2005

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AIP Physics of Fluids

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Citation: Physics of Fluids **17**, 025109 (2005); doi: 10.1063/1.1849184
View online: http://dx.doi.org/10.1063/1.1849184
View Table of Contents: http://scitation.aip.org/content/aip/journal/pof2/17/2?ver=pdfcov
Published by the AIP Publishing

A Lagrangian stochastic model for dispersion in stratified turbulence

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(Received 31 August 2004; accepted 19 November 2004; published online 24 January 2005)

In this paper we discuss the development of a Lagrangian stochastic model (LSM) for turbulent dispersion of a scalar (species). Given any tensorally linear second-moment closure (SMC) turbulence model we show how to derive a mathematically equivalent set of stochastic differential equations (SDEs), i.e., the second-moment equations constructed from these SDEs are exactly the same (within a realizability constraint) as the given SMC. This set of equations forms the LSM. Both turbulence anisotropy and buoyancy effects are incorporated by this method. In order to achieve the correct critical Richardson number and to obtain the simplest Lagrangian formulation, a revised set of constants for the isotropization of production model is proposed. They improve agreement with experiments. The LSM is applied to homogeneous shear flow with varying degrees of stratification. Our model is shown to capture important physics associated with buoyant flows and we also parametrize our results. Finally the form of the current model is compared with a few of the well-known Lagrangian stochastic models. © *2005 American Institute of Physics*.
[DOI: 10.1063/1.1849184]

I. INTRODUCTION

Taylor[1] introduced the Lagrangian stochastic model (LSM) for turbulent dispersion in the atmosphere. His seminal model was valid only for homogeneous turbulence. Over time, variants have been explored. Legg and Raupach[2] made an important revision by adding a term that corrects a spurious drift which occurred when the velocity variance was not homogeneous. Thomson[3] reviewed LSMs and formulated a *well mixed* criterion as a further method of assessing different formulations. He also described how to design LSMs to meet his criterion. Wilson and Sawford[4] provide a brief review of models that meet this constraint. Most of these models did a fairly good job for unstratified flows but they were not designed for thermal stratification and proved unsatisfactory in strongly stably stratified flows.[4]

Pearson *et al.*[5] proposed a theoretical model for dispersion in horizontal mean flow with stably stratified, stationary turbulence. They added a separate equation for the fluctuating density, containing a parameter γ that was described as a measure of molecular mixing processes. With no molecular mixing ($\gamma=0$) the mean square displacement of the released fluid particles ceased to grow after a certain time whereas nonzero, positive values of γ produced a linear increase at large times. Venkatram *et al.*[6] proposed a semiempirical model that did not support the role of molecular mixing in turbulent dispersion in stably stratified atmospheric flows. Comparison of both these models with experiments was not conclusive about the role of molecular mixing. Although these models were designed for stratification, they did not take other complexities such as mean shear and turbulence inhomogenity into account.

Lagrangian dispersion has largely been pursued in the context of atmospheric dispersion. By nature it is a statistical closure. The individual, random trajectories are an artifice. Their purpose is to produce statistics via Monte Carlo simulation. In some sense there should be a parallel between LSMs and Eulerian second-moment closure models, which is the theme of this paper.

Second-moment closure models have been designed for complex engineering flows. They can treat complexities such as turbulence anisotropy, inhomogenity, mean shear, buoyancy, etc. This suggests that such effects might be incorporated into Lagrangian formulations by developing a correspondence between the Lagrangian and Eulerian closures. Essentially, the aim is to incorporate stratification into the LSM by making it consistent with the Eulerian formulation. The premise is that the Eulerian closure provides acceptable predictions or, perhaps, that the latter is a vehicle for developing the empirical modeling, which then can be exploited by the LSM.

Pope[7] examined the relation between a generalized Langevin model and second-moment closures. In his approach, the Langevin model is essentially an Eulerian stochastic equation that implements a probability density function (pdf) closure. He showed how the second moment of the Langevin equation was a Reynolds stress closure. Hence, he explored the relation between stochastic models and second-moment closure models. Durbin and Speziale[8] constructed stochastic differential equations whose second moment would exactly reproduce a given Reynolds stress closure—up to a realizability constraint. They did not address stratified turbulence.

The objective of the present paper is to extend the approach of Durbin and Speziale;[8] that is, to develop a Lagrangian model that accounts for stratification effects by devising it to reproduce a given second-moment closure (SMC) model. This is an alternative to previous methods[5] for devising buoyant components. We show how to construct a set of stochastic differential equations (SDEs) whose second moments equal to a given, general form of SMC equations for Reynolds stress, Reynolds temperature flux, and temperature

variance. Again, this is done up to a realizability constraint: the stochastic model must produce realizable statistics. Most SMC models do not ensure realizability; indeed, by deriving them from a valid stochastic equation they can be revised to ensure realizablity.[8] Heinz[9] derived stochastic models that included an equation for potential temperature and, hence, are suited for thermally stratified flows. However, his formulation did not reproduce the well-known SMC models, such as that of Gibson and Launder.[10]

We choose the general linear formulation as the SMC. This is widely used with the Gibson–Launder coefficients.[10] Recently, Ji and Durbin[11] have analyzed this model and found a few deficiencies. It produces a critical Richardson number that is significantly too large. We propose a different set of values for constants for the Reynolds scalar flux and variance closures. The constants of the Reynolds stress equations retain their accepted values. The recalibration of scalar transport is not essential to our formulation, however, a critical Richardson number of about 0.25 is desirable for stratified flow applications. The present constants improve agreement with experimental and numerical data.

II. MATHEMATICAL FORMULATION

A. Turbulence second-moment closure

The general linear model forms the framework for the stochastic model. This closure of the Reynolds stress transport equations is contained in the right side of

$$\begin{aligned}\frac{d\overline{u_iu_j}}{dt} &= -c_1\frac{\epsilon}{k}\left(\overline{u_iu_j}-\frac{2}{3}k\delta_{ij}\right)-c_2\left(\mathcal{P}_{ij}-\frac{2}{3}\underline{\mathcal{P}}\delta_{ij}\right)\\ &\quad -c_3\left(\mathcal{D}_{ij}-\frac{2}{3}\underline{\mathcal{P}}\delta_{ij}\right)-c_sk\mathcal{S}_{ij}+\mathcal{P}_{ij}-\frac{2}{3}\epsilon\delta_{ij}\\ &\quad +(1-c_5)\mathcal{G}_{ij}+\frac{2}{3}c_5\underline{\mathcal{G}}\delta_{ij},\\ \frac{d\overline{\theta u_i}}{dt} &= -c_{1\theta}\frac{\epsilon}{k}\overline{\theta u_i}-(1-c_{2\theta})\overline{\theta u_k}\frac{\partial U_i}{\partial x_k}+c_{3\theta}\overline{\theta u_k}\frac{\partial U_k}{\partial x_i}\\ &\quad -(1-c_{4\theta})\overline{u_iu_k}\frac{\partial\Theta}{\partial x_k}-(1-c_{5\theta})\beta g_i\overline{\theta^2},\\ \frac{d\overline{\theta^2}}{dt} &= -2\overline{\theta u_k}\frac{\partial\Theta}{\partial x_k}-\mathcal{R}\frac{\epsilon}{k}\overline{\theta^2}.\end{aligned} \tag{1}$$

These are the equations for homogeneous turbulence. In (1)

$$\mathcal{S}_{ij}=\frac{1}{2}\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right),$$

$$\mathcal{P}_{ij}=-\overline{u_iu_k}\frac{\partial U_j}{\partial x_k}-\overline{u_ju_k}\frac{\partial U_i}{\partial x_k},$$

$$\mathcal{D}_{ij}=-\overline{u_iu_k}\frac{\partial U_k}{\partial x_j}-\overline{u_ju_k}\frac{\partial U_k}{\partial x_i},$$

$$\mathcal{G}_{ij}=-\beta(g_i\overline{u_j\theta}+g_j\overline{u_i\theta}),$$

$$\underline{\mathcal{P}}=\tfrac{1}{2}\mathcal{P}_{kk},\quad \underline{\mathcal{G}}=\tfrac{1}{2}\mathcal{G}_{kk}.$$

U_i and u_i are the mean and fluctuating velocities, Θ and θ are the mean and fluctuating temperatures, t is the time, x_i is the spatial coordinate, g_i is the acceleration due to gravity, β is the thermal expansion coefficient, k is the turbulent kinetic energy, ϵ is its dissipation rate, and $\mathcal{R}$ is a *time-scale ratio* of mechanical to scalar time scales. Terms with an overbar mean that they are ensemble averaged quantities. $\mathcal{R}$ is not a universal constant, its value may vary for different flows. According to Warhaft,[12] in the presence of a uniform mean scalar gradient, $\mathcal{R}$ is found to be very nearly constant and equal to 1.5.

This model can be derived by expansion about isotropy. The general linear expansion allows the constants c_1, c_2, c_3, c_s, c_5, $c_{1\theta}$, $c_{2\theta}$, $c_{3\theta}$, $c_{4\theta}$, $c_{5\theta}$, and $\mathcal{R}$. Their values have been derived mostly by calibration against experiments and by theoretical reasoning. Further details can be found in Durbin and Pettersson Reif.[13]

B. Stochastic differential equations

Our goal is to derive a set of Langevin stochastic differential equations that will have (1) as their second moment. First we review how to construct the second-moment equation of a given Ito-type stochastic differential equation. For more information the reader is referred to texts such as those by Arnold[14] and Øksendal.[15]

Let us take the case of the simplest Langevin equation

$$du_i=-\frac{u_i}{T}dt+(c_0\epsilon)^{1/2}d\mathcal{W}_i(t), \tag{2}$$

where u_i is the dependent variable—a random function of t—T is a time scale, c_0 is a constant, ϵ is a deterministic function of t, and $\mathcal{W}_i(t)$ is the Wiener stochastic process. For derivation of the second-moment equation we need the following properties of $d\mathcal{W}_i(t)$:

$$\begin{aligned}&\overline{d\mathcal{W}_i}=0,\quad \overline{d\mathcal{W}_id\mathcal{W}_j}=dt\delta_{ij},\quad \overline{u_jd\mathcal{W}_i}=0,\\ &d\mathcal{W}=O(dt)^{1/2}.\end{aligned} \tag{3}$$

Then the derivation of the second-moment equation proceeds as follows. Evaluate the differential, keeping terms to order $(du)^2$:

$$\begin{aligned}d(u_iu_j)&=(u_i+du_i)(u_j+du_j)-u_iu_j\\ &=u_idu_j+u_jdu_i+du_idu_j.\end{aligned}$$

Average the above using (3) to get

$$\frac{d\overline{u_iu_j}}{dt}=-2\frac{\overline{u_iu_j}}{T}+c_0\epsilon\delta_{ij}. \tag{4}$$

This is the second-moment closure corresponding to (2). In essence this is the procedure used herein to derive second-moment turbulence closure equations from the stochastic differential equations of our Lagrangian model. Subsequently, we will not detail the steps.

C. Lagrangian stochastic model

If we choose the values of $c_{2\theta}$, $c_{3\theta}$, and $c_{5\theta}$ in Eq. (1) as equal to c_2, c_3, and c_5, respectively, and set $c_s=0$, then the simplest form of our model results. The standard isotropization of production (IP) model uses $c_s=0$. The general form of our LSM will be described in the following section where the motive for these specifications of the constants will become clear. The simplified form is

$$\begin{aligned} du_i &= -\frac{c_1}{2}\frac{\epsilon}{k}u_i dt + (c_{2\theta}-1)u_k\frac{\partial U_i}{\partial x_k}dt + c_{3\theta}u_k\frac{\partial U_k}{\partial x_i}dt \\ &\quad - (1-c_{5\theta})\beta g_i\theta dt + \sqrt{c_0\epsilon}d\mathcal{W}_i, \\ d\theta &= -\left(c_{1\theta}-\frac{c_1}{2}\right)\frac{\epsilon}{k}\theta dt - (1-c_{4\theta})u_k\frac{\partial\Theta}{\partial x_k}dt + \sqrt{c_\theta}d\mathcal{W}_\theta. \end{aligned} \tag{5}$$

The coefficients c_0 and c_θ are specified as

$$\begin{aligned} c_0 &= \frac{2}{3}\left[c_1 - 1 + (c_2+c_3)\frac{\mathcal{P}}{\epsilon} + c_5\frac{\mathcal{G}}{\epsilon}\right], \\ c_\theta &= -2c_{4\theta}\overline{\theta u_k}\frac{\partial\Theta}{\partial x_k} + \frac{\epsilon}{k}(2c_{1\theta}-c_1-\mathcal{R})\overline{\theta^2}. \end{aligned} \tag{6}$$

Realizabilty takes the form of requiring these to be nonnegative, so that the square roots in Eq. (5) are real valued. If $c_{1\mathrm{SMC}}$ is a standard value of the constant c_1, the Langevin model will be well posed if the return to isotropy constants are replaced by[8]

$$\begin{aligned} c_1 &= \max\left[c_{1\mathrm{SMC}}, 1-(c_2+c_3)\frac{\mathcal{P}}{\epsilon} - c_5\frac{\mathcal{G}}{\epsilon}\right], \\ c_{1\theta} &= \max\left[c_{1\theta\ \mathrm{SMC}}, 0.5\left[2\frac{k}{\epsilon\overline{\theta^2}}c_{4\theta}\overline{\theta u_k}\frac{\partial\Theta}{\partial x_k} + (c_1+\mathcal{R})\right]\right]. \end{aligned}$$

The method of the preceding section shows how (5) with (6) reproduces (1).

Although (5) is contrived only to reproduce (1) mathematically, it inherits certain physical attributes. Oscillatory motion is produced by the restoring force $\beta g\theta$ in the first equation. The natural frequency is less than the Brunt–Väisälä frequency. It equals $\sqrt{(1-c_{5\theta})\beta g S_\theta}$, S_θ being the mean temperature gradient in the negative direction of gravity. Pearson *et al.*[5] argue that internal wave radiation can be modeled in this way. The frequency of radiated internal waves is the Brunt–Väisälä frequency times the cosine of the angle to the direction of gravity. The empirical constant $(1-c_{5\theta})$ plays the role of the average over radiation angles in the physical reasoning of Pearson *et al.*[5]

The density fluctuations of fluid elements relax toward the mean state by mixing with their environment. The second of equations (5) can be characterized as describing this via linear damping of the temperature fluctuation of the fluid particle. It might be questioned whether it is valid to assume that the particle relaxes toward the ensemble averaged environment. That rationale was not invoked in (5), we only required it to reproduce the statistics of the SMC. However, this physical interpretation is available.

A calibration of the constants and discussion of the properties of this model are presented in a later section.

D. General case

The Langevin equation of the general linear model is somewhat more involved than (5). The white noise forcing is no longer isotropic. A device introduced by Durbin and Speziale[8] can be used to ensure the desired second moment. We present the equation without derivation. To a large extent it is a matter of working backward from the SMC to the stochastic equation. However, the latter is not unique; the second moment does not uniquely determine the stochastic process. The following is a form that has (1) as its moment equation:

$$\begin{aligned} du_i &= -\frac{c_1}{2}\frac{\epsilon}{k}u_i dt + (c_{2\theta}-1)u_k\frac{\partial U_i}{\partial x_k}dt + c_{3\theta}u_k\frac{\partial U_k}{\partial x_i}dt \\ &\quad - (1-c_{5\theta})\beta g_i\theta dt + M_{ik}d\mathcal{W}_k' + P_{ik}d\mathcal{W}_k'' + D_{ik} \\ &\quad \times d\mathcal{W}_k''' + G_{ik}d\mathcal{W}_k^{iv} + (c_0\epsilon)^{1/2}d\mathcal{W}_i, \\ d\theta &= -\left(c_{1\theta}-\frac{c_1}{2}\right)\frac{\epsilon}{k}\theta dt - (1-c_{4\theta})u_k\frac{\partial\Theta}{\partial x_k}dt + c_\theta^{1/2}d\mathcal{W}_\theta. \end{aligned} \tag{7}$$

The matrices multiplying the white noise terms are devised to produce requisite terms of (1). In order to do so, they must satisfy the following:

$$\begin{aligned} M_{ik}M_{kj} - \lambda_{\mathcal{S}}\delta_{ij} &= -c_s k\mathcal{S}_{ij}, \\ P_{ik}P_{kj} - \lambda_{\mathcal{P}}\delta_{ij} &= -(c_2-c_{2\theta})\mathcal{P}_{ij}, \\ D_{ik}D_{kj} - \lambda_{\mathcal{D}}\delta_{ij} &= -(c_3-c_{3\theta})\mathcal{D}_{ij}, \\ G_{ik}G_{kj} - \lambda_{\mathcal{G}}\delta_{ij} &= -(c_5-c_{5\theta})\mathcal{G}_{ij}. \end{aligned} \tag{8}$$

The right-hand sides of the above equations are the terms that appear in the SMC model equations. In order to get those terms when second-moment equations are generated from the general form of the LSM, the matrices given in the first terms on the left of Eqs. (8) are required. The λ's which are the maximum eigenvalues of the matrices on the right achieve the equality.

The coefficients c_0 and c_θ are now given by

$$\begin{aligned} c_0 &= \frac{2}{3}\left[c_1 + (c_2+c_3)\frac{\mathcal{P}}{\epsilon} + c_5\frac{\mathcal{G}}{\epsilon} - 1\right] \\ &\quad - \frac{1}{\epsilon}(\lambda_{\mathcal{S}}+\lambda_{\mathcal{P}}+\lambda_{\mathcal{D}}+\lambda_{\mathcal{G}}), \\ c_\theta &= -2c_{4\theta}\overline{\theta u_k}\frac{\partial\Theta}{\partial x_k} + \frac{\epsilon}{k}(2c_{1\theta}-c_1-\mathcal{R})\overline{\theta^2}. \end{aligned} \tag{9}$$

Realizability requires that each term under the square root in the SDEs be positive. The turbulence constants are such that this is satisfied in most situations. But sometimes c_0 and c_θ, as calculated by the above equations, may become negative. As previously noted, unconditional realizability is enforced by defining c_1 and $c_{1\theta}$ as

$$c_1 = \max\left[c_{1\,\mathrm{SMC}}, \frac{1.5}{\epsilon}(\lambda_{\mathcal{S}} + \lambda_{\mathcal{P}} + \lambda_{\mathcal{D}} + \lambda_{\mathcal{G}}) - (c_2 + c_3)\frac{\mathcal{P}}{\epsilon} - c_5\frac{\mathcal{G}}{\epsilon} + 1 \right],$$

$$c_{1\theta} = \max\left\{ c_{1\theta\ \mathrm{SMC}}, 0.5\left[2\frac{k}{\epsilon\overline{\theta^2}} c_{4\theta}\overline{\theta u_k}\frac{\partial\Theta}{\partial x_k} + (c_1 + \mathcal{R}) \right] \right\}, \tag{10}$$

where $c_{1\,\mathrm{SMC}}$ and $c_{1\theta\ \mathrm{SMC}}$ are the constants c_1 and $c_{1\theta}$ of the original SMC model.

The matrices M, P, D, and G can be regarded as generalized square roots of the matrices in the right-hand side of (8). We show the procedure to calculate M. The rest can be calculated by the same method. Matrix $c_s k\mathcal{S}$ can be diagonalized by the orthogonal matrix U of eigenvectors as follows:

$$c_s k\mathcal{S} = U \cdot \mathrm{diag}[\lambda_1, \lambda_2, \lambda_3] \cdot U^t, \tag{11}$$

where $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3$. It is not very difficult to show that the generalized square root M is then given by

$$M = U \cdot \mathrm{diag}[0, (\lambda_1 - \lambda_2)^{1/2}, (\lambda_1 - \lambda_3)^{1/2}] \cdot U^t. \tag{12}$$

In stationary, nonhomogeneous flow, the mean Lagrangian time derivative is

$$\overline{D_t u_i} = \frac{\partial \overline{u_i u_k}}{\partial x_k}, \quad \overline{D_t \theta} = \frac{\partial \overline{\theta u_k}}{\partial x_k}.$$

These terms must be included in the Lagrangian equation to make it consistent with the Eulerian mean.[16] Legg and Raupach[2] derived such terms by attributing them to a mean pressure gradient. They are needed to avoid spurious drift and to satisfy the well mixed condition. After adding these terms, the final and most general form of our stochastic equation is

$$\begin{aligned} du_i &= -\frac{c_1}{2}\frac{\epsilon}{k}u_i dt + (c_{2\theta} - 1)u_k\frac{\partial U_i}{\partial x_k}dt + c_{3\theta}u_k\frac{\partial U_k}{\partial x_i}dt \\ &\quad - (1 - c_{5\theta})\beta g_i\theta dt + \frac{\partial \overline{u_i u_k}}{\partial x_k}dt + M_{ik}d\mathcal{W}'_k + P_{ik}d\mathcal{W}''_k \\ &\quad + D_{ik}d\mathcal{W}'''_k + G_{ik}d\mathcal{W}^{iv}_k + (c_0\epsilon)^{1/2}d\mathcal{W}_i, \\ d\theta &= -\left(c_{1\theta} - \frac{c_1}{2}\right)\frac{\epsilon}{k}\theta dt - (1 - c_{4\theta})u_k\frac{\partial\Theta}{\partial x_k}dt + \frac{\partial\overline{\theta u_k}}{\partial x_k}dt \\ &\quad + c_\theta^{1/2}d\mathcal{W}_\theta. \end{aligned} \tag{13}$$

The second-moment equations constructed from these stochastic differential equations can be shown (after a fair bit of algebra) to be similar to the Eulerian closure equations. In inhomogeneous turbulence, the SMC model contains triple correlation terms whereas in the Lagrangian approach these terms are a natural part of the Lagrangian derivative. So no extra term is required. However, in the Eulerian models, pressure diffusion terms need to be modeled; usually they are clubbed together with the turbulent transport terms and are modeled collectively. In the current approach, the pressure diffusion is neglected. Also, as mentioned before, the above equation set (13) is not unique. SDEs, other than those given by (13), can be constructed that can generate the same second moments. Indeed, a unique set of SDEs cannot be constructed by consideration of second moments alone.

Heinz[9] also derived Lagrangian equations for turbulent motion and buoyancy in inhomogeneous flows. He derived the corresponding Fokker–Planck equation for the pdf, generated moment equations from it, and evaluated the unknown terms of his SDEs by comparing terms with the conservation equations of momentum and potential temperature and transport equations of second moments. But these second-moment equations were not any of the well-known SMC models and hence his LSM could not reproduce the category of Eulerian closure models that are considered here.

III. MODEL CALIBRATION

The IP model is one of the simplest and most widely established SMC turbulence models. But until recently it had not been tested properly for buoyant flows. Ji and Durbin,[11] while studying the structural equilibrium behavior of SMC models in stably stratified, spanwise rotating, homogeneous shear flows, found that the IP model did not perform well for values of gradient Richardson number around 0.25. This is the critical value of Ri_g at which turbulence becomes stationary. Ji and Durbin[11] felt that SMC turbulence models in general should be calibrated to have the correct stabilization point, and proceeded to do so.

In this section we propose another set of constants (different from theirs) to use with our simplified model (5). Rotation is not taken into account, as this is not our focus. Only those constants that are associated with active scalar transport in the standard IP model will be altered, leaving the other constants untouched. Here, the choice is made with the Lagrangian formulation as a guideline. From the general form of the LSM given by Eqs. (13) and (8), it is clear that if $c_s = 0$ and $c_{2\theta}$, $c_{3\theta}$, and $c_{5\theta}$ are made equal to c_2, c_3, and c_5, respectively, then the simplified form of the LSM is arrived at. The proposed values of the set of constants is given in Table I.

The next step is to test these coefficients against experimental and numerical (DNS and LES) data for stratified flows. These are experiments of Tavoularis and Corrsin[17] and Rohr *et al.*,[18] direct numerical simulations of Rogers *et al.*,[19]

TABLE I. Model constants for IP and this model.

Constants	c_1	c_2	c_3	c_5	c_s	$c_{1\theta}$	$c_{2\theta}$	$c_{3\theta}$	$c_{4\theta}$	$c_{5\theta}$	$\mathcal{R}$
IP model	1.8	0.6	0.0	0.6	0.0	2.5	0.4	0.0	0.0	0.4	1.6
Our model	1.8	0.6	0.0	1/3	0.0	2.5	0.6	0.0	0.0	1/3	1.5

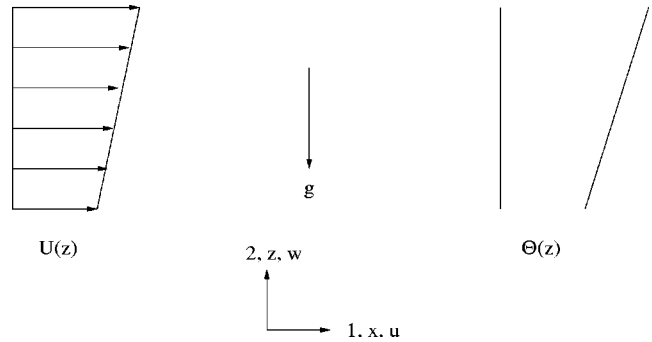

FIG. 1. Schematic for flow configuration.

Gerz and Schumann,[20] Holt *et al.*,[21] and Shih *et al.*,[22] and large eddy simulations of Kaltenbach *et al.*[23] They have all focused on homogeneous stratified shear flow cases.

Homogeneous shear flow with varying degrees of stable stratification characterized by different values of Ri_g is computed. The mean velocity is unidirectional, with a specified constant value of dU/dz. The mean temperature gradient $d\Theta/dz$ is positive and constant. A schematic for the flow is given in Fig. 1.

Ji and Durbin[11] have specified the problem, the governing differential equations, and the initial conditions in greater detail. We do not repeat those details here, instead the reader is referred to their work for more information. We show test results for both the original IP model and the constants that we are proposing.

Figure 2 shows the turbulent kinetic energy evolution. Time is nondimensionalized as St where $S \equiv dU/dz$, and turbulent kinetic energy has been normalized by its initial value k_0. Other parameters appearing in the figures are defined as $u' \equiv \sqrt{\overline{u^2}}$, $R_{uw} \equiv \overline{uw}/(u'w')$, and $R_{w\theta} \equiv \overline{w\theta}/(w'\theta')$, where $\theta' \equiv \sqrt{\overline{\theta^2}}$.

It is clear that at $\mathrm{Ri}_g = 0.25$ the IP model shows an increase in turbulent kinetic energy with time, while it neither grows nor decays for our model. In fact Ji and Durbin[11] reported that the IP model predicts the critical Ri_g at 0.48 whereas in our model it is predicted at around 0.24 which is extremely close to the experimentally observed value of 0.25. Figure 3 shows the evolution of the rms velocity u'. The models do not predict the initial transient ($St < 4$) which may be due to mismatch between the initial conditions of the experiments and the model calculations. But it is clearly seen that our model performs much better than the IP model after the initial transients. Figure 4 compares the evolution of R_{uw} and $R_{w\theta}$ with experimental and numerical (DNS and LES) data. The prediction of this model is given in the time interval $8 < St < 17$. Since all the experimental and numerical data were taken during the time $8 < St < 15$, the performance of this model seems reasonable.

IV. DISPERSION IN HOMOGENEOUS STABLY STRATIFIED SHEAR FLOW

In dispersion analysis, the Reynolds stress is given and the statistics of the dispersing particles are to be computed. For the simplified model, only k, ε, $\mathcal{P}$, and $\mathcal{G}$ are needed. They are obtained by solving the ordinary differential equations of the SMC turbulence model given by Eqs. (1). The values of the constants are specified in Table I. For this problem the LSM reduces to

$$du = -\frac{c_1}{2}\frac{\epsilon}{k}u\,dt + (c_{2\theta} - 1)w\frac{dU}{dz}dt + (c_0\epsilon)^{1/2}d\mathcal{W}_u,$$

$$dw = -\frac{c_1}{2}\frac{\epsilon}{k}w\,dt + (1 - c_{5\theta})\beta g\theta\,dt + (c_0\epsilon)^{1/2}d\mathcal{W}_w, \qquad (14)$$

$$d\theta = -\left(c_{1\theta} - \frac{c_1}{2}\right)\frac{\epsilon}{k}\theta\,dt - w\frac{d\Theta}{dz}dt + c_\theta^{1/2}d\mathcal{W}_\theta,$$

where the constants c_0 and c_θ are given by

$$c_0 = \frac{2}{3}\left(c_1 - c_2\frac{\overline{uw}}{\epsilon}\frac{dU}{dz} + c_5\frac{\beta g}{\epsilon}\overline{w\theta} - 1\right),$$

$$c_\theta = \frac{\epsilon}{k}(2c_{1\theta} - c_1 - \mathcal{R})\overline{\theta^2}. \qquad (15)$$

Realizability is ensured by calculating c_1 and $c_{1\theta}$ as follows:

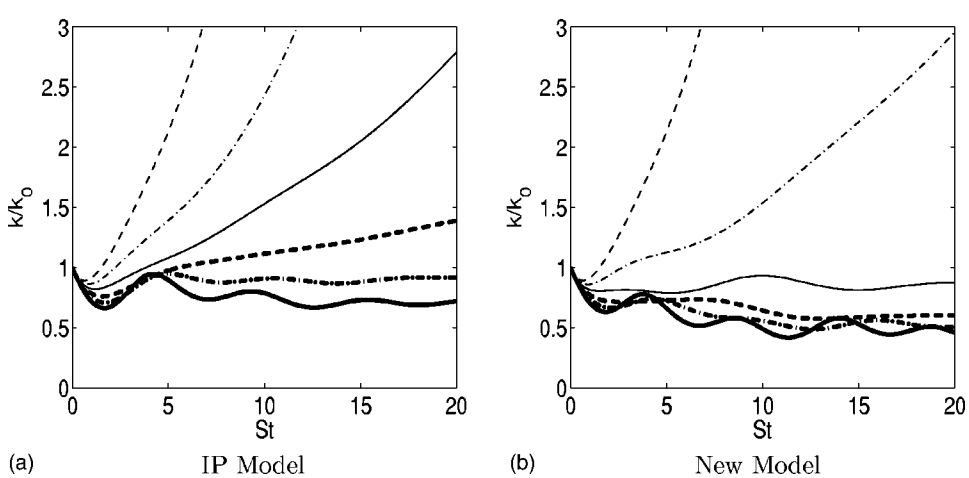

FIG. 2. Evolution of turbulent kinetic energy with time at different Ri_g. Lines: dash, 0; dash dot, 0.13; solid, 0.25; thick dash, 0.37; thick dash dot, 0.48; thick solid, 0.60.

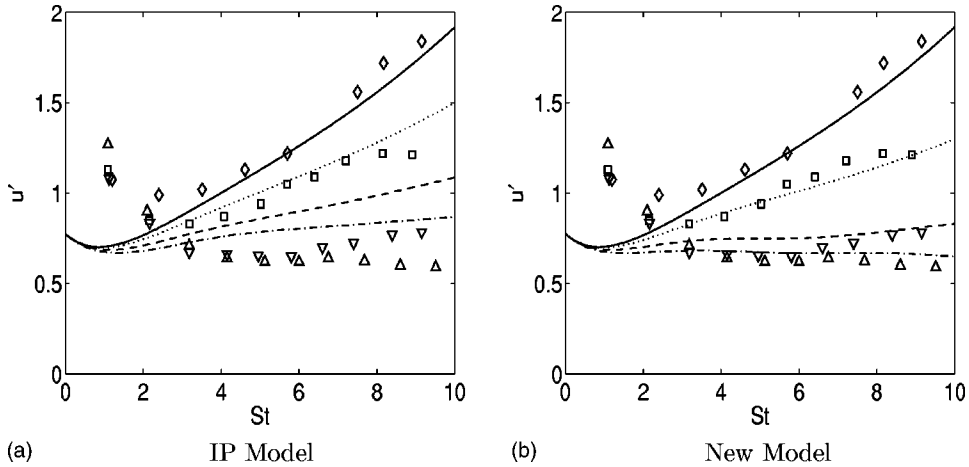

FIG. 3. Evolution of u rms velocity with time at different Ri_g. Lines (model predictions): solid, 0; dotted, 0.075; dash, 0.21; dash dot, 0.37. Symbols [experimental data of Rohr *et al.* (1988)]: ◇, 0; □, 0.075; ▽, 0.21; △, 0.37.

$$c_1 = \max\left[c_{1\,\mathrm{SMC}}, 1 + c_2\frac{\overline{uw}}{\epsilon}\frac{dU}{dz} - c_5\frac{\beta g}{\epsilon}\overline{w\theta}\right],$$
$$c_{1\theta} = \max[c_{1\theta\,\mathrm{SMC}}, 0.5(c_1 + \mathcal{R})]. \tag{16}$$

Initially the focus is on the case where turbulence is stationary. As mentioned before, the SMC turbulence model given by (1) predicts stationary turbulence at $\mathrm{Ri}_g = 0.24$. The advantage with stationary turbulence is that while solving the LSM we deal with fixed values of turbulence statistics and do not have to worry about these values changing with time. It is to be noted though that the LSM in general is capable of handling nonstationary turbulence, in that case the Eulerian statistics that are to be fed in our SDEs will be varying in time.

In this problem we are particularly interested in the variation of dispersion length squared, $\overline{Z^2}(t)$ with time t. $\overline{Z^2}(t)$ is calculated as the mean of the $Z^2(t)$ over a large number of trajectories, where $Z(t)$ for each particle is defined as

$$Z(t) = \int_0^t w\, dt.$$

For statistically stationary turbulence we have $\overline{Z^2}(t)$ evaluated as

$$\begin{aligned}\overline{Z^2}(t) &= \int_0^t\int_0^t \overline{w(t')w(t'')}dt''dt' \\ &= \overline{w^2}\int_0^t\int_0^t R_{ww}(t''-t')dt''dt' \\ &= 2\overline{w^2}\int_0^t (t-\tau)R_{ww}(\tau)d\tau.\end{aligned} \tag{17}$$

So if the vertical velocity autocorrelation R_{ww} is known then the vertical dispersion length can be readily calculated. It turns out that for this problem an analytical closed form solution of our model exists. To proceed further it is necessary to find out an equation for R_{ww}. In order to achieve this the w equation needs to be manipulated. Substituting $T_L = 2k/(c_1\epsilon)$ and $c_{5\theta} = 1/3$ in the w equation it can be written as

$$dw = -\frac{w}{T_L}dt + \frac{2}{3}\beta g\theta\, dt + (c_0\epsilon)^{1/2}d\mathcal{W}_w. \tag{18}$$

Multiplying both sides of this equation by $w(t-\tau)$, taking the mean and finally dividing by $\overline{w^2}(0)$ gives

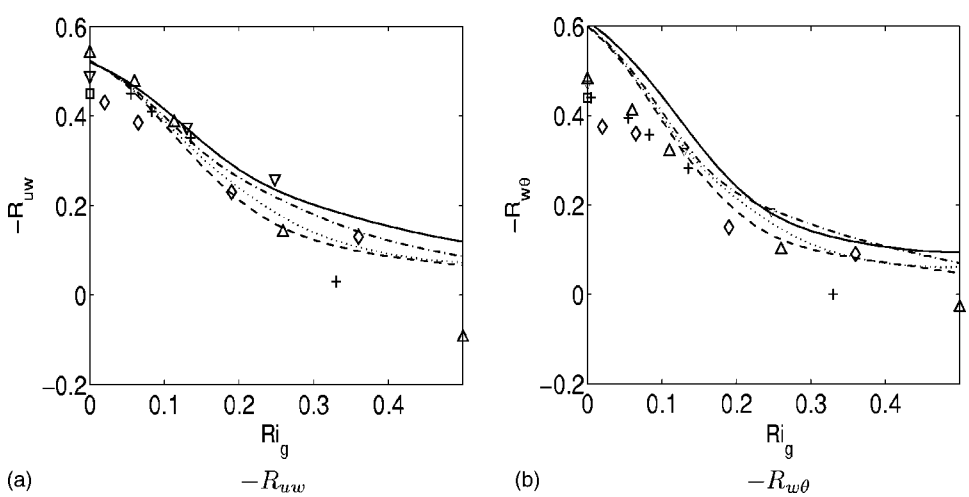

FIG. 4. $-R_{uw}$ and $-R_{w\theta}$ vs Ri_g. Lines (model predictions): solid, $St=8$; dash dot, $St=11$; dot, $St=14$; dash, $St=17$. Symbols: ◇, Rohr *et al.* (1988); □, Tavaoloris and Corrsin (1981); △, Holt *et al.* (1992); +, Gerz and Schumann (1991); ▽, Kaltenbach *et al.* (1994).

$$\frac{dR_{ww}}{dt} = -\frac{1}{T_L}R_{ww} + \frac{2}{3}\beta g R_{\theta w}. \tag{19}$$

The derivation invokes the nonanticipating property $\overline{w(t-\tau)d\mathcal{W}_t}=0$ for $\tau \geqslant 0$. To find an equation for $R_{\theta w}(\tau)[\equiv \overline{\theta(t)w(t-\tau)}/\overline{w^2(0)}]$, a similar procedure is followed for the θ stochastic equation, to find

$$\frac{dR_{\theta w}}{dt} = -\frac{1}{T_L'}R_{\theta w} - S_\theta R_{ww}, \tag{20}$$

where $T_L'=2k/[(2c_{1\theta}-c_1)\epsilon]$ and $S_\theta = d\Theta/dz$. In matrix notation the above two equations can be written as

$$\frac{d\overline{\mathcal{R}}}{dt} = -\mathcal{A}\overline{\mathcal{R}}, \tag{21}$$

where

$$\overline{\mathcal{R}} = \begin{bmatrix} R_{ww} \\ R_{\theta w} \end{bmatrix}, \quad \mathcal{A} = \begin{bmatrix} 1/T_L & -\frac{2}{3}\beta g \\ S_\theta & 1/T_L' \end{bmatrix}.$$

The solution of (21) is

$$\overline{\mathcal{R}}(t) = e^{-\mathcal{A}t}\overline{\mathcal{R}}(0). \tag{22}$$

It is not very difficult to show that

$$\begin{aligned} R_{ww}(t) &= Ae^{-\lambda_A t} + Be^{-\lambda_B t}, \\ \overline{Z^2}(t) &= 2\overline{w^2}(0)\left[\left(\frac{A}{\lambda_A} + \frac{B}{\lambda_B}\right)t + \frac{A}{\lambda_A^2}(e^{-\lambda_A t} - 1) \right. \\ &\quad \left. + \frac{B}{\lambda_B^2}(e^{-\lambda_B t} - 1)\right], \end{aligned} \tag{23}$$

where

$$\lambda_A = 0.5\left[\left(\frac{1}{T_L} + \frac{1}{T_L'}\right) + \sqrt{\left(\frac{1}{T_L} - \frac{1}{T_L'}\right)^2 - \frac{8}{3}N^2}\right],$$

$$\lambda_B = 0.5\left[\left(\frac{1}{T_L} + \frac{1}{T_L'}\right) - \sqrt{\left(\frac{1}{T_L} - \frac{1}{T_L'}\right)^2 - \frac{8}{3}N^2}\right],$$

$$N^2 = \beta g S_\theta,$$

$$A = p[sR_{ww}(0) - qR_{\theta w}(0)]/(ps - qr),$$

$$B = q[pR_{\theta w}(0) - rR_{ww}(0)]/(ps - qr),$$

$$p = (\lambda_A - 1/T_L')/\sqrt{(\lambda_A - 1/T_L')^2 + S_\theta^2},$$

$$q = (\lambda_B - 1/T_L')/\sqrt{(\lambda_B - 1/T_L')^2 + S_\theta^2},$$

$$r = S_\theta/\sqrt{(\lambda_A - 1/T_L')^2 + S_\theta^2},$$

$$s = S_\theta/\sqrt{(\lambda_B - 1/T_L')^2 + S_\theta^2}.$$

The factor of $8/3$ multiplying N^2 is $4(1-c_{5\theta})$.

λ_A and λ_B are eigenvalues of the matrix $\mathcal{A}$ which appears in Eq. (21). N is the Brunt–Väisälä, or buoyancy, frequency. So in addition to the turbulent time scale, another due to buoyancy has made an appearance in the solution. This enters through the additional SDE for θ. For moderate to strongly stable stratification $NT_L \geqslant 1$, so in general the eigenvalues λ_A and λ_B can become complex, especially for strongly stable stratification. As given in Eqs. (23), R_{ww} and $\overline{Z^2}$ contain terms such as $e^{-\lambda_A t}$ and $e^{-\lambda_B t}$, so we expect to see wavelike oscillations in the solution; these are effects of internal gravity waves in the flow field.

Consider the short time and long time behaviors of $\overline{Z^2}$. As $t \to 0$, $\overline{Z^2} \to \overline{w^2}(0)t^2$ from the solution (23). This is the standard short time behavior expected from all Lagrangian models. As $t \to \infty$,

$$\overline{Z^2} \to 2\overline{w^2}(0)\left[\left(\frac{A}{\lambda_A} + \frac{B}{\lambda_B}\right)t - \left(\frac{A}{\lambda_A^2} + \frac{B}{\lambda_B^2}\right)\right].$$

Hence, the model predicts a linear increase of $\overline{Z^2}$ at large times. Differentiating (17) with respect to t gives

$$\frac{d\overline{Z^2}}{dt} = 2\overline{w^2}(0)\int_0^t R_{ww}(\tau)d\tau.$$

As $t \to \infty$ the integral becomes the Lagrangian time scale of turbulence, which in cases of buoyant flows is expected to have positive values. Thus, at large times, $\overline{Z^2}$ is expected to grow linearly, as the model predicts.

As mentioned before, the solution of Eqs. (1) gives the Reynolds stresses for stationary, stratified, homogenous shear flow. The value of the dissipation rate ϵ is obtained from DNS studies,[22] which state that at high Reynolds number the value of the dimensionless shear rate Sk/ϵ becomes constant at around 5.5. Figure 5 shows plots of normalized vertical dispersion length squared, $\xi^2\,[\equiv \overline{Z^2}N^2/\overline{w^2}(0)]$ and vertical velocity autocorrelation R_{ww} with normalized time Nt at critical Richardson number. At short times some small oscillations are seen which are due to internal gravity waves but they get damped out pretty quickly. In order to see their effect more clearly the turbulent time scale is increased by changing the value of Sk/ϵ to 20. The results are plotted in Fig. 6 where the effect of the waves are clearly seen in both the ξ^2 and R_{ww} plots as more pronounced damped oscillations. After they decay away, ξ^2 shows a linear increase with Nt as predicted by our analytical solution.

In order to further explore our model, the LSM is solved for a range of values of Ri_g other than the critical one. It is well known that for this problem the so-called *moving equilibrium* solution to the SMC equations exists, i.e., the ratios of all the Reynolds stresses, scalar fluxes, and variance to the turbulent kinetic energy are steady whereas only the turbulent kinetic energy itself varies with time. In Fig. 2 it is seen that at values of Ri_g greater than $\mathrm{Ri}_{g\,crit}$ the turbulent kinetic energy tends to show much less variation in time than for cases where $\mathrm{Ri}_g < \mathrm{Ri}_{g\,crit}$. Hence the Eulerian statistics for these cases will be varying quite slowly with time. So just for illustration purposes it seems plausible to feed constant values of these statistics into our LSM for values of Ri_g higher than critical.

The LSM is solved numerically for values of $\mathrm{Ri}_g = 0.25$, 0.30, 0.35, and 0.40. The Eulerian statistics correspond to constant turbulent kinetic energy which is the same for all

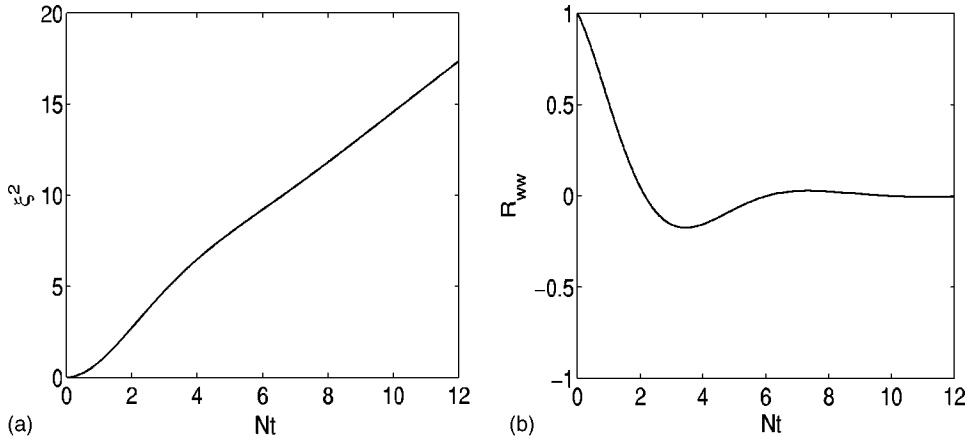

FIG. 5. (a) Normalized vertical dispersion length squared $\xi^2\,[\equiv\overline{Z^2}N^2/\overline{w^2}(0)]$ and (b) vertical autocorrelation R_{ww} vs normalized time Nt at critical Ri_g with $Sk/\epsilon=5.5$.

cases. The problem specification is $dU/dz=1.0\ \mathrm{s}^{-1}$, $d\Theta/dz=5.0\ \mathrm{K/m}$, $g=9.81\ \mathrm{m/s}^2$, and the value of β is adjusted for different Ri_g. The value of k is fixed at $3.75\times10^{-3}\ \mathrm{m}^2/\mathrm{s}^2$ and Sk/ϵ at 20. The values of the rest of the turbulence statistics are obtained from the moving equilibrium solution of the SMC model.

Figure 7 shows the results. Part (a) shows how the vertical dispersion is reduced as stability is increased. From part (b) it is apparent that the frequency of the internal gravity waves follows the $0.8N$ curve quite closely. Mathematically the imaginary part of the complex eigenvalues λ_A and λ_B, given by Eq. (23), gives the frequency of the internal gravity waves for stationary turbulence. Assuming the integral time scale of turbulence to be much larger than the buoyancy time scale (a very reasonable assumption) the imaginary part of the eigenvalues becomes $0.82N$. It can be interpreted to mean that the internal gravity waves are radiated at an angle of about arccos(0.8), i.e., 37° with the horizontal. Pearson *et al.*[5] assumed in their model that internal gravity waves were radiated at an angle of arccos(0.8) for stably stratified flows. They explicitly specified the value of 0.8 as a constant to capture the angle of radiation; in our case the value comes from the specification of the constant c_5 in the SMC model.

We also parametrize the dispersion curves. In this problem there are two time scales, viz. the integral time scale T_L and the buoyancy time scale $1/N$. Figure 8(a) shows a plot of the dimensionless dispersion length ξ with time nondimensionalized as Nt. The curves do collapse at small times but at large times they separate. The frequencies of the oscillations of the curves match quite well. In Fig. 8(b) the time is nondimensionalized by the integral time scale T_L. Overall the curves collapse onto each other but there is no match with the frequencies. So it is clear from the figures that only as long as the internal gravity waves have an effect on the dispersion, Nt is a good time parameter; for very short times it does an excellent job. However, the integral time scale controls the overall dispersion, especially at large times. The same conclusion can also be arrived at mathematically from the analytical solution for $\overline{Z^2}$ given by Eq. (23). The internal gravity waves come only through the exponential terms and at large times those terms become neglible. On the other hand the real part of the eigenvalues contain the integral time scale and though it has an effect throughout the process, it becomes relatively much more important at large times.

V. COMPARISON WITH PREVIOUS MODELS

The random force model of Legg and Raupach[2] consisted of a single equation for w which in differential form can be written as

$$dw=-\frac{w}{T_L}dt+\frac{d\overline{w^2}}{dz}dt+\left(\frac{2\overline{w^2}}{T_L}\right)^{1/2}d\mathcal{W}_w. \tag{24}$$

The w equation of the current LSM for one-dimensional neutral flows reduces to

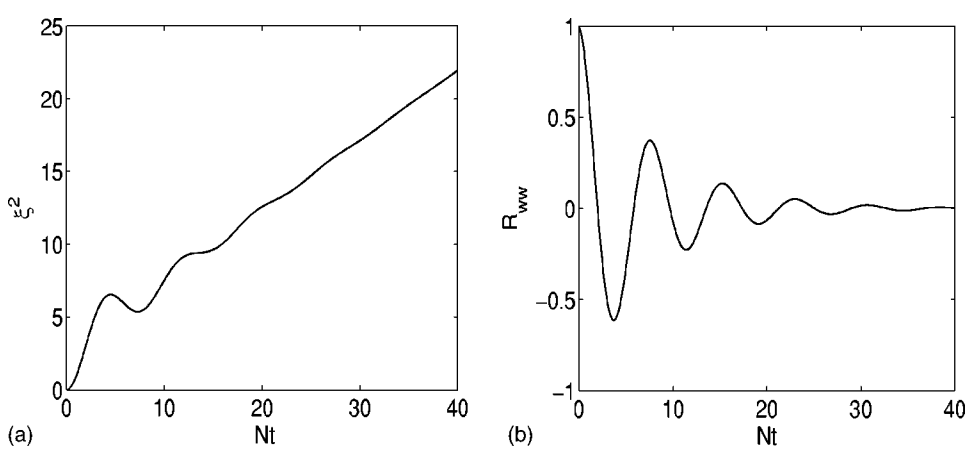

FIG. 6. (a) Normalized vertical dispersion length squared ξ^2 and (b) vertical autocorrelation R_{ww} vs normalized time Nt at critical Ri_g with $Sk/\epsilon=20.0$.

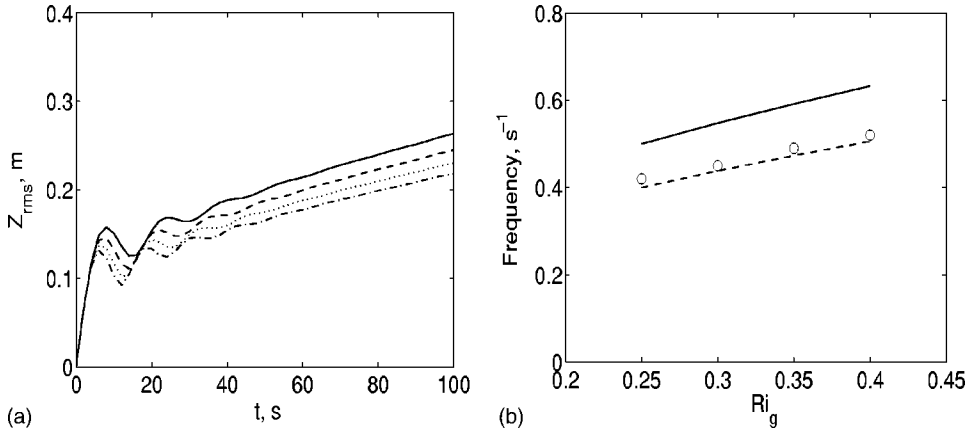

FIG. 7. (a) Vertical dispersion length $Z_{rms}(\equiv\sqrt{\overline{Z^2}})$ vs time t at different Ri_g. Lines: solid, $\mathrm{Ri}_g=0.25$; dash, $\mathrm{Ri}_g=0.30$; dot, $\mathrm{Ri}_g=0.35$; dash dot, $\mathrm{Ri}_g=0.40$. (b) Frequency of the internal gravity waves vs Ri_g. Symbol: ○, frequency from LSM. Lines: solid, N; dash, $0.8N$.

$$dw = -\frac{c_1}{2}\frac{\epsilon}{k}w\,dt + \frac{d\overline{w^2}}{dz}dt + (c_0\epsilon)^{1/2}d\mathcal{W}_w. \tag{25}$$

If we assume $2k/(c_1\epsilon)=T_L$ and $c_0=c_1\overline{w^2}/k$ then our w equation becomes exactly (24). Furthermore if the turbulence inhomogenity term is dropped then the LSM reverts back to Taylor's model.[1]

Pearson *et al.*[5] developed a model for horizontal mean flow with stably stratified, statistically stationary turbulence that consisted of equations for w and ρ' (fluctuating density). After converting to temperature from density their equations are given by

$$\begin{aligned} dw &= -2\phi N w\,dt + g\beta\theta\,dt + H(t)dt, \\ d\theta &= -\gamma N\theta dt - w\frac{d\Theta}{dz}dt, \end{aligned} \tag{26}$$

where ϕ and γ are constants and $H(t)$ is a stationary random function which represents the fluctuating pressure gradient. They claimed that $\gamma[\sim O(1)]$ was dependent on molecular mixing process and the constant ϕ (=0.8) set the angle of propagation of the radiated internal gravity waves. Different forms of the pressure gradient function were assumed in their work. Its representation as white noise is an assumption of a flat frequency spectrum. It is seen that their model contains only one time scale, the Brunt—Väisälä, or buoyancy frequency, in their deterministic terms. However the form of $H(t)$ can be chosen to contain the turbulence time scale in the random component.

Equation (14) is the present LSM for this case. Substituting T_L, T_L', and $c_{5\theta}$ gives

$$\begin{aligned} dw &= -\frac{w}{T_L}dt + \frac{2}{3}\beta g\theta dt + (c_0\epsilon)^{1/2}d\mathcal{W}_w, \\ d\theta &= -\frac{\theta}{T_L'}dt - w\frac{d\Theta}{dz}dt + c_\theta{}^{1/2}d\mathcal{W}_\theta. \end{aligned} \tag{27}$$

Unlike (26) a turbulence time scale T_L (or T_L') is explicitly present in the model. The analytical solution given in Eq. (23) shows the presence of the Brunt–Väisälä frequency as well. In turbulent dispersion problems in a stratified environment it is expected to have time scales both due to turbulence and buoyancy present in the solution.

The two time scales are related in the following way:

$$\begin{aligned} T_L &= \frac{c_1}{2}\frac{k}{\epsilon} = \frac{c_1}{2}\frac{S^*}{S} \quad \left(\text{where } \frac{Sk}{\epsilon} = S^*\right), \\ &= \frac{c_1}{2}S^*\frac{\mathrm{Ri}_g^{1/2}}{N} \quad \left(\text{since } \mathrm{Ri}_g = \frac{N^2}{S^2}\right). \end{aligned}$$

For stationary stratified turbulence S^* approaches a constant value of about 5.5. As mentioned before, many researchers have predicted the critical value of $\mathrm{Ri}_g=0.25$. So T_L (and

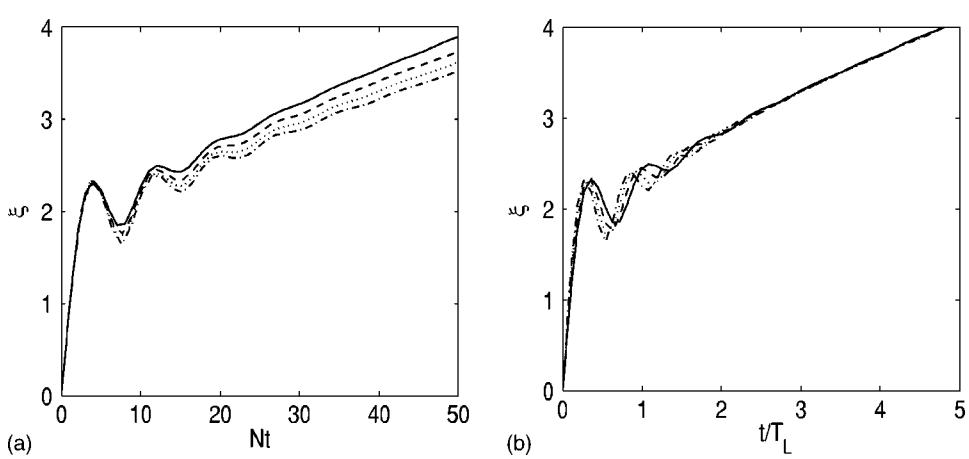

FIG. 8. (a) Normalized vertical dispersion length $\xi[\equiv\sqrt{\overline{Z^2}}N/\sqrt{\overline{w^2}}(0)]$ vs dimensionless time Nt at different Ri_g. (b) Normalized vertical dispersion length ξ vs dimensionless time t/T_L at different Ri_g. Lines: solid, $\mathrm{Ri}_g=0.25$; dash, $\mathrm{Ri}_g=0.30$; dot, $\mathrm{Ri}_g=0.35$; dash dot, $\mathrm{Ri}_g=0.40$.

similarly T_L') $\sim 1/N$ under critical conditions. Aside from this, the present model differs from the model of Pearson *et al.*[5]

VI. CONCLUSION

The main objective of the paper is to devise a method to obtain Lagrangian stochastic models for dispersion, given a SMC. The motive is that prediction of turbulent dispersion in atmospheric flows can be divorced from prediction of Eulerian statistics. Indeed, the latter are often prescribed as surface layer similarity profiles. Given the general, tensorally linear Reynolds stress model, the corresponding Lagrangian model is a set of stochastic differential equations reproducing it as their second moment.

A set of constants was proposed for the general linear model. They were selected to provide a simple form of LSM, while providing the correct critical Richardson number, and reasonable agreement to experimental and simulation data. The stochastic formulation also ensures realizability, although that is effected by constraints on the return to isotropy coefficients.

The model was illustrated by computations of homogeneous shear flow with varying degrees of stable stratification. Depending on the ratio of buoyancy to turbulence time scale, oscillatory dispersion can be observed. That might at first seem to be unphysical. A rationale is that particles released at a given height will move randomly, either upward, or downward. Those moving upward will experience negative buoyancy. At a later time, they will have a tendency to move downward. Hence the correlation function will oscillate: upward velocity tends to be correlated with downward velocity after one buoyancy time scale. The dispersion formula (17) connects the correlation function to the variance of dispersing particles. Oscillations of the correlation function translate into nonmonotonic dispersion.

Although the current model has been formulated following a very different approach its form has been shown to become very similar to other well known LSMs when one or more of various simplifying assumptions such as neutral conditions, turbulence homogenity, and absence of mean shear are applied. So this LSM is expected to give better results for more complex flows.

The proposed LSM has a strong physical and mathematical basis but further tests, especially for unstably stratified flow, are needed. Even for stably stratified flows further experiments are needed to test the model. One merit of the approach is that it inherits the empiricism of the second moment model.

ACKNOWLEDGMENTS

This work was funded by NASA Ames Research Center, with R. Miraflor being the contract monitor. S.K.D. would like to thank M. Ji for his helpful discussion on calibration of SMC models and also for providing his codes for doing the same.

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