On the necessity of including the turbulence experienced by an inertial particle in Lagrangian random-walk models

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Abstract

Many Lagrangian models have been developed in the literature in order to simulate the dispersion of particles in turbulent gas and liquid flows. The purpose of the present study is to critically analyze the impact of different fluid autocorrelation functions on the behavior of the dispersed phase in homogeneous isotropic turbulence. The “purely Lagrangian” autocorrelation, well-appropriate for turbulent diffusion problems, needs to be modified by other more sophisticated autocorrelation coefficients, including either space–time characteristics or better particle parameters to obtain appropriate numerical dispersion results in concordance with a recent theory.

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1. Introduction

As it is well-known, Lagrangian models based on Monte-Carlo processes or the random walk principle are well appropriate for predicting the turbulent dispersion in dilute two-phase flows. In these models, a significant large number of individual particle trajectories are simulated in order to obtain statistical mean values which characterize the turbulent dispersion of a cloud of particles. However, the use of the random walk models, based on the Langevin equation using dependent variables, as well as the use of Monte-Carlo methods, based on independent random variables is conditioned by the knowledge of an ensemble of parameters of the flow field, among with the fluid autocorrelation coefficient \( R_{F-u}^p(\tau) \) along the particle's trajectory which is explicitly included in Langevin's equation. Unfortunately, no universal expression exists for \( R_{F-u}^p(\tau) \) which is moreover, because of its Lagrangian nature, difficult to reach by the experimental techniques, even those now really available and very sophisticated non-intrusive techniques.

The aim of this paper is to establish the necessity of taking into account in Lagrangian modeling of particulate dispersion, the spatio-temporal turbulent fluid field experienced by an inertial particle instead of...
the classical turbulent fluid characteristics seen by a fluid element, which may be named “purely Lagrangian” and are generally found valid only for diffusion of tracers like heat, gases or small not inertial particles, droplets or bubbles. An illustration of this necessity is proposed here by comparing a recent theory to the numerical results obtained with random walk models, in which we consider either “purely Lagrangian” fluid autocorrelation coefficients or fluid autocorrelation coefficients including particle’s parameters such as density, diameter which can lead to high-inertia and drift velocity due to gravity effects.

2. Fluid autocorrelation coefficient as experienced by the particle

Considerations on the general case of particles submitted to external forces such as gravity and dispersing in a turbulent flow field allows, with the aid of physical analysis, to establish that the fluid autocorrelation coefficients \( R_{F,ii}^p(\tau) \) along the particle’s trajectory has to be a function of the particle’s characteristics (inertia and drift velocity, see Launay (1998)). In case of low inertia particles behaving like fluid particles and when the particle’s drift velocity \( v_{ch} \) tends to 0 (is small compared to the mean velocity of the carrier fluid), these functions will be close to the fluid Lagrangian correlation coefficient \( R_{L,ii}(\tau) \). In opposite, when \( v_{ch} \) is very large (for high inertia or heavy particles), an rms estimation of the random particle position change from time zero to \( \tau \) will be small compared to \( v_{ch} \), and \( R_{F,ii}^p(\tau) \) will behave as spatio-temporal Eulerian functions. Further considering that, for the range of studied fall velocities, eddy vanishing within time \( \tau \) can be neglected compared to spatial correlation changes, \( R_{F,ii}^p(\tau) \) have to be close to pure Eulerian spatial correlation functions. For this limiting case, the Eulerian spatial correlation coefficients have also to exhibit negative loops in the directions perpendicular to the fall/gravity direction, due to the continuity equation as formulated by Csanady (1963). Indeed, in homogeneous isotropic turbulence for instance, if the Eulerian longitudinal space coefficient \( f(r) \), \( r \) being a distance, has no negative loop, necessarily the corresponding lateral function \( g(r) \) must have one, see Hinze’s textbook (1975). In conclusion, \( R_{F,ii}^p(\tau) \) will range between the pure Lagrangian \( R_{L,ii}(\tau) \) and an Eulerian function which might have a negative loop.

Under these conditions, we are able to discuss the apparent validity of the expressions proposed by Frenkiel (1948), Csanady (1963), Zhuang et al. (1989) and Wang and Stock (1993) for the fluid autocorrelation coefficient seen by the particle. Frenkiel (1948) has proposed correlation coefficients which mainly depend on two parameters, a form positive constant \( q \) and the integral Lagrangian time scales \( T_{L,ii} \):

\[
R_{Frenkiel,ii}(\tau) = \exp \left( -\frac{\tau}{(q^2 + 1)T_{L,ii}} \right) \cos \left( \frac{q\tau}{(q^2 + 1)T_{L,ii}} \right)
\]

(1)

The case \( q = 0 \) corresponds to the simple exponential expression, often met in literature. \( q \) allows to control the number and the amplitude of negative loops. Unfortunately, the Frenkiel parameters do not integrate any particle characteristic. Zhuang et al. (1989) have proposed a more physically appropriate expression involving both time and space correlations in order to simulate eddy-particle crossing trajectory effects (Csanady, 1963):

\[
R_{Zhuang,ii}(s, \tau) = \exp \left( -\frac{\tau}{T_{L,ii}} \right) \exp \left( -\frac{s}{L_{E,ii}} \right)
\]

(2)

where \( L_{E,ii} \) are Eulerian spatial integral scales, \( s \) is the distance between the centre of an eddy and the particle position (two particle models, Launay, 1998). In so far, (2) depends implicitly on the particle behavior (drift and inertia) through distance \( s \). But, Csanady (1963) has derived autocorrelation coefficients which contain explicitly the particle’s drift velocity \( v_{ch} \):
\[ R_{\text{Csadvy,} f}(\tau) = \exp \left( -\frac{\tau}{T_{L,f}} \sqrt{1 + \left( \frac{T_{L,f}v_{ch}}{L_f} \right)^2} \right) \]  

(3)

where \( L_f \) is the Eulerian integral longitudinal scale and \( T_{L,f} \) is the corresponding Lagrangian time scale for the fluid field. However, its expression is only valid for zero inertia particles.

That is why, Wang and Stock (1993) have corrected Csanady’s theory by replacing the fluid integral time scale by the fluid integral time scale seen by the particle (Eqs. (4)–(6)). Wang and Stock’s fluid autocorrelation coefficients verify the whole of the previous announced criteria:

\[ R_{F,11}^p(\tau) = R_{F,22}^p(\tau) = \left( 1 - \frac{v_{ch}\tau}{2L_f} \right) \exp \left( -\frac{\tau}{T_F^p} \sqrt{1 + \left( \frac{v_{ch}T_F^p}{L_f} \right)^2} \right) \]  

(4)

\[ R_{F,33}^p(\tau) = \exp \left( -\frac{\tau}{T_F^p} \sqrt{1 + \left( \frac{v_{ch}T_F^p}{L_f} \right)^2} \right) \]  

(5)

where \( T_F^p \) is the true fluid time scale experienced by a heavy particle without gravity (Wang and Stock, 1993):

\[ T_F^p(St) = T_{\text{mE}} \left( 1 - \frac{1 - T_L/T_{\text{mE}}}{(1 + St)^{0.4(1 + 0.03St)}} \right) \]  

(6)

\( St \) is the particle Stokes number (ratio of the particle relaxation time \( \tau_s \) to the moving Eulerian time), direction 3 corresponding to gravity.

For small inertia, the particle autocorrelation functions are quite the same in the three directions and close to the purely Lagrangian fluid autocorrelation coefficient in so far as, for \( \tau_s \to 0 \) and \( v_{ch} \to 0 \), \( T_F^p \to T_L \). With increasing inertia, \( R_{F,i,i}^p(\tau) \) differ more and more with respect to the different considered directions, the lateral ones, in direction perpendicular to gravity, exhibiting a negative loop which is as more effective as the particle relaxation time \( \tau_s \), representative of the inertia, is large. For important drift velocities, or more exactly for \( L_f/v_{ch} < \min(T_{\text{mE}}, T_L) \) (meaning a small time for crossing the largest eddies), the correlation functions in lateral directions \( (R_{F,11}^p, R_{F,22}^p) \) and that in gravity direction \( (R_{F,33}^p) \) approach respectively the Eulerian lateral space correlation \( g(v_{ch}\tau) \) and the corresponding longitudinal function \( f(v_{ch}\tau) \).

### 3. Results and discussion

In order to establish the necessity of inserting in the random walk model, the real turbulence seen by the particle, we compare the normalized dispersion coefficients (fluid elements diffusion coefficient/particles dispersion coefficient) computed by using successively the Frenkiel (\( q = 0 \)), the Zhuang et al. and the Wang and Stock expressions for the fluid autocorrelation coefficients seen by the particle.

The numerical studies are made in a Galilean frame moving with the mean fluid velocity, the turbulent field is homogeneous isotropic and stationary. Assuming that the particle to fluid density ratio verifies \( \rho_p/\rho_f > 100 \), the equations of motion reduce to (Maxey and Riley, 1983)

\[ \frac{dv_i(t)}{dt} = \frac{\left[ u_i^p(\vec{y}(t), t) - v_i(t) \right]}{\tau_s} f + g\delta_{i3} \quad i = 1, 2, 3 \]  

(7)
\[
\frac{dv_i(t)}{dt} = v_i(t) \quad i = 1, 2, 3
\]

where \( f = C_d/C_{ds} \) is the ratio of the real drag to Stokesian drag coefficient, \( v_i(t) \) and \( y_i(t) \) are the instantaneous particle velocity and position, \( g \) the gravity acceleration and \( u_i^p(\tilde{y}(t), t) \) the fluid velocity at the heavy particle location. The last is obtained by the discretized Langevin equation in homogeneous isotropic turbulence given by:

\[
u_i^p(t + \tau) = u_i^p(t)R_{F,ii}^p(\tau) + u_0\tilde{\zeta}_i\sqrt{1 - (R_{F,ii}^p)^2} \quad i = 1, 2, 3
\]

where \( u_0 \) is the rms scale of the turbulent fluid velocity and \( \tilde{\zeta}_i \) represents an ensemble of random centred Gaussian variables.

The equations are numerically solved by a fourth order Runge–Kutta method and the long time dispersion coefficients \( D_{p,11} \) are statistically derived from 50,000 random trajectories of spherical water droplets (density \( \rho_p = 1000 \text{ kg/m}^3 \)) moving in air (\( \rho_f = 1275 \text{ kg/m}^3 \) and \( v_t = 1.36 \times 10^{-5} \text{ m/s}^2 \)). The fluid turbulent scale \( u_0 = 0.131 \text{ m/s} \) and the moving Eulerian time scale verifies \( T_{mE} = 0.182 \text{ s} \) and \( T_L = 0.5 \ T_{mE} \).

In Fig. 1, we report the case of heavy particles dispersing in homogeneous, isotropic and stationary turbulence but not submitted to the gravitational field. Because of the small particle Reynolds number (induced by the small turbulent intensity), the drag law can be assumed Stokesian. The three dispersion coefficients normalized by the fluid diffusivity \( u_0^2 \ T_L \) are, as they have to be for \( g = 0 \), identical (the dispersion tensor is spherical) and noted \( D_{p,11} = D_{p,22} = D_{p,33} = D_p \) for the three cases. They are compared to the theoretical curve established by Wang and Stock (1993). They show three different trends according to the fluid autocorrelation coefficients used in the Langevin equation (Eq. (9)): indeed, for the Zhuang et al. Expression (2), the calculations predict that the inertial particles disperse much less than fluid elements \( (u_0^2 \ T_L/D_p > 1) \). This feature is often obtained by other less recent classical Lagrangian models as earlier experienced and pointed out by Launay et al. (1998). Frenkel’s exponential correlations (without negative loop, case \( q = 0 \)) lead to a constant normalized dispersion coefficient. On the contrary, the use of the more complex Wang and Stock expression brings to a particles dispersion coefficient larger than the fluid elements diffusion coefficient. Since theoretical (Reeks, 1977; Pismen and Nir, 1978; Wang and Stock, 1993), numerical (Squires and Eaton, 1991; Deutsch, 1992; Graham, 1996) and experimental studies (Wells and Stock, 1983) have proved that the high-inertia particles disperse faster than the fluid elements (this is the inertia effect), the necessity of using, in the Langevin equation, a fluid autocorrelation coefficient de-
pending on the particles characteristics is clearly showed. The inertia effect is only really confirmed for the case of the autocorrelations proposed by Wang and Stock (1993). The same result has been found out to with a Monte-Carlo process correlated to the Wang and Stock theory (Launay et al., 1998).

Then, we study the dispersion of particles submitted to the gravitation (Fig. 2). In this case, particles acquire a mean velocity equal to the mean fluid velocity superimposed by the drift velocity: in that case, a non-linear drag law must be used, the present choice was to consider a Schiller and Nauman drag (see Clift et al., 1978) given by \( f = 1 + 0.15 \cdot Re_p^{0.687} \) in Eq. (7). The dispersion is known to be non-isotropic too: the particles disperse faster in the fall direction than in the perpendicular directions to gravity. This phenomena is called the continuity effect (Yudine, 1959; Csanady, 1963). In the computations, this effect is not restored by the random walk model using the Frenkiel correlation coefficient. On the contrary, the continuity effect as well as the crossing trajectories effect, integrating in fact inertia and gravity (which leads to particle dispersion decrease with larger Stokes number), are well-restored when the Zhuang et al. or the Wang and Stock autocorrelation coefficients are used. Nevertheless, the functions derived by Wang and Stock (1993) seem much better than the one derived by Zhuang et al. (1989) mainly according to the bad predictions obtained with these correlation coefficients for the case of particles not submitted to the gravity (Fig. 1).

In so far, it clearly appears that a random-walk model based on Wang and Stock’s correlation functions is much better suited to predict with accuracy the true dispersion of heavy particles in homogeneous isotropic turbulence with or without gravity effects. The main feature of that method is that it takes into account explicitly the particle parameters and so is able to ‘reestablish the true turbulence experienced along the particle trajectory’.

4. Conclusion

The performance of a Lagrangian approach depends on the knowledge of the fluid autocorrelation coefficient seen by the particle. Besides, this study has clearly shown that the obtained predictions are different according to the correlation coefficient used. As a consequence, in order to be sure to obtain statistical characteristics of the dispersion which close to reality, it is necessary to use a fluid correlation coefficient which has itself an appropriate physical meaning. This was enabled by inserting in the random walk model, relationships for the fluid autocorrelation coefficients depending on the particle’s and fluid
characteristics (depending on fluid viscosity, fluid and particle density, particle diameter), derived by Wang and Stock (1993). Then, the obtained numerical results testify to the necessity to take into account for the ‘turbulence really experienced by the inertial particles’.

References