, even though the moments $\langle \mathbf{U}\rangle_s$ and $\langle u_iu_j\rangle_s$ vary with position. We maintain that such a specification is physically incorrect: it does not occur in a turbulent flow governed by the Navier–Stokes equations.

The justification for this assertion is that in inhomogeneous turbulence the triple correlation $\langle u_iu_ju_k\rangle$ is nonzero, and hence the turbulence is not Gaussian. In the transport equation for $\langle u_iu_ju_k\rangle$ there is a source term $(\partial/\partial x_m)\langle u_iu_ju_ku_m\rangle$, which is nonzero for inhomogeneous Gaussian turbulence. Thus even if the turbulence is Gaussian initially it becomes non-Gaussian. Experimental evidence clearly shows that in shear flows,[19] and in inhomogeneous turbulence without shear[20] the triple correlations are nonzero, and hence the turbulence is non-Gaussian.

In summary, if the true pdf is specified (i.e., $f_s = f$) then it is desirable to satisfy the consistency condition. Otherwise ($f_s \neq f$) there is no good reason to satisfy the consistency condition. In particular, there is no reason to regard a model as being defective if it violates the consistency condition for the unphysical test case of inhomogeneous Gaussian turbulence.

B. Nonlinear Gaussian model

It is shown here that the model function $\mathbf{H}(\hat{\mathbf{U}})$ can be chosen to make the nonlinear Gaussian model [Eq. (8)] completely consistent.

If the complete consistency condition ($f_c = f_s$) is satisfied at a general time t, and if at that time $\partial f_c/\partial t$ equals $\partial f_s/\partial t$, then the consistency condition is satisfied for all time. Consequently, the complete consistency condition is satisfied if Eq. (11) is satisfied by f_s (in place of f_c). This can be achieved by a suitable choice of $\mathbf{H}(\mathbf{V})$.

Since $\mathbf{H}(\mathbf{V})$ appears in Eq. (11) as the divergence (in $\mathbf{V}$ space) of the vector $f_c\mathbf{H}$, the rotational component of $f_c\mathbf{H}$ is irrelevant. Hence we can write

$$f_cH_i(\mathbf{V}) = -\frac{\partial}{\partial V_i}\Phi(\mathbf{V}), \quad (18)$$

where $\Phi(\mathbf{V})$ is a scalar. Substituting this relation into Eq. (11), with f_s replacing f_c, we obtain the Poisson equation

$$\frac{\partial^2}{\partial V_i\,\partial V_i}\left(\Phi + \frac{1}{2}Df_s\right) = \frac{\partial f_s}{\partial t} + V_i\frac{\partial f_s}{\partial x_i} + M_i\frac{\partial f_s}{\partial V_i}. \quad (19)$$

As $|\mathbf{V}|$ tends to infinity, f_c approaches zero rapidly, and hence Φ approaches a constant (zero, say). The Poisson equation [Eq. (19)] uniquely determines Φ with this boundary behavior. The right-hand side of Eq. (19) tends to zero as $|\mathbf{V}|$ tends to infinity, and its integral over all $\mathbf{V}$ is zero. [In principle f_s can be identically zero in some region where Φ is not uniform. Hence a finite value of $\mathbf{H}$ cannot satisfy Eq. (18). But for f_s corresponding to the pdf of velocity in a turbulent flow, this circumstance is ruled out.]

In summary, the nonlinear Gaussian model [Eq. (8)] can be completely consistent. Indeed, for given f_s, the part of $\mathbf{H}$ that affects the evolution of the pdf is uniquely determined by this condition.

In our view, if the consistency condition is to be satisfied, it is better to do so by modifying the deterministic term rather than the random term. That the random term is Gaussian is not the key issue. The important point is that (in view of Kolmogorov's hypotheses) the mean dissipation rate ϵ is the only physical parameter on which the random term should depend. Suggested modifications to the random term[13,14] have not been in accord with this principle.

C. Linear Gaussian model

The linear Gaussian model (or the generalized Langevin equation) [Eqs. (8) and (10)] contains three coefficients. The coefficient D of the random term is determined from consistency with Kolmogorov's hypothesis, Eq. (14); while the mean drift $\mathbf{M}$ is determined from consistency with the mean of the Navier–Stokes equation, Eq. (16), and (coincidentally) from the requirement that mean continuity equation be satisfied, Eq. (17). We now consider the choice of the remaining coefficient G—a second-order tensor.

An evolution equation for the calculated Reynolds stresses is obtained by substituting Eq. (10) into Eq. (11), multiplying by $(V_j - \langle U_j \rangle_c)(V_k - \langle U_k \rangle_c)$, and integrating:

$$\frac{\partial \langle u_j u_k \rangle_c}{\partial t} + \langle U_i \rangle_c \frac{\partial \langle u_j u_k \rangle_c}{\partial x_i} + \frac{\partial \langle u_i u_j u_k \rangle_c}{\partial x_i} + \langle u_i u_k \rangle_c \frac{\partial \langle U_j \rangle_c}{\partial x_i} + \langle u_i u_j \rangle_c \frac{\partial \langle U_k \rangle_c}{\partial x_i} = G_{kl} \langle u_l u_j \rangle_c + G_{jl} \langle u_l u_k \rangle_c + C_0 \epsilon \delta_{jk}. \tag{20}$$

By comparing Eq. (20) with the exact Reynolds stress equation, some constraints on the tensor G are obtained.[6,7] But these constraints fall far short of uniquely determining G. Instead, Haworth and Pope[7,8] have constructed models for G and assessed their performance in homogeneous turbulence with mean velocity gradients,[7] and in free shear flows.[8]

In the pdf approach, the generalized Langevin equation can be used to calculate the one-point joint pdf of the Eulerian velocity f_c in inhomogeneous flows. In a dispersion study, on the other hand, we may use the generalized Langevin equation to calculate the trajectories of fluid particles through a specified turbulent field. The field may be specified by the dissipation $\epsilon(\mathbf{x},t)$ and the specified Eulerian pdf of velocity $f_s(\mathbf{V};\mathbf{x},t)$, or some of its moments. The question then is: can G be chosen so that the calculated pdf f_c is the same as that specified f_s?

It is clear that there is no choice of G that can yield an arbitrarily specified evolution of the Eulerian joint pdf. [At given $(\mathbf{x},t)$, G is comprised of nine numbers, whereas the Eulerian joint pdf f_s is a function of three independent variables.] But we now show that it may be possible to choose G so that the generalized Langevin equation yields the required evolution of the mean velocity and Reynolds stresses. Then the consistency condition is satisfied to second order.

It is assumed that the moments of f_s are consistent with the Navier–Stokes equations. So $\langle \mathbf{U} \rangle_s$ and $\langle u_i u_j \rangle_s$ satisfy

$$\frac{\partial}{\partial x_i} \langle U_i \rangle_s = 0, \tag{21}$$

$$\frac{\partial \langle U_j \rangle_s}{\partial t} + \frac{\partial}{\partial x_i} (\langle U_i \rangle_s \langle U_j \rangle_s + \langle u_i u_j \rangle_s) = \nu \nabla^2 \langle U_j \rangle_s - \frac{1}{\rho} \frac{\partial \langle p \rangle_s}{\partial x_j}, \tag{22}$$

and

$$\nabla^2 \langle p \rangle_s = -\rho \frac{\partial^2}{\partial x_i \, \partial x_j} (\langle U_i \rangle_s \langle U_j \rangle_s + \langle u_i u_j \rangle_s). \tag{23}$$

These equations are identical to those satisfied by $\langle \mathbf{U} \rangle_c$ and $\langle u_i u_j \rangle_c$ [Eqs. (15), (17), and the mean momentum equation obtained from (11)]. Given $\langle u_i u_j \rangle_s$ at all $(\mathbf{x},t)$, and given initial and boundary conditions on $\langle \mathbf{U} \rangle_s$, then Eqs. (21)–(23) determine the evolution $\langle \mathbf{U} \rangle_s$. Hence if the consistency condition is satisfied for the second moments, i.e.,

$$\langle u_i u_j \rangle_s = \langle u_i u_j \rangle_c, \tag{24}$$

then the evolution of $\langle \mathbf{U} \rangle_c$ is the same as that of $\langle \mathbf{U} \rangle_s$ (with the same initial and boundary conditions). In other words, if the consistency condition is satisfied for the second moments, it is satisfied for the first moments also.

To determine the consistency condition for second moments, we examine the evolution equation for the calculated Reynolds stresses, Eq. (20). Clearly, with the initial condition $\langle u_j u_k \rangle_c = \langle u_j u_k \rangle_s$, if the equation

$$\frac{\partial \langle u_j u_k \rangle_c}{\partial t} = \frac{\partial \langle u_j u_k \rangle_s}{\partial t} \tag{25}$$

is satisfied everywhere, then $\langle u_j u_k \rangle_c$ equals $\langle u_j u_k \rangle_s$ and hence (as argued above) $\langle \mathbf{U} \rangle_c$ equals $\langle \mathbf{U} \rangle_s$. Thus from Eq. (20) a necessary and sufficient condition for the consistency of the first and second moments is

$$G_{kl} \langle u_l u_j \rangle_s + G_{jl} \langle u_l u_k \rangle_s = Q_{jk}, \tag{26}$$

where

$$Q_{jk} = \frac{\partial \langle u_j u_k \rangle_s}{\partial t} + \langle U_i \rangle_s \frac{\partial \langle u_j u_k \rangle_s}{\partial x_i} + \frac{\partial \langle u_i u_j u_k \rangle_c}{\partial x_i} + \langle u_i u_k \rangle_s \frac{\partial \langle U_j \rangle_s}{\partial x_i} + \langle u_i u_j \rangle_s \frac{\partial \langle U_k \rangle_s}{\partial x_i} - C_0 \epsilon \delta_{jk}. \tag{27}$$

It is important to note that Q is determined by specified quantities (ϵ and moments of f_s) except for the term in $\langle u_i u_j u_k \rangle_c$.

In homogeneous turbulence the triple correlations are zero, and then Q is known in terms of specified quantities. The consistency condition is then satisfied to second order if the tensor G satisfies Eq. (26). It is shown in the Appendix that a tensor G can always be found that satisfies Eq. (26). More precisely, Eq. (26) removes six degrees of freedom in the choice of the nine components of G. Thus in homogeneous turbulence there are choices of G for which the generalized Langevin equation is consistent to second order.

For Gaussian homogeneous turbulence the generalized Langevin model is completely consistent (with an appropriate choice of G). This follows because a Gaussian distribution is uniquely determined by its first and second moments, and because for homogeneous turbulence the generalized Langevin equation yields a Gaussian distribution. [In principle non-Gaussian homogeneous turbulence can exist, at least as an initial condition. But experiments on homogeneous turbulence (e.g., Ref. 21) strongly suggest Gaussianity.]

For inhomogeneous turbulence, Eq. (26) remains the consistency condition. But to deduce simple algebraic constraints on G is less straightforward since Q depends on G through $\langle u_i u_j u_k \rangle_c$. In practice one might expect that $\langle u_i u_j u_k \rangle_s$ would be a good approximation to $\langle u_i u_j u_k \rangle_c$, and hence a choice of G that approximately satisfies Eq. (26) could be obtained. In principle this choice could be refined iteratively, by evaluating $\langle u_i u_j u_k \rangle_c$ based on the current choice of G, and then using Eq. (26) to obtain an improved choice. The convergence of this iteration is not established.

In summary, in the generalized Langevin equation, if the coefficients G are chosen to satisfy Eq. (26), then the consistency condition is satisfied to second order. For homogeneous turbulence such a choice always exists; and if, further, the turbulence is Gaussian, then the consistency condition can be completely satisfied. For inhomogeneous turbulence Eq. (26) remains the consistency condition, but it has not been proved that G can be chosen to satisfy it.

IV. SUMMARY AND CONCLUSIONS

For turbulent dispersion models, we have examined the thermodynamic constraint and introduced consistency conditions. For a given flow, it is essential to distinguish between three turbulent fields: $f(\mathbf{V};\mathbf{x},t)$ is the true one-point Eulerian pdf that in principle can be determined by error-free measurement or from exact solutions to the Navier–Stokes equations; $f_s(\mathbf{V};\mathbf{x},t)$ is the pdf specified in the dispersion calculations; and $f_c(\mathbf{V};\mathbf{x},t)$ is the pdf calculated from the random-walk model. A dispersion model is completely consistent if the calculated pdf f_c equals that specified f_s. Or, it is consistent to order m if the moments of f_c, up to order m, are equal to those of f_s.

The main conclusions to be drawn from this work are now summarized.

(i) A necessary and sufficient condition for the satisfaction of the thermodynamic constraint is that the calculated mean velocity $\langle \mathbf{U}\rangle_c$ satisfy the continuity equation. This, in turn, requires that the mean pressure gradient be properly incorporated in the random-walk model. The appropriate mean pressure gradient is that of the calculated field: this is the same as the specified mean pressure gradient only if the dispersion model is consistent to second order.

(ii) The additional constraints deduced by Sawford[14] can be interpreted as consistency conditions. They are not necessary to the satisfaction of the thermodynamic constraint.

(iii) According to Kolmogorov's hypotheses,[15,17] for time intervals s corresponding to the inertial subrange, the Lagrangian structure function $D_{ij}^{L}(s)$ is given by Eq. (13). Irrespective of the deterministic term the nonlinear Gaussian model [Eq. (8)] is consistent with Kolmogorov's hypotheses, whereas some models with a generalized random term[13,14] are not. Whether the random term is Gaussian or not is not the key issue: what is important is that the mean dissipation rate ϵ is the only parameter on which it depends.

(iv) The nonlinear Gaussian model [Eq. (8)] can be made completely consistent. For given f_s, the part of the model function **H** that affects the evolution of the pdf is uniquely determined by this condition.

(v) The linear Gaussian model (i.e., the generalized Langevin equation) is consistent to second order if the coefficients G satisfy an algebraic relation, Eq. (26). For homogeneous turbulence this relation can always be satisfied: its satisfaction removes six degrees of freedom from the choice of the nine components of G. For homogeneous Gaussian turbulence, complete consistency is possible.

(vi) A dispersion model should not be regarded as defective if it is inconsistent ($f_c \neq f_s$) when applied to an unphysical turbulent field ($f_s \neq f$). The previously used test problem of inhomogeneous Gaussian turbulence is an example of an unphysical specification.

APPENDIX: DETERMINATION OF THE TENSOR G TO SATISFY EQ. (26)

In this Appendix we employ matrix notation. Let R be the matrix of Reynolds stresses with components

$$R_{ij} = \langle u_i u_j \rangle_s. \tag{A1}$$

Since R is symmetric, there is a real unitary matrix L, and a diagonal matrix Λ such that

$$\mathsf{R} = \mathsf{L}^T \Lambda \mathsf{L}. \tag{A2}$$

The components of Λ are the eigenvalues of R—$\lambda^{(1)}$, $\lambda^{(2)}$, and $\lambda^{(3)}$. It is assumed that the turbulence is three dimensional so that the eigenvalues are strictly positive.

Equation (26) can be rewritten

$$\mathsf{GR} + \mathsf{RG}^T = \mathsf{Q}, \tag{A3}$$

or

$$\mathsf{GL}^T \Lambda \mathsf{L} + \mathsf{L}^T \Lambda \mathsf{LG}^T = \mathsf{Q}. \tag{A4}$$

Now premultiplying by L and postmultiplying by L^T we obtain

$$(\mathsf{LGL}^T)\Lambda + \Lambda(\mathsf{LG}^T\mathsf{L}^T) = \mathsf{LQL}^T, \tag{A5}$$

or

$$\widetilde{\mathsf{G}}\Lambda + \Lambda\widetilde{\mathsf{G}}^T = \widetilde{\mathsf{Q}}, \tag{A6}$$

where

$$\widetilde{\mathsf{G}} \equiv \mathsf{LGL}^T, \tag{A7}$$

and $\widetilde{\mathsf{Q}}$ is defined similarly. Now, in component form (without an implied summation convention) Eq. (A6) is

$$\widetilde{\mathsf{G}}_{kj}\lambda_j + \lambda_k \widetilde{\mathsf{G}}_{jk} = \widetilde{\mathsf{Q}}_{kj}. \tag{A8}$$

In order to satisfy Eq. (A8), the diagonal components of $\widetilde{\mathsf{G}}$ must be

$$\widetilde{\mathsf{G}}_{jj} = \tfrac{1}{2}\widetilde{\mathsf{Q}}_{jj}/\lambda_j \tag{A9}$$

(no summation). The upper-triangular components ($\widetilde{\mathsf{G}}_{jk}, k>j$) can be chosen arbitrarily, but then to satisfy Eq. (A8) the lower-triangular components must be

$$\widetilde{\mathsf{G}}_{jk} = (\widetilde{\mathsf{Q}}_{kj} - \lambda_j \widetilde{\mathsf{G}}_{kj})/\lambda_k \quad (k<j) \tag{A10}$$

(no summation).

In summary Eq. (26), or equivalently Eq. (A3), is satisfied by any tensor

$$\mathsf{G} = \mathsf{L}^T \widetilde{\mathsf{G}} \mathsf{L}, \tag{A11}$$

where the diagonal components of $\widetilde{\mathsf{G}}$ are given by Eq. (A9), and the lower-triangular components are related to the upper-triangular components by Eq. (A10). Thus the constraint [Eq. (26)] removes six degrees of freedom from the choice of the nine components of G.

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