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A new lagrangian model for the particle rotation effects on turbulent dispersion

A. Echchelh
Département de Mathématique et Informatique, Université Hassan I^{er}, Faculté des Sciences et Techniques, B. P. 577, route de Casablanca, Settat, Maroc.
E-mail: echeladil@yahoo.fr

K. Gueraoui
Groupe de Mécanique des Fluides et des Structures, Laboratoire de Mécanique, Faculté des Sciences de Rabat, Avenue Ibn Batouta, B. P. 1014, Rabat, Maroc.

Taibi
Groupe de Mécanique des Fluides et des Structures, Laboratoire de Mécanique, Faculté des Sciences de Rabat, Avenue Ibn Batouta, B. P. 1014, Rabat, Maroc.

A. Mrabti
Groupe de Mécanique des Fluides et des Structures, Laboratoire de Mécanique, Faculté des Sciences de Rabat, Avenue Ibn Batouta, B. P. 1014, Rabat, Maroc.

M. Y. Haddad
Département de Génie Mécanique, Université d'Ottawa, Ottawa, Canada.

D. Huilier
Institut de Mécanique des Fluides URA CNRS 854, Université Louis Pasteur de Strasbourg, France.

Abstract
A new model is proposed in order to study the particle rotation effects on turbulent dispersion. When turbulent structures interact with heavy inertial particles suspended in a turbulent flow, it is believed that 'turbulent' rotation of the dispersing particles is generated, hence producing lift forces that modified their trajectories. A model is proposed to simulate the random rotational motion of the turbulent eddies. It is then applied to the prediction of the dispersion of spherical solid particles in a grid turbulent. Particle rotation is found to have effect on turbulent dispersion.

Résumé
Un nouveau modèle est proposé dans le but d'étudier l'effet de la rotation particulaire sur la dispersion turbulente. En effet, les structures turbulentes interagissent avec les particules inertielles en mouvement dans l'écoulement turbulent. Il faut noter que la rotation 'turbulente' des particules dispersées est ainsi générée, produisant ainsi les forces qui modifient leurs trajectoires.
Le modèle est ensuite appliqué à la dispersion des particules sphériques dans un écoulement turbulent de grille. La rotation des particules a un effet sur la dispersion turbulente.

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1. INTRODUCTION

In recent years several, Monte Carlo methods have been proposed in order to simulate the dispersion of inertial particles in turbulent flows. These so called Lagrangian models are well suited to track the motion of a representative ensemble of particles within the carrier flow. The calculation of an individual trajectory is achieved by solving numerically an equation of motion in which the fluid velocity, as viewed by the particle, is a combination of the local mean velocity and a random turbulent component. The turbulent structures interacting with the particles are also modelled by a Lagrangian formalism including the stochastic properties of the local turbulent of the carrier flow (Ormancey and Martinon [12], Shuen and al. [16], Milojevic and al. [9], Berlemont [1]).

In the case of the heavy particle motion, usually only the drag force, the buoyancy and gravity term, and eventually an added mass and the Basset history terms are considered together with a model which accounts for the interaction of individual particles with the turbulent eddies in the flow. However, in many situations, this is not sufficient since, for example, lift forces may become important when strong shear layers are locally present.

A recent theory proposed by Lee and Durst [7], based on their own experiments, demonstrates that the particle motion and diffusion in a turbulent flow field have to be numerically simulated by including the Saffman lift force [15]. Furthermore, the Magnus or lift force may have a significant influence on the particle motion under the effect of the shear turbulent flow. A relation for the rotation lift force has been analytically derived by Rubinow and Keller [14].

Further, large particle rotation velocities may also be induced by particle-wall collisions or particle-particle collisions as observed in dense and confined two-phase flows. These phenomena were reported by Matsumoto and Saito [8], Sommerfeld [18] and Oesterle [11] for instance. It is now commonly admitted that these effects have to be included in models capable to numerically predict the motion of particles in turbulent flows.

But it is believed that these lift forces also depend on turbulent quantities, such as the fluctuating velocity gradient and the fluctuating rotational, which are generally unknown. In so far, a formal description of these turbulent characteristics is necessary and should be incorporated into the equation of motion.

The goal of this article is to present an original model with inertial particles dispersion in a turbulent flow such as a nearly homogeneous and isotropic turbulence. This model will be used to study numerically the influence of additional lift forces induced by such turbulent vorticity field on the particle dispersion and to compare the numerical results to those obtained experimentally in similar conditions by Snyder and Lumley [17].

2. LAGRANGIAN MODEL

2.1 Lagrangian trajectography

The Lagrangian model is able to reproduce the trajectory of an inertial particle. Such model has been initially developed by Burnage and Moon [2] and the main philosophy will be presented here, enhanced by a module for fluid vorticity.

The fluid velocity field as 'viewed' by the particle is considered as a series of discrete turbulent spherical structures, which have each a diameter λ related to a length scale Λ and a life time τ related to a Lagrangian time scale T_L . The material particle will 'jump' from structure to structure in time. In order to simplify the problem, we make the hypothesis that the velocity $(\vec{U} + \vec{u}')$ f the fluid structure stays constant when the inertial particles moves inside it. We assume that the mean velocity field, the

fluctuating velocities, and the Lagrangian correlation are known. In fact, these quantities are derived, in the cases that we treat here, by experimental results, but they can also be defined by a turbulent model (K-ε,…) for instance.
The fluid particle characteristics λ, τ and translation fluctuating velocity $\vec{u}'$ are randomly sampled according to the properties of the turbulent field.
Where λ and τ are drawn at random from Poisson distributions with appropriate local mean length Λ and Lagrangian time scale T_L, fitting roughly an exponential for the autocorrelation function.
The eddy fluctuating velocity u' is randomly drawn from a Gaussian distribution with respect to the local Reynolds stress tensor.
Since the model tracks at the same time the material and fluid particles, it takes into account the crossing trajectory effects, due to a slip velocity between the carrier fluid and the particle, induced by gravity or inertia effects.
The inertial particle is 'carried' by successive fluid elements: when a solid particle enters in a turbulent structure, its trajectory is computed by solving the equation of motion of the particle. The trajectories are computed steps by steps. Each step is corresponding to an effective fluid-particle interaction time: At time t_0, marking the beginning of a step, we assume that the discrete particle coincides with a fluid particle at the centre of a structure. The properties $(\lambda, \tau, \vec{u}')$ of the latter being drawn at random. The equation of motion is then integrated with respect to time, as long as the time scale is less than the eddy life time τ or that the fluid particle distance does not exceed the interaction length λ.
According to [2], it is reasonable to take λ as a random variable obeying to a Poissonian distribution for which the mean value is given by $\Lambda = L_{E22}$. Further, the random lifetime distribution has a mean value of T_L. This Lagrangian time scale T_L can be obtained from Hinze's relationship [19].

$$T_L = \frac{2}{C} . \frac{\overline{u'^2}}{\varepsilon} \tag{1}$$

Where C is a constant adapted to the turbulence concerned, and ε the turbulent dissipation rate, other relations can be used.

2.2 Turbulent vorticity model

The Eulerian-Lagrangian model, initially developed by Burnage and Moon [2], has been modified to take into account the non-isotropy of the turbulent flow. It is here completed by a new code simulating the turbulent vorticity [4] of the fluid structures interacting with the particles. These fluid particles are not only characterized by a Lagrangian lifetime τ, a fluid-particle interaction length scale λ and a translation velocity $\vec{u}'$ but also by a velocity vector $\vec{\omega}'$. A dimensional analysis conducts us to postulate that the turbulent shear can be modelled [4] as the ratio of a typical scale of the turbulent velocity by a length scale representative of the turbulent scales. The turbulent shear rate can be then expressed as:

$$\frac{\partial u_i'}{\partial x_j} = \frac{\left(\overline{u_{\underline{i}}'^2}\right)^{1/2}}{\lambda_j} Q_{\underline{i}} \tag{2}$$

where the underlined lower index must not be summed as with Einstein's rule. $\overline{u_i'^2}$ is the variance of the velocity fluctuations which distributions are supposed to be Gaussian, Q_i is a random variable with normal distribution and λ_j is taken as an Eulerian length scale in j direction.
By extension of (2), one can further postulate that a turbulent vorticity vector $\vec{\omega}'$ can be written as:

$$\omega_k' = \frac{1}{2}\varepsilon_{ijk}\frac{\partial u_i'}{\partial x_j} \tag{3}$$

where ε_{ijk} is the unit alternating tensor and $\frac{\partial u_i'}{\partial x_j}$ is given by equation (2)

2.3 Equation of motion

The trajectory of an inertial particle is obtained by integrating a nonlinear system of differential equations. The rotation effect and the Odar & Hamilton's equation [10] are omitted. These equations were completed here by Echchelh [4], in order to take into account the Saffman shear lift force [15] and the rotation forces of Rubinow & Keller [14] in the transverse direction.
On one hand, we assume there is no influence of the particle rotation and velocity gradient of the flow on the drag coefficient for small Reynolds number. Therefore, we use the classical drag force, corrected nevertheless, as classically made, by Schiller and Nauman (see Clift and al.) [3], in order to take into account for larger Reynolds number (non Stokesian drag).
On the other hand, the expression of the Saffman's lift force and Rubinow and Keller's rotation force have been initially established for small Reynolds numbers. Nevertheless, as shown respectively by Rubin [13] experimentally for the Saffman's force and by Laquerbe [6] for Rubinow and Keller's force, these forces can also be used for larger Reynolds number (2<Re<1000).
In vectoriel form, the equations of motion are written:

For the particle position:

$$\frac{d\overrightarrow{X_p}}{dt} = \vec{V} \tag{4}$$

For momentum balance :

$$\frac{\pi D_P^3}{6}(\rho_P + C_A\rho)\frac{d\vec{V}}{dt} = -\frac{1}{2}C_D\frac{\pi D_P^2}{4}\rho\left\|\vec{V}-\vec{U}\right\|\left(\vec{V}-\vec{U}\right) + \frac{\pi D_P^3}{6}(\rho_P - \rho)\vec{g}$$

$$-\frac{1}{2}C_L\frac{\pi D_P^2}{4}\rho\frac{\left\|\vec{V}-\vec{U}\right\|^2}{\left\|\left(\frac{1}{2}\mathrm{rot}(\vec{U})-\vec{\Omega}_p\right)\wedge\left(\vec{V}-\vec{U}\right)\right\|}\left(\frac{1}{2}\mathrm{rot}(\vec{U})-\vec{\Omega}_p\right)\wedge\left(\vec{V}-\vec{U}\right) \tag{5}$$

$$-1.615\rho\upsilon^{1/2}D_p^2\left(\vec{V}-\vec{U}\right)_{\perp n}\frac{\partial U_{\perp n}/\partial\vec{n}}{\left\|\partial U_{\perp n}/\partial n\right\|^{1/2}}$$

The component of $D_p^2\left(\vec{V}-\vec{U}\right)_{\perp n}$ and $U_{\perp n}$ are perpendicular to $\vec{n}$ vector. In our case, the based flow is parallel to x-direction, $\vec{n}$ has two directions n = y or z, then the Saffman's lift forces have two components in the y and z directions.

Therefore, the following set of equations of the positions $\vec{X}_p\left(x_p, y_p, z_p\right)$, velocity $\vec{V}\left(u_p, v_p, w_p\right)$ and rotation rate $\vec{\Omega}_p\left(\Omega_x, \Omega_y, \Omega_z\right)$ of the particles has to be solved:

$$\frac{d}{dt}\begin{bmatrix} x_p \\ y_p \\ z_p \end{bmatrix} = \begin{bmatrix} u_p \\ v_p \\ w_p \end{bmatrix} \tag{6.1}$$

In the x direction:

$$\frac{\pi D_P^3}{6}\left(\rho_P + C_A\rho\right)\frac{du_p}{dt} = -\frac{1}{2}C_D\frac{\pi D_P^2}{4}\rho\left\|\vec{V}-\vec{U}\right\|\left(u_p - u\right) - \frac{\pi D_P^3}{6}\left(\rho_P - \rho\right)g$$

$$-\frac{1}{2}C_L\frac{\pi D_P^2}{4}\rho\frac{\left\|\vec{V}-\vec{U}\right\|^2}{\left\|\left(\frac{1}{2}rot(\vec{U})-\vec{\Omega}_p\right)\wedge\left(\vec{V}-\vec{U}\right)\right\|}\left[\left(\omega_y-\Omega_y\right)\left(w_p-w\right)-\left(\omega_z-\Omega_z\right)\left(v_p-v\right)\right] \tag{6.2}$$

In the y direction:

$$\frac{\pi D_P^3}{6}\left(\rho_P + C_A\rho\right)\frac{dv_p}{dt} = -\frac{1}{2}C_D\frac{\pi D_P^2}{4}\rho\left\|\vec{V}-\vec{U}\right\|\left(v_p - v\right) - 1.615\rho\upsilon^{1/2}D_p^2\left(u_p - u\right)\frac{\partial u/\partial y}{\left\|\partial u/\partial y\right\|^{1/2}}$$

$$-\frac{1}{2}C_L\frac{\pi D_P^2}{4}\rho\frac{\left\|\vec{V}-\vec{U}\right\|^2}{\left\|\left(\frac{1}{2}rot(\vec{U})-\vec{\Omega}_p\right)\wedge\left(\vec{V}-\vec{U}\right)\right\|}\left[\left(\omega_y-\Omega_y\right)\left(u_p-u\right)-\left(\omega_z-\Omega_z\right)\left(w_p-w\right)\right] \tag{6.3}$$

In the z direction:

$$\frac{\pi D_P^3}{6}\left(\rho_P + C_A\rho\right)\frac{dw_p}{dt} = -\frac{1}{2}C_D\frac{\pi D_P^2}{4}\rho\left\|\vec{V}-\vec{U}\right\|\left(w_p - w\right) - 1.615\rho\upsilon^{1/2}D_p^2\left(u_p - u\right)\frac{\partial u/\partial z}{\left\|\partial u/\partial z\right\|^{1/2}}$$

$$-\frac{1}{2}C_L\frac{\pi D_P^2}{4}\rho\frac{\left\|\vec{V}-\vec{U}\right\|^2}{\left\|\left(\frac{1}{2}\mathrm{rot}(\vec{U})-\vec{\Omega}_p\right)\wedge\left(\vec{V}-\vec{U}\right)\right\|}\left[(\omega_x-\Omega_x)(v_p-v)-(\omega_y-\Omega_y)(u_p-u)\right] \quad (6.4)$$

Where: $\vec{U}(u,v,w)$ and $\vec{\omega}=\mathrm{rot}\vec{U}/2$ are the instantaneous velocity and vorticity of the fluid which interact with the inertial particle, their turbulent contribution are randomly sampled as previously stated, their mean value are supposed to be known explicitly. υ is the kinematic viscosity of the carrier fluid and D_p the particle diameter. ρ_p and ρ are respectively the particle and fluid density. C_A is the added mass coefficient as derived by Odar and Hamilton [10], the history Basset term is here neglected since, on one hand ρ_p/ρ is assumed to be large and, on the other hand, the accelerations of the particles, mainly due to volume forces, are in practice relatively small. The gravitation force is taken anti parallel to the X direction of the flow.
The empirical correlations for the drag and lift coefficients are given by:

$$C_D=\frac{24}{Re}\left[1+0.15Re^{0.687}\right] \quad \text{when } Re<1000 \quad \text{(Schiller et Naumann 1931)} \quad (7.1)$$

$$C_D=0.44 \quad \text{when } Re>1000 \quad \text{(Rubin 1977)} \quad (7.2)$$

$$C_L=2\gamma \quad \text{when } Re<10 \quad \text{(Laquerbe 1970)} \quad (7.3)$$

$$C_L=2\gamma\, Re^{-1/2} \quad \text{when } 10\le Re\le 130 \;\; \& \;\; 1\le\gamma\le 5 \quad (7.4)$$

where *Re* is the particle Reynolds number based on the fluid-particle slip velocity expected by:

$$Re=\frac{D_p\left\|\vec{V}-\vec{U}\right\|}{\upsilon} \quad (7.5)$$

and γ the ratio of the rotational velocity at the surface of the spherical particle to the slip velocity, is given by:

$$\gamma=\frac{D_p\left\|\vec{\omega}-\vec{\Omega}_p\right\|}{2\left\|\vec{V}-\vec{U}\right\|} \quad (7.6)$$

The added mass coefficient is given by

$$C_A=1.05-\frac{0.066}{A_C^2+0.12} \quad (7.7)$$

where:

$$A_C = \frac{\left\|\vec{V} - \vec{U}\right\|^2}{D_p \left\| \frac{d\vec{V}}{dt} - \frac{d\vec{U}}{dt} \right\|^2} \tag{7.8}$$

The change of the particle angular momentum due to its interaction with the surrounding fluid is given by a torque equation, first derived by Stokes and Faxen, and then completed by Rubinow & Keller [14] and Gatignol [5]:

$$\frac{d\vec{\Omega}_P}{dt} = \frac{60\mu}{D_P^2 \rho_P} \left[\frac{1}{2}\vec{\omega} - \vec{\Omega}_P \right] \tag{8}$$

where μ is the dynamical viscosity of the carrier fluid.
Equation (8) is valid without restriction in so far as the relative rotation Reynolds number is small as well as the translation Reynolds number Re based on the mean particle-fluid slip velocity V_g.
We can remember that at the same time, the trajectory of the fluid particle is computed by the integration of Equation (6.1).
The system constituted by the previous equations is numerically solved by a fourth-order Runge-Kutta procedure. The time step must be smaller than the particle relaxation time, τ_p, and a relevant time scale for turbulence. The equations (2) are numerically linearized by taking the particle Reynolds number at the previous time step as well as the drag, lift and added mass coefficients. In a similar way, the relative velocity is also treated as an explicit variable.

3. NUMERICAL RESULTS

The model was tested on a standard well recognized test experiment, that of Snyder and Lumley [17], which describes the turbulent dispersion of different kind of inertial particles in a grid turbulent flow. The characteristics of the grid turbulence are well known. Firstly, we recall the experimental context and then we present some comparisons between experimental results and simulation computations including or not the particle rotation in order to quantify its effect on the dispersion.
The Snyder and Lumley experiment was performed in an upwind grid turbulent flow. The mean fluid velocity was $U_x = U = 6.55$ m/s, $U_y = U_z = 0$. The turbulence decay vertical upwind direction x and transverse direction y are fitted by the two following equations, classically expressed for small decaying grid turbulence (M mesh size, X distance from the grid) as:

$$\frac{U^2}{\overline{\overline{u_x'^2}}} = 42.4\left(\frac{X}{M} - 16\right) \quad \text{and} \quad \frac{U^2}{\overline{\overline{u_y'^2}}} = 39.4\left(\frac{X}{M} - 12\right) \tag{9}$$

Applying Taylor's frozen flow hypothesis, a good estimate of the energy dissipation rate ε is given by:

$$\varepsilon = -U\frac{dk}{dX} = \frac{1}{2}\frac{U^3}{M}\left[\frac{1}{42.4}\left(\frac{X}{M} - 16\right)^{-2} + \frac{1}{39.4}\left(\frac{X}{M} - 12\right)^{-2}\right] \tag{10}$$

considering that the turbulent kinetic energy $k=\frac{1}{2}\left(\overline{u_x'^2}+2\overline{u_y'^2}\right)$. Referring to the turbulence measurements of Snyder and Lumley, the relations $L_{E11}= 2.58L_{E22}$ and $L_{E33}= L_{E22}$ were used for the Eulerian integral length scales. Further, a fair estimation of the Lagrangian time scale T_L can be obtained by using Hinze's relationship:

$$T_L=\frac{2}{C}\frac{\overline{u_x'^2}}{\varepsilon} \tag{11}$$

Where C=8.5.

According to the generalized theory of turbulent diffusion initially derived by Taylor, a statistical treatment of the trajectories of a representative number of individual particles can lead to a meaningful description of the turbulent dispersion such as the evolution of the lateral mean square displacement $\langle Y^2 \rangle$ with time.

The average, for a given kind of particle, is here made for 5000 trajectories, satisfying so the order one tenth of the Stokesian relation time $\tau_p=\frac{D_p^2}{18\upsilon}$; the particles are released without an initial slip velocity and without spin.

The criteria of particle rejection, defined experimentally has been numerically applied in the first time.

For all kind of particles used (corn pollen, glass, hollow glass and copper), the particle rotation induced by the turbulence reduces the turbulent lateral dispersion as indicated by the particle dispersion curves. The calculations yield a better fit with the experimental results when they take the rotation into account, as shown on figure 1 & 2, which represent lateral particle dispersion. The calculations are performed for two values of the constant C. Classically C is taken equal to 8.5 in our model, but the value C=7.2 better fits the fluid particle integral scale extrapolated from the measurements performed by Snyder & Lumley at X/M = 73, yielding T_L of 91 ms. In the latter case, the dispersion should be increased compared to the use of C=8.5 this was verified numerically.

For corn pollen and hollow glass, the computed dispersions coincided with the experimental data, whereas for copper and solid glass beads, the lateral square displacements are somewhat overestimated.

Considering the particle autocorrelation functions at $\frac{X}{M}=73$

$$R_{L22}(\tau)=\frac{\langle v_p'(t).v_p'(t+\tau)\rangle}{\langle v_p'(t).v_p'(t)\rangle}$$

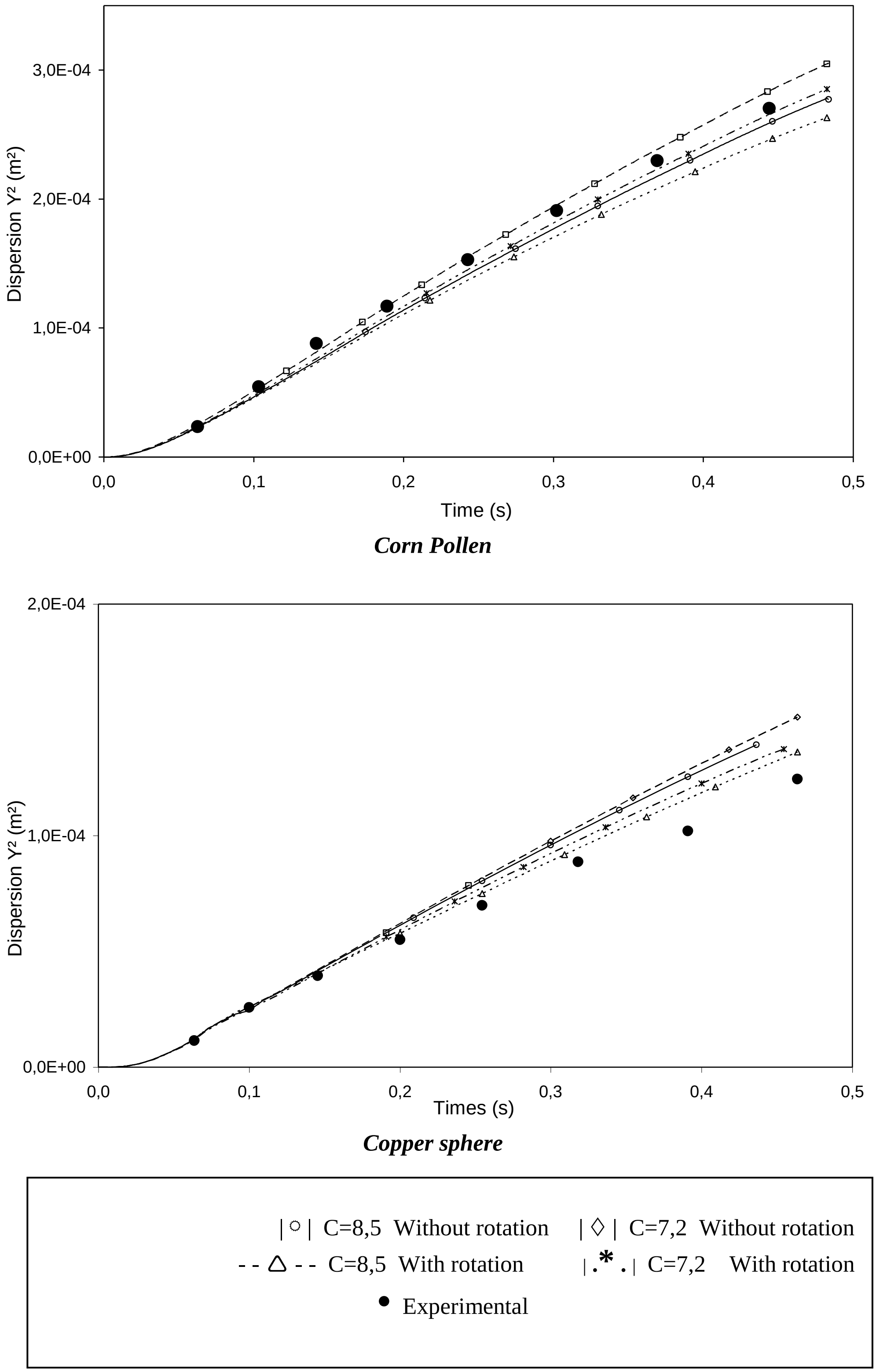
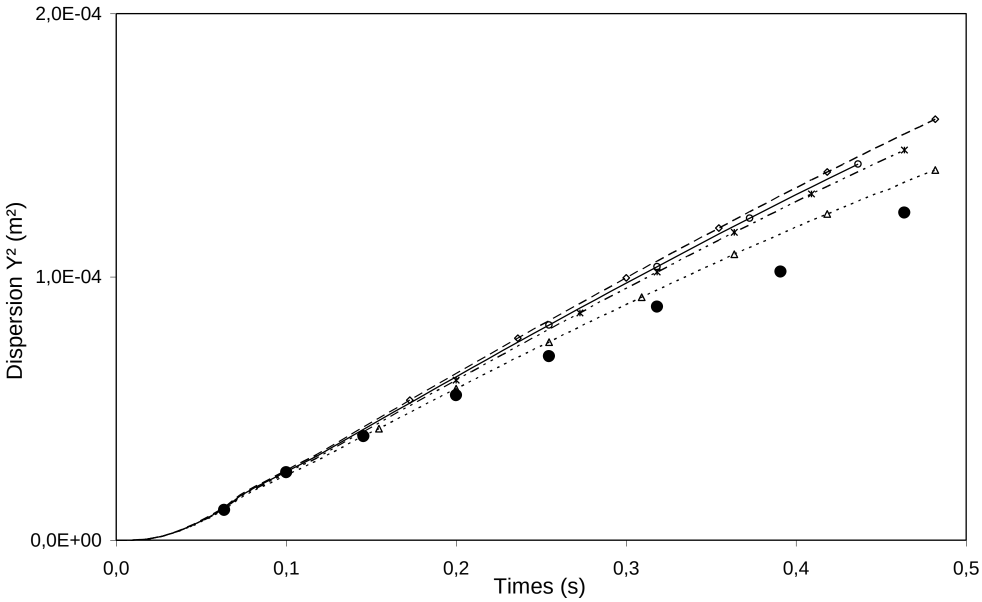
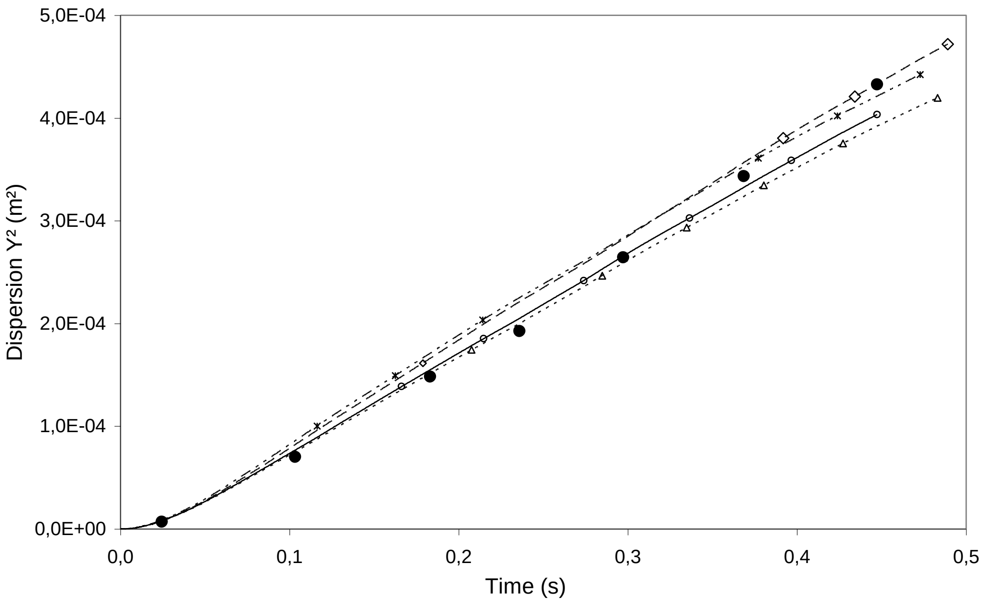


Figure 1 : Particle dispersion [Snyder and Lumley experiment]



Solid glass



Hollow glass

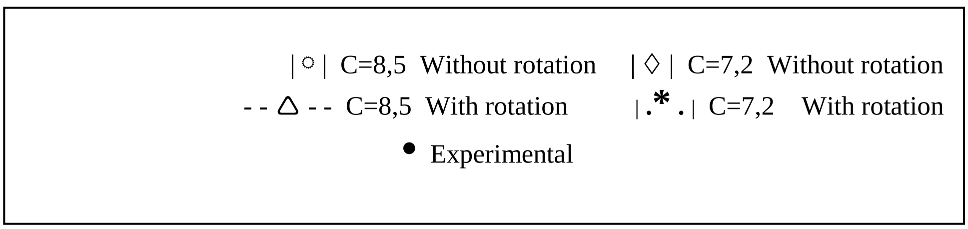


Figure 2 : Particle dispersion [Snyder and Lumley experiment]

The computations of particle autocorrelation are presented on figure 3 & 4, which represent the effect of rotation on the Lagrangian autocorrelation. The results show that the turbulent rotation decreases the correlation by 10 to 15 % and the Lagrangian time scale. This still has to be explained.

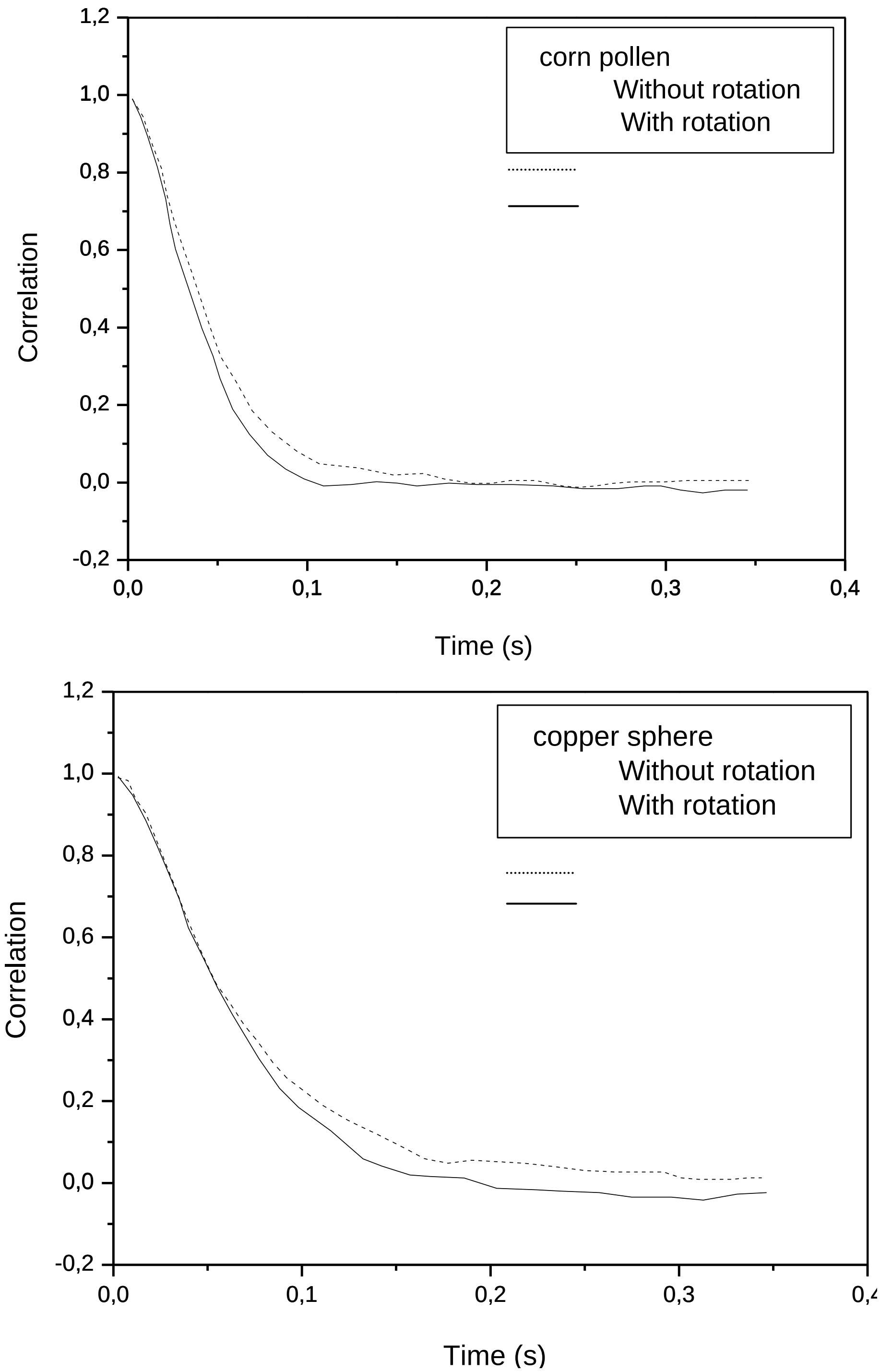


Figure 3 : Particle autocorrelation

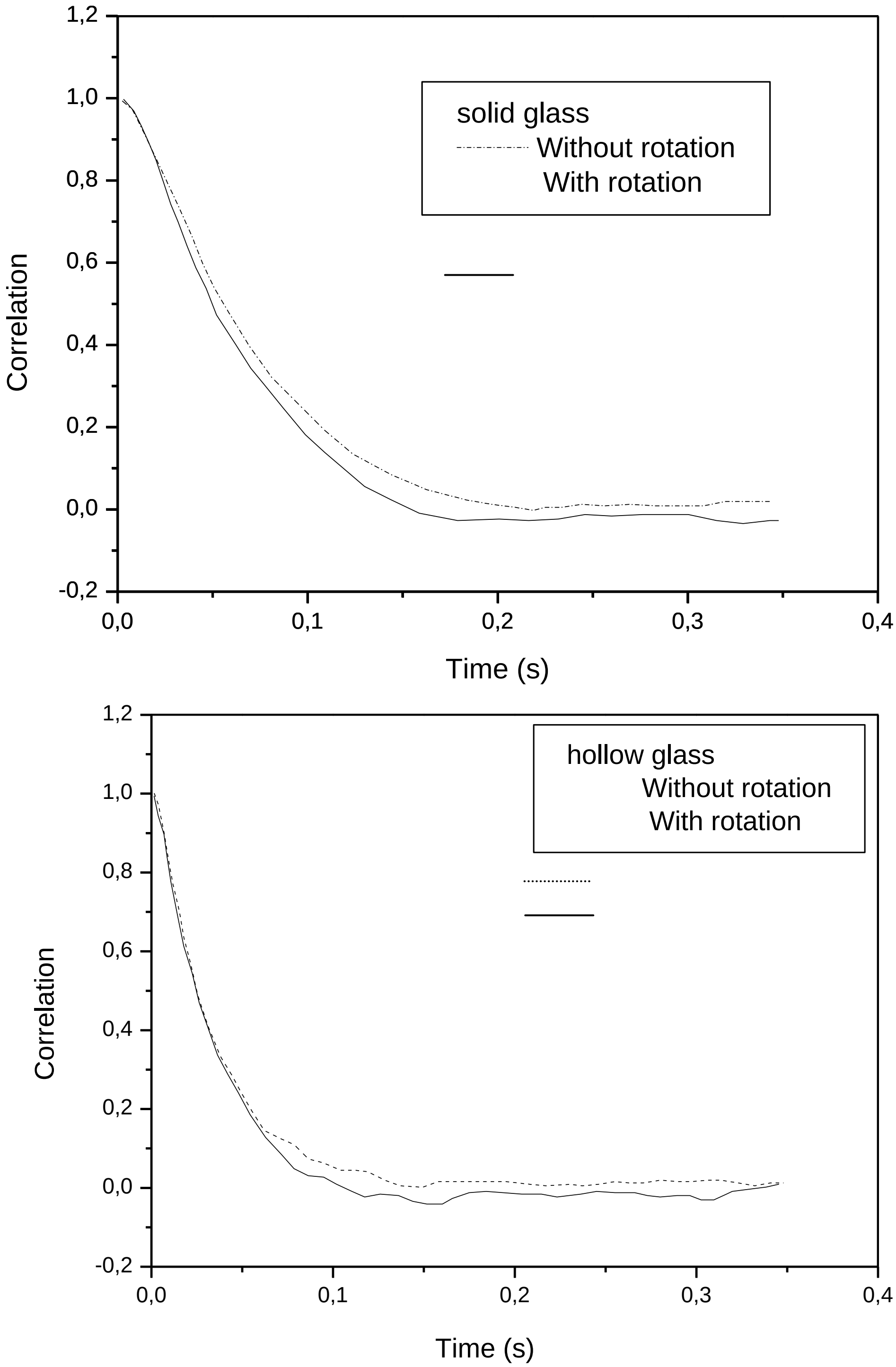


Figure 4 : Particle autocorrelation

Nature	T_L (ms) with rotation	T_L (ms) without rotation
Hollow glass	31.49	35.52
Corn pollen	38.93	45.11
Solid glass	59.32	68.16
Copper	61.65	71.86

Table 1: Particles Lagrangian autocorrelation time T_L with and Without rotation effects. (C=8.5)

The influence of rotation can also be characterised by generalizing Taylor's diffusion theory, according to Batchelor, in term of $D_{T\Omega}$ and D_{To} which denote turbulent diffusivities with and without rotation effects for long diffusion times as shown in the following table.

Nature	$\rho_p(kg/m^3)$	$D_p(\mu m)$	$\tau_p(ms)$	$V_g(cm/s)$	$\frac{D_{T\Omega}}{D_{T0}} * 100$	R_{ep}
Hollow glass	260	46.5	1.9	1.67	96	0.517
Corn pollen	1000	87.0	25.6	19.8	94	1.148
Solid glass	2500	87.0	62.6	44.2	91	2.563
Copper	9800	46.5	63.6	48.3	84	1.497

Table 2: Particles relevant parameters and ratio between turbulent dispersion coefficients with ($D_{T\Omega}$) and without (D_T) rotation effects. (C=8.5).

For the light corn particles, the dispersion is only slightly modified by rotation whereas for heavier beads, $D_{T\Omega}$ decreases with increasing particle density, slip velocity Vg and particle relaxation time τ_p (or inertia). This is directly related to inertia and crossing trajectory effects (see Wells & Stock, [19]) which increase with slip velocity, inertia and rotation. The slip velocity is the terminal particle velocity as a result of the force balance between drag and buoyancy.

4. CONCLUSIONS

It has been shown that numerical simulations of turbulent particulate two phase flows by a Lagrangian-statistical method are able to predict effects associated with transverse lift forces acting on the particles in grid turbulence.

Furthermore the particle rotation induces transverse lift forces which modify the trajectories and dispersion when it moves in a turbulent flow. Using the new model for the turbulent vorticity of the carrier flow, it was demonstrated that the resulting effects are enhanced for the heavier or more inertial particles, which are less sensitive to the carrier fluid fluctuations. As a first result, the turbulent dispersion is reduced by these effects due to rotation.

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