

A Three-Dimensional Stochastic Model for Concentration Fluctuation Statistics in Isotropic Homogeneous Turbulence

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A three-dimensional model for prediction of concentration fluctuations in isotropic homogeneous turbulence is presented. The model is based on calculating the Lagrangian trajectories of a particle pair, taking into account the interaction between the particle velocities. The velocity correlation function at a given instant is taken as the Eulerian one. This correlation function is constrained to obey the continuity condition, due to the fluid incompressibility. The proposed model was used to study concentration fluctuations for three different sources: An uniform sphere, a plane source, and a line source. Results for the plane source differ from those predicted by the one-dimensional model. This difference may be attributed to the compressibility condition in the one-dimensional model (P. A. Durbin, *J. Fluid Mech.* **100**, No. 2, 279 (1980)). © 1988 Academic Press, Inc.

1. INTRODUCTION

The statistics of concentration fluctuations of a passive scalar in a turbulent medium is a problem of wide ranging interest with applicability to air quality modelling, smoke obscuration, chemical reactions, hazard estimation of toxic gases, and combustion problems.

The techniques to predict these fluctuations are divided into two classes. The first one includes all models based on the Eulerian approach, i.e., the diffusion and the flow field are looked at fixed points in space. Examples of such models are the gradient transfer approximation or higher order closure to the diffusion and the flow equations ([3, 18, 12], and others). In this approach the length scale of the turbulent field must be small compared with that of the contaminant cloud, a restriction which is not always satisfied. In addition, these models are based on unverified closure assumptions. The other class of techniques is the Lagrangian approach, based on assumptions concerning the Lagrangian statistics of the particles. In both approaches those assumptions cannot be verified directly, and the models are judged by their success in predicting a measured quantity. There are

many Lagrangian models that are able to predict the first moment of the concentration fluctuations ([19, 8] and others), some of them applicable to three-dimensional inhomogeneous turbulence [20]. On the other hand, there exist only one-dimensional models which are able to predict the second moment of concentration fluctuations, taking into account the interaction among the particles. These models are based on two approaches for estimating the relative velocity. The first approach [15, 13] is based on the assumption that the relative diffusion of a pair of particles is a function of the ensemble averaged mean square relative separation [1]. The assumption results in a Gaussian distribution for the relative separation of the pair of particles that causes the fluctuation intensity to decrease inversely proportional to the square root of time [16]. This result contradicts experimental features.

The other approach [14] relates the relative velocity of the particle pairs to their instantaneous separation. This assumption formulated in the one-dimensional model of Durbin [4], and in the authors' model [9], leads to a non-Gaussian distribution of the relative distances and thus results in a fluctuation intensity that tends asymptotically to a constant value as time increases.

In spite of the fact that one-dimensional models give valuable information on experimental features, one must be cautious in calculating statistical fluctuation concentrations. This care is required because one-dimensional models describe compressible flow, and the effects of this condition on the results cannot be isolated.

We found it interesting to formulate the Richardson assumption in a three-dimensional flow, constrained to be incompressible. In this way, we could verify the consequences of Durbin's model, that the Richardson assumption leads to concentration fluctuation intensity that depends on source size, but in contrast to Durbin's results, the fluctuation intensity calculated by our model, decreases slowly with time.

In Section 2, we describe the statistics of concentration fluctuations emphasizing the influence of compressibility of the flow. In Section 3, we formulate a three-dimensional model for the Lagrangian motion of particles in a turbulent field including the interaction among them. This model is constrained to describe incompressible flow. In this paper, we discuss only the case of homogeneous isotropic turbulence.

In Section 4, a numerical method for calculating concentration moments is described. Results of our calculations for special sources are represented in Section 5.

2. CONCENTRATION FLUCTUATIONS

2.1. *Definition at a Given Point*

We adopt the definition of concentration fluctuations suggested by Durbin [4]. According to this definition the concentration at a given point r at time t is given

by averaging the instantaneous concentration over a small volume V_η of order η around r , i.e.,

$$C(\mathbf{r}, t) = \frac{1}{V_\eta} \int_{V_\eta} \tilde{c}(\mathbf{r}', t) d^3r' \tag{2.1}$$

where $\tilde{c}(\mathbf{r}, t)$ is the instantaneous point concentration and η the Kolmogorov length scale. By taking the limit $V_\eta \rightarrow 0$ we mean that $(V_\eta/L^3) \rightarrow 0$, where L is the turbulent integral length scale. This definition takes into account smearing by molecular action and by finite measurement probe size. The concentration fluctuations are determined primarily by the dynamic of eddies in the subinertial range.

2.2. Statistics

The moments of concentration fluctuations can be calculated in terms of forward or reversed diffusion [16, 4, 6]. We define the N -particle probability function for the forward diffusion,

$$P_N(r_1, \dots, r_N, t; r'_1, \dots, r'_N, 0) d^3r'_1 \dots d^3r'_N$$

as the probability that N particles located at time $t=0$ at r'_1, \dots, r'_N will arrive at time t at locations r_1, \dots, r_N , respectively. The N -particle probability function for the reversed diffusion,

$$P_N(r'_1, \dots, r'_N, 0; r_1, \dots, r_N, t) d^3r'_1 \dots d^3r'_N$$

is defined as the probability that N particles which are located at r_1, \dots, r_N at time t came from locations r'_1, \dots, r'_N at time $t=0$. For incompressible flow, it was proved by Egbert and Baker [6] that

$$P_N(r_1, \dots, r_N, t; r'_1, \dots, r'_N, 0) = P_N(r'_1, \dots, r'_N, 0; r_1, \dots, r_N, t) \tag{2.2}$$

and that the N th moment of the concentration fluctuations is given by

$$\begin{aligned} \langle C^N(r, t) \rangle &= \lim_{r_1, \dots, r_N \rightarrow r} \iint \dots \int S(r') P_N(r_1, \dots, r_N, t; r'_1, \dots, r'_N, 0) d^3r'_1 \dots d^3r'_N \\ &= \lim_{r_1, \dots, r_N \rightarrow r} \iint \dots \int S(r') P_N(r'_1, \dots, r'_N, 0; r_1, \dots, r_N, t) d^3r'_1 \dots d^3r'_N \end{aligned} \tag{2.3}$$

where $S(r') = S(r'_1) \dots S(r'_N)$ is the source function.

It is more convenient to calculate the N th moment, using reversed diffusion. This can be done by Monte Carlo methods. One has to follow trajectories of N particles backward in time and to find their location r'_1, \dots, r'_N at time $t=0$. Then assign the

particles the concentration $S(r'_1), \dots, S(r'_N)$ correspondingly. If one repeats this procedure M times the integral in Eq. (2.3) is given by

$$\langle C^N(r, t) \rangle = \frac{1}{M} \sum_{k=1}^M S(r'_1)^{(k)} \dots S(r'_N)^{(k)} \quad (2.4)$$

where $r_i^{(k)}$ denotes the values of r_i in the k th realization. To solve the trajectories of the particles, one has to know their Lagrangian velocity equations, including the correlations between them. The particle trajectories are computed in reversed time, but because the turbulence is stationary, we did not reverse the evolution of the turbulence. In Section 3, our model assumption for the two-particle equations of motion are formulated and the procedure to calculate first and second moments of the concentration fluctuation distribution is described. The procedure of reversed diffusion is valid because of the incompressibility of the flow.

In compressible flow

$$P_N(r_1, \dots, r_N, t; r'_1, \dots, r'_N, 0) \neq P_N(r'_1, \dots, r'_N, 0; r_1, \dots, r_N, t);$$

therefore a different interpretation should be given to the integral

$$\lim_{r_1, r_2 \rightarrow r} \iint S(r'_1) S(r'_2) \cdot P_2(r_1, r_2, t; r'_1, r'_2, 0) d^3 r'_1 d^3 r'_2 \quad (2.5)$$

and to the integral

$$\lim_{r_1, r_2 \rightarrow r} \iint S(r'_1) S(r'_2) \cdot P_2(r'_1, r'_2, 0; r_1, r_2, t) d^3 r'_1 d^3 r'_2 \quad (2.6)$$

The first integral is the second moment of the concentration fluctuation distribution, while the concentration is defined as the number of contaminant particles per unit volume [6]. The second integral is the second moment of the mass-specific concentration fluctuations, while the mass-specific concentration is defined as the ratio of the number of contaminant particles to the number of fluid particles in unit volume [17]. The use of either the first definition for concentration or the second in compressible flow depends on the specific problem that one is investigating.

In Durbin's [4] one-dimensional model and its generalization to include molecular diffusivity [17], the flow field represented by the equation of motion of particles is compressible [6, 16]. Therefore the fluctuation intensity calculated by this model using the technique of reversed diffusion is for the mass-specific concentration. On the other hand, concentration fluctuations calculated using the forward diffusion technique in the one-dimensional model [9] includes contribution from compressible fluctuations. Therefore one should be careful in applying the results of both models to analyze the fluctuation statistics in incompressible flow.

The physical concepts formulated in Durbin's model and in its generalization [9] for the 1-D case can be generalized to the three-dimensional model constrained to fulfill the incompressibility condition. This is done in Section 3.

3. PARTICLE MOTION IN THE TURBULENT FIELD

3.1. Equation of Motion for the Particles

We assume that two particles move in a homogeneous isotropic three-dimensional incompressible turbulence field. The Lagrangian velocities of the particles v_1, v_2 are described by the equations

$$\begin{aligned}
 v_1(t + \Delta t) &= R_L(\Delta t) v_1(t) + \sqrt{1 - R_L^2(\Delta t)} \theta(r_1(t)), \\
 v_2(t + \Delta t) &= R_L(\Delta t) v_2(t) + \sqrt{1 - R_L^2(\Delta t)} \theta(r_2(t)), \\
 r_1(t + \Delta t) &= r_1(t) + v_1(t) \Delta t, \\
 r_2(t + \Delta t) &= r_2(t) + v_2(t) \Delta t, \\
 v_1(0) &= \theta(r_1(0)), \\
 v_2(0) &= \theta(r_2(0))
 \end{aligned} \tag{3.1}$$

where $R_L(\Delta t) = \exp(-\Delta t/T_L)$ is the Lagrangian-time correlation function and in stationary turbulence depends on the time lag Δt . $\theta(r)$ is a random field. For convenience, we shall omit the vector notation throughout this paper to avoid confusion. We assume that at a given instant the spatial correlation between the components of $\theta(r)$ is equal to the spatial Eulerian velocity correlation of the turbulence field. Therefore the covariance matrix C of the random field $\theta(r)$ is equal to the covariance matrix of the Eulerian field. We show in detail in Appendix B that the Lagrangian motion of fluid particles described in Eq. (3.1) is equivalent to the motion of fluid particles in an incompressible Eulerian velocity field in the subinertial range, i.e., where viscosity forces can be neglected. If we assume that the part of the Eulerian field which is not correlated in time is responsible for the random part of the particles' acceleration, it is reasonable to take the covariance of $\theta(r')$ to be equal to that of the Eulerian field. However, in our model this was taken as an assumption and has no theoretical rigorous justification, except that it is compatible with the Eulerian distribution function (see Appendix B).

Following Durbin [4] we define two variables,

$$\begin{aligned}
 A &= (r_1 - r_2)/\sqrt{2}, \\
 Y &= (r_1 + r_2)/\sqrt{2}
 \end{aligned} \tag{3.2}$$

where r_1, r_2 are the locations of the two particles, A is proportional to the relative distance between the particles, and Y is proportional to their center-of-mass

location. The constant of proportionality is chosen only for simplicity of the calculations.

The equations of motions for Δ and Y are

$$\begin{aligned} \frac{d\Delta}{dt}(t + \Delta t) &= R_L(\Delta t) \frac{d\Delta}{dt}(t) + \sqrt{1 - R_L^2(\Delta t)} [\theta(r_1(t)) - \theta(r_2(t))] / \sqrt{2}, \\ \frac{dY}{dt}(t + \Delta t) &= R_L(\Delta t) \frac{dY}{dt}(t) + \sqrt{1 - R_L^2(\Delta t)} [\theta(r_1(t)) + \theta(r_2(t))] / \sqrt{2}. \end{aligned} \quad (3.3)$$

In homogeneous turbulence, the covariance of the velocities at two different points depends only on the distance between those points. If we assume that $\theta(r)$ has a trinormal distribution function, the sum of $\theta(r_1)$ and $\theta(r_2)$ and their difference also have a trinormal distribution function with covariance that depends only on the relative distance between the particles. We have to specify the covariance matrix of the Eulerian field. The homogeneous isotropic turbulent field is easy to treat because the covariance tensor of the velocities $C(\Delta)$ is invariant to displacement or rotation of the coordinate system. Therefore [11], the correlation tensor has the form

$$C_{ij}(\Delta) = A(|\Delta|) \Delta_i \Delta_j + \delta_{ij} B(|\Delta|) \quad (3.4)$$

where $|\Delta| = (\Delta_1^2 + \Delta_2^2 + \Delta_3^2)^{0.5}$.

The incompressibility of the fluid yields another condition through the continuity equation:

$$\sum_j \frac{\partial}{\partial \Delta_j} C_{ij}(\Delta) = 0. \quad (3.5)$$

This implies that the whole covariance tensor is expressed in terms of a scalar function of r . This scalar function can be determined by the one-dimensional correlation function:

$$C(\Delta, 0, 0) = \sigma_v^2 f(|\Delta|) \quad (3.6)$$

where σ_v^2 is the velocity variance and f a 1-D function.

Using (3.4), (3.5), and (3.6), we get

$$C_{ij}(\Delta) = \sigma_v^2 \left[-0.5 \frac{\Delta_i \Delta_j}{|\Delta|} f'(|\Delta|) + \delta_{ij} (f(|\Delta|) + 0.5 |\Delta| f'(|\Delta|)) \right]. \quad (3.7)$$

This is the expression for the Eulerian covariance matrix of the points whose relative distance is Δ . Let us define

$$\begin{aligned} \Psi &= (\theta(r_1) - \theta(r_2)) / \sqrt{2}, \\ \Phi &= (\theta(r_1) + \theta(r_2)) / \sqrt{2}. \end{aligned} \quad (3.8)$$

Ψ is a random field with covariance matrix $\sigma_v^2 I - C$ and Φ is a random field with covariance matrix $\sigma_v^2 I + C$ where I is the unit matrix. Equation (3.8) and the expression for C (Eq. (3.7)) completely determine the two-particle motion in the field.

4. NUMERICAL PROCEDURE

4.1. Algorithm for Calculating Particle Trajectories

The numerical technique for the solution of Eq. (3.3) is divided into two steps. In the first stage, the relative distance Δ of the particle pair and its center-of-mass coordinate Y are changed, given their derivatives at time t :

$$\begin{aligned}\Delta(t + \Delta t) &= \Delta(t) + v_{\Delta}(t) \cdot \Delta t, \\ Y(t + \Delta t) &= Y(t) + v_c(t) \cdot \Delta t.\end{aligned}\tag{4.1}$$

Then the relative velocity v_{Δ} and the center-of-mass velocity v_c are determined according to the equations

$$\begin{aligned}v_{\Delta}(t + \Delta t) &= v_{\Delta}(t) \exp(-\Delta t/T_L) + \sqrt{1 - \exp(-2\Delta t/T_L)} \Psi, \\ v_c(t + \Delta t) &= v_c(t) \exp(-\Delta t/T_L) + \sqrt{1 - \exp(-2\Delta t/T_L)} \Phi\end{aligned}\tag{4.2}$$

where Ψ and Φ are random vectors, the components of which are normally distributed with covariance which depends on Δ , and defined by (3.7). The procedure to generate those random vectors is given in Appendix A. The main steps of the algorithm at a given time t are therefore:

- (1) Calculate the matrix C_{ij} according to (3.7).
- (2) Calculate the matrices λ_{ϕ} , λ_{ψ} , Eq. (A.5).
- (3) Draw ζ_1 , ζ_2 , two random vectors with independent random components, each of which is normally distributed with zero mean and variance 1.
- (4) Calculate Ψ and Φ according to Eq. (A.6).
- (5) Calculate v_{Δ} , v_c according to Eq. (4.2).
- (6) Calculate $\Delta(t + \Delta t)$, $Y(t + \Delta t)$ according to Eq. (4.1).

4.2. Calculation of Concentration Moments

For calculating concentration moments, we have used the process of reversed diffusion [2] in the same way it is used in Durbin's [4] model. We solve for the initial position of the particles r_1 , r_2 given their position at time t , where they nearly coincide. r_1 and r_2 are given in terms of Δ and Y :

$$\begin{aligned}r_1 &= (Y + \Delta)/\sqrt{2} \\ r_2 &= (Y - \Delta)/\sqrt{2}.\end{aligned}\tag{4.3}$$

To particle 1 we assigned the concentration $C_1(r, t) = S(r_1)$ and to particle 2 the concentration $C_2(r, t) = S(r_2)$ where $S(r)$ represents the initial source distribution. The moments of the concentration (see [4]) are given by

$$\bar{C}_i = \frac{1}{M} \sum_{n=1}^M C_{in}, \quad i = 1, 2, \quad (4.4)$$

$$\bar{C} = (\bar{C}_1 + \bar{C}_2)/2,$$

$$\overline{C^2} = \frac{1}{M} \sum_{n=1}^M C_{1n} C_{2n}, \quad (4.5)$$

$$C_v = (\overline{C^2} - \bar{C}_1 \bar{C}_2) / (\bar{C}_1 \bar{C}_2).$$

C_v represents the fluctuation intensities, and C_{in} is the value of $C_i(r, t)$ in the n th realization.

4.3. Numerical Values of the Parameters

The values chosen for the parameters in this work are the Lagrangian time scale $T_L = 1$ (sec), the Eulerian length scale $L_E = 1$ (m), and the Eulerian velocity standard deviation $\sigma_v = 0.6$ (m/sec). These values are connected by the nondimensional equation

$$L_E \sigma_v / T_L = 0.6$$

(see [8, 9]). The value of Δt is chosen as

$$\Delta t = 0.05 T_L.$$

The number of realizations $M = 100,000$. $f(|A|)$ is the one-dimensional correlation function which appears in Eq. (3.7), and was chosen to be the same as in the one-dimensional model of Durbin [4]:

$$f(|A|) = 1 - (|A|^2 / (|A|^2 + L_E^2))^{1/3} \quad (4.6)$$

5. RESULTS AND DISCUSSIONS

Averaged concentration and fluctuation intensity of concentration fluctuations were calculated using the numerical technique described in Section 4. These quantities were calculated for three different sources: a three-dimensional Gaussian source with standard deviation σ_0 , an infinite line source with cross section of a bi-Gaussian shape, and a plane source with a Gaussian shape with standard deviation σ_0 . Different values were chosen for σ_0 : $0.7L_E$, $0.35L_E$, $0.17L_E$, and $0.08L_E$, where L_E is the Eulerian length scale of the velocity fluctuation field. In Fig. 1, we represent the averaged concentration at point $(0, 0, 0)$ as a function of time. The one-particle probability function described in our model is calculated

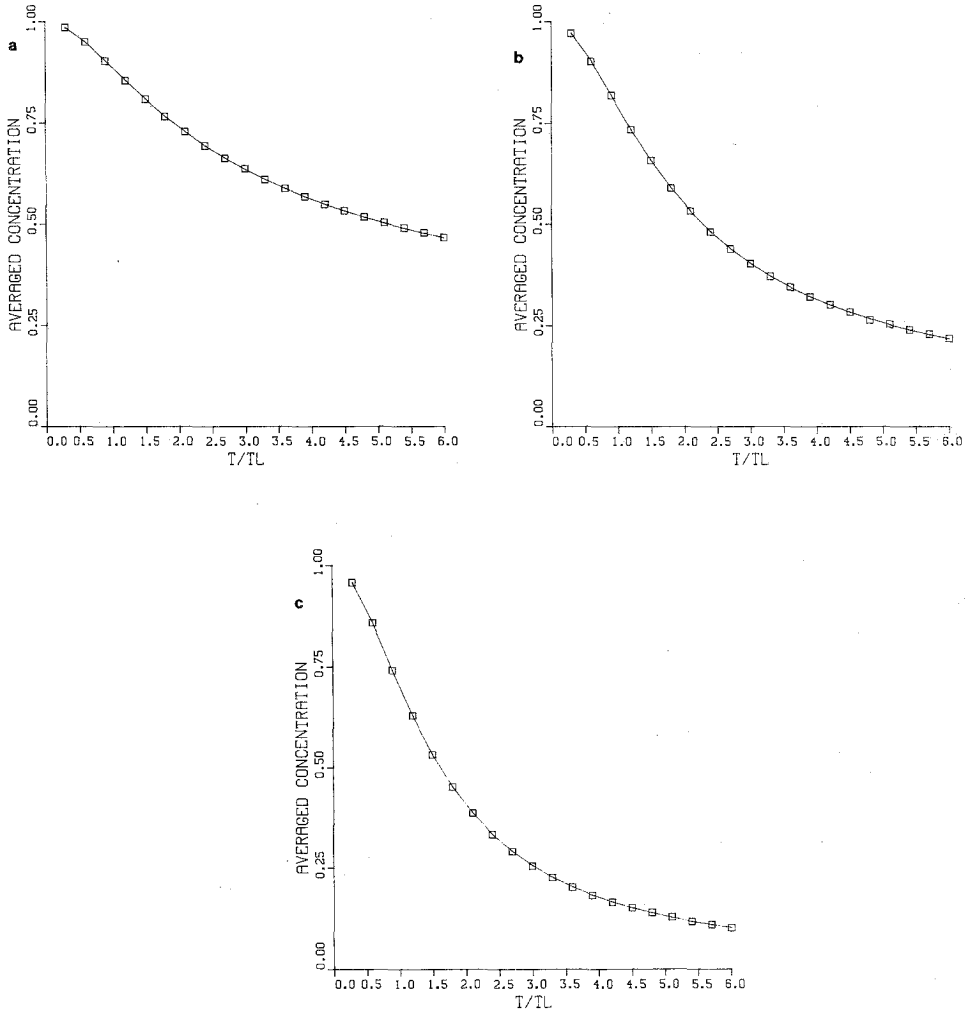


FIG. 1. The average concentration at the source center as a function of time: (a) for plane source; (b) for line source; (c) for sphere source. Theoretical predictions are denoted by lines, simulated values are denoted by □ ($\sigma_0 = 0.7L_E$).

using the trajectories of one particle. Equations (3.3) and (3.7) show that each component of the velocity field is a Uhlenbeck–Ornstein process, independent of the other component. Therefore, the one-particle probability density function $\phi_1(000, xyz)$ [22] is given by

$$\phi_1(000, xyz) = \exp(-(x^2 + y^2 + z^2)/(2\sigma_{v_p}^2(t)))/((\sqrt{2\pi})^3 \sigma_{v_p}^3(t)) \quad (5.1)$$

where

$$\sigma_{v_p}(t) = \sqrt{2\sigma_v T_L} (\exp(-t/T_L) + t/T_L - 1)^{1/2}$$

where σ_{v_p} is the standard deviation of ϕ_1 .

The averaged concentrations for the three sources are easily calculated, and are given by

$$\begin{aligned} C_{\text{plane}} &= \exp(-0.5x^2/(\sigma_0^2 + \sigma_{v_p}^2)) / \sqrt{2\pi(\sigma_0^2 + \sigma_{v_p}^2)}, \\ C_{\text{line}} &= \exp(-0.5(x^2 + y^2)/(\sigma_0^2 + \sigma_{v_p}^2)) / [\sqrt{2\pi(\sigma_0^2 + \sigma_{v_p}^2)}], \\ C_{\text{sphere}} &= \exp(-0.5(x^2 + y^2 + z^2)/(\sigma_0^2 + \sigma_{v_p}^2)) / [\sqrt{2\pi(\sigma_0^2 + \sigma_{v_p}^2)}]^{3/2}. \end{aligned} \tag{5.2}$$

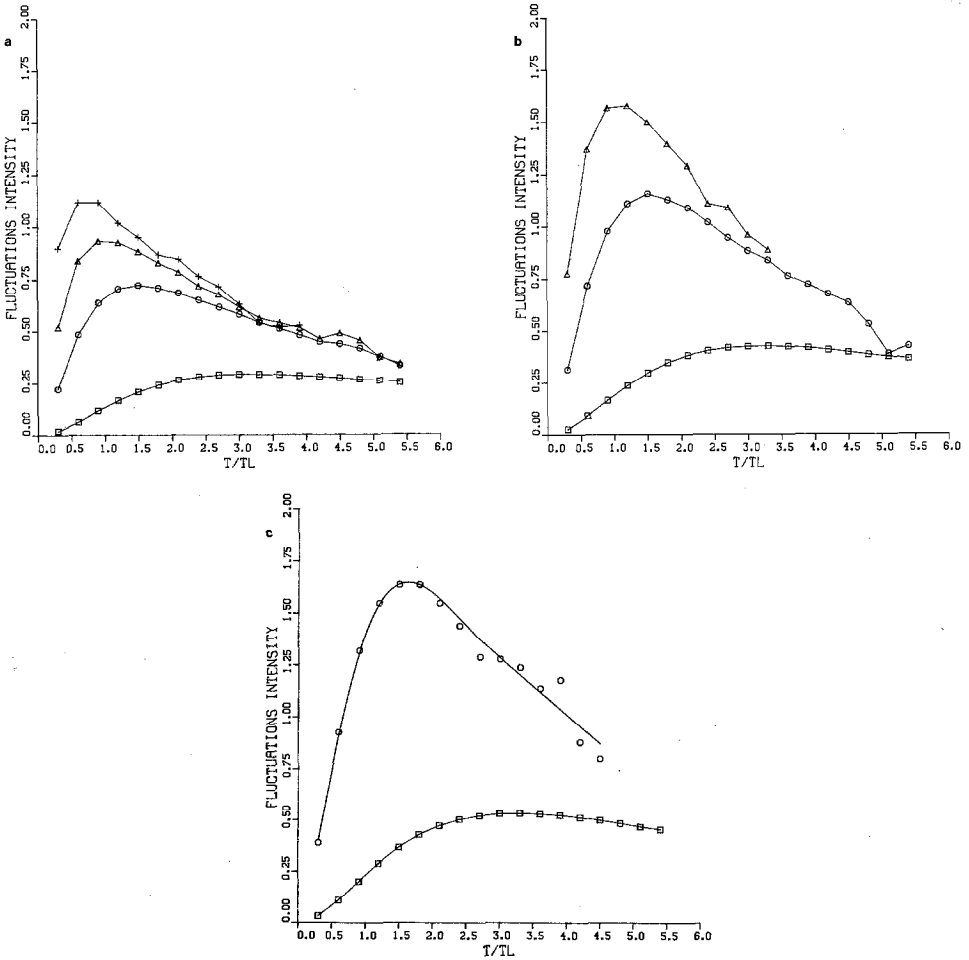


FIG. 2. Fluctuation intensity σ_0/C at point (0,0,0) as a function of time: (a) For plane source: □, $\sigma_0/L_E = 0.7$; ○, $\sigma_0/L_E = 0.35$; △, $\sigma_0/L_E = 0.17$; +, $\sigma_0/L_E = 0.08$. (b) For line source: □, $\sigma_0/L_E = 0.7$; ○, $\sigma_0/L_E = 0.35$; △, $\sigma_0/L_E = 0.17$. (c) For sphere source: □, $\sigma_0/L_E = 0.7$; ○, $\sigma_0/L_E = 0.35$.

In Fig. 1, we compare the theoretical predictions with the simulated value at the source center. The theoretical predictions are denoted by lines and the simulated values are denoted by squares.

In Fig. 2 results for the fluctuation intensity σ_c/C at point $(0, 0, 0)$ are presented as functions of time. In contrast to the one-dimensional case [4], our results show that the fluctuation intensity decreases with time. This decreasing is very slow, as time tends to infinity. Dependence of fluctuation intensity on the source size was found in our results, only up to $t = 3T_L$ for the case of plane source and the line source. Then the cloud forgets its initial dimensions and the behaviour of the fluctuation intensity is about the same for the four source sizes. In the case of the sphere source, there is dependence of the fluctuations on the source size, even for t larger than $4.5T_L$. Our model was also compared with wind tunnel experiments performed by Warhaft [21]. Remarkable agreement was found between calculated and measured values of the fluctuation intensity as a function of time [10].

In order to show that this behaviour of fluctuation intensity is a result of the incompressibility of the flow, we ran our model for the 1-D case. The equations of motion for this case are

$$\begin{aligned} \frac{d\Delta}{dt}(t + \Delta t) &= \exp(-\Delta t/T_L) \frac{d\Delta}{dt}(t) + \sqrt{1 - \exp(-2 \Delta t/T_L)} \sqrt{1 - R(\Delta)} \xi, \\ \frac{dY}{dt}(t + \Delta t) &= \exp(-\Delta t/T_L) \frac{dY}{dt}(t) + \sqrt{1 - \exp(-2 \Delta t/T_L)} \sqrt{1 + R(\Delta)} \xi \end{aligned} \tag{5.3}$$

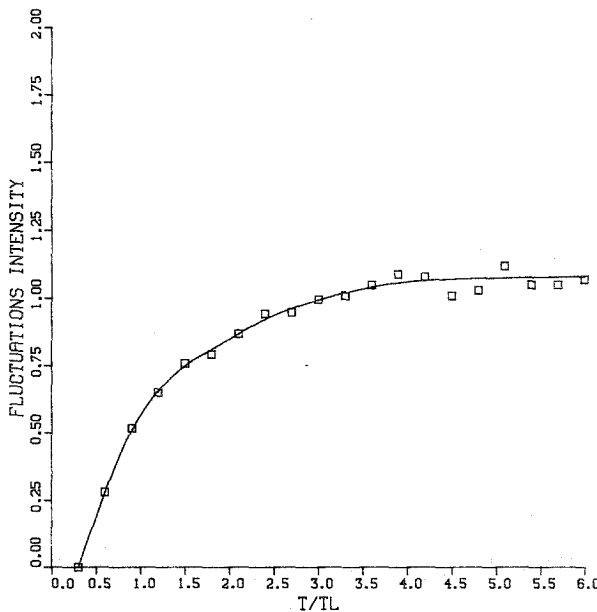


FIG. 3. Fluctuation intensity σ_c/C at the source center as function of time for the 1-D mode (Eq. (5.3)).

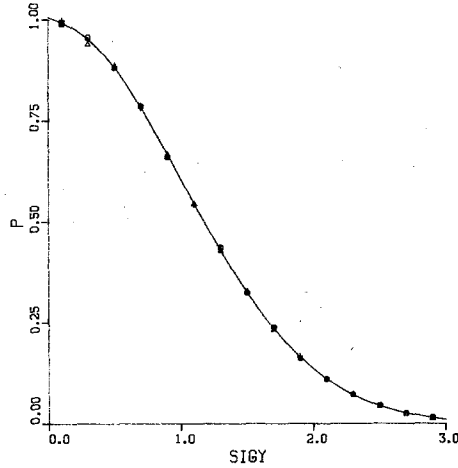


FIG. 4. Distribution of the center-of-mass location as a function of time. The center-of-mass variable Y is scaled by $\sigma_v(t)$ given in formula (5.1). —, Gaussian shape; \square , at time $t/T_L = 0.3$; \circ , at time $t/T_L = 3$; \triangle , at time $t/T_L = 6$.

where $R(\Delta)$ is the Eulerian correlation used by Durbin [4], and given in Eq. (4.6) and ξ is a random variable normally distributed with zero mean and standard deviation σ_v . These equations are different from Durbin's equations [4].

Results of our calculations for the 1-D model are presented in Fig. 3; it is also found in our model that the fluctuation intensity tends to a constant value as time increases. We claim that this behavior is a result of the compressibility of the 1-D model.

In Fig. 4, we represent the distribution of the center-of-mass variable (in the 3-D case) as a function of time (Y is scaled by $\sigma_{v_p}(t)$ given in formula (4.6)). The full line is Gaussian and the points are Monte Carlo results for different time values. We see that the dependency of Y on Δ is very weak and the Gaussian distribution is a very good approximation for the distribution of Y .

6. SUMMARY

In this work, we represent a three-dimensional model for prediction of concentration fluctuations in isotropic homogeneous turbulence. The velocity field is constrained to obey the continuity equation, due to the fluid incompressibility. Results show that this constraint is very important in coupling the three components of the velocity field. Therefore, even problems of one-dimensional symmetry like diffusion of an infinite plane source cannot be solved following only one component of the velocity field (see, e.g., Durbin [4] and Sawford and Hunt [17]).

Our results show that for small sources, fluctuation intensity depends on source size, up to $t = 6T_L$.

Our theory can be expanded to the inhomogeneous case, but the main problem is to specify the three-dimensional Eulerian correlation in space.

APPENDIX A: PROCEDURE FOR GENERATING THE RANDOM VECTORS Ψ, Φ

A.1. *A Procedure for Generating a Tri-Gaussian Normally Distributed Variable with a Given Covariance Matrix C_{ij}*

Since C_{ij} is symmetric, a unitary matrix U exists ($U^T U = I$), such that $U^T C U$ is diagonal, i.e.,

$$U^T C U = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \tag{A.1}$$

where $\lambda_1, \lambda_2, \lambda_3$ are the eigenvalues of C_{ij} and the columns of U are the corresponding eigenvectors.

Let $\zeta_1, \zeta_2, \zeta_3$ be three independent random variables, each of which is normally distributed with zero mean and variances $\lambda_1, \lambda_2, \lambda_3$, respectively. We define

$$x = U \cdot \zeta, \quad \zeta = (\zeta_1, \zeta_2, \zeta_3). \tag{A.2}$$

Being a linear combination of normally distributed variables, x is also normally distributed and its covariance matrix is given by

$$\begin{aligned} \langle x_i x_j \rangle &= \left\langle \sum_{kk'} U_{ij}^T \zeta_k U_{jk'} \zeta_{k'} \right\rangle \\ &= \sum_{kk'} U_{ik}^T U_{jk'} \langle \zeta_k \zeta_{k'} \rangle = \sum_k U_{ik}^T U_{jk} \lambda_k = C_{ij}. \end{aligned} \tag{A.3}$$

Therefore x has the desired properties.

A.2. *The Unitary Matrix That Diagonalizes the Covariance Matrix C_{ij} (Eq. 3.7)*

The covariance matrix described in Eq. (3.7) can be split into a sum of two matrices. A scalar matrix

$$\sigma_v^2 [f(|\Delta|) + 0.5 |\Delta| f'(|\Delta|)] I$$

and a matrix whose elements are given by

$$0.5 f'(|\Delta|) \sigma_v^2 \Delta_i \Delta_j / |\Delta|.$$

Therefore, the unitary matrix that diagonalizes $\Delta_i \Delta_j$ will also diagonalize C_{ij} . The matrix $\Delta_i \Delta_j$ has a double zero eigenvalue and a single eigenvalue $|\Delta|^2$. The unitary

matrix U which diagonalizes $A_i A_j$, is the matrix that rotates the coordinate system in such a way that one of the principal axes is aligned along the vector A . This matrix is not unique, and one of the choices which we have used in our procedure is

$$U = \begin{bmatrix} -A_2/\tilde{A} & A_1 A_3/(\tilde{A} |A|) & A_1/|A| \\ A_1/\tilde{A} & A_2 A_3/(\tilde{A} |A|) & A_2/|A| \\ 0 & -\tilde{A}/|A| & A_3/|A| \end{bmatrix} \quad (\text{A.4})$$

where $\tilde{A} = (A_1 + A_2)^{0.5}$. For $A \rightarrow 0$, $U \rightarrow I$.

It can be easily seen that the matrix C_{ij} will therefore have a double eigenvalue $\sigma_v^2(f(|A|) + 0.5 |A| f'(|A|))$ and a single eigenvalue $\sigma_v^2 f(|A|)$.

A.3. Calculation of the Random Variables Φ and Ψ (Eq. (3.8))

The two random variables Ψ and Φ (Eq. (3.8)) have covariances $\sigma_v^2 \delta_{ij} - C_{ij}$ and $\sigma_v^2 \delta_{ij} + C_{ij}$, respectively. Therefore their covariance matrix is diagonalized by the unitary transformation U given in (A.4), and its eigenvalues are given by

$$\begin{aligned} \lambda_{\Psi}^{(1)} &= \lambda_{\Psi}^{(2)} = (1 - f(|A|) - 0.5 |A| f'(|A|)) \sigma_v^2, \\ \lambda_{\Psi}^{(3)} &= (1 - f(|A|)) \sigma_v^2, \\ \lambda_{\Phi}^{(1)} &= \lambda_{\Phi}^{(2)} = (1 + f(|A|) + 0.5 |A| f'(|A|)) \sigma_v^2, \\ \lambda_{\Phi}^{(3)} &= (1 + f(|A|)) \sigma_v^2. \end{aligned} \quad (\text{A.5})$$

Given those eigenvalues, the procedure to calculate Ψ and Φ as described in (A.1) is as follows: We draw ζ_1, ζ_2 , two random vectors with independent components, each of which is normally distributed with zero mean and variance 1:

$$\begin{aligned} \Psi &= U(A) \sqrt{\lambda_{\Psi}(A)} \zeta_1, \\ \Phi &= U(A) \sqrt{\lambda_{\Phi}(A)} \zeta_2 \end{aligned} \quad (\text{A.6})$$

where

$$\begin{aligned} \sqrt{\lambda_{\Psi}} &= \begin{bmatrix} \sqrt{\lambda_{\Psi}^{(1)}} & 0 & 0 \\ 0 & \sqrt{\lambda_{\Psi}^{(2)}} & 0 \\ 0 & 0 & \sqrt{\lambda_{\Psi}^{(3)}} \end{bmatrix}, \\ \sqrt{\lambda_{\Phi}} &= \begin{bmatrix} \sqrt{\lambda_{\Phi}^{(1)}} & 0 & 0 \\ 0 & \sqrt{\lambda_{\Phi}^{(2)}} & 0 \\ 0 & 0 & \sqrt{\lambda_{\Phi}^{(3)}} \end{bmatrix}. \end{aligned} \quad (\text{A.7})$$

APPENDIX B: INCOMPRESSIBILITY OF THE VELOCITY FIELD DEFINED IN (3.1)

We shall prove that (3.1) describes the Lagrangian motion of particles in an incompressible Eulerian field by two stages.

First we shall show that any Eulerian distribution of velocities with zero first-order moments and second moments $C_{\alpha\beta} = (r_l - r_m)$ satisfying

$$\sum_{\alpha=1}^3 \frac{\partial}{\partial A_{lm}^\alpha} C^{\alpha\beta}(A_{lm}) = 0, \tag{B.1}$$

$$A_{lm} = r_l - r_m = (r_l^1 - r_m^1, r_l^2 - r_m^2, r_l^3 - r_m^3),$$

describes incompressible flow (Lemma 1). Then we shall show that the Lagrangian process Eq. (3.1) describes an Eulerian distribution function with $C^{\alpha\beta}(r_l - r_m)$ which fulfills Eq. (B.1).

LEMMA 1. *We have to show*

$$\nabla^{(k)}\theta(r) = 0 \tag{B.2}$$

at any point r , for each realization k of the field.

Proof. Suppose (B.1) is not true; then for some r_l and some k

$$a^{(k)}(r_l) \equiv \nabla \cdot \theta^{(k)}(r_l) \neq 0. \tag{B.3}$$

If we multiply (B.3) by $\theta^{\beta(k)}(r_m)$ and take ensemble averages, we obtain after some algebra:

$$\frac{1}{k} \sum_{j=1}^k a^{(j)}(r_l) \cdot \theta^{\beta(j)}(r_m) = \sum_{\alpha} \frac{\partial}{\partial r_l^\alpha} C^{\alpha\beta}(A_{lm}) \equiv 0. \tag{B.4}$$

Taking the divergence of (B.4), we get

$$\frac{1}{k} \sum_{j=1}^k a^{(j)}(r_l) \nabla \cdot \theta^{(j)}(r_m) = \frac{1}{k} \sum_{j=1}^k a^{(j)}(r_l) a^{(j)}(r_m) = 0 \tag{B.5}$$

due to the continuity of the velocity and its derivatives; it follows (for $r_m \rightarrow r_l$) that

$$\frac{1}{k} \sum_{j=1}^k [a^{(j)}(r_l)]^2 = 0. \tag{B.6}$$

This contradicts (B.3) and then (B.1) is true.

LEMMA 2. *The Lagrangian process (3.1) is compatible with the Eulerian distribution function in the subinertial range.*

Proof. Assuming that the process (3.1) describes the Lagrangian motion of fluid particles, let us denote the distribution of fluid particles in phase space at time t by $g_t(\mathbf{r}_1 \cdots \mathbf{r}_n, v_1 \cdots v_n)$. We would like to show that if at $t=0$

$$g_t(\mathbf{r}_1 \cdots \mathbf{r}_n, \mathbf{v}_1 \cdots \mathbf{v}_n) = g_E(\mathbf{r}_1 \cdots \mathbf{r}_n, \mathbf{v}_1 \cdots \mathbf{v}_n)$$

where g_E is the Eulerian distribution function, then the covariance of g_t is equal to that of g_E at any time. We shall use the following properties of g_E :

(a) All its first moments are zero:

$$\mu'_\alpha(\mathbf{r}_i) = 0 \quad \forall i, \alpha. \quad (\text{B.7})$$

This is due to the definition of the fluctuating part of velocities as the deviation from the average,

$$(b) \quad \mu^2_{\alpha\beta}(r_i, r_k) = C^{\alpha\beta}(r_i - r_k) \quad (\text{B.8})$$

where $C^{\alpha\beta}(r_i - r_k)$ is a tensor which satisfies (B.1). This is due to homogeneity and incompressibility of the flow.

$$(c) \quad \frac{\partial C^{\alpha\beta}(\Delta_{kl})}{\partial t} = T^{\alpha\beta}(\Delta_{kl}) + 2\nu C^{\alpha\beta}(\Delta_{kl}) \quad (\text{B.9})$$

where ν is the fluid viscosity and

$$T^{\alpha\beta}(\Delta_{kl}) = \sum_\varepsilon \frac{\partial}{\partial \Delta_{kl}^\varepsilon} (\mu^3_{k'l\varepsilon} + \mu^3_{k'l\varepsilon})$$

(see Batchelor [1, pp. 86, 100]).

In the subinertial range where the third term in (B.9) can be neglected, we get

$$\frac{\partial C^{\alpha\beta}(\Delta_{kl})}{\partial t} = \sum_\varepsilon \frac{\partial}{\partial \Delta_{kl}^\varepsilon} (\mu^3_{k'l\varepsilon} + \mu^3_{k'l\varepsilon}). \quad (\text{B.10})$$

In stationary turbulence the right-hand side of (B.10) is zero.¹

(d) For any $k \neq l \neq m$,

$$\sum_\varepsilon \frac{\partial}{\partial r_m^\varepsilon} \mu^3_{k'l\varepsilon} = 0. \quad (\text{B.11})$$

The proof is done by mathematical induction.

¹ For the Eulerian field, we made the somewhat unrealistic assumption of a homogeneous stationary isotropic turbulence.

Assume that at time t , g_t fulfills conditions (B.8), (B.9), and

$$\sum_{\varepsilon} \frac{\partial}{\partial \Delta_{kl}^{\varepsilon}} (\mu_{klk}^{3\alpha\beta\varepsilon} + \mu_{kll}^{3\alpha\beta\varepsilon}) = O(\Delta t). \tag{B.12}$$

Then at any time g_t fulfills these conditions.

We split the time evolution of particles in phase space into two steps. In the first step, the locations of particles are changed according to

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i. \tag{B.13}$$

The new distribution of particles in phase space after this step is $g'(\mathbf{r}_1 \cdots \mathbf{r}_N, \mathbf{v}_1 \cdots \mathbf{v}_N)$. To first order in Δt the relation between g_t and g' is given by

$$g'(\mathbf{r}_1 \cdots \mathbf{r}_N; \mathbf{v}_1 \cdots \mathbf{v}_N) = g_t(\mathbf{r}_1 \cdots \mathbf{r}_N; \mathbf{v}_1 \cdots \mathbf{v}_N) - \Delta t \sum_{k=1}^N \sum_{\alpha=1}^3 v_k^{\alpha} \frac{\partial g_t}{\partial r_k^{\alpha}}. \tag{B.14}$$

Let us define the moments generating function by

$$\hat{g}(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) = \int g(\mathbf{r}_1 \cdots \mathbf{r}_N; \mathbf{v}_1 \cdots \mathbf{v}_N) \exp \left[\sum_{k=1}^N (\boldsymbol{\theta}_k \cdot \mathbf{v}_k) \right] d^3v_1 \cdots d^3v_N. \tag{B.15}$$

It follows from (B.13) that

$$\hat{g}'(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) = \hat{g}_t(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) - \Delta t \sum_{k=1}^N \sum_{\alpha=1}^3 \frac{\partial^2 \hat{g}_t}{\partial r_k^{\alpha} \partial \theta_k^{\alpha}}. \tag{B.16}$$

In the second step, we change the velocities of particles according to

$$\mathbf{v}_i(t + \Delta t) = \left(1 - \frac{\Delta t}{T_L} \right) \mathbf{v}_i(t) + \sqrt{\frac{2 \Delta t}{T_L}} \boldsymbol{\theta}(\mathbf{r}_i(t + \Delta t)). \tag{B.17}$$

Since the moment-generating function of a sum of independent random variables is equal to the product of the moment-generating function of each variable, we obtain, to first order in Δt ,

$$\begin{aligned} \hat{g}_{t+\Delta t}(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) &= \hat{g}' \left(\mathbf{r}_1 \cdots \mathbf{r}_N; \left(1 - \frac{\Delta t}{T_L} \right) \boldsymbol{\theta}_1 \cdots \left(1 - \frac{\Delta t}{T_L} \right) \boldsymbol{\theta}_N \right) \\ &\quad \cdot \hat{f}(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) \end{aligned} \tag{B.18}$$

where \hat{f} is the moment-generating function of $\sqrt{2 \Delta t / T_L} \boldsymbol{\theta}(\mathbf{r})$. Using (B.16), we finally obtain

$$\hat{g}_{t+\Delta t}(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) = \hat{F}(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) \cdot \hat{f}(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) \tag{B.19}$$

where

$$\begin{aligned} \hat{F}(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) &= \hat{g}_t(\mathbf{r}_1 \cdots \mathbf{r}_N; \boldsymbol{\theta}_1 \cdots \boldsymbol{\theta}_N) - \Delta t \sum_{k=1}^N \sum_{\alpha=1}^3 \frac{\partial^2 \hat{g}_t}{\partial r_k^\alpha \partial \theta_k^\alpha} \\ &\quad - \frac{\Delta t}{T_L} \sum_{k=1}^N \sum_{\alpha=1}^3 \theta_k^\alpha \frac{\partial \hat{g}_t}{\partial \theta_k^\alpha}. \end{aligned} \quad (\text{B.20})$$

The moments of \hat{F} are given by

$$\begin{aligned} \mu_{l'}^{1\beta} &= \left. \frac{\partial \hat{F}}{\partial \theta_{l'}^\beta} \right|_{\boldsymbol{\theta}=0} = \left. \frac{\partial \hat{g}_t}{\partial \theta_{l'}^\beta} \right|_{\boldsymbol{\theta}=0} - \Delta t \sum_{k=1}^N \sum_{\alpha=1}^3 \left. \frac{\partial^3 \hat{g}_t}{\partial r_k^\alpha \partial \theta_{l'}^\beta \partial \theta_k^\alpha} \right|_{\boldsymbol{\theta}=0} \\ &\quad - \frac{\Delta t}{T_L} \sum_{k=1}^N \sum_{\alpha=1}^3 \theta_k^\alpha \left. \frac{\partial^2 \hat{g}_t}{\partial \theta_{l'}^\beta \partial \theta_k^\alpha} \right|_{\boldsymbol{\theta}=0} - \frac{\Delta t}{T_L} \left. \frac{\partial \hat{g}_t}{\partial \theta_{l'}^\beta} \right|_{\boldsymbol{\theta}=0}. \end{aligned} \quad (\text{B.21})$$

The first and fourth terms are zero because the first moment of g_t is zero. The third term is zero substituting $\boldsymbol{\theta}=0$. The second term is zero by the induction assumption that at time t , g_t fulfills conditions (B.1).

$$\begin{aligned} \mu_{lm}^{2\gamma\beta} &= \left. \frac{\partial^2 \hat{F}}{\partial \theta_m^\gamma \partial \theta_{l'}^\beta} \right|_{\boldsymbol{\theta}=0} = \left. \frac{\partial^2 \hat{g}_t}{\partial \theta_m^\gamma \partial \theta_{l'}^\beta} \right|_{\boldsymbol{\theta}=0} - \Delta t \sum_{k=1}^N \sum_{\alpha=1}^3 \left. \frac{\partial}{\partial r_k^\alpha} \frac{\partial^3 \hat{g}_t}{\partial \theta_m^\gamma \partial \theta_{l'}^\beta \partial \theta_k^\alpha} \right|_{\boldsymbol{\theta}=0} \\ &\quad - \frac{\Delta t}{T_L} \sum_{k=1}^N \sum_{\alpha=1}^3 \theta_k^\alpha \left. \frac{\partial^3 \hat{g}_t}{\partial \theta_m^\gamma \partial \theta_{l'}^\beta \partial \theta_k^\alpha} \right|_{\boldsymbol{\theta}=0} - \frac{2 \Delta t}{T_L} \left. \frac{\partial^2 \hat{g}_t}{\partial \theta_{l'}^\beta \partial \theta_m^\gamma} \right|_{\boldsymbol{\theta}=0}. \end{aligned} \quad (\text{B.22})$$

Using the properties of g_t we get, to first order in Δt ,

$$\mu_{lm}^{(2)\gamma\beta} = \left(1 - \frac{2 \Delta t}{T_L} \right) C^{\alpha\beta}(\Delta_{lm}), \quad (\text{B.23})$$

$$\begin{aligned} \mu_{nml}^{(3)\delta\gamma\beta} &= \left(1 - \frac{2 \Delta t}{T_L} \right) \left. \frac{\partial^3 \hat{g}_t}{\partial \theta_n^\delta \partial \theta_m^\gamma \partial \theta_{l'}^\beta} \right|_{\boldsymbol{\theta}=0} - \Delta t \sum_{k=1}^N \sum_{\alpha=1}^3 \left. \frac{\partial}{\partial r_k^\alpha} \frac{\partial^4 \hat{g}_t}{\partial \theta_n^\delta \partial \theta_m^\gamma \partial \theta_{l'}^\beta \partial \theta_k^\alpha} \right|_{\boldsymbol{\theta}=0} \\ &\quad - \frac{\Delta t}{T_L} \left. \frac{\partial^3 \hat{g}_t}{\partial \theta_m^\gamma \partial \theta_{l'}^\beta \partial \theta_n^\delta} \right|_{\boldsymbol{\theta}=0} - \frac{\Delta t}{T_L} \sum_{k=1}^N \sum_{\alpha=1}^3 \theta_k^\alpha \left. \frac{\partial^4 \hat{g}_t}{\partial \theta_n^\delta \partial \theta_m^\gamma \partial \theta_{l'}^\beta \partial \theta_k^\alpha} \right|_{\boldsymbol{\theta}=0}. \end{aligned} \quad (\text{B.24})$$

Equation (B.24) proves that (B.12) is satisfied.

The moment-generating function \hat{g} of $g_{t+\Delta t}$ is a product of \hat{F} and \hat{f} . Therefore $g_{t+\Delta t}$ is the distribution of the sum of two independent random variables. Its covariance satisfies

$$\left(1 - \frac{2 \Delta t}{T_L} \right) C^{\alpha\beta}(\Delta_{lm}) + \frac{2 \Delta t}{T_L} C^{\alpha\beta}(\Delta_{lm}) = C^{\alpha\beta}(\Delta_{lm}). \quad (\text{B.25})$$

Since at time $t=0$, $g_t = g_E$ and g_E fulfill (B.8), (B.9), and (B.12), the lemma is proved.

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