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EDITOR Borhani, N.

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11th October 2010

Instituto Superior Tecnico, Lisbon, Portugal.

ERCOFTAC SPC, IPC & MB-GA Meetings

12th October 2010

Instituto Superior Tecnico, Lisbon, Portugal.



The ERCOFTAC Best Practice Guidelines for Industrial Computational Fluid Dynamics

The Best Practice Guidelines (BPG) were commissioned by ERCOFTAC following an extensive consultation with European industry which revealed an urgent demand for such a document. The first edition was completed in January 2000 and constitutes generic advice on how to carry out quality CFD calculations. The BPG therefore address mesh design; construction of numerical boundary conditions where problem data is uncertain; mesh and model sensitivity checks; distinction between numerical and turbulence model inadequacy; preliminary information regarding the limitations of turbulence models etc. The aim is to encourage a common best practice by virtue of which separate analyses of the same problem, using the same model physics, should produce consistent results. Input and advice was sought from a wide cross-section of CFD specialists, eminent academics, end-users and, (particularly important) the leading commercial code vendors established in Europe. Thus, the final document can be considered to represent the consensus view of the European CFD community.

Inevitably, the Guidelines cannot cover every aspect of CFD in detail. They are intended to offer roughly those 20% of the most important general rules of advice that cover roughly 80% of the problems likely to be encountered. As such, they constitute essential information for the novice user and provide a basis for quality management and regulation of safety submissions which rely on CFD. Experience has also shown that they can often provide useful advice for the more experienced user. The technical content is limited to single-phase, compressible and incompressible, steady and unsteady, turbulent and laminar flow with and without heat transfer. Versions which are customised to other aspects of CFD (the remaining 20% of problems) are planned for the future.

The seven principle chapters of the document address numerical, convergence and round-off errors; turbulence modelling; application uncertainties; user errors; code errors; validation and sensitivity tests for CFD models and finally examples of the BPG applied in practice. In the first six of these, each of the different sources of error and uncertainty are examined and discussed, including references to important books, articles and reviews. Following the discussion sections, short simple bullet-point statements of advice are listed which provide clear guidance and are easily understandable without elaborate mathematics. As an illustrative example, an extract dealing with the use of turbulent wall functions is given below:

- Check that the correct form of the wall function is being used to take into account the wall roughness. An equivalent roughness height and a modified multiplier in the law of the wall must be used.
- Check the upper limit on y^+ . In the case of moderate Reynolds number, where the boundary layer only extends to y^+ of 300 to 500, there is no chance of accurately resolving the boundary layer if the first integration point is placed at a location with the value of y^+ of 100.

- Check the lower limit of y^+ . In the commonly used applications of wall functions, the meshing should be arranged so that the values of y^+ at all the wall-adjacent integration points is only slightly above the recommended lower limit given by the code developers, typically between 20 and 30 (the form usually assumed for the wall functions is not valid much below these values). This procedure offers the best chances to resolve the turbulent portion of the boundary layer. It should be noted that this criterion is impossible to satisfy close to separation or reattachment zones unless y^+ is based upon y^* .
- Exercise care when calculating the flow using different schemes or different codes with wall functions on the same mesh. Cell centred schemes have their integration points at different locations in a mesh cell than cell vertex schemes. Thus the y^+ value associated with a wall-adjacent cell differs according to which scheme is being used on the mesh.
- Check the resolution of the boundary layer. If boundary layer effects are important, it is recommended that the resolution of the boundary layer is checked after the computation. This can be achieved by a plot of the ratio between the turbulent to the molecular viscosity, which is high inside the boundary layer. Adequate boundary layer resolution requires at least 8-10 points in the layer.

All such statements of advice are gathered together at the end of the document to provide a 'Best Practice Checklist'. The examples chapter provides detailed expositions of eight test cases each one calculated by a code vendor (viz FLUENT, AEA Technology, Computational Dynamics, NUMECA) or code developer (viz Electricité de France, CEA, British Energy) and each of which highlights one or more specific points of advice arising in the BPG. These test cases range from natural convection in a cavity through to flow in a low speed centrifugal compressor and in an internal combustion engine valve.

Copies of the Best Practice Guidelines can be acquired from:

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DISPERSED MULTIPHASE FLOW: FROM MICRO-SCALE TO MACRO-SCALE NUMERICAL MODELLING

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The sizes of particles in nature and technical or industrial multiphase flow processes may range from several nano-meters to several centimetres. On the other hand the transport and interaction of particles (representing solid particles, droplets or bubbles) in turbulent flows is governed by a number of physical processes occurring on a wide range of different scales. Such processes are exemplarily summarised in Table 1. The direct interaction between particles occurs on very small length scales which are only a small fraction of the particle size. This is for example the film thickness between colliding bubbles or the distance over which the adhesive van der Waals force is acting. The transport of particles by turbulence may be affected by the entire spectrum of eddy sizes ranging from the dissipation length scale (Kolmogorov length scale) to the dimension of the device inducing the flow (e.g. stirrer blade). The importance of particle transport by turbulence normally is characterised by the Stokes number, being the ratio of particle response time to the relevant turbulent time scale.

From these considerations it is obvious that a numerical calculation of dispersed multiphase flow systems is not possible by just using one numerical approach. Anticipating the prediction of an industrial process requires the use of a number of models describing sub-grid scale processes, which are smaller than the mesh size used for discretising the flow system. A real multi-scale simulation is hardly possible and limited to a few orders of magnitude in the scale dimension. One example is the method proposed by Tomiyama (2002) where a hybrid approach combining an interface tracking method with a multi-fluid model for a certain number of particle size classes was developed. An ideal application of this multi-scale hybrid approach was a heterogeneous bubbly flow.

Normally, however different numerical methods have to be used in order to resolve a certain scale range. With high resolution simulations (micro-scale simulations) the considered process can be analysed, understood and hence models can be derived which may be used in methods resolving only larger scales, i.e. macro-scale simulations. An essential step in the model development is the validation based on experiments or high resolution simulations. Some of the numerical methods being mostly used for analysing particle behaviour and transport on different scales are summarised in Table 2. Due to the limitation in computational resources micro-scale simulations (e.g. particle resolved DNS) are limited to small computational domains and only a few hundreds of particles. On the other hand RANS-based methods (based on the Reynolds-averaged conservation equations combined with turbulence modelling) allow macro-scale simulations of an entire process with limited spatial resolution. Here the particles are treated as point masses.

Furthermore, models are needed for all the sub-grid-scale processes, such as turbulence effects or inter-particle collisions. Multiphase flows are treated using either the multi-fluid model (also referred to Euler/Euler model) or the Euler/Lagrange approach where the particle phase is simulated by tracking a large number of representative point-particles through the flow field for obtaining the properties of the dispersed phase. It is clear, that the degree of modelling increases with reduced scale resolution.

Diffusive mass transport within the particle and in the bulk flow	Molecular scale
Film thickness between coalescing bubbles or droplets	10nm - 100nm
Range of van der Waals forces in solid particle interaction	0.4nm - 50nm
Particle transport by turbulence in the dissipation regime	Kolmogorov lengthscale $\eta = (v^3/\varepsilon)^{1/4}$
Particle transport by large scale eddies L	$L/\eta = Re_L^{3/4}$
Flow structure around particles	Particle size
Particle interaction (collision)	Particle size

Table 1: *Comparison of physical processes and relevant length scales.*

Molecular dynamics simulation	Simulation of molecular motion
Particle resolving DNS	Resolving the particle and the flow around it
Point-particle DNS	Resolving the dissipation scale of turbulence, particles are treated as point masses
LES	Resolves large-scale vortices and the spectrum of larger turbulence, particles treated as point-masses
RANS-methods	Resolves only the mean flow structure, particles treated as point-masses

Table 2: *Comparison of numerical methods and their resolution.*

The present special issue of the ERCOFTAC Bulletin tries to address the above described issues and presents numerical methods and results obtained with different scale resolution. With exception of molecular dynamic

simulations, contributions using all the other numerical methods are included. Regarding the latter methods in Table 2, contributions are included using the two-fluid approach and the Euler/Lagrange method. The special issue gives a good overview of the present research activities within the special interest group 12: ‘Dispersed Turbulent Two-Phase Flow’.

References

Tomiyama, A., *Some attempts for the improvement of computational bubble dynamics*, CD-ROM-Proceedings 12th Workshop on Two-Phase Flow Predictions, Merseburg, Germany, 9-12th. April 2002.

DIRECT NUMERICAL SIMULATION OF HIGH SCHMIDT NUMBER MASS TRANSFER FROM AIR BUBBLES RISING IN LIQUIDS USING THE VOLUME-OF-FLUID-METHOD

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Abstract

We present a combined VOF-based approach for the direct numerical simulation of mass transfer across deformable fluidic interfaces in 3D. For this purpose and in order to resolve all relevant length scales for moderate Reynolds and Schmidt numbers in convection dominated cases, several computational techniques are employed. In particular, we build on a subgrid-scale model for the concentration boundary layer at the interface, a moving frame of reference technique, and a local mesh refinement around the bubble. Furthermore, we show a first result employing so-called artificial boundary conditions to reduce the size of the computational domain in lateral direction.

1 Introduction

In Chemical Engineering, dispersed gas / liquid mass transfer operations are often realized in bubble column reactors, especially for performing chemical reactions like hydrogenations, oxidations, or chlorinations. The overall process evidently involves multiple scales. On the macro-scale, the bubbly flow circulates depending in particular on the reactor design and on the operating conditions. This leads, on the one hand, to dispersion of the gas content and, on the other hand, to segregation. The resulting velocity gradients close to the reactor walls lead to a lift force acting on each individual bubble. This lift force shows a change of sign under variation of the bubble diameter resulting in the fact that small bubbles move to the reactor walls where larger gradients in the relative velocity appear, whereas large bubbles move to the opposite direction, i.e. to the center of the column. This behavior leads to a gas plume which itself can become unstable and move around. On the meso-scale, bubble fragmentation and bubble / bubble interactions such as bouncing and coalescence without and with subsequent fragmentation occur. These processes determine the bubble population's size distribution and, hence, influence massively the efficiency of the overall process. The bubble diameter distribution determines not only the volume specific interfacial area, which is significant for the transfer rates, but also the local velocity field around the bubble. In particular the wake structure is of immense importance since it is responsible for the convective transport of the transfer component away from the interface, hence keeping a driving concentration gradient at the bubble surface. Moreover, in case of reactive mass transfer, the bubble wake can be considered as a mini reactor since chemical reaction takes place mainly there. The (diffusive) inter-phase mass transfer and the

micro-mixing process as well as the chemical reaction itself occur on the micro-scale.

A detailed continuum mechanical model of the full process has to be based on the two-phase Navier-Stokes equations complemented by two-phase species equations and, if necessary, by the two-phase energy balance equation. However, it is not possible to numerically solve the full model resolving the full phase topology and all relevant scales in detail. Hence different CFD models of this process are required and used at the different scales (Figure 1).

For the overall process with a large gas hold-up, the Euler / Euler formulation is the common approach; here both phases, i.e. the continuous as well as the dispersed phase, are treated as interpenetrating continua. In this model most of the local information concerning individual bubble shape and size is lost and modeling assumptions are necessary.

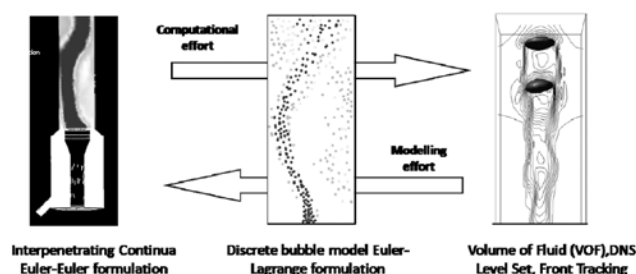


Figure 1: *Model hierarchy for CFD simulations.*

For smaller gas hold up, the Euler / Lagrange formulation is possible where ordinary differential equations of motion are solved for individual dispersed particles (Lagrangian formulation) whereas the flow of the continuous phase is solved in the Eulerian frame. Here certain information concerning location and velocity of representative particles is available, but local information concerning bubble shape and inner velocity field is still missing. For both the Euler / Euler as well as the Euler / Lagrange formulation closure terms are needed to account for the exchange of mass and momentum between the phases. As sketched in Figure 1, the modeling effort and the computational effort change in opposite directions. Once a closure model is assumed, its model parameters can be obtained from experiments, but also from computational analysis based on results from Direct Numerical Simulation (DNS). The latter refers to the detailed model based on first principles and its numerical simulation with sufficient resolution in time and

space in order to resolve all present scales. DNS is desired if operating conditions are not experimentally feasible, e.g. a defined velocity gradient for determining the lift force coefficient, or if local information is not accessible by measurements. However, due to the limits of current (super-)computers in computational power, only few fluid particles can be treated by means of a true DNS. Furthermore, a combined experimental and DNS analysis is possible in certain cases. For example the experimental analysis of the mass transfer from a rising bubble requires an adequate resolution of the velocity and the concentration fields in the continuous phase. This is not possible today, especially for the velocity field near the interface with available experimental techniques. Contrary, the relevant hydrodynamic scales can be resolved by DNS while the resolution of the concentration boundary layer is hardly possible. The smallest length scale for species transport is the Batchelor length scale, which is $1/\sqrt{Sc}$ times the hydrodynamic length scale; here the Schmidt number is defined as $Sc = \nu/D$ and has typical values of several hundred for aqueous systems. But for mass transfer the thin concentration layer at the region above the equator is crucial, since most of the transfer takes place there. For DNS of two-phase flow several numerical techniques are available which are able to resolve the free phase boundary like the Volume of Fluid (VOF), Level Set or Front Tracking method.

In the present paper a VOF-based approach for simulating mass transfer of dilute components from rising bubbles is presented [BKA09, ABKW09] and combined with several computational techniques for capturing the thin concentration boundary layer at least for moderate Reynolds and Schmidt numbers. In particular, we employ a subgrid-scale model for the concentration profile, a moving frame of reference technique, and a local mesh refinement around the bubble [WHW09]. While the second technique is to reduce the computational domain in rise direction, we currently also develop so-called artificial boundary conditions to reduce the lateral computational domain size.

2 Mathematical model and numerical method

2.1 Hydrodynamics

The mathematical model is based on the one-field formulation of the isothermal, incompressible momentum balance in the buoyancy formulation:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\begin{aligned} \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = & -\nabla p_{dyn} \\ & + \nabla \cdot (\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \\ & + (\rho - \rho_c) \mathbf{g} + \mathbf{f}_\sigma \end{aligned} \quad (2)$$

The buoyancy formulation is chosen because no solid wall but an outflow boundary condition is applied at the bottom of the computational domain such that no hydrostatic pressure can be build up. For the numerical solution of (1) and (2), the Volume-of-Fluid (VOF) method by Hirt and Nichols [HN81] is employed. There the phase volume is tracked by solving the additional transport equation

$$\frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{u}) = 0 \quad (3)$$

for the phase indicator function f , which in the context of a Finite Volume discretization corresponds to the volume fraction of dispersed phase inside computational cells. For the given f -distribution, the local density and the viscosity of the fluids are calculated by

$$\rho = f \rho^d + (1 - f) \rho^c, \quad \mu = f \mu^d + (1 - f) \mu^c \quad (4)$$

Simulations are performed using the ITLR inhouse code Free Surface 3D (FS3D) [Rieb04]. The surface tension is represented by a volume force $\mathbf{f}_\sigma$ in the momentum equation, which is computed using the conservative continuum surface stress (CSS) model by Lafaurie et al. [LNSZZ94]. The reconstruction of the interface, which is used for convection of the volume fraction, is based on the piecewise linear interface calculation (PLIC) method by Rider and Kothe [RK98]. FS3D uses a structured finite volume scheme on a staggered (MAC) grid. The spatial discretization is of second order accuracy and the temporal discretization is of first order accuracy.

2.2 Mass transfer

Under the additional assumptions that the transfer species are ideally diluted regarding the mass and momentum balances, no phase change like evaporation or condensation occurs, the transfer component is not surface active and local thermodynamical equilibrium holds at the interface $\Sigma(t)$, the two-phase species equations read as

$$\partial_t c_k + \nabla \cdot (c_k \mathbf{u} + \mathbf{j}_k) = R_k \quad \text{in } \Omega^c(t) \cup \Omega^d(t) \quad (5)$$

$$[\mathbf{j}_k] \cdot \mathbf{n}_\Sigma = 0 \quad \text{and} \quad c_k^d / c_k^c = H_k \quad \text{on } \Sigma(t) \quad (6)$$

$$\mathbf{j}_k = D_k \nabla c_k, \quad D_k > 0 \quad (7)$$

Here the source term R_k stands for the overall production rate of the chemical component k if chemical reactions take place. Local thermodynamical equilibrium is modeled by Henry's law with constant distribution coefficient H_k . From the first assumption it follows that the diffusive flux $\mathbf{j}_k$ can be calculated according to Fick's law and that the transfer component has no influence on the local momentum such that the common barycentric fluid velocity $\mathbf{u}$ is governed by a single set of two-phase Navier-Stokes equations. Due to the last assumptions and the isothermal conditions, no surface tension gradients are present, i.e. no Marangoni stresses appear at the interface.

Our numerical approach is based on the VOF method and uses two scalar variables for the concentration field of any transfer component, one for each phase according to

$$\phi_k^j(\mathbf{x}, t) = \begin{cases} c_k & \text{for } \mathbf{x} \text{ in } \Omega^j(t) \\ 0 & \text{otherwise} \end{cases} \quad (8)$$

Note that these variables are similar to the VOF variable f . Hence the convective transport of molar mass can be directly intertwined with the convective transport of the phase volume employing the PLIC reconstruction of the interface. In this manner artificial mass transfer induced by numerical diffusion due to the convective transport step is prevented.

Mass transfer across the interface is modeled by an interchange term accounting for local thermodynamical

equilibrium at the phase boundary. According to (6), the normal component of the diffusive flux is continuous at the interface since no accumulation occurs at the interface. Therefore only a single one-sided limit of the concentration gradient is needed for the calculation of the local flux across the interface. In case of rising gas bubbles, the concentration gradient on the continuous liquid phase side is more suitable for this purpose due to the larger mass transfer resistance there. Applying directional splitting, the normal component of the mass transfer flux inside an interfacial cell V_i is given as

$$\mathbf{j}_{\Sigma_i} \mathbf{n}_{\Sigma_i} |A_{\Sigma_i}| = (j_{\Sigma_i,x} n_{\Sigma_i,x} + j_{\Sigma_i,y} n_{\Sigma_i,y} + j_{\Sigma_i,z} n_{\Sigma_i,z}) |A_{\Sigma_i}| \quad (9)$$

where $|A_{\Sigma_i}|$ is the area of that part of the interface lying in V_i ; for better readability, the species index k is dropped in (9) and below. As well as for all other transport schemes in FS3D which employ directional splitting, the three spatial directions are processed successively and the order of this sequence is altered in each time step in order to prevent systematic errors. Only directions to neighboring cells completely filled with the continuous phase are considered. For the 1D calculation of the one-sided limit of the concentration gradient appearing in the components of the Fickian fluxes, i.e. $j_{\Sigma_i,x} = D_k^c dc_k/dx|_{\Sigma_i}$, the intermediate values $\phi_{k,i}^d/H_k$ and $\phi_{k,nb}^c$ are used. The x -coordinate $n_{\Sigma_i,x}$ of the interface normal as well as the interfacial area $|A_{\Sigma_i}|$ of that part of the interface lying in V_i are determined from the phase volume distribution. The approach is conservative concerning the molar mass of all transfer components and allows for variable distribution coefficients without artificial mass transfer due to convection of the discontinuous concentration fields.

However, in case of aqueous systems with Schmidt numbers of the order of 100 and well above, the concentration gradient is extremely steep in convection dominated cases and it is therefore a big challenge to capture this thin concentration boundary layer. In the following, additional computational and modeling techniques are described which help to increase the resolution near the interface.

2.3 Subgridscale Model

The concentration profiles result from the two-phase species equations (5) which are invariant under a transformation into a coordinate system moving with the barycenter of the bubble. Therefore, a flow passing around the fluid particle is considered for the derivation of an appropriate subgrid-scale model. Zooming into the interface region around the equator of the bubble, where most of the mass transfer takes place, the situation can be approximated by a planar fluidic interface moving without slip to the adjacent liquid. In the latter phase a concentration layer is build up by convection and diffusion. In this simplified 1D model, it is assumed that the interface and the adjacent liquid move parallel and laminar with constant velocity $\mathbf{u}$, diffusion in flow direction is negligible, and the dispersed gaseous phase is homogeneously mixed. Due to the last assumption, the jump condition (6) can be substituted by a Dirichlet condition for the liquid phase concentration. Figure 2 illustrates this setting.

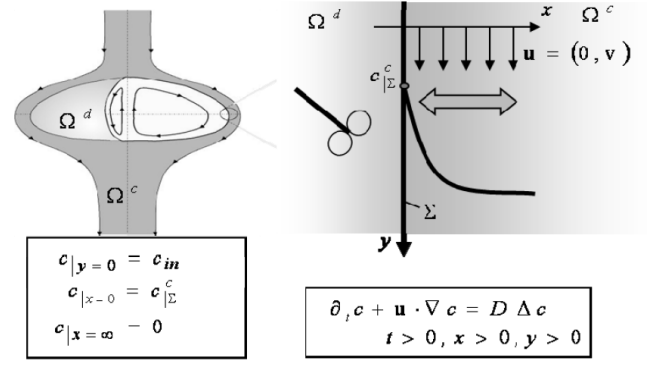


Figure 2: *Simplified 1D model.*

For the stationary case and for an inflow concentration of $c_{in} = 0$, the analytical solution for the concentration profile is

$$c(x, y) = c_{\Sigma}^c \left(1 - \operatorname{erf} \left(\frac{x}{\delta(y)} \right) \right) \quad \text{with} \quad \delta(y) = 2 \sqrt{\frac{D^c y}{v}} \quad (10)$$

and the concentration gradient at the interface (in normal direction) is

$$\frac{\partial c}{\partial x}|_{\Sigma} = -\frac{2}{\sqrt{\pi}} \frac{c_{\Sigma}^c}{\delta} \quad (11)$$

Equation (10) is used to determine the characteristic length δ by a Newton iteration using discrete intermediate values of ϕ_j^c after the convective transport step of the considered interfacial cell i and the neighbor cell if the latter lies completely in the continuous phase. Then, the x -component of the flux $j_{\Sigma_i,x}$ is computed from (11), thus accounting for nonlinearities of the concentration profile at the interface. Again, in both steps the relation $c_{\Sigma_i}^c = c_{\Sigma_i}^d/H$ is employed.

The diagram in Figure 3 shows the decrease of (initially normalized) molar mass inside a fluid particle rising in a liquid with a Schmidt number of $Sc = 10$ with time obtained from 2D simulations with different resolutions. Curves obtained without subgrid-scale model, i.e. with a linear concentration gradient (grey line), at resolution level B and C as well as curve obtained with subgrid-scale model (dark line) at resolution A are congruent but steeper than the curve obtained without subgrid-scale model at resolution A. These results indicate firstly, that grid independency is already reached with grid B. With the coarse grid A the concentration layer is not fully resolved so that the linear gradient calculation leads to a too small transfer rate. Secondly, a factor of at least 2 (in each direction) is saved when using the subgrid-scale model. Similar results are obtained for $Sc = 100$ but there one more refinement of a factor 2 is required to reach grid independency. Here, the time saving due to subgrid-scale model is huge. A 2D simulation with double fine resolution as with grid C already lasts about three weeks while simulation with grid resolution C runs only four to five days on the present computer cluster in Darmstadt. The cluster consists of 20 nodes with two Intel Xeon Quad Core processors per node and 4 GB of main memory per core. For physical 3D simulations further techniques are needed to reduce cell number.

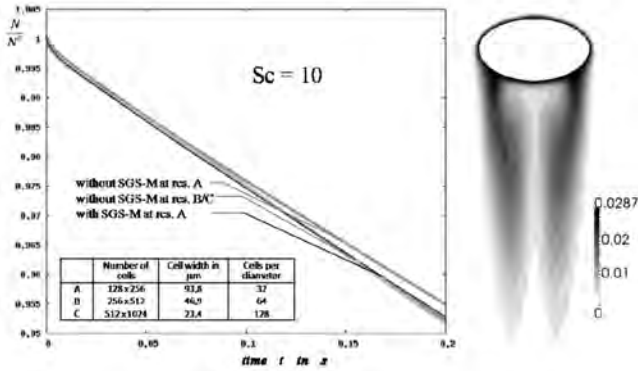


Figure 3: Change of normalized molar mass inside a 3mm fluid particle rising in a liquid with $Sc = 10$ without (grey) and with subgrid-scale model (dark) obtained by 2D simulations with different grids.

2.4 Moving Frame of Reference

In order to observe the rise behaviour of gaseous bubbles over a large period of time and thus over a long rising path, a moving frame of reference is employed. This technique induces a counter flow in the computational domain, which is adapted dynamically over time depending on the motion of the centre of mass of the gaseous phase. The motion of the centre of mass is considered as a damped oscillation of a point mass around its initial position. Depending on the displacement and the velocity of the centre of mass a correcting body force $\rho \mathbf{k}_C$ is imposed to the flow field by adding it to the right hand side of the momentum equation (2). This keeps the bubble close to its initial position in computational domain, or, from the view of a fixed observer, moves the computational domain along with the bubble. The correction force is calculated every time step for all three spatial dimensions by

$$\mathbf{k}_C = 2\omega \frac{\mathbf{P}_g}{m^*} + C_1 \omega^2 \Delta \mathbf{x}_g \quad (12)$$

with the momentum of the bubble, $\mathbf{P}_g$, divided by the virtual mass of the gaseous phase, m^* , and the displacement vector $\Delta \mathbf{x}_g$. The displacement vector and the momentum of the gaseous phase refer to the moving frame of reference. The value of C_1 is switched from 1 to 0 if the centre of mass of the gaseous phase approaches its initial position. This avoids overshoots in the displacement. The angular frequency ω , governing the hardness of the dampening and the magnitude of the oscillation around the initial position, is calculated by

$$\omega = C_2 \sqrt{\frac{\rho_f}{\rho_g}} \pi \omega_{res} = C_2 \sqrt{\frac{\rho_f}{\rho_g}} \pi \sqrt{\frac{12\sigma}{d_e^3 \rho_f}} \quad (13)$$

where ω_{res} is the first mode of the bubble eigenfrequencies, which is multiplied by π and a constant value C_2 in order to avoid that ω becomes a higher mode of the surface resonance frequencies.

This method requires an outflow boundary condition, allowing eddies to leave the computational domain. For this reason, the domain is somewhat enlarged by addition of a damping zone in front of the outflow. This avoids backflow at the domain boundary while eddies can leave the undamped main part of the computational domain. The setup of a cubic domain using the moving frame of reference is illustrated in Figure 4.

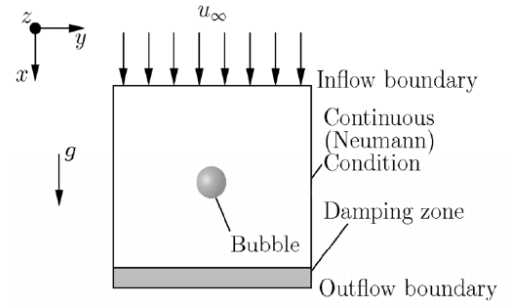


Figure 4: Numerical setup and coordinate system.

2.5 Mass transfer Local mesh refinement

In the past, various approaches have been made to increase the grid resolution at the free surface of two phase flows (e.g. [TB04], [Sus05]). FS3D was extended to generate an interlaced hierarchy of refined patches with doubled resolution with indices $0 \leq l \leq l_{max}$ in the vicinity of the bubble. Grid level $l = 0$ is the coarsest level and contains the entire computational domain (Figure 5), so the general setup of this level is similar to Figure 4. Each finer patch l is completely embedded in the next coarser grid level $l - 1$. The solution on all patches is advanced with the same time step, i.e. we do not use subcycling in the cases presented. The boundary conditions for the refined patch l are taken from the solution of the coarser patch $l - 1$ and the solution of patch l is interpolated to patch $l - 1$. Both, the interpolation of the boundary conditions and of the solution are conservative. A solution cycle of one time step reads:

1. begin of time step
2. loop over l from 0 to l_{max}
 - a. for $l \neq 0$: obtain boundary conditions from level $l - 1$
 - b. solve the governing equations on level l
3. loop over l from l_{max} to 1
 - a. interpolate solution of volume fraction field and velocity field to $l - 1$
4. Calculate time step size for next time step (stability constraints)

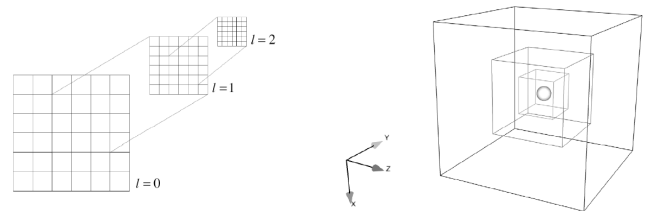


Figure 5: Hierarchy of refined patches for $l_{max} = 2$.

The left side of Figure 6 shows the fine grid result of a simulation of a rising $d_e = 2\text{mm}$ air bubble in water using two fine patches. The setup is similar to that in Figure 5. The coarsest level (outer box in Figure 5) is bubble diameters wide. Each finer patch l (intermediate and inner box in Figure 5) has the half width of the underlying patch $l - 1$ and every patch is resolved by 32 computational cells. On the right side the solution of a

calculation without refined patches is shown. This case is resolved by 32 cells in every direction, so in both simulations there is the same spatial resolution at the interface. The free surface is shown using the corresponding colour for both cases.

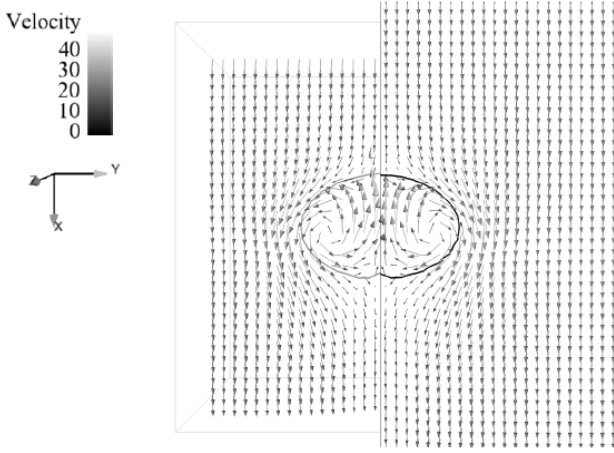


Figure 6: Velocity field and interface with $l_{max} = 2$ (left) and $l_{max} = 0$ (right).

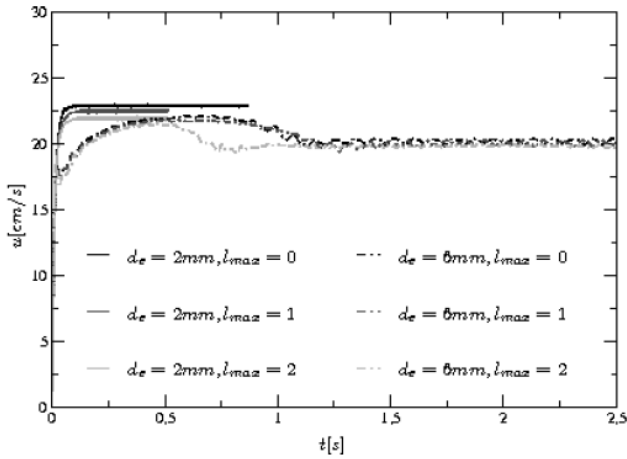


Figure 7: Rise velocities of 2mm and 6mm bubble using $l_{max} = 0$, $l_{max} = 1$ and $l_{max} = 2$.

The computed rise velocities for both cases are plotted along with the result of a third simulation ($l_{max} = 1$ in dark grey) which is resolved by 64 cells in every direction (Figure 7). The difference between $l_{max} = 0$ and $l_{max} = 2$ is less than 5%, whereas the total number of computational cells and thus the computational effort are reduced by the factor of 21. Additionally, the results of simulations using the three different values of l_{max} on a 6mm bubble are plotted. The $l_{max} = 1$ and $l_{max} = 0$ simulation are predicting the same rise behaviour, whereas the rising path of the $l_{max} = 2$ case changes much earlier from the rectilinear regime, indicated by the plateau at the maximum velocity, to a three dimensional trajectory, indicated by the decrease in the velocity and the oscillation around a mean value. The magnitude of this oscillation is much weaker for the

$l_{max} = 2$ simulation than for the other two. This behaviour indicates that the distance between the boundary of the finest patch and the free surface was chosen too small in this simulation. With a sufficient number of computational cells between the patch boundaries and the bubble, this method allows an immense reduction of computational effort.

2.6 Artificial boundary conditions

A high resolution usually requires a large number of computational cells. To reduce the necessary computational effort, the computational domain has to be as small as possible. FS3D is restricted to structured grids with cubic cells due to the geometric multigrid solver. This in turn allows only rectangular computational domains which implies an unsymmetrical influence especially of the lateral boundaries on the flow field and, hence, to the concentration profile if slip or slip free boundary conditions are used. The closer the lateral boundaries are, the higher is of course their influence. But the goal is to quantify the mass transfer from gas bubbles rising in an infinite liquid. Therefore, in simulations presented above, for both the flow and the concentration field, homogeneous Neumann boundary condition is applied allowing fluid to enter and leave the domain. However, this condition does not account for the decay behavior of the velocity field with increasing lateral distance from the particle. Basis of the current approach for the artificial boundary condition is the outer velocity field of the Hadamard-Rybczinski (H-R)-solution [Lev63]. Although the latter describes only the creeping flow ($Re < 1$) around a fluid particle, there are hints that stream lines of H-R-type are valid up to Reynolds numbers of $Re = 200$ [RK66]. Higher-order terms in $1/r$ in the (H-R)-solution are neglected, yielding the asymptotic relation

$$\frac{\partial u_\xi}{\partial \mathbf{r}} + \frac{1}{r} u_\xi = 0 \quad \text{as } r \rightarrow \infty \quad (14)$$

for the spherical velocity coordinates (u_r , u_θ , u_φ) which can be used as a Robin type boundary condition.

Figure 8 shows stream lines from 2D VOF-simulations obtained with different boundary conditions for the Navier-Stokes equations. The bubble rises with a Reynolds number of about 10. The grey curves correspond on both sides to stream lines from a reference solution with slip boundary condition at the lateral boundaries and a wall distance of 8 bubble diameters. The black curves correspond to stream lines obtained from computations with smaller wall distance of 3 bubble diameters. In the left half again the slip condition is applied, while in the right half the artificial boundary condition from above is applied. Especially at the equator of the fluid particle, the stream lines obtained with the artificial boundary condition are in much better accordance with the reference streamlines than those obtained with slip condition for small wall distance. The result presented in Figure 8 is obtained with homogeneous pressure boundary condition, but it should be mentioned that, in general, each boundary condition for the velocity field corresponds to a specific pressure boundary condition which has not been accounted for so far. The work on this topic is under development and it is expected that improved pressure boundary conditions will yield even better results, allowing for smaller domains or higher resolutions.

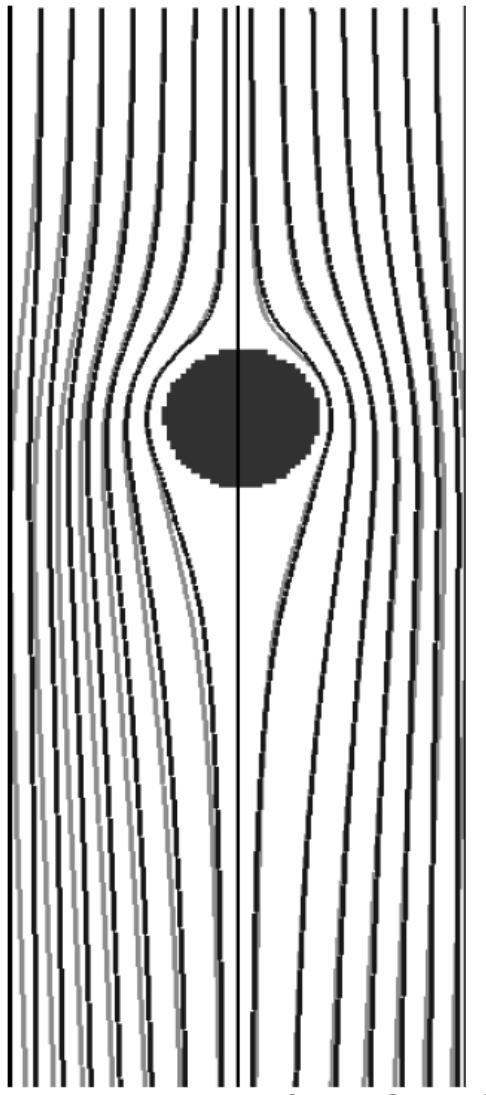


Figure 8: Stream lines obtained from 2D simulations with different wall distances and boundary conditions.

3 Conclusion and Outlook

It is shown how mass transfer from a deformable single bubble rising over a long distance in a liquid with almost realistic Schmidt number can be simulated. This is important in order to obtain local information for closure models used in scale-reduced CFD approaches. For this purpose a recent VOF-based mass transfer approach is combined with additional techniques such as a moving frame of reference, local grid refinement and artificial lateral boundary conditions. With this overall method, Schmidt numbers of the order of 100 can be handled for single bubbles under moderate bubble Reynolds numbers. The applied techniques are under development and will be combined and further improved in future work.

Acknowledgements

The authors gratefully acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) within the project cluster 'Reactive mass transfer from rising gas bubbles' (PAK-119). The authors from the TU Darmstadt also acknowledge financial support within the cluster of excellence 'Smart Interfaces' (EXC-259).

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ANALYSIS OF THE BEHAVIOUR OF CYLINDERS IN HOMOGENEOUS ISOTROPIC TURBULENCE BY LATTICE-BOLTZMANN METHOD

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Abstract

Direct numerical simulations of the motion of resolved volume equivalent single cylindrical particles with axis ratios of 1, 2, 3, and 4 and Stokes numbers of 1, 2, 4, and 40 in a homogeneous isotropic turbulent flow field are presented. The forced turbulent flow is simulated using the Lattice-Boltzmann-Method (LBM). The particles are allowed to freely move according to the forces acting on them obtained from the direct interaction of fluid elements with the particle surface. First the temporal evolution and the PDF's of the forces and moments acting on the particles and the resulting velocities in the axial and radial direction are analysed in dependence of axis ratio and Stokes number. It is observed that the rms velocity and the rms angular velocity in longitudinal and in radial direction are not very different for the considered particles, even though the rms forces can differ more than 100% and the rms torque more than 1000% in both directions. The forces and moments in the radial direction and their fluctuations increase with the axis ratio, as the projected area of the particles in the radial direction becomes larger than that in the axial direction. This is clearly observed in the correlations between the forces in the axial and radial direction, which are random for all considered particles. Furthermore, it is found that the rms particle velocity decreases with increasing axis ratio and the rms particle angular velocity has a maximum at an axis ratio of about 2.0. The ratio of the rms velocity of the particle to that of the fluid decreases with increasing Stokes number. The ratio between the rms angular velocities also decrease, but at a much lower rate.

Introduction

The numerical computation of particle-laden flows relies mostly on the assumption that the particles are spherical and smaller than the Kolmogorov scale. However, quite often particles are considerable larger and may therefore not be considered as point masses. Consequently the particles and the flow around it need to be resolved by the numerical grid. Such kind of simulations are so far mainly done for laminar flows using finite element approaches with adaptive grids or the force coupling method (often also called immersed boundary method). The finite element method is computationally very expensive since the grid has to be adapted to the surface of the particle at every time step (Hu 1996). The immersed boundary method approximately resolves the particle surface by an additional force term in the Navier-Stokes equations. This method is numerically more efficient since the numerical grid is fixed and may have a

simple structure (Lomhold et al. 2002). The motion of resolved spherical particles in turbulent flows including particle collisions was studied by Ten Cate et al. (2004) applying the Lattice-Boltzmann-Method which allows for a rather simple treatment of the boundary condition at the particle surface.

Numerical simulations on the behaviour of non-spherical particles in laminar or turbulent flows, which are from the practical point of view more important, are however found less frequent. Laminar flows around fixed non-spherical particles (i.e. mostly ellipsoids) were simulated in order to evaluate the forces acting on such particles as a function of orientation (e.g. Dwyer and Dandy 1990, Comer and Kleinstreuer 1995 and Hölzer and Sommerfeld 2009). Such kind of simulations is for example necessary for evaluating the resistance coefficients of non-spherical particles at larger particle Reynolds numbers. An analysis of the motion and oscillation behaviour of resolved non-spherical particles (i.e. ellipsoidal particles and cylinders) in a simple shear flow was performed by Ding and Aidun (2000) and in a Couette flow by Qi and Luo (2003).

Numerical simulations of turbulent particle-laden flows are so far mainly performed on the basis of the point-particle assumption, implying that the non-spherical particles are smaller than the Kolmogorov length scale and hence Stokes flow applies where analytic relations for the different forces are available. The flow field is generated by a random process or direct numerical simulations (DNS). The particle motion is calculated accounting for translation and rotation which implies that also the change of particle orientation is obtained. In the work of Olson and Kerekes (1998) as well as Olson (2001) the motion of fibres in turbulent flow was studied and the dispersion coefficients of these particles were derived. It was shown that the dispersion coefficient decreases as the ratio of fibre length to integral length scale increases. A similar result was also obtained by Fan and Ahmadi (1995) for a pseudo-turbulence field simulated by a Gaussian random model. The dispersion and deposition of ellipsoidal particles in turbulent channel flow was analyzed by Zhang et al. (2001) on the basis of DNS and assuming point-like particles, where translation, rotation and orientation are tracked. For different size and aspect ratio the particle fluctuating behaviour and their dispersion was studied.

Hence, for turbulent flow conditions detailed studies on the dispersion of non-spherical particles are not available. Therefore, the Lattice-Boltzmann-Method was applied to analyse the behaviour of resolved cylindrical particles in homogeneous isotropic turbulence. The ratio of the volume equivalent particle diameter to the Kolmogorov length scale studied here is about 12. In a first

step, the difference in motion of elongated cylindrical particles in longitudinal and radial direction is analyzed. Secondly, the dependence of the particle rms velocity and rms angular velocity on the Stokes number and the axis ratio is determined.

Numerical method

The fluid flow is simulated by the Lattice-Boltzmann-Method (LBM) which is an alternative approach to conventional methods for numerically solving the conservation equations. Whereas conventional models are based on the conservation laws formulated at the macroscopic level, the Boltzmann equation describes the behaviour of fluids at a microscopic level (i.e. the discrete motion of small fluid elements). The Lattice-Boltzmann-Method is based on the Boltzmann equation (He and Luo 1997) which describes the change of state of the fluid using a probability distribution function $f = f(\underline{x}, \underline{e}, t)$, declaring the probability of a fluid element to be present at position $\underline{x}$ moving with a velocity of $\underline{e}$ at a certain instant of time t :

$$\left(\frac{\partial}{\partial t} + \underline{e} \cdot \nabla \right) f(\underline{x}, \underline{e}, t) = -\frac{1}{\tau} \left(f(\underline{x}, \underline{e}, t) - f^{(0)}(\underline{x}, \underline{e}, t) \right) \quad (1)$$

The three-dimensional phase space is discretised into cubic cells and nineteen discrete velocities in this case (called D3Q19 model, Qian et al. 1992), i.e. one velocity vector for fluid elements at rest ($\sigma = 0$), six vertical or horizontal velocity vectors ($\sigma = 1$), and twelve diagonal velocity vectors ($\sigma = 2$). The velocity vectors are illustrated in Fig. 1 and read:

$$\underline{e}_{\sigma i} = \begin{cases} (0, 0, 0), & \sigma = 0, i = 1 \\ (\pm 1, 0, 0)c, (0, \pm 1, 0)c, (0, 0, \pm 1)c, & \sigma = 1, i = 1 \dots 6 \\ (\pm 1, \pm 1, 0)c, (\pm 1, 0, \pm 1)c, (0, \pm 1, \pm 1)c, & \sigma = 2, i = 1 \dots 12 \end{cases} \quad (2)$$

with c being the lattice constant which is the ratio of space to time step ($c = \Delta x / \Delta t$). The discretised lattice Boltzmann equation with single relaxation time (BGK-model, Qian et al. 1992; Chen et al. 1992) used in the present work reads:

$$f_{\sigma i}(\underline{x} + \underline{e}_{\sigma i} \Delta t, t + \Delta t) - f_{\sigma i}(\underline{x}, t) = -\frac{\Delta t}{\tau} (f_{\sigma i}(\underline{x}, t) - f_{\sigma i}^{eq}(\underline{x}, t)) \quad (3)$$

where $f_{\sigma i}(\underline{x}, t)$ is the discrete distribution function representing the probability of finding a number of fluid elements with the velocity $\underline{e}_{\sigma i}$ at the position $\underline{x}$ and the time t , $f_{\sigma i}^{eq}(\underline{x}, t)$ being the discrete equilibrium distribution function, and τ the relaxation time. For the present simulations the relaxation time is $\tau = 0.515$. In the D3Q19 model the discrete equilibrium distribution function is:

$$f_{\sigma i}^{eq}(\underline{x}, t) = \omega_{\sigma} \rho \left(1 + \frac{3\underline{e}_{\sigma i} \cdot \underline{u}(\underline{x}, t)}{c^2} + \frac{9(\underline{e}_{\sigma i} \cdot \underline{u}(\underline{x}, t))^2}{2c^4} - \frac{3\underline{u}^2(\underline{x}, t)}{2c^2} \right) \quad (4)$$

with:

$$\omega_{\sigma} = \begin{cases} 1/3, & \sigma = 0, i = 1 \\ 1/18, & \sigma = 1, i = 1 \dots 6 \\ 1/36, & \sigma = 2, i = 1 \dots 12 \end{cases} \quad (5)$$

The macroscopic properties of the fluid, i.e. density and momentum are obtained through the equations:

$$\rho(\underline{x}, t) = \sum_{\sigma} \sum_i f_{\sigma i}(\underline{x}, t) \quad (6)$$

and

$$\rho(\underline{x}, t) \underline{u}(\underline{x}, t) = \sum_{\sigma} \sum_i \underline{e}_{\sigma i} f_{\sigma i}(\underline{x}, t) \quad (7)$$

The relaxation time determines the kinematic viscosity via the relation:

$$\nu = \frac{1}{6} c^2 (2\tau - \Delta t) \quad (8)$$

In the present study a homogeneous isotropic turbulence in a cubic box is considered. Periodic boundary conditions are imposed at the faces of the computational domain. Single cylindrical particles are moving through the computational domain according to the forces and moments acting on them. The curved no-slip boundary condition introduced by Bouzidi et al. (2001) is applied on the particle surface. This boundary condition considers the exact contour of the particle surface within a cell. The fluid forces acting on the particle are directly evaluated from the momentum exchange between the fluid elements and the particle surface (Bouzidi et al. 2001, Mei et al. 2002).

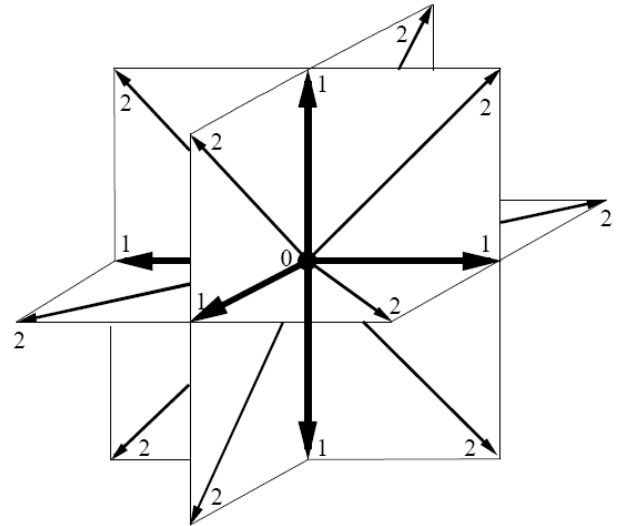


Figure 1: Discrete velocity vectors in the D3Q19 model.

Turbulence forcing

Isotropic turbulence is forced by a spectral method (Eswaran and Pope 1988), where a turbulent motion is excited at small wave numbers (large length scales). For this purpose, a force $\underline{f}$ is generated via the Fourier transformation:

$$\begin{aligned} \underline{f}(\underline{x}) &= \frac{\underline{a}_0}{2} + \sum_{k=1}^{\infty} \underline{a}_k \cos(\omega \underline{k} \cdot \underline{x}) + \sum_{k=1}^{\infty} \underline{b}_k \sin(\omega \underline{k} \cdot \underline{x}) \\ \underline{a}_k &= \frac{2}{L} \int_0^L \underline{f}(\underline{x}) \cos(\omega \underline{k} \cdot \underline{x}) d\underline{x} \\ \underline{b}_k &= \frac{2}{L} \int_0^L \underline{f}(\underline{x}) \sin(\omega \underline{k} \cdot \underline{x}) d\underline{x} \end{aligned} \quad (9)$$

where L is the length of one period and $\omega = 2\pi/L$ the angular frequency. In this study the forcing acceleration is defined by wave numbers $k_i \leq 2$, $\underline{a}_0$ is set equal to zero, and $\underline{a}_k$ and $\underline{a}_{-k}$ are determined by a Gaussian random process. The generated turbulence intensity is characterised by the standard deviation of a Gaussian distribution. Typical turbulence parameters are the turbulent kinetic energy k , the dissipation rate ε , the Kolmogorov, Taylor and integral length and time scales, and the Taylor Reynolds number Re_τ . The values obtained for the considered homogeneous isotropic turbulence in a cubic box of $60 \times 60 \times 60$ equidistant cells are summarized in Table 1. All values are made dimensionless by using Δx and Δt , respectively. For the present simulations the Kolmogorov length scale is about one half of the mesh size. Fig. 2 shows a turbulent flow field including a single cylindrical particle and Fig. 3 the corresponding energy spectrum. As mentioned above, the forcing is applied at the first two wave numbers. The $-5/3$ line associated with the inertial sub-range (Kolmogorov spectrum) is additionally plotted in Fig. 3. However, a true inertial sub-range does not exist due to the rather low Reynolds number of the simulation.

v	0.05
k	0.00075
ε	1.10E-06
λ_K	0.5806
λ_T	5.8387
λ_{Int}	8.9
τ_K	67.42
τ_T	314.11
τ_{Int}	398.02
Re_T	26.112

Table 1: *Properties of the homogeneous isotropic turbulence (made dimensionless by Δx and Δt).*

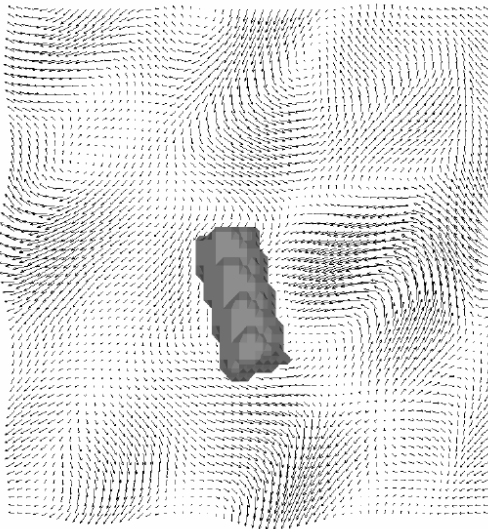


Figure 2: *Instantaneous velocity field of a turbulent flow including a single particle for an arbitrary slice through the computational domain (the ruggedness of the particle is a result of the plotting software).*

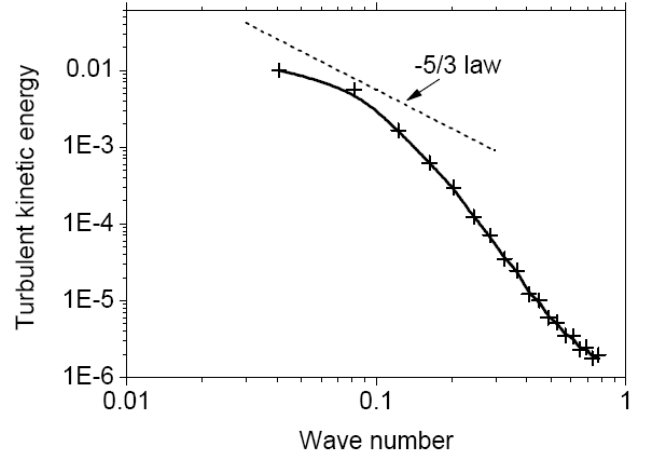


Figure 3: *Energy spectrum of the turbulent flow field.*

Results

In the present simulation cylindrical single particles were suspended in a homogeneous isotropic turbulent flow field and were allowed to translate and rotate freely with linear velocity $\underline{u}_{Pa}$ and angular velocity $\underline{\omega}_{Pa}$. Four cylindrical particles with a length to diameter ratio of $l/d = 1, 2, 3$, and 4 are considered. All particles have an identical volume equivalent diameter d_{Pa} of 12 cells. For changing the particle Stokes number, which describes the ability of a particle to follow the fluid flow, the particle material density was adjusted accordingly (i.e. $\rho_p = 250, 500, 1,000$ and $10,000 \text{ kg/m}^3$). The Stokes number used is based on the integral time scale (see Table 1) and is defined as:

$$St = \frac{\rho_{Pa} d_{Pa}^2}{18 \nu \tau_{int}} \quad (10)$$

With a fluid density of 1000 kg/m^3 , four particle Stokes numbers, i.e. 1, 2, 4, and 40, are obtained.

All the simulations were run over more than 250,000 time steps to guaranty a reliable statistical averaging. For analysing the particle behaviour, first the distribution functions of normalised forces, torques, linear velocities and angular velocities are considered. They are more or less Gaussian distributed, as particle motion is induced by the Gaussian fluid turbulence. The frequency distributions of the forces and moments acting on the particle strongly depend on the length to diameter ratio. For a small Stokes number particles with $l/d = 4$, the frequency distribution of the radial force and moment are wider than those in the axial direction (Fig. 4). The radial and axial directions are determined for a coordinate system fixed to the major axes of the particle. This behaviour is a consequence of the fact that the projected area of the particle in the radial direction is considerable larger than in axial direction whereby the particle views a larger spectrum of fluid fluctuations in the radial direction. This yields much broader frequency distributions for the radial components, where the momentum acting on the particle is more sensitive to this effect (Fig. 4). For an axis ratio of $l/d = 1$ (not shown here) the frequency distributions of the axial and radial forces are almost identical for all Stokes numbers. However, the radial momentum distributions are nevertheless remarkably wider than the axial ones.

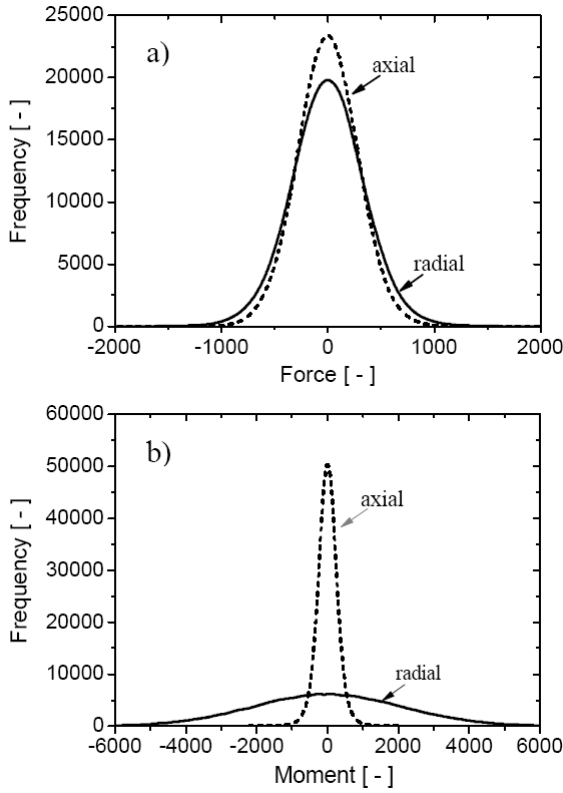


Figure 4: Frequency distributions of the radial and axial forces (a) and moments (b) for a cylindrical particle with $St = 1$ and $l/d = 4$.

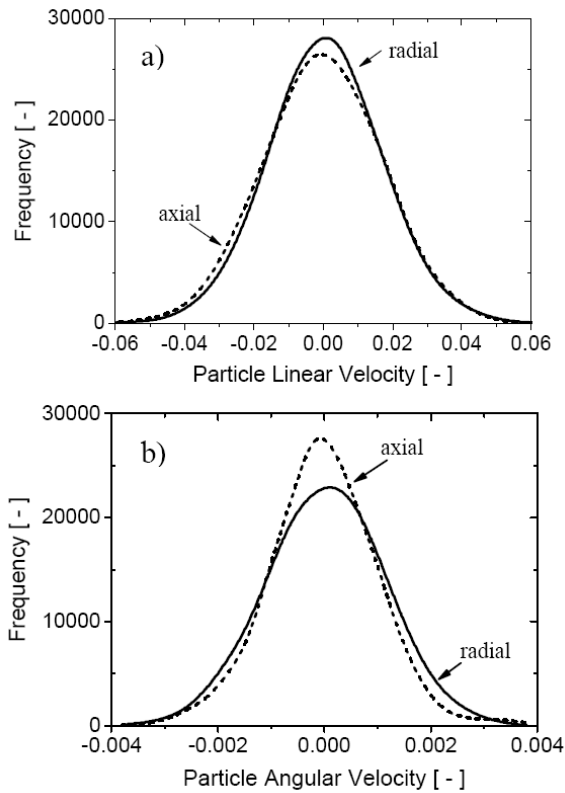


Figure 5: Frequency distributions of the radial and axial linear (a) and angular (b) velocities for a cylindrical particle with $St = 1$ and $l/d = 4$.

As inertial particles need some time to respond to the force and moment actions, their velocities (linear and angular) are changing with some delay and exhibit less fluctuations than the forces and moments (filtering effect). Hence, the particle velocity histories (see Fig. 6) and the shape of the velocity distributions depend additionally on the response behaviour of the particles, i.e. the particle Stokes number. The resulting frequency distributions for the cylindrical particle with $St = 1$ and $l/d = 4$ are almost identical for the linear velocity components (Fig. 5a), since these particles follow the fluid fluctuations reasonably well. The angular velocity components are however still slightly anisotropic similar to the moments. Here the angular velocity around the axial main axis of the cylinder is slightly narrower distributed than the angular velocity around one of the radial directions. Similar observations are made for the cylindrical particles with larger Stokes numbers, but the linear and angular velocity distributions are narrower as they are not able to follow the fluid fluctuations completely.

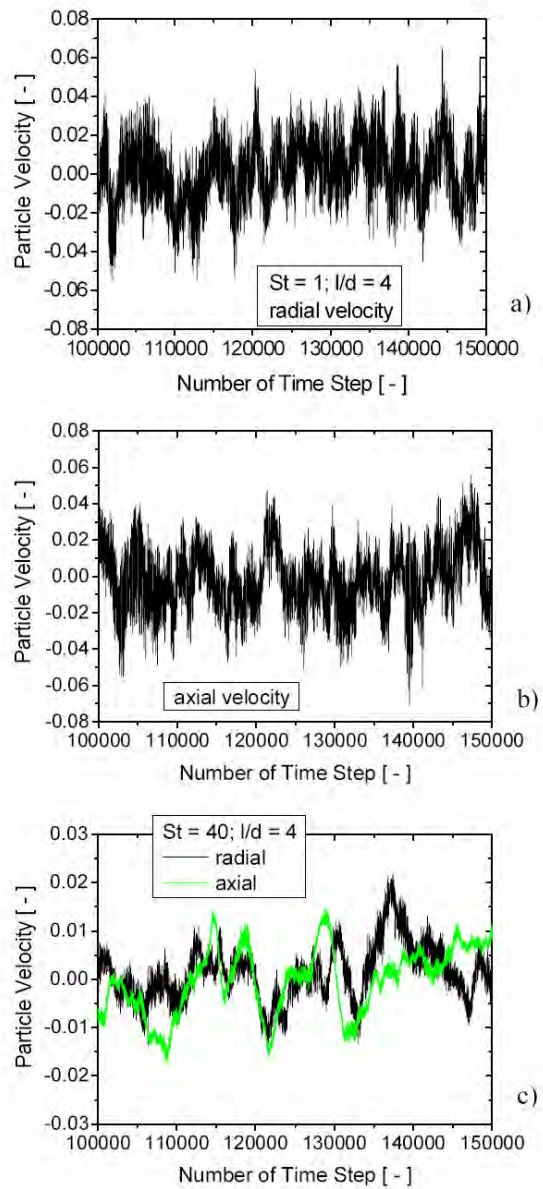


Figure 6: Temporal evolution of particle linear velocities over 50,000 time steps: a) radial velocity for $St = 1$ and $l/d = 4$, b) axial velocity for $St = 1$ and $l/d = 4$, c) radial and axial velocities for $St = 40$ and $l/d = 4$.

The particle behaviour may be also visualised by looking at the temporal history of the particle velocities (Fig. 6). For the small Stokes number particle ($St = 1$, $l/d = 4$) the fluctuations of the axial and radial velocity components are much stronger and more noisy than those for the large Stokes number particle ($St = 40$, $l/d = 4$). Although the small Stokes number particle is quite long, the axial velocity component is very similar to the radial one (Fig. 6a and b). The corresponding axial velocity component of the long heavy cylindrical particle shows clearly less noise than its radial component, but the large-scale fluctuations are almost identical (Fig. 6c). This is again caused by the larger projected area of the particle in the radial direction, whereby it views a wider spectrum of fluid fluctuations.

The interrelation between forces and linear particle velocities is illustrated in Fig. 7 based on scattering diagrams for the correlation between radial and axial components of forces and velocities. The forces (i.e. $F_{rad} = f(F_{ax})$) are randomly distributed around zero for $l/d = 1$ forming an almost symmetric three-dimensional normal distribution for all Stokes numbers (only shown for $St = 1$ in Fig. 7). For the particles with $l/d = 4$, the distribution of the forces is squeezed with the scatter of the radial component being larger than that of the axial one as already indicated by the frequency distributions (Fig. 4). The correlations between the radial and axial velocity components are not random, but exhibit a continuous behaviour for all Stokes number particles. The shape of these orbits depends on the particle response behaviour, i.e. the Stokes number. For small values of St the velocities are almost symmetrically distributed around zero in a range of -0.06 to 0.06 (Fig. 7) and do not show any specific tendency to respond to the different scales of turbulence. Large Stokes number particles are not able to follow the fluid fluctuations completely and have much lower velocities (i.e. ± 0.02). Their orbits show some large-scale structure coming from the reaction on the most energetic turbulent eddies. The small amplitude variations of the particle velocities are due to the interaction of small eddies with the particle. Again these variations are larger in the radial direction than in the axial one for elongated cylinders.

In a second step, the influence of the axis ratio and the Stokes number on the particle response to the turbulent fluctuations was analysed by sampling their velocity over the entire computational time. Since the fluctuations of the particles may be anisotropic the considered rms values are the averages of all three components. The relative particle rms values (i.e. relative to the fluid rms velocities) of the linear and angular velocity at $St = 1, 2, 4$ and 40 are plotted over l/d in Fig. 8 and 9, respectively. Naturally the relative particle rms values of the linear and angular velocity decrease with increasing St . Fig. 10 shows this behaviour more clearly for particles with $l/d=1$. It is obvious, that the relative rms of the linear velocity decreases much stronger than that of the angular velocity with increasing Stokes number.

Fig. 8 shows that the particle rms velocity clearly decreases with increasing l/d . This trend is somewhat stronger for lower St . In contrast, the particle rms angular velocity (Fig. 9) first increases with l/d , reaches a maximum at about $l/d = 2.0$ and then decreases again. This behaviour is observed mainly for the smaller Stokes numbers. At the highest Stokes number considered (i.e. $St = 40$), the relative rms angular velocity is almost independent of l/d .

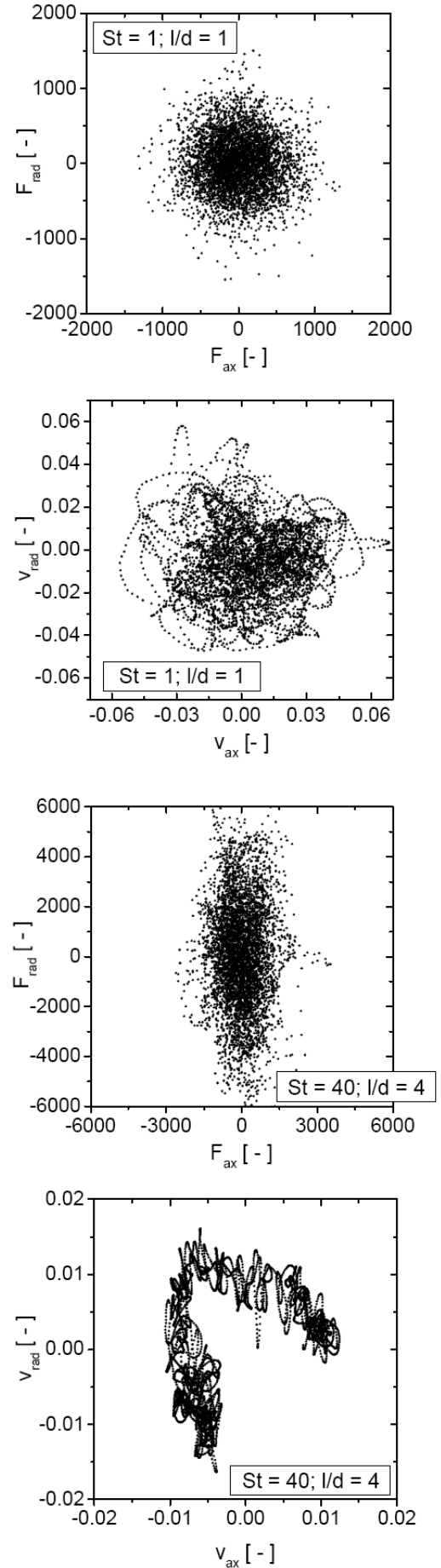


Figure 7: Correlations between radial and axial components of particle forces and velocities; upper two graphs: $St=1$ and $l/d=1$; lower two graphs: $St=40$ and $l/d=4$.

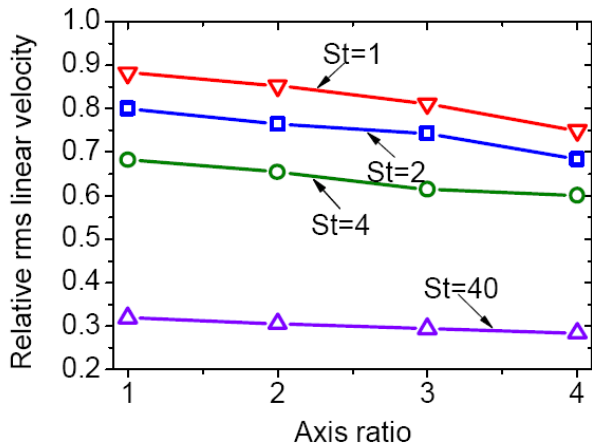


Figure 8: Relative rms linear velocity of a cylindrical particle as a function of the axis ratio at $St = 1, 2, 4$, and 40 .

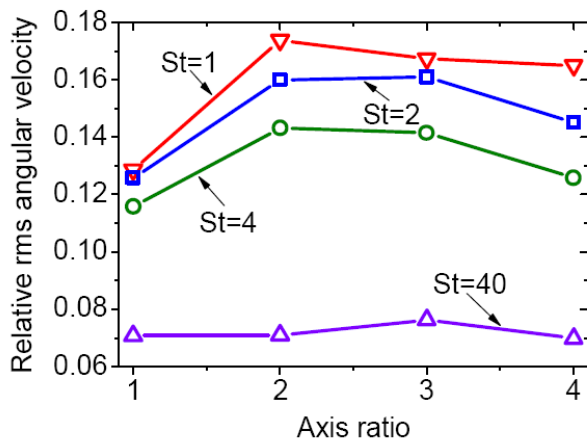


Figure 9: Relative rms angular velocity of a cylindrical particle as a function of the axis ratio at $St = 1, 2, 4$, and 40 .

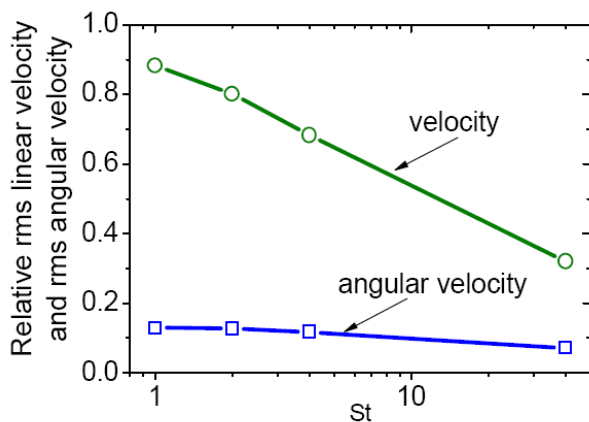


Figure 10: Relative rms velocity and angular velocity of cylindrical particles with $l/d = 1$ as a function of the Stokes number.

Conclusions

The rms velocity of elongated cylindrical particles decreases with increasing axis ratio, all particles having the same volume. This is due to the averaging of the turbulent fluid fluctuations over the particle surface which increases with increasing axis ratio. Thus, it can be concluded that the best dispersion of particles suspended in a turbulent flow is achieved for spherical particles, since they have the smallest surface area per volume. In contrast, the particle rms angular velocity first increases to a maximum at about $l/d = 2.0$ and then decreases. This is probably caused by the additional effect of the change of the moment of inertia with l/d . The value of the moment of inertia around the longitudinal axis decreases and around the radial axis increases with increasing l/d , which would lead to higher and lower rms angular velocities, respectively.

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AN IMMERSED BOUNDARY METHOD FOR INTERACTING PARTICLES

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Abstract

This paper describes a novel implicit immersed boundary method (IBM) implementation for simulating the detailed flow around arbitrary moving bodies. An implicit immersed boundary method (Mark and van Wachem (2008)) uses a non-boundary conforming grid in the whole domain, to enable efficient solution of the flow equations, and a Lagrangian representation of the boundary of an arbitrary particle (the immersed boundary) to determine the behaviour of the particle. The boundary of the particle is triangulated and at the intersections of the triangles with the grid, so-called immersed boundary conditions are applied. The implicit immersed boundary condition used in this work, mirrors the velocity field along the normal of the local triangulated immersed boundary (IB) segments such that the fluid exactly follows the IB. As a result, a fictitious velocity field inside the immersed boundary is developed, which is excluded from the discretized Navier-Stokes equations to preserve mass. The numerical method is based on a finite volume approach on a collocated variable arrangement with a fully coupled pressure-velocity solver.

The validation of the method presented in this paper is determining the lift force of a rotating sphere in a low Reynolds number flow. Due to the rotation, a lift force develops called the Magnus effect, see Rubinow and Keller (1961). In the simulations, the Reynolds number, the diameter of the sphere, and the mesh spacing are varied to show the method has a second order accurate prediction of the drag and lift force on the sphere.

Introduction

Multiphase flow problems occur in a wide range of industrial processes as well as in many natural environments. Multiphase flow is most often characterized by a range of different length scales which results in difficulty in understanding such flow problems, both from a physical as well as from a numerical point of view. Although still very much under development for multiphase flows, computational fluid dynamics (CFD) has been shown to be a valuable research tool in the multiphase flow area. CFD can be used to gain insight of flow phenomena at large scales, but can also be used as an accurate tool to study phenomena at the scales of individual particles. Currently, multiphase CFD at the large scale relies heavily on closure models, often empirically determined, and is far from mature. A thorough understanding of the physical phenomena at the particle scale is required to understand and control the global process, leading to new insights and closure models which can be employed to develop and validate closure models applicable at the large scales. This paper focusses on deriving models to accurately describe and predict the flow at the scale up to that of a few particles. This requires a framework to capture the flow around a number of complex

interfaces.

There are different approaches that can deal with the flow around moving complex geometries, probably the first and most well-known is the Arbitrary Lagrange-Euler (ALE) formulation, originally presented by Hirt et al. (1974). In Hu (1996); Hu et al. (2001) an ALE method is derived and validated to accurately predict the behaviour of two-dimensional fluid-solid flows. The method employs a Galerkin finite element method based on a moving unstructured mesh. The method works well and is stable for relatively high Reynolds numbers, but the regeneration of the mesh is computationally very expensive. Moreover, the necessity of projecting the solution from one grid to another may lead to loss of accuracy. To avoid the re-meshing, three new non-boundary conforming methods have been developed: Cartesian, (e.g. Noh (1964); Kirkpatrick et al. (2003)) Lagrange multiplier, (e.g. Glowinski et al. (2001, 1994)) and the immersed boundary method, (e.g. Peskin (1977); Lai and Peskin (2000); Goldstein et al. (1993); Silva et al. (2003); Oliveira et al. (2005); Mark and van Wachem (2008)). This paper will focus on the immersed boundary method (IBM).

The immersed boundary methods have been pioneered by Hirt et al. (1974) and Peskin (1977), and are capable of simulating the flow around a body using a mesh which does not conform to the geometry of the body. With this methodology, it is in principle possible to determine the flow around an arbitrary geometry while employing a simple discretisation grid. The mesh used to represent the immersed body is independent of the fluid grid, which allows the body to displace relative to the fixed grid used to discretize the fluid equations. The IBM becomes an efficient alternative to the classical body-fitted/re-meshing methods to handle moving boundaries problems. The immersed boundary method has been successfully applied in many fields.

The Implicit Method: MIBM

A new method called mirroring immersed boundary method (MIBM) recently published by Mark and van Wachem (2008) was implemented in a fully coupled framework. This method imposes effect of the immersed body on the flow by directly modifying the Navier-Stokes coefficients obtained from the discretization process, which includes the desirable boundary condition at the first time-step iteration; there are no outer iterations required.

In the MIBM method the interface, Γ , is used to map the fluid mesh defining a three subsets of points (see Figure 1): $\vec{x}_i$ points inside the interface, $\vec{x}_{ib}$ points inside and near the IB interface and $\vec{x}_e$ points outside the interface.

The method directly mirrors the external velocity over the interface Γ . The internal immersed-boundary velocities, $\vec{u}_{ib}$, are set in the opposite direction of the exterior normal velocities, $\vec{u}_e$, plus the immersed-boundary velocity, $\vec{u}_{ib}$, such that

the velocity constraint is enforced at the interface Γ :

$$\vec{u}_{iib} + \vec{u}_e = 2\vec{u}_{ib}. \quad (1)$$

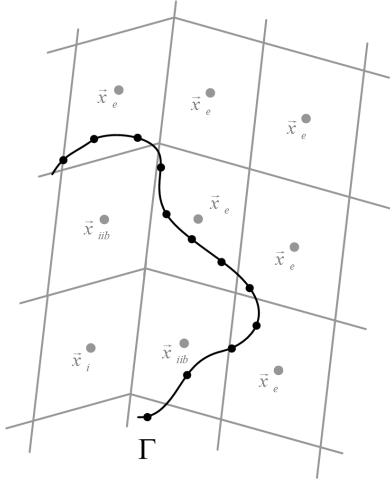


Figure 1: Mapping of the cell centered fluid cells, MIBM method.

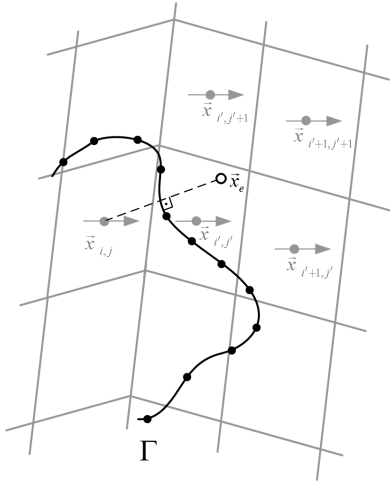


Figure 2: A 2D representation of the MIBM method, the exterior normal point $\vec{p}_e$ with its surrounding interpolation points.

This is done by setting a fictitious exterior normal point, as depicted in Figure 2. The mirror point is defined as the $\vec{x}_{iib}$ mirrored along the normal of its closest interface point. Hence the smallest distance between the interface and the fictitious point $\vec{x}_e$ are the same.

$$\vec{x}_e = \vec{x}_{iib} + 2d\vec{n} \quad (2)$$

If the exterior normal point coincides with a discrete velocity point, the application of the Dirichlet condition is trivial. More generally, the exterior normal point lies between the discrete velocity points and therefore the velocity needs to be implicitly interpolated using the surround points. The IIB velocity can then be set to the reversed interpolated velocity plus the boundary velocity. The interior velocities are set to the boundary (IB) velocity.

Interpolation of various variables in the three dimensional discretized spaces is frequently required. In this working an inverted weighted interpolation is used. The inverse distance weighted methods are based on the assumption that the interpolating points should be influenced most by the nearby points and less by the more distant points. Several options are

available for inverse distance weighted interpolation; the simplest form is referred to as Shepard's method. The equation used is as follows:

$$w_i = \frac{h_i^{-2}}{\sum_{j=1}^n h_i^{-2}} \quad (3)$$

where h_i is the distance from the scatter point to the interpolation point.

The inverse weighted distance is forced to have a minimum number of the data points, however the choice of the maximum number of data points is arbitrary. In this work a fixed amount of eight points ($n = 8$), that define an interpolation box surround the interpolation point, is employed.

Calculation of the Forces

The total force on the immersed object consists of two contributions, i.e. the pressure force and the viscous force. These forces are integrated over the interface Γ .

$$F_i = \int_{\Gamma} (-p\delta_{ij} + \tau_{ij}) n_j dS \quad (4)$$

In order to proceed with the numerical calculation of the forces acting at the body, the interface Γ must be discretized. In our work, we have used a triangulation process to discretize the immersed boundary. The contribution of each individual triangle of the triangulated immersed boundary is determined and summed up to get the total surface force acting on the body. In order to discretize the force terms, auxiliary points are introduced, as is shown in Figures 3 and 4.

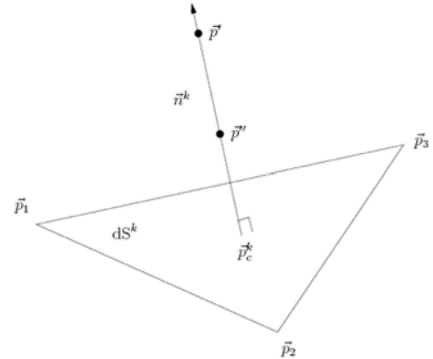


Figure 3: Triangle k in the triangulation of the immersed-boundary interface Γ with the exterior points, $\vec{p}'$ and $\vec{p}''$.

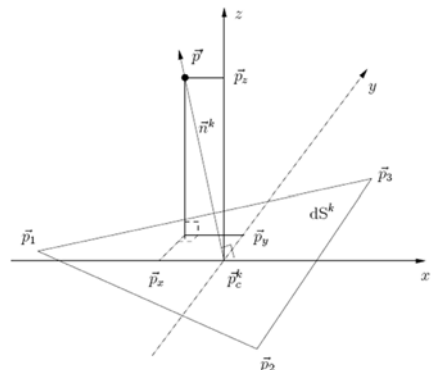


Figure 4: Triangle k with the projection of $\vec{p}_p$ onto the coordinate axes ($\vec{p}_x, \vec{p}_y, \vec{p}_z$).

The evaluation of the pressure force is done with the help of two auxiliary points $\vec{p}'$ and $\vec{p}''$ which lie on the normal of the triangle. The pressure is interpolated onto the auxiliary points and then extrapolated onto the centre of the triangle,

$$P_c = 2P'' - P' \quad (5)$$

To evaluate the viscous part, the tensor τ_{ij} is needed at the center of each triangle. This is done by introducing three new points, $\vec{p}_x'$, $\vec{p}_y'$ and $\vec{p}_z'$ which are the projections of auxiliary point $\vec{p}'$ onto the Cartesian axes. The fluid velocities are interpolated onto these points.

Fully Implicit Solving of Flow Equations

The flow outside of the immersed objects is modeled by the Navier-Stokes equations. The continuity equation, equation 6, and the momentum equation, equation 7, for viscous and incompressible flows can be written as:

$$\frac{\partial u^i}{\partial x^i} = 0, \quad (6)$$

$$\rho \frac{\partial u^j}{\partial t} + \rho \frac{\partial}{\partial x^i} (u^i u^j) = -\frac{\partial p}{\partial x^j} + \frac{\partial \tau_{ij}}{\partial x^i} - R u^j - S^j, \quad (7)$$

where source terms are given by S^j , which is a general source term and a linearized source term R . The τ_{ij} represents the stress tensor:

$$\tau_{ij} = \mu \left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} \right). \quad (8)$$

The cell centered finite volume discretization at P of the velocity terms for one direction of the equation 7, is of the form:

$$\left[\frac{\rho V_P}{\Delta t} + a_P^{(u^j)} + V_P R_P^{(u^j)} \right] u_P^j = \left[\sum_{nb} a_{nb}^{(u^j)} u_{nb}^j \right]_P - V_P \left[\sum_{nb} b_{nb}^{(j)} P_{nb} + S^{u^j} \right] + \left[\frac{\rho V_P}{\Delta t} \right]_P u_P^{j,O},$$

where a is a coefficients that combines the convective and shear terms, and b is obtained from the discretization of the pressure gradient.

Discretization of the Continuity Equation

Considering the single phase flow continuity equation, equation 6, in its discretized form

$$\sum_{f=\text{faces}} M_f = \sum_{f=\text{faces}} u_f^i s_f^i = 0 \quad (9)$$

The coefficients for the continuity equation are determined by the momentum weighted interpolation. The objective is to obtain an expression for the face velocity u_f^i from the averaged momentum equations. The net force driving the flow in equation 9 is given by, and now is redefined as

$$\widetilde{\frac{\partial p}{\partial x^j}} = \left[\frac{\partial p}{\partial x^j} + S^{u^j} \right] \quad (10)$$

It is important to treat the pressure gradient and the sources similar, as their sum is the contribution to accelerating the fluid. With this, equation 11 becomes

$$\left[1 + \frac{\rho}{\Delta t} \frac{V_P}{a_P^{(u^j)} + V_P R_P^{(u^j)}} \right] u_P^j = \frac{\left[\sum_{nb} a_{nb}^{(u^j)} u_{nb}^j \right]_P}{a_P^{(u^j)} + V_P R_P^{(u^j)}} - V_P \frac{\left[\frac{\partial p}{\partial x^j} \right]_P}{a_P^{(u^j)} + V_P R_P^{(u^j)}} + \left[\frac{\rho}{\Delta t} \right]_P \frac{V_P}{a_P^{(u^j)} + V_P R_P^{(u^j)}} u_P^{j,O} \quad (11)$$

After which a number of abbreviations are introduced,

$$c = \frac{\rho}{\Delta t} \quad (12)$$

$$d^{(u^j)} = \frac{V_P}{a_P^{(u^j)} + V_P R_P^{(u^j)}} \quad (13)$$

$$\tilde{u}^j = \left\{ \frac{\left[\sum_{nb} a_{nb}^{(u^j)} u_{nb}^j \right]_P}{a_P^{(u^j)} + V_P R_P^{(u^j)}} \right\} \quad (14)$$

With this discretization stencil, an equation for the velocity at all nodal points can be expressed. To proceed with discretization of the continuity equation, the values of the velocities are required at cell faces or integration points. In our approach, a weighted, analogous equation can be written down for the velocity at the cell faces,

$$\left[1 + c_{e'} d_{e'}^{(u^j)} \right] u_{e'}^j = \tilde{u}_{e'}^j - d_{e'}^{(u^j)} \left[\frac{\partial p}{\partial x^j} \right]_{e'} + c_{e'} d_{e'}^{(u^j)} u_{e'}^{j,O} \quad (15)$$

The point e' lies in the center of the line connecting the nodes P and E , therefore the weighting coefficient will be exactly $\frac{1}{2}$. An expression for the velocity $\tilde{u}_{e'}^j$ is obtained by linear interpolation using the velocity expressions for points E and P .

$$\tilde{u}_{e'}^j = \frac{1}{2} (\tilde{u}_P^j + \tilde{u}_E^j) \quad (16)$$

The expression for $\tilde{u}_{e'}^j$, can be substituted in equation 15. This equation can then directly be used to close the discretized continuity equation outside of the region occupied by the immersed boundary. At the immersed boundary, the interpolation coefficients from the MIBM are employed to find the velocity. This approach leads to a fully coupled system in the form of

$$\begin{pmatrix} \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ p \end{pmatrix} = \begin{pmatrix} RH_{u_1} \\ RH_{u_2} \\ RH_{u_3} \\ RH_p \end{pmatrix} \quad (17)$$

which can be solved iteratively.

Results and Discussion

To validate the method, simulations of an isolated rotating sphere in a uniform crossflow are performed for different rotation velocities, fluid velocities, and mesh resolution. The computational domain is a unitary cube, with an inflow condition on one side, an outflow condition on the other side, and a mirroring boundary condition on all walls. The sphere in all simulations has 1280 trigangles. The sphere center is placed at the center of computational domain and it has a diameter between $D = 0.1 \text{ m}$ and $D = 0.25 \text{ m}$. The timestep in the simulation is taken to correspond with a CFL number of 0.99.

However, for the steady-state solution which exists for these low Re number cases, the size of the timestep did not matter.

The lift force develops due to the rotation of the sphere, and is shown in figure 5. This lift force is caused by the Magnus effect. The sphere rotation produces an asymmetry in the velocity field causing a pressure differential between the two sides of the sphere.

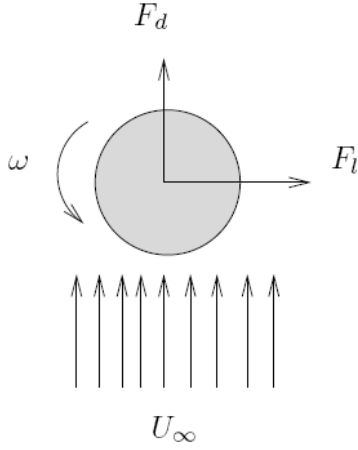


Figure 5: Magnus force (lift) due to sphere rotation.

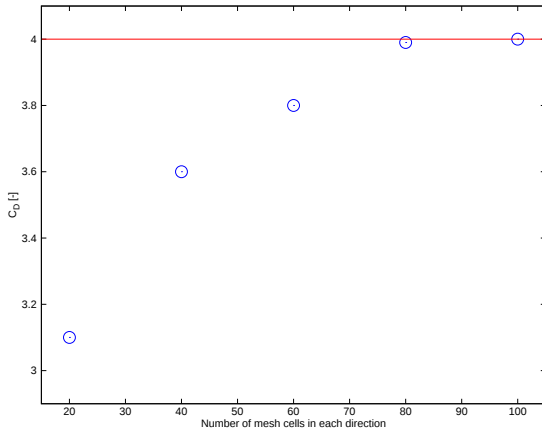


Figure 6: The prediction of the lift coefficient for $Re_D = 0.5$ as a function of the number of cells in each direction. The top line indicates the theoretical prediction of Rubinow and Keller (1961).

The rotational speed of the sphere is usually represented by a ratio of the tangential velocity of the sphere to the fluid stream velocity

$$\gamma = \frac{d\omega}{2U_\infty} \quad (18)$$

A theoretical solution for $Re_D < 1$ has been developed by Rubinow and Keller (1961) and shows that the lift force, for a rotating sphere, can be expressed in terms of the rotational speed (γ),

$$C_l = 2\gamma \quad (19)$$

The lift force coefficient calculated numerically is given by

$$C_l = \frac{2f_l}{\rho_f \mu A U_\infty^2} \quad (20)$$

Figure 6 shows the predicted lift coefficient of the mesh refinement study performed for the rotating sphere. The coarsest mesh consisted out of 20^3 cells in each direction, and the finest mesh out of 100^3 cells. The line corresponds with the Rubinow and Keller theory. The figure shows that the drag improves quickly as the mesh is refined. A curve fit shows the convergence behaviour with respect to mesh spacing is second order.

In figure 7, the symbols show the prediction of the lift coefficient for various sphere diameters and the line shows the prediction given by equation 20. In these simulations, the flow velocity at the inlet was kept constant and the size of the domain scaled with the diameter of the sphere. The number of discretisation points in each direction is 60, leading to 216,000 mesh cells.

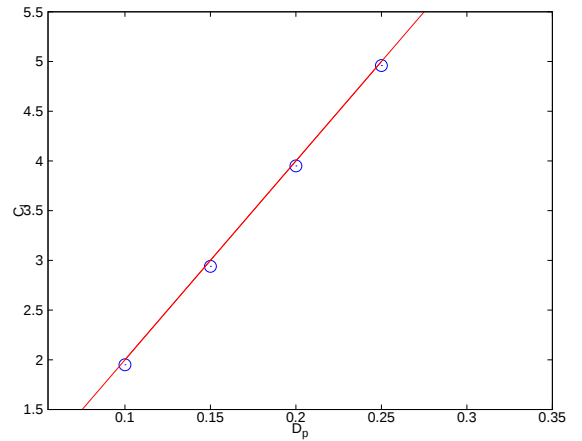


Figure 7: The prediction of the lift coefficient with a fixed inlet velocity for various sizes of spheres (symbols) compared to the theoretical prediction of Rubinow and Keller (1961) as depicted by the line.

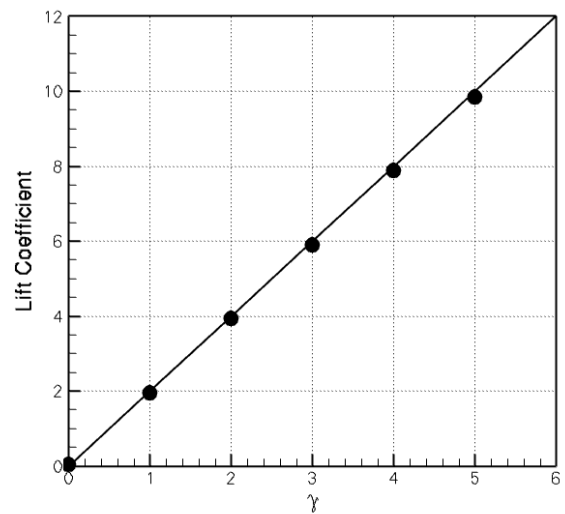
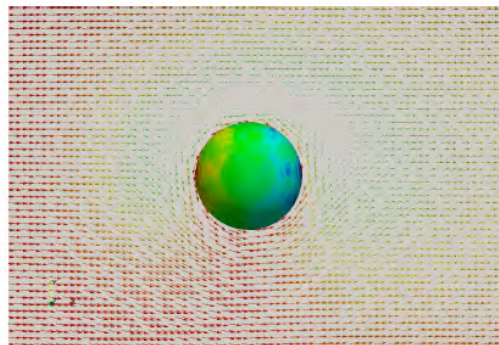


Figure 8: Comparison between theoretical and simulated results for C_l at $Re_D = 0.5$.

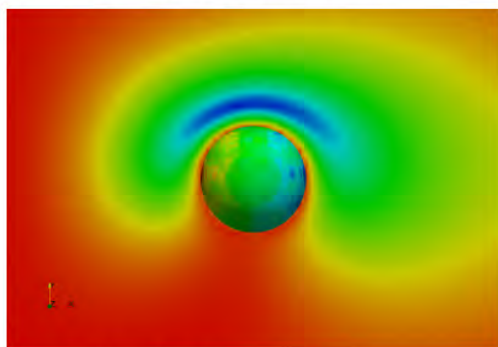
Figure 8 shows a comparison between lift coefficients predicted by numerical simulation using the MIBM method, for $Re_D = 0.5$ and the theoretical data. These predictions agree well with theory. This confirms a good accuracy of

the method to impose a desirable boundary condition at the interface.

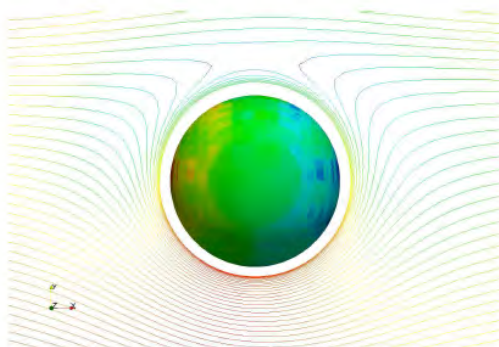
The flow pattern is shown in Figure 9. From this figure, the appropriately achieved no-slip boundary condition on the surface of the sphere can be clearly seen. The velocity of the fluid near the sphere is gradually modified by the influence of the rotation of the sphere, producing a strong flow asymmetry.



fluid velocity vectors



fluid velocity magnitude



fluid streamlines

Figure 9: Representations of the flow around the rotating sphere with $Re_D = 0.5$.

Computational Performance

The implementation of the IB methods implies an extra computational cost to perform all interpolation procedures and setup the appropriated IB coefficients. The impact of this implementation depends, of course, of the refinement of the triangulation in the interface. Considering a fluid grid of $40 \times 40 \times 40$ at Reynolds 1, the extra cost to insert a immersed sphere with 1280 triangles is about 13%, including the calculation of the forces in each time step. The cost only due to setting the IB coefficients is less than 4% for this simulation.

Conclusions

This paper describes the derivation, implementation and validation of a transient immersed boundary method implemented in a fully coupled framework; *i.e.* each time-step advancement requires inverting only one matrix. The method is validated with the theoretical findings of a rotating sphere in a fluid, described by Rubinow and Keller (1961), and the results show the method is accurate already for a relatively course mesh. The next steps will be to perform multiple moving particles a moderate Reynolds numbers.

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MODELLING HIERARCHIES IN DISPERSED MULTIPHASE FLOWS

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1 Introduction

A major challenge in the area of dispersed multiphase flows is to be able to describe the entire flow field generated by collections of large number of discrete elements (droplets, particles, bubbles) moving relative to an incident flow. There are various degrees of representation from fully resolved to point-particle representation, through to distributed drag formulations. In this paper we consider the problem of flow past a fixed array of bodies in a uniform unbounded flow. The aim is to develop a rational criterion for deciding when each of these modelling approaches can be applied. The theory and discussion we introduce is valid for both two and three-dimensional flows. The comparison we make is quite a severe as it involves inertially dominated planar flow past a group of cylinders, where the flow interaction is much stronger than for instance, sphere, and where recent fully numerical results enable us to examine these questions in much more detail.

2 Hierarchy of mathematical models

Consider N_C rigid bodies (diameter D) within a localised region V_G (diameter D_G) held in an incident flow U (figure 1(a)). In this section we define the different modelling approaches which are used. The Reynolds numbers based on the group and individual bodies are $Re_G = D_G U / \nu$, $Re = D U / \nu$, respectively.

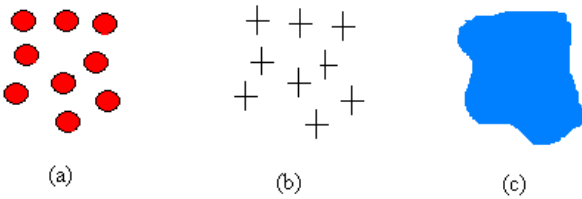


Figure 1: *Schematic of the three modelling approaches: (a) fully resolved, (b) point-particle representation and (c) distributed drag approach.*

2.1 Fully resolved calculations

The fully resolved calculation of the flow $\mathbf{u}$ past a group of bodies involves solving

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau}, \quad (1)$$

over the whole domain where p is pressure and $\boldsymbol{\tau}$ is the stress-tensor. The boundary conditions applied are $\mathbf{u} \cdot \hat{\mathbf{n}} = 0$, $\mathbf{u} \times \hat{\mathbf{n}} = \mathbf{0}$, on each of the surfaces S_i ($i = 1, \dots, N_C$). The kinematic and no-slip boundary conditions each play different roles in the impact of a

body on the ambient flow, with the kinematic leading to a localised blocking while the no-slip generates the vorticity at the surface which is advected downstream. The force on the i -th body located at $\mathbf{x}_i$ is

$$\mathbf{F}_i = \int_{S_i} (p\mathbf{I} - \boldsymbol{\tau}) \cdot \hat{\mathbf{n}} dS. \quad (2)$$

2.2 Point-particle description

The point-particle description has been applied extensively in computational studies of dispersed multiphase flows (see Prosperetti & Tryggvason 2007, Chp 9) - see figure 1(b). The reduced set of equations are

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} - \sum_{i=1}^{N_C} \mathbf{F}_i \mathcal{S}(\mathbf{x}, \mathbf{x}_i). \quad (3)$$

The source function $\mathcal{S}$ satisfies $\int \mathcal{S} dV = 1$ and can take a number of forms depending on the particle diameter compared to the grid size h . For $D \ll h$, it is usual to assume

$$\mathcal{S}(\mathbf{x}, \mathbf{x}_i) = \delta(\mathbf{x} - \mathbf{x}_i). \quad (4)$$

Computationally, it is difficult to treat delta-functions and an alternative (to cope with finite sized bodies) when the bodies are larger than the element size (eg $d \geq h$) is to use a Gaussian source function, such as

$$\mathcal{S}(\mathbf{x}, \mathbf{x}_i) = \frac{1}{(2\pi l^2)^{n/2}} \exp\left(-\frac{|\mathbf{x} - \mathbf{x}_i|^2}{2l^2}\right), \quad (5)$$

where $n = 2, 3$ for two- and three-dimensional problems and the source size l is taken to be slightly larger than the particle. For $D \ll h$ and $N_C \rightarrow \infty$, while ϕ is held constant, it is usual to computationally smear out the forces and weight them according to distance from the nearest node. For $d \gg h$, the contribution is weighted by integrating over each element. The major challenge is in the choice of the force closure $\mathbf{F}_i$ which depends on the local velocity field relative to the particles and the local velocity gradient tensor ($\nabla \mathbf{u}$).

Going from the full solution to the reduced model requires replacing particles by a point forces which can be made to have both the same drag and the same downstream wake signature. Closures and estimates of the unperturbed flow are usually discussed in terms of subtracting the Stokes flow perturbation from the flow local to the particle or spatially averaging the flow in the vicinity of the particle. The most successful application of the point-particle approach is in the limit of $Re < 10$, for three-dimensional flows (Maxey & Patel 2001). In this limit, diffusive effects are strong and locally the flow is dominated by Stokeslet and dipole contributions. Stokes flow descriptions are valid within a distance $O(D/Re)$ from the body, beyond which the flow is dominated by a source term. Bevilaqua & Lykoudis (1978) contrasted the wake of a rigid and porous sphere (with the same

drag force), show that it is turbulent wake intensity distribution depends on factors other than just drag.

Previous attempts to replace bodies by point forces have tended to focus on the low Reynolds numbers based on the slip velocity. Here we attempt to extend this approach to the case of inertially dominated flows ($Re \gg 1$) and develop a first order analysis of the global effect of a group of bodies on the ambient mean flow. The effect of a point force on a uniform flow is well-known (eg Batchelor 1967, Bretherton 1962). In three-dimensional flows, the velocity deficit decays sufficiently fast (far downstream) that the momentum equation can be linearised (since $|\mathbf{u} - U\hat{\mathbf{x}}_1|/U \ll 1$). We consider the dominant effect of drag on the steady flow which generates a flow distribution estimated to be

$$\mathbf{u} = U\hat{\mathbf{x}}_1 + \sum_{i=1}^{N_C} Q_i \nabla \Phi_S(\mathbf{x} - \mathbf{x}_i) + \mu_i \frac{\partial}{\partial x_1} \nabla \Phi_S(\mathbf{x} - \mathbf{x}_i) \quad (6)$$

$$-(1, 0)H(x - x_i) \frac{Q_i U}{4\pi\nu(x_1 - x_{1i})} \exp\left(\frac{-R_i(x_2, x_3)^2 U}{4\nu(x_1 - x_{1i})}\right) \hat{\mathbf{x}}_1,$$

where $R_i(x_2, x_3) = \sqrt{(x_2 - x_{2i})^2 + (x_3 - x_{3i})^2}$. For two-dimensional laminar flows, the downstream velocity and vorticity fields are

$$\mathbf{u} = U\hat{\mathbf{x}}_1 + \sum_{i=1}^{N_C} Q_i \nabla \Phi_S(\mathbf{x} - \mathbf{x}_i) + \mu_i \frac{\partial}{\partial x_1} \nabla \Phi_S(\mathbf{x} - \mathbf{x}_i) \quad (7)$$

$$+(1, 0)H(x - x_i) \frac{Q_i}{\sqrt{2\pi\nu(x_1 - x_{1i})/U}} \exp\left(\frac{-(x_2 - x_{2i})^2 U}{4\nu(x_1 - x_{1i})}\right) \hat{\mathbf{x}}_1.$$

The effect of multiple bodies can then be estimate to leading order by summing up the contributions from each body. The vorticity maximum behind an isolated body decreases as x^{-1} and $x^{-3/2}$ for two- and three-dimensional laminar flows. This is a faster decay of the maximum concentration of a passively diffusing material (as $x^{-1/2}$, x^{-1} respectively) because of vorticity annihilation. For planar flows, the presence of von Karman vortex streets means that positive and negative vorticity are well separated (until a distance $\sim DRe$ or $D_G Re_G$ downstream) so that the decay is much slower. For collections of bodies, vorticity annihilation is caused by wakes intermingling which leads to an exponential decrease of the velocity deficit (White & Nepf 2005) over a distance $l_D = (l_{sep}^2 - D^2/4)u_E/2\nu \sim dRe_L\pi/8(1/\phi - 1)$ for planar laminar wakes and $l_D = l_{sep}^2 u_E/2\nu \sim dRe_L\pi/12(1/\phi^{2/3} - 1)$ for three-dimensional wakes, where u_E is a measure of the average flow in the vicinity of the bodies. (For turbulent wakes, ν is placed by a nominal turbulent viscosity). As ϕ increases, the local Reynolds number $Re_L = Du_E/\nu$, defined in terms of the Eulerian average velocity within the array, decreases because the average flow u_E is reduced. When l_D/D_G is much less than unity the individual wake signatures are lost and a distributed model is applicable.

2.3 Distributed drag models

This modelling approach is usually applied when the geometry and number of the bodies is complex and large, for instance, in the urban terrain (see figure 1(c)). In this class of models, the effect of the collection of bodies is smeared over the flow, through

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} - \langle \mathbf{F}(\mathbf{x}, t) \rangle. \quad (8)$$

For most inertially dominated flows, the applied drag force is assumed to take the form

$$\langle \mathbf{F} \rangle = \frac{2\rho C_D \mathbf{u} |\mathbf{u}|}{\pi D_G} S(\mathbf{x}), \quad (9)$$

where $S(\mathbf{x}) = 1$ for $\mathbf{x} \in V_B$, and 0 otherwise and C_D is a closure drag coefficient (eg. see Belcher et al. 2003). The total force on the array is $\mathbf{F}_T = \int_{V_G} \mathbf{F} dV$. Looking again at the vorticity field, we see

$$\rho \frac{D\boldsymbol{\omega}}{Dt} = \rho \boldsymbol{\omega} \cdot \nabla \mathbf{u} - \nabla \times \langle \mathbf{F} \rangle. \quad (10)$$

Providing, $|\langle \mathbf{F} \rangle|/|\nabla \langle \mathbf{F} \rangle| D_G \ll 1$, vorticity is largely generated at the leading edge and sides of the region V_B . This type of modelling approach predicts large shear layers at the edge of the array. Since the positive and negative vorticity are well separated in the near field, the maximum vorticity decays slowly as $x^{-1/2}$ in both 2D and 3D until the flow becomes unstable. In the near wake region, the streamwise velocity field has a top hat profile and the maximum velocity deficit decays slowly with distance.

3 Model evaluation and comparison

We illustrate the three modelling approaches described above in the context of the two-dimensional flow past a localised group of bodies and draw on the recent high-resolution calculations of Nicolle (2009). In this work, an array of circular cylinders of diameter $D = 1$ is organised in concentric circles forming a circular group of diameter $D_G = 21$. The cylinders forming the group are equally spaced from one another. The number of cylinders in each group is varied from $N_C = 7$ to 133 which results in a void fraction from $\phi = 0.0023$ to 0.3016. The Reynolds numbers of these simulations are $Re = 100$ and $Re_G = 2100$. The point-particle and distributed drag model uses the same flow and geometric characteristics as well as applying the point particles at the same cylinder positions as used for the full numerical calculations. Figure 2(a) shows the resolved flow past a group of 95 cylinders.

Three distinct regimes were identified as the solid fraction was increased. For $\phi < 0.045$, the cylinders were well separated and the vortices shed from each cylinder could be identified. For $0.045 < \phi < 0.145$, the flow inside the array was steady and a distinct shear layer was generated at the edge of the array. Beyond $\phi > 0.145$, the wake was attached to the array and the flow behaved in a similar fashion to a rigid cylinder.

To compare the full calculations against a point-particle model, we apply closure expressions for drag forces based on estimating the local velocity when the i -th cylinder is removed. The drag force closure expression applied to each body cylinder (Clift & Weber 1978)

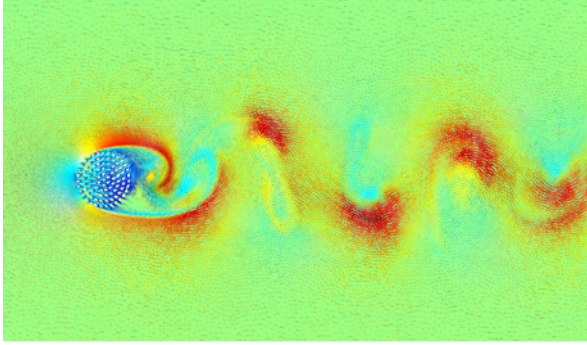
$$C_{D_i} = \begin{cases} 9.689 Re^{-0.78} (1 + 0.147 Re^{0.82}) & Re_i < 5, \\ 9.689 Re^{-0.78} (1 + 0.227 Re^{0.55}) & 5 < Re_i \leq 40 \\ 9.689 Re^{-0.78} (1 + 0.083 Re^{0.82}) & Re_i > 40 \end{cases}$$

The local Reynolds number, $Re_i = D|\mathbf{u}|/\nu$ is obtained from the velocity at the center of cylinder i which is removed from the flow. A number of iterations were applied to ensure convergence. A comparison of the mean (time-averaged) drag coefficient on the cylinders (in figure 2) calculated from the inertially dominated point-particle model and the full numerical results, are shown

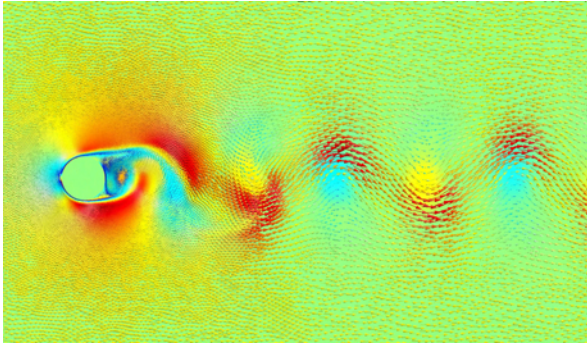
N_C	1	7	20	39	64	95	133
ϕ	0.0023	0.0159	0.0454	0.0884	0.1451	0.2154	0.3016
Predicted $\langle C_D \rangle$	0.0592	0.3435	0.8324	1.3691	1.6926	1.9271	2.1496
Numerical calculations	0.0619	0.3707	0.8155	0.9694	1.1063	1.6460	1.7678
Percentage error	4.3	7.3	2.1	41.2	53.0	17.1	21.6

Table 1: Comparison between numerically calculated and predicted array drag as a function of solid fraction ϕ .

in Table 1. The agreement between the numerical calculations and point-particle model is good up to about $\phi \sim 0.1 - 0.15$.



(a)



(b)

Figure 2: Numerical results at $Re_G = 2100$ for (a) fully resolved flow past 95 cylinders in a circular grouped where $\phi = 0.2154$, and (b) for a circular region of distributed drag which has a similar total drag to (a) (using (9) with $C_D = 1.6$).

At low solid fractions the bodies are too close for the point-particle model to be practically applied (largely because $|\mathbf{u}|/D||\nabla\mathbf{u}||_E \sim O(1)$). Beyond this range, $l_{sep}/D \sim O(1)$ and the individual flow signature from individual bodies is annihilated. In this regime and at high solid fractions, distributed drag models should be applied as they are capable of reproducing the attached shear layers (described previously). Figure 2(b) shows the results from a distributed drag model calculation. The leading coefficient $2C_D/\pi D_G$ was chosen to be 0.043 (based on $C_D = 1.6$). The field wake structure is similar to the fully resolved calculations, but the near field structure is different.

4 Conclusion

We have compared and contrasted the three main modelling approaches which can be applied to dispersed mul-

tiphase flows: fully resolved, point-particle models and distributed drag formulation in the limit of $Re \gg 1$.

We have extended the point particle approach to the case of $Re \gg 1$ and two- and three-dimensional groups of bodies. The comparison between the forces on a group of cylinders predicted from the point-particle and the full numerical calculations is quite good until $\phi \sim 0.06$ when the spacing between the bodies is comparable to their diameter.

The point-particle approach shows that as ϕ increases, the lengthscale over which the wake signature is annihilated becomes comparable to the size of the array. In this case, individual flow signatures are annihilated and a distributed drag model is more appropriated. This gives support to the point-particle approach generally applied within the turbulence literature.

When individual wakes are annihilated and it is then appropriate to apply a distributed drag model. In such flows, the deflection of the mean flow means that $\int F_i S dV$ is less than the drag on the body. The inherent problem of the distributed drag model is that the usual force closures are no longer appropriate and may necessitate the use of drag coefficients which many seem unphysical (ie > 1). One future direction, largely unexplored, is the development of a rational basis for the force closures applied to distributed drag models.

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POINT-PARTICLE DNS OF SUSPENDED SEDIMENT TRANSPORT

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Abstract

In this paper we evaluate the use of the point-particle approach in direct numerical simulations (DNS) of suspended sediment transport with a dilute particle-concentration. We perform a comparison between the simulations and PIV/PTV experiments in a horizontal open water channel flow, with a dilute concentration of small spherical particles (diameter of the same order of the Kolmogorov length-scale) with a density slightly larger than the density of the fluid. Overall, the results indicate that, provided a resuspension mechanism at the bottom wall is included, point-particle direct numerical simulations give accurate results. The results show that the inclusion of a resuspension mechanism is crucial; however, the details of it are not important, provided that it is strong enough to promote an adequate resuspension of the particles. For the dilute concentration considered here, the key resuspension mechanisms are associated with the lift force near the wall, which can be easily incorporated within the point-particle formalism using standard lift-force models. Alternatively, a simple ad-hoc resuspension model, using a virtual particle-bouncing wall, also gives good results.

1 Introduction

The transport of suspended sediment in wall-bounded turbulent flows is important in numerous situations. A common situation involves the transport and sedimentation of sand-like particles in turbulent water-flows. The sedimentation of the particles depends strongly on the interaction between the particles and the turbulence, and there is a lack of good understanding about it. Most of the work on particle-turbulence interactions has been done for solid particles in air, with a density ratio between the particle and the fluid of the order of 1000, whereas in this case we are interested in a density ratio of the order of 1.

One of the techniques used to simulate the motion of particles in a turbulent flow is the point-particle approach [1, 2]. In the point-particle approach the interaction between a particle and the surrounding fluid is modeled through a force located at the center of the particle. When doing point-particle DNS, all the scales of the continuous phase are computed and the level of modeling is kept to a minimum. Therefore, point-particle DNS is extremely useful in gaining a better understanding of the interactions between the particles and the turbulence. However, in principle, the point-particle approach requires that the particles be much smaller than the smallest flow scales, and it is not clear to what extent the restriction on the particle size can affect the accuracy of the simulations. In many situations involving

sediment transport the particles have a diameter of the same order of the Kolmogorov length-scale, hence it is important to know to what extent the restriction on the particle size can affect the accuracy of the simulations. In this work, we perform point-particle DNS, and compare the results with PIV/PTV experiments in a horizontal open water channel flow. The particles have a diameter of the same order of the Kolmogorov length-scale, therefore, even though they are ‘small’, they are not ‘much smaller’ than the smallest flow scales. As much as possible, all the conditions in the simulations and the experiments were exactly the same.

First, the simulations were performed assuming one-way coupling, with drag, gravity, added mass and the surrounding fluid stresses acting on the particles. The comparison between the experiments and the simulations, presented in Cargnelutti et al. [3], showed a good agreement for the profiles of the particle mean-velocity in the streamwise direction, and for the profiles of the particle velocity-fluctuation. However, there was a mismatch in the profiles of the particle mean-velocity in the normalwise direction, and in the profiles of the particle-concentration. The difference between the numerical and experimental results can be related to a lack of a re-suspension process in the simulations. In the point-particle approach, the force acting on a particle is obtained using the fluid-velocity interpolated at the center of the particle. Therefore, in the simulations, once the particle reaches the bottom of the channel, the only normalwise forces that oppose gravity are due to the velocity fluctuations at a distance of one radius from the wall, which are very small and cannot resuspend the particles. The actual resuspension process is due to physical mechanisms not included in the simulations presented in Cargnelutti et al. [3]. In order to check the importance of the different resuspension mechanisms, in this work the simulations were also performed with: (i) the inclusion of ad-hoc resuspension models, and (ii) the inclusion of the lift force.

First, we present the equations of motion, the lift force models and the resuspension mechanisms. Then, we present the numerical and experimental setups. Finally, the results for the different resuspension mechanisms are presented and compared with the experimental data, and some conclusions are drawn.

2 Equations of motion and resuspension mechanisms

Considering a one-way coupling situation, where the influence of the particles on the fluid is neglected, the equations of motion of the continuous phase are given by the continuity and Navier-Stokes equations for an incompressible flow:

$$\nabla \bullet \vec{U} = 0 \quad (1)$$

$$\frac{D\vec{U}}{Dt} = -\frac{\nabla P}{\rho_f} + \nu \nabla^2 \vec{U} \quad (2)$$

where $\vec{U}$ is the fluid velocity, P the pressure, ρ_f the fluid density, and ν the fluid kinematic viscosity.

The forces acting on a small particle were described by Maxey and Riley [4]. In addition to the forces considered by Maxey and Riley, we also include the lift force, and, following the results of Armenio and Fiorotto [5], we neglected the history (Basset) force. Considering Stokes drag, gravity, added mass, the particle surrounding fluid stresses and the lift force, the particle equation of motion is given by:

$$\begin{aligned} \frac{d\vec{V}}{dt} = & \frac{1}{\tau_a} (\vec{U} - \vec{V}) + \frac{\beta-1}{\beta+\frac{1}{2}} \vec{g} \\ & + \frac{3}{2} \frac{1}{\beta+\frac{1}{2}} \frac{D\vec{U}}{Dt} + \frac{\beta}{\beta+\frac{1}{2}} \vec{f}_L \end{aligned} \quad (3)$$

where d_p and ρ_p are the particle diameter and density, $\vec{g}$ is the acceleration of gravity, $\beta = \rho_p/\rho_f$ is the particle-fluid density ratio, $\vec{f}_L = 6\vec{F}_L/\rho_f\pi d_p^3$ is the lift force per unit of mass, $\tau_a = \frac{\beta+\frac{1}{2}}{\beta}\tau_p$, and the particle relaxation time τ_p is given by:

$$\tau_p = \beta \frac{d_p^2}{18\nu} \quad (4)$$

The lift force, acting in the direction perpendicular to the wall, needs to be modeled. In principle, the lift force can also have components in the streamwise and spanwise directions, however, their values are much smaller than the normalwise component, and, following the usual practice, we model only the lift force in the normalwise direction. There exist many models, with different ranges of validity according to the particle distance from the wall. Wang et al. [6] formulated an ‘optimal’ lift force, as a compilation of different models available in the literature. This ‘optimal’ lift force can be expressed as:

$$F_L = 6\pi a_p \mu V_r f(G, V_r, \mu, \rho_f, \ell) \quad (5)$$

where a_p is the radius of the particle, μ and ρ_f are the viscosity and density of the fluid, V_r is the absolute value of the streamwise velocity difference between the particle and the surrounding fluid, G is the wall-normal gradient of the streamwise velocity of the fluid at the position of the center of the particle, and ℓ is the distance between the particle center and the wall. The function $f(G, V_r, \mu, \rho_f, \ell)$ depends on the lift model used, and the details can be found in Wang et al. [6]. The model proposed by Wang et al. [6] does not consider the case when the particles are in contact with the wall. Leighton and Acrivos [7] gave a model for the lift force acting on a particle at rest, in contact with a wall, in the presence of a shear flow:

$$F_L = 9.22\rho_f a_p^4 G^2 \quad (6)$$

Krishnan and Leighton [8] extended this model for the cases when the particle is still in contact with the wall but no longer at rest (the corrected formulation can be found in King and Leighton [9]); neglecting the particle rotation, the lift force is given by:

$$\begin{aligned} F_L = & 9.257\rho_f a_p^4 G^2 + 1.755\rho_f a_p^2 V_p^2 \\ & - 9.044\rho_f a_p^3 V_p G \end{aligned} \quad (7)$$

where V_p is the streamwise particle velocity.

Very close to the wall, there is no agreement on which model to use for the lift force. According to King and Leighton [9], the model proposed by Wang et al. [6] is valid when the distance of the center of the particle to the wall is larger than $1.1a_p$, and tends asymptotically to the model of Krishnan and Leighton [8] as the particle approaches the wall. As we will see below, the choice of the lift-force model when the distance from the particle center to the wall is between a_p and $1.1a_p$ can affect the results.

Inter-particle collisions can also produce particle entrainment into suspension. A collision algorithm can be very time consuming and an alternative, often used in ‘engineering simulations’, is to use a resuspension model. One important feature of the inter-particle collision process, besides the energy and momentum transfer, is the fact that two particles cannot occupy the same space at the same time. This led us to include a very simple ‘ad-hoc’ resuspension model: a virtual particle-bouncing wall located at a short distance from the bottom wall. This mimics in a simple way the bouncing of the particles on the top of other particles lying at the bottom wall. We should note, however, that here we are considering a very dilute particle concentration, where, a priori, inter-particle collisions are not expected to play a significant role.

3 Numerical setup

The numerical setup, consisting of a particle-laden open channel flow driven by a streamwise pressure gradient, is shown schematically in figure 1. The continuous phase was solved with a standard finite-volume code on a staggered grid, using a predictor-corrector solver with a second-order Adams-Bashforth scheme; the time-step was obtained using the Courant stability criterion. At the top wall was imposed a free-slip boundary condition and at the bottom wall a no-slip boundary condition. Periodic boundary conditions were used in the streamwise and spanwise directions.

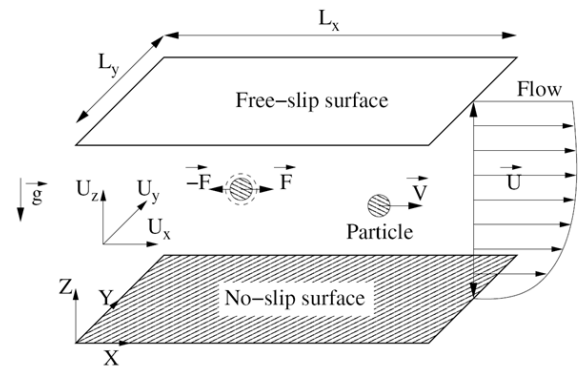


Figure 1: *Numerical setup.*

The equations of motion were made dimensionless using the friction velocity u_τ and the height of the channel h . With these parameters, the Reynolds number was set to $Re_\tau = 500$ which corresponds to a bulk Reynolds number $Re_b = 10 \times 10^3$. The length of the computational domain in the streamwise, spanwise and normalwise directions was equal to, respectively, $L_x^+ = 2500$, $L_y^+ = 1000$ and $h^+ = 500$ with, respectively, 256, 192 and 128 grid points. The grid was uniform in the streamwise and

spanwise directions, and a hyperbolic-tangent stretching was used in the normalwise direction ($\Delta z^+ \approx 0.9$ at the wall and $\Delta z^+ \approx 7$ at the center). The superscript + is used to denote a value in wall-units (i.e. non-dimensionalized using u_τ and ν).

For the discrete phase, the particle equation of motion was integrated with an explicit method, using the point-particle approach, with the fluid velocity at the particle position given by a tri-linear interpolation. When a particle left the domain on one side, it was inserted in the opposite side with the same velocity. At the top and bottom walls it was used specular reflection for the particles. When an ad-hoc resuspension model consisting of a virtual particle-bouncing wall was used, the specular reflection occurred at a short distance from the bottom wall, determined by the position of the virtual particle-bouncing wall. Details of the code can be found in [2].

4 Experimental setup

The experiments were performed in an open channel, with a channel length of 23.5m, a width of 0.495m, and a height of 0.5m (figure 2). The walls and bottom were made of glass in order to have a hydraulically smooth boundary. The water was pumped from a buffer into the flume. At the downstream side, the water level was controlled with an adjustable weir, followed by three pipes allowing the water to return to the buffer. In order to perform the fluid velocity measurements, the water was seeded with 10 micron hollow glass spheres.

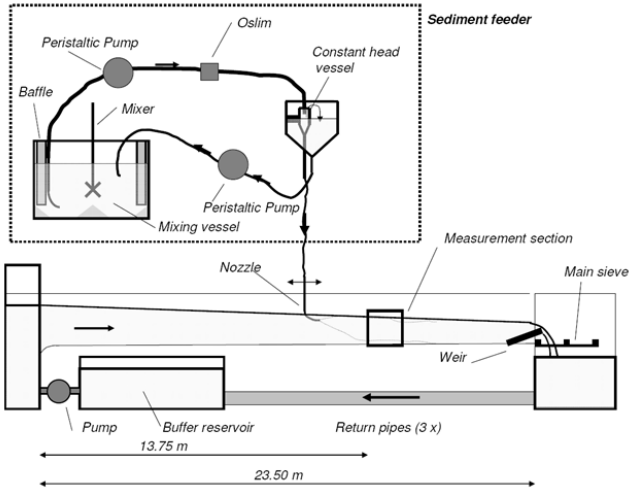


Figure 2: *Experimental setup.*

As pseudo-sediment, $d_p=347$ micron ($\sigma=45$ micron) polystyrene particles were used, which had a density ρ_p of 1035kg/m^3 . The value measured for the terminal velocity ($v_T=2.2\text{mm/s}$) compared well with the theoretical estimate of 2.1mm/s ($Re_p = v_T d_p / \nu = 0.71$). The particles were fed to the channel with a particle feeder, and the volumetric sediment concentration in the mixing vessel was equal to 1.2×10^{-2} . The sediment mixture entered the channel through a nozzle with an inner diameter of 1cm, placed at the channel centerline and with its center located at 0.7cm below the free surface. The inflow velocity was adjusted to match the channel velocity.

The measurement section was located at a distance of 14.25m from the channel entrance. At this location, a combination of both PIV and PTV was used to measure

the velocities of the polystyrene particles and the fluid. The data were processed with a modified version of the method of Kiger and Pan [10] to discriminate between sediment and tracer particles. Then, a PTV algorithm was used to calculate the position and velocity of the tracer particles, whereas the fluid velocity was calculated from the tracer image with PIV.

A more complete description of the experimental setup is presented in Breugem and Uijttewaalt [11]. All the results presented here were measured at $Re_b=10 \times 10^3$, which was obtained by setting the centerline velocity to $U_{cl} = 0.2\text{m/s}$ and the water depth to $h=0.05\text{m}$. Four sets of data were collected, corresponding to different nozzle positions with respect to the measurement section: $x/h=16$, $x/h=35$, $x/h=75$ and $x/h=160$.

4 Results

Three types of one-way coupling simulations were performed: (i) without lift force and without a virtual particle-bouncing wall, (ii) without lift force and with a virtual particle-bouncing wall, and (iii) with lift force and without a virtual particle-bouncing wall.

For the simulations of type (ii), two cases were considered: (a) *resusp1* and (b) *resusp2*, with the particle-bouncing virtual wall located one and two particle diameters above the bottom wall, respectively. For the simulations of type (iii), different cases were considered: (a) *l&a*, using the model of Leighton and Acrivos [7] (equation 6) for the lift force when the distance between the center of the particle and the bottom wall was smaller or equal to the threshold $L_{l\&a}$ (two values were used: $L_{l\&a}=1.2a_p$, $L_{l\&a}=1.05a_p$) and without lift force in the rest of the channel, (b) *k&l*, using the model of Krishnan and Leighton [8] (equation 7) for the lift force when the distance between the center of the particle and the bottom wall was smaller or equal to the threshold $L_{k\&l}$ (three values were used: $L_{k\&l}=1.1a_p$, $L_{k\&l}=1.05a_p$ and $L_{k\&l}=1.0a_p$) and without lift force in the rest of the channel, and (c) *full*, using a 'full lift force', with the model of Krishnan and Leighton [8] (equation 7) when the distance between the center of the particle and the bottom wall was smaller or equal to the threshold L_{full} (four values were used: $L_{full}=1.1a_p$, $L_{full}=1.05a_p$, $L_{full}=1.0a_p$ and $L_{full}=0.0$) and with the model of Wang et al. [6] (equation 5) in the rest of the channel.

Obviously, for $L_{full}=0.0$ the model of Wang et al. [6] is applied over the entire channel. Note also that when the threshold distance is equal to $1.0a_p$, in principle, the lift force is applied only when the particle is exactly touching the bottom wall, therefore, formally, $L_{full}=1.0$ and $L_{full}=0.0$ are the same case, and $L_{k\&l}=0.0$ is, formally, the same as the absence of lift force over the entire channel. The cases with the threshold distance equal to $1.0a_p$ were considered in order to check the consistency of the results. Indeed, only small differences were observed between the cases that are formally the same, which can be attributed to the details of the implementation and to the slight differences between the runs (initial fields, run times, etc.).

The simulations of type (i), without lift force and without a virtual particle-bouncing wall, are presented in Cargnelutti et al.[3]. Overall, the agreement between the simulations and the experiments, both for the fluid and the particles, was very good. The only exception was for the particle concentration and the particle mean normalwise velocity profile, which indicated that a fully-developed situation could not be reached, and the particles kept accumulating at the bottom wall.

The reason why a fully-developed concentration profile is not reached in simulations of type (i) can be understood by a balance of forces in the vertical direction. For the situation considered here, when the particle is at rest at the bottom wall, in order to have a vertical drag force larger than the gravitational force the velocity of the surrounding fluid needs to be larger than $0.24u_\tau$, however, the root-mean-square value of the vertical velocity fluctuation of the fluid at one radius from the bottom wall is $u'_z \approx 0.03u_\tau$. Since in the point-particle approach the velocity of the surrounding fluid is given by the velocity of the fluid at the position of the center of the particle, the chance of having a fluid velocity large enough to resuspend the particle is extremely small.

The experimental profiles at $x/h=75$ and $x/h=160$ are not very different, indicating that the profiles at $x/h=160$ can be considered fully-developed, and they are both used for comparison with the numerical data (denoted by *exp75* and *exp160* in the figures).

The concentration profiles are shown in figure 3, with the ‘theoretical’ Rouse profile also shown as a ‘rough reference’. For the simulations of type (ii), with the virtual particle-bouncing wall, we can see a good agreement with the experimental data for case (c) with $L_{full}=1.1a_p$ and $L_{full}=1.05a_p$, and for case (a) (both with $L_{l\&a}=1.2a_p$ and $L_{l\&a}=1.05a_p$), but not for the other cases.

The results shown in figure 3 indicate that a ‘full lift force’ is enough to promote an adequate resuspension of the particles, and that, provided an adequate resuspension is promoted, the lift force does not play a significant role in the simulations. They also indicate that the details of the near-wall resuspension mechanism are not important, provided that is strong enough to promote an adequate resuspension of the particles. Note that the lift force model of Leighton and Acrivos [7] is known to overestimate the lift force at the wall; therefore its use near the wall is enough to promote an adequate resuspension of the particles, without the need to use the lift force in the rest of the channel.

The mean normalwise particle velocity profiles are shown in figure 4 (since several of the cases gave approximately the same results, not all the cases are shown). The results are consistent with the concentration profiles of figure 3, showing that the case where a good agreement with the experimental data was obtained have a mean normalwise velocity profile close to zero, indicating a fully-developed profile. The other cases have a non-zero mean normalwise velocity towards the bottom wall, indicating that the near-wall resuspension mechanisms are not strong enough.

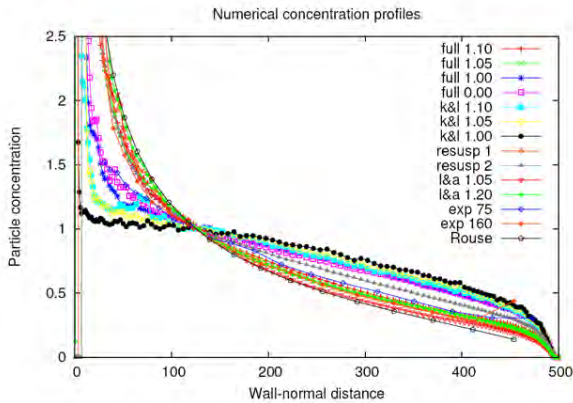


Figure 3: Particle concentration normalized by the value at $z/h=0.125$ ($z^+=125$), as a function of the distance to the wall (in wall-units).

Apart from the concentration and the mean normalwise velocity profile, all the other particle statistics profiles obtained from the different numerical simulations showed a good agreement between themselves and with the experimental data, regardless of the type of simulation. The results for the mean streamwise velocity, streamwise velocity fluctuation, normalwise velocity fluctuation, and Reynolds shear-stress, are shown in figures 5 to 8. From the results it is clear that both the lift force and the near-wall resuspension mechanism do not play a significant role.

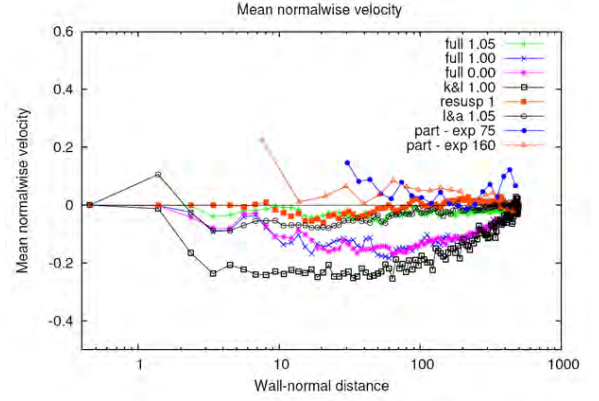


Figure 4: Mean normalwise particle velocity (in wall-units) as a function of the distance to the wall (in wall-units).

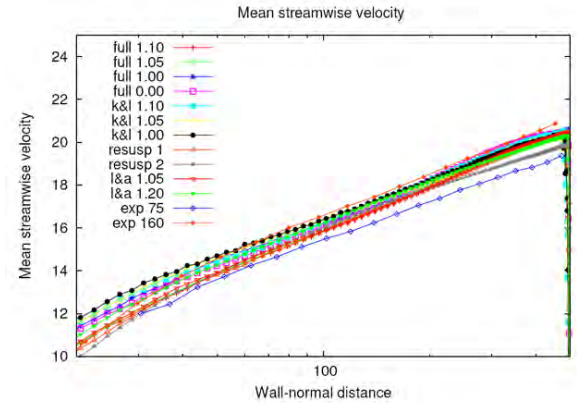


Figure 5: Mean streamwise particle velocity (in wall-units) as a function of the distance to the wall (in wall-units).

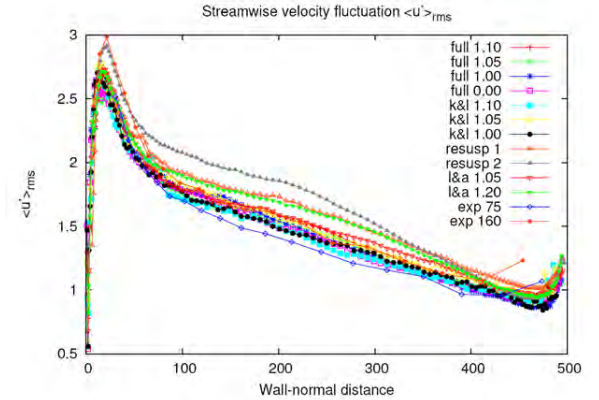


Figure 6: Root-mean-square of the streamwise particle velocity fluctuation (in wall-units), as a function of the distance to the wall (in wall-units).

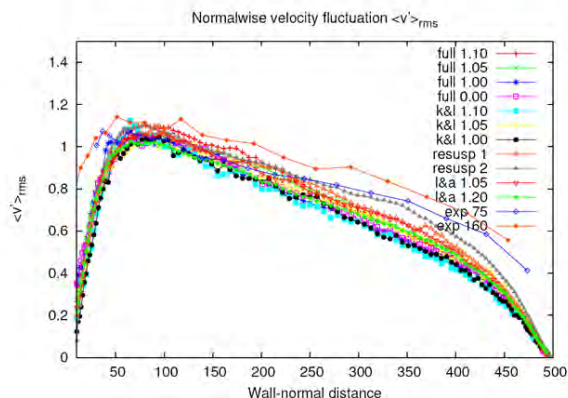


Figure 7: Root-mean-square of the normalwise particle velocity fluctuation (in wall-units), as a function of the distance to the wall (in wall-units).

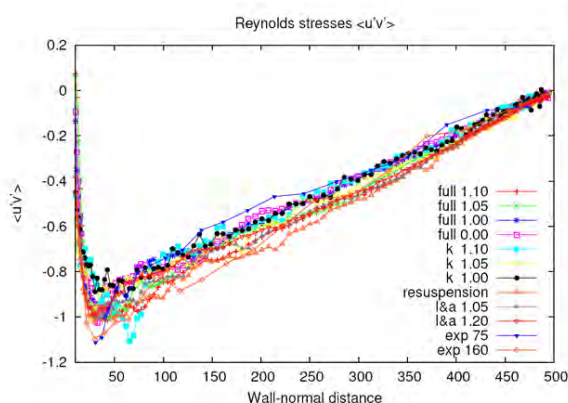


Figure 8: Particle Reynolds shear-stress (in wall-units), as a function of the distance to the wall (in wall-units).

4 Conclusions

The results from standard point-particle direct numerical simulations were compared with PIV/PTV experiments in a horizontal open water channel flow with a dilute particle-concentration, for small spherical particles with a density slightly above the fluid density. The comparison shows a good agreement between the simulations and the experiments, provided a strong enough near-wall resuspension mechanism is present.

The use of a ‘full lift force’ model is adequate to promote a strong enough resuspension mechanism. However, the details of the near-wall resuspension mechanism are not important, and good results are obtained with both a simple ad-hoc resuspension model, consisting of a virtual particle-bouncing wall, and the near-wall Leighton and Acrivos model [7], which is known to overestimate the lift force at the wall.

Except for its role in providing a resuspension mechanism, and therefore ensuring that a fully-developed or statistically-steady situation is reached, the lift force does not play an important role and similar results are obtained with and without the lift force, except for the particle concentration and the particle mean normalwise velocity. Also, except for the particle concentration and the particle mean normalwise velocity, similar results are obtained regardless of the resuspension mechanism (a lift force, an ad-hoc virtual particle-bouncing wall, or none).

The good agreement between the simulations and the experiments, and the lack of sensitivity of the results

to particular model choices, indicates the adequacy and robustness of point-particle DNS, even when the particles are no longer ‘much smaller’ than the Kolmogorov length-scale. From a pragmatic perspective this is particularly important, because from a strict formal perspective the point-particle approach is valid only in the limit when the particles are ‘much smaller’ than the smallest flow scales, whereas in many situations of interest the particle size is of the same order of magnitude of the smallest length scales of the flow; like the situation considered here, where the particle size is of the same order of magnitude of the Kolmogorov length-scale.

Acknowledgements

The numerical simulations were performed by Marcos Cargnelutti and the experimental results were obtained by Alexander Breugem, as part of their Ph.D. research, financed by STW (Dutch Foundation for Technology Research).

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MEASURING AND CONTROLLING LOCAL SEGREGATION OF DISPERSED PARTICLES IN TURBULENT FLOWS

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Abstract

Transport, dispersion and segregation of inertial particles in turbulent flows are crucial phenomena in a number of technological applications. From a physical viewpoint, whichever the geometry of the flow, particle dynamics is controlled by turbulent flow structures whose time scale is comparable to the particle relaxation time. In previous works focusing on dispersed flow in channels and pipes (see Soldati and Marchioli (2009), and references therein for a review), we have shown that there is a strong correlation between coherent wall structures, local particle segregation and subsequent deposition. This is true also in more complex configurations. As discussed in Campolo et al. (2005), for instance, particle dispersion in a transverse jet is controlled by specific flow structures and the extent of this interaction can be used to improve/reduce dispersion (Campolo et al., 2008). A statistical characterization of particle preferential segregation is thus important to provide a sound physical picture of the dispersion mechanisms and to develop accurate predictive models. In this paper we consider well-known case studies, namely turbulent channel flow and jet in cross-flow, to survey two statistical tools, the segregation parameter and the correlation dimension, that suite the purpose. We will also show how these tools may be used to devise strategies for particle segregation control in practical applications.

1 Statistical tools for quantification of particle segregation

The instantaneous location of particles in a turbulent flow field can provide relevant information about the nature of the dispersion process if we look at it using suitable tools. Due to their inertia, particles are never uniformly distributed: they accumulate preferentially in specific regions and avoid some other regions of the flow. By simply counting the number of particles within given subspaces of the flow domain, the statistical distribution of the local particle number density can be obtained and used to measure particle relative tendency to segregate and preferentially concentrate in a turbulent flow field. One way to do so is given by the segregation parameter, D , also referred to as deviation from randomness (Fessler et al., 1994). The segregation parameter is calculated as:

$$D = \frac{\sigma - \sigma_{Poisson}}{\mu}, \quad (1)$$

where σ represents the standard deviation for the actual particle number density distribution and $\sigma_{Poisson}$ represents the standard deviation for a Poisson distribution,

which corresponds to a purely random distribution of the same average number of particles. The parameter μ is the mean particle number density. According to Eq. (1), the value $D = 0$ corresponds to a random particle distribution, $D < 0$ corresponds to a uniform particle distribution, and $D > 0$ indicates segregation of particles. In this latter case, the larger is the value of D , the stronger is segregation. The segregation parameter has been applied to homogeneous isotropic turbulence (Février et al., 2005) and to the centerline of a turbulent channel flow (Fessler et al., 1994): attention was focused on two-dimensional regions of nearly homogeneous flow to quantify the degree of organization of particle patterns due to particle response to small-scale turbulent motions. In our works, we have extended the use of the D parameter to three-dimensional regions of more complex configurations, characterized by flow inhomogeneities and by a wider range of spatial and temporal turbulent scales.

Technical details on the calculation of D are given in Soldati and Marchioli (2009). Here, it suffices to remark that the value calculated for D depends on the cell size. Because of this dependency, the segregation parameter can not provide an absolute, clearcut quantification of particle segregation; rather it should be used just to identify and compare differences in the tendency of particles to segregate in a turbulent flow field according to their inertia. Taking this into account, the cell size dependency can be partially overcome by computing the particle number density distribution for several values of the cell size and keeping only the largest value of D , referred to as D_{max} hereinafter (Picciotto et al., 2005; Février et al., 2005). This choice is justified by the fact that the cell size for which D is a maximum provides information about the length scales on which particles are being clustered.

In several previous numerical works (see Soldati and Marchioli (2009), and references therein), we have tried to extend the use of D to Turbulent Channel Flow (TCF) to characterize inhomogeneities arising in particle distribution along the wall-normal direction. To this aim, the flow domain was divided into wall-parallel bins of equal thickness and a local value of the segregation parameter was computed applying Eq. (1) for each slab. In this way, the wall-normal behavior of D can be evaluated. In Campolo et al. (2008) we further applied D to a transverse jet flow. Even if this flow is strongly inhomogeneous and intrinsically time-dependent due to the quasi periodic formation of large scale vortices, the time behavior of D computed for swarms of particles injected at different instants proved useful to evaluate differences in the dispersion behavior induced by the different time of injection.

In the problems just mentioned, the analysis on par-

ticle segregation was complemented by providing a single quantitative measure rather than the two numbers, D and the length scale for that value of D . Such measure is given by the correlation dimension, introduced by Grassberger and Procaccia (1983) to quantify the fractal dimension of the subspace in which particles cluster. In its three-dimensional formulation needed to study non-isotropic flows, this parameter can be computed by choosing one base particle and counting the fraction, $N_p(r)$, of particles within a distance r from the base particle. The correlation dimension, ν , is defined as the slope of $N_p(r)$ as a function of r in a log-log plot. The probability distribution of the distance between the neighboring particles and the base particle is obtained repeating this count for all possible values of r , thus removing any dependence on the length scale used. To compute results significant from a statistical perspective, the procedure can be repeated for different randomly chosen base particles and different times, averaging the results. In general, $N_p(r)$ will scale with r^ν such that smaller values of ν indicate greater preferential concentration: if particles are uniformly distributed in the volume surrounding the base particle, $N_p(r)$ will scale with r^3 (namely with the volume of the sphere centered on the base particle) and the correlation dimension will be 3; if particles are uniformly distributed over a surface, $N_p(r)$ will scale with r^2 (namely with the area of the circle centered on the base particle) and the correlation dimension will be 2; whereas if particles are concentrated into a line, $N_p(r)$ will scale linearly with r and the correlation dimension will be 1. For more complex particle distributions, the correlation dimension will be a non integer value.

In the following, we will show how the segregation parameter and the correlation dimension were used both to characterize from a fundamental viewpoint local particle segregation in wall-bounded turbulence and to control particle dispersion in more *practical* flow configurations.

2 Case studies

A. Quantification of local particle segregation in turbulent channel flow

Results shown in this section refer to a particle-laden turbulent Poiseuille flow of air (incompressible and Newtonian) in a channel at $Re_\tau = u_\tau h / \nu_f = 150$, where u_τ is the friction velocity, ν_f is fluid viscosity and h is the channel half-height. TCF was chosen as it represents a well-known archetype of wall-bounded shear flow. We used pseudo-spectral direct numerical simulation to compute the flow field in a reference geometry consisting of two infinite vertical flat parallel walls with periodic boundary conditions in the streamwise (x) and spanwise (y) directions and no-slip conditions at the walls. The computational domain, sketched in Fig. 1a), is $1885 \times 942 \times 300$ wall units (*i.e.* in terms of variables identified with the superscript “+” made dimensionless using ν_f and u_τ) in x , y and z , discretized with $128 \times 128 \times 129$ grid nodes.

We tracked five swarms – $O(10^5)$ – of heavy particles, characterized by diameters in the range $9 \div 228 \mu\text{m}$ corresponding to values of the Stokes number, St , equal to 0.2, 1, 5, 25 and 125. In wall turbulence, the Stokes number may be expressed as particle response scale, $\tau_p = \rho_p d_p^2 / 18 \mu_f$, made dimensionless using ν_f and u_τ . To characterize the collective behavior of particles, we chose a simplified numerical setting in which *i*) particle mass fraction and volume fraction are small enough to neglect

inter-particle collisions and particle feedback onto the gas flow (one-way coupling approach), and *ii*) particles are pointwise, rigid spheres that rebound elastically at the wall. The Lagrangian equation of particle motion includes only the effects of particle inertia and Stokes drag, with non-linear correction of the drag coefficient applied for particle Reynolds numbers larger than unity. Initially, particle number concentration is uniform and particle position is chosen randomly.

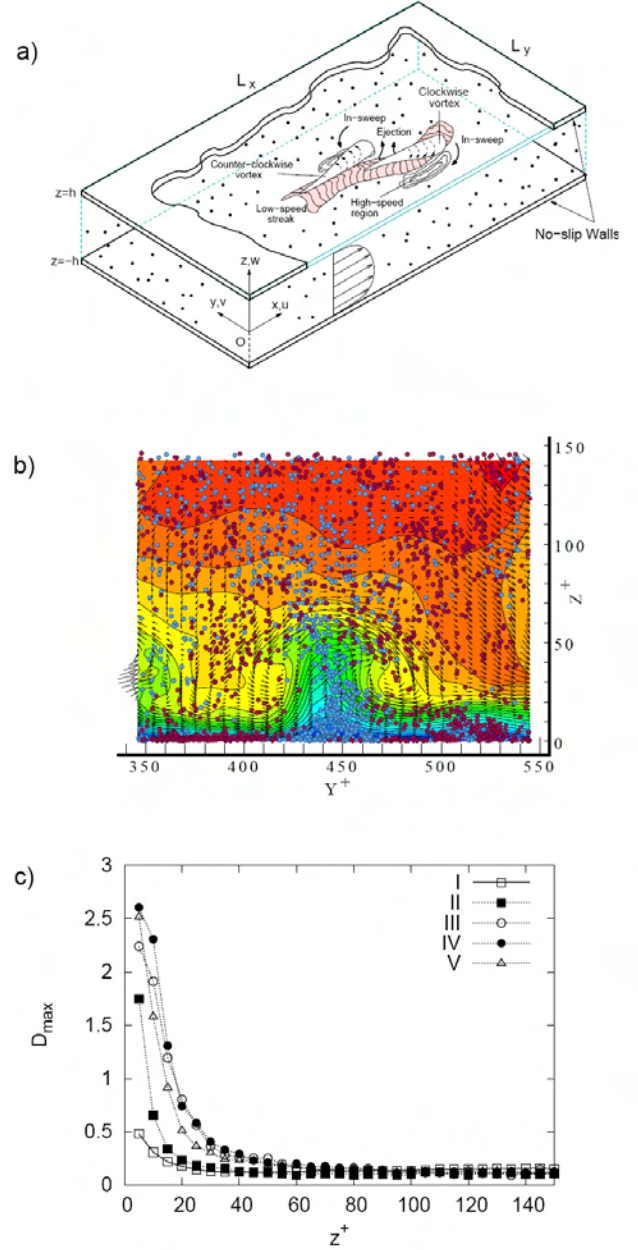


Figure 1: *Particle dispersion measurements in turbulent channel flow. Panels: a) Particle-laden turbulent gas flow in a channel: sketch of the computational domain and minimal schematics of near-wall turbulent coherent structures. Strong causal relationship links low-speed streaks to ejections generated by quasi-streamwise vortices, which also generate in-sweeps of high streamwise momentum fluid to the wall in the high velocity regions. b) Cross-section of the flow field and front view of particles in the region of particle accumulation. c) Maximum deviation from randomness, $D_{\max}$, as function of the wall-normal coordinate, z^+ , at different time intervals (I, II, III, IV and V) for $St=25$ particles.*

As mentioned, particle transfer processes are dominated by the dynamics of turbulent structures in the proximity of the wall. A pictorial view of particle transport mechanisms is provided in Fig. 1b), where one instantaneous snapshot of particle distribution and turbulent coherent structures in the near-wall region of the channel is shown. Here, we focus on a cross-sectional window ($y-z$ plane) of the computational domain having thickness equal to one streamwise cell, where strong particle accumulation takes place between two subsequent vortices. Vectors represent the fluid velocity in the plane and grayscale isocontours map the values of the streamwise velocity component. A strongly coherent ejection of low-momentum fluid is apparent in the middle of the figure, where one low-speed streak is lifted and flanked by two counter-rotating vortices. In-sweeps of high-momentum fluid are also visible on the downwash side of the vortices. Particle position is identified with the circles – larger than the real scale for ease of visualization. Light gray particles have wall normal velocity directed away from the wall whereas dark gray particles have wall-normal velocity directed toward the wall. The structures depicted in Fig. 1b) control the deposition process: (i) they accumulate particles in a region not far from the wall; (ii) they produce the sweeps which bring particles to the wall; (iii) they may trap particles in the wall region or (iv) they may entrain particles again in the outer flow. It was shown previously that particles are either re-entrained immediately by the same vortex which brought them to the wall or confined for very long times in the viscous region (Narayanan et al., 2003). As a consequence, particle transfer fluxes toward the wall have higher intensity than particle transfer fluxes away from the wall. In turn, unbalanced fluxes lead to nonuniform (preferential) distribution of particles within the flow and produce near-wall particle accumulation (Marchioli and Soldati, 2002).

To provide a trend in the temporal behavior of particle preferential distribution, Fig. 1c) shows the maximum values of the segregation parameter, D_{max} , along the wall-normal direction for five subsequent time intervals. Intervals are indicated with Roman numbers and correspond to different stages of the dispersion process. Each profile was obtained averaging D_{max} over 1000 non-dimensional units. For brevity, only results for the $St = 25$ particles are shown. Confirming the anisotropic nature of particle preferential distribution, D_{max} increases in the near-wall region, and particularly in the viscous sublayer where profiles develop a sharp peak corresponding to the last point in the plot. This behavior is common to all particle sets investigated (Marchioli et al., 2006).

Fig. 2 shows the maximum value of the segregation parameter, D_{max} (black circles), as a function of the particle Stokes number, St , in the viscous sublayer ($0 < z^+ < 5$). Values indicate that the maximum segregation is obtained for the $St = 25$ particles, which exhibit the strongest tendency to sample preferentially the flow field. This indicates that particle dynamics in the viscous sublayer is controlled by flow structures with non-dimensional timescale $\tau_f^+ \simeq 25$. Considering that τ_f^+ scales linearly with wall distance and decreases progressively as the turbulence structures lie closer to the wall, we can infer that this value corresponds to the circulation time of the turbulence structures in the buffer layer ($5 < z^+ < 30$). The correlation dimension calculated for the same particle sets is also shown in Fig. 2 (open circles). The correlation dimension is always smaller than 2, indicating that, regardless of their size, particles never attain a uniform spatial distribution. It

is confirmed that, while nearly random distribution is observed for the smaller particles, preferential concentration is maximum for particles with Stokes numbers around 25. In particular, the minimum value $\nu \simeq 1.53$ indicates that the preferential accumulation of these particles mainly occurs in elongated structures.

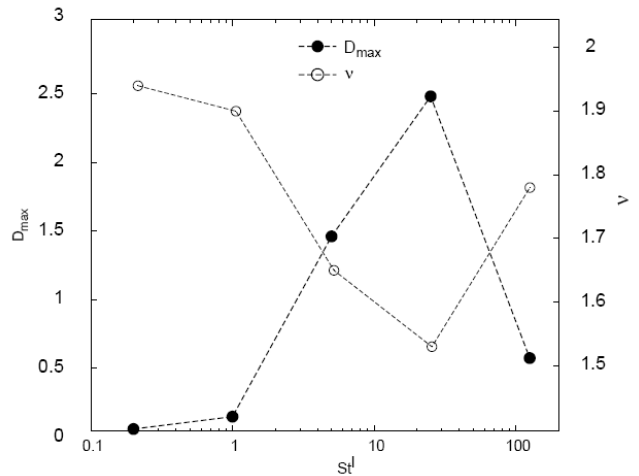


Figure 2: Maximum deviation from randomness, D_{max} (black circles), and correlation dimension, ν (open circles), in the viscous sublayer as a function of the particle Stokes number, St . Data are relative to the no-gravity, no-lift flow.

B. Quantification and control of local particle segregation in transverse jet

Transverse jets are used in many industrial flow configurations to achieve effective mixing between a dispersed phase (particles or droplets) and a main stream (e.g. fuel injection in combustion chambers, post-combustion control devices): species are injected by a carrier fluid normal to the main, transverse stream and the desired mixing effect some distance away from the jet exit can be obtained by tuning the jet flow and/or the crossflow.

The flow field generated by the jet is characterized by the instability of the jet shear layer which, even under steady state conditions (i.e. constant velocity profile for the jet and the transverse stream), promotes the (quasi periodical) formation of large-scale roll-up structures (shear layer vortices, SLVs) at the jet interface, as sketched in Figure 3. SLVs dominate the initial portion of the jet, the downstream side of which is characterized by formation of wake vortices; farther downstream, streamwise counter-rotating vortices dominate the flow field.

In a previous work (Campolo et al., 2005) we used the correlation dimension analysis to demonstrate that preferential accumulation of particles into specific patterns is selectively observed depending on the particle size. Since the characteristic time of segregated particles fits with the time scales of the SLVs, we concluded that these structure are those controlling mixing in the transverse jet. In our opinion, this suggests the possibility to modulate the dispersion of species exploiting the time-dependent nature of the mixing structures, instead of controlling “actively” their generation through jet forcing techniques –see Shapiro et al. (2003), and Karagozian et al. (2005) for details on jet forcing. In

Campolo et al. (2008) we proposed to use pulsed injection of particles and precise synchronization between injection time and flow structures dynamics. To prove the idea we performed a numerical experiment (a coarse DNS) in which the Eulerian-Lagrangian approach is used to simulate the dispersion of packets of $5 \mu\text{m}$ particles, those more responsive to the SLVs. Each packet is made of 5000 particles, transported into the crossflow by the jet. The Stokes number of these particles can be given as $St = \tau_p/T_{slv} = 0.64$, where T_{slv} is the time of circulation of SLVs. The jet Reynolds number and the cross-flow Reynolds number are $Re_{jet} = U_{jet}D/\nu_f = 2000$ and $Re_{cf} = U_{cf}D/\nu_f = 400$, where D is the jet exit diameter, and U_{cf} is the unperturbed crossflow velocity. The computational domain, sketched in Fig. 3a), is $12D \times 8D \times 9D$ in the streamwise, spanwise and vertical directions, respectively, discretized using $92 \times 58 \times 51$ finite volumes. Smaller volumes are used to describe the jet exit region. For further details on boundary and initial conditions for both phases, see Campolo et al. (2005) and Campolo et al. (2008).

We focused specifically on the effect produced on particle dispersion by different time delays of injection. Figure 3 sketches schematically the particle injection times. Time zero (not indicated in the sketch) corresponds to the injection of the first (of 490 simulated) particle packet. Top-down grayscale arrows identify the time of injection of four (out of 490) significant particle packets chosen for the analysis. The solid line represents the spanwise vorticity signal sampled shortly downstream of the jet exit. This signal allows to monitor in real time the formation of SLVs (Megerian and Karagozian, 2005), eventually adjusting the time shift between the pulsed injection of particle and the formation of mixing vortices. Black arrows identify the time at which the snapshot shown in Figure 3 were taken. Injection times for particle packets (a), (b), (c) and (d) differ by $T = T_{roll-up}/2$ each, $T_{roll-up}$ being the frequency of formation of SLVs. This choice is made to evaluate variations in particle dispersion due to the interaction of the four particle packets with a couple of spanwise SLVs at different stages of their evolution. Figures 3b-c) show four snapshots of particles from packets (a)-(d) about $2 T_{roll-up}$ after the injection of each packet. Only particles contained in the jet symmetry plane (i.e. within the slab $\|y/D\| < 0.25$) are shown, superposed to spanwise vorticity isocontours, which are used to visualize SLVs. Particles belonging to packets (a) and (c) seem to be effectively entrained by SLVs, being wrapped backward around the vortex in the jet symmetry plane. Particles belonging to packets (b) and (d) seem to escape this strong interaction, moving downstream slightly faster than packets (a) and (c). This has consequences on the dispersion of particles.

We tried to quantify the preferential accumulation of particles injected at different times using the segregation parameter (D_{max}): the statistical distribution of the local particle number density was obtained for different subspace dimension, and the segregation parameter was defined as D_{max} , i.e. the largest value obtained over the different subspace dimensions. We should remark here that in the jet in crossflow the random distribution of particles in the whole computational domain does not represent a “realizable” state for the particle/flow system, since (i) the particles are initially clustered at the point of injection and (ii) some regions of the flow (for instance, the region of the crossflow which is upstream the jet orifice) can never be explored. This poses some interesting issues on the use of D as a robust indicator of particle segregation: the quantifier is biased because the

random distribution can not be obtained, and can not discriminate between the clustering generated by injection and the clustering resulting from mixing/de-mixing by vortical structures. However, our focus is to identify *differences* in preferential segregation among particle packets which should definitely be ascribed to the effect of clustering by mixing/de-mixing vortical structures. Furthermore, the length scale at which clustering occurs allows to discriminate if the clustering is the result of initial segregation or if it is generated by vortical structures. From our calculation we found that the length scale associated with D increases over time, indicating that while at the starting time clustering is controlled by injection conditions, at later times it is associated with the mixing/de-mixing action of specific flow structures (SLVs).

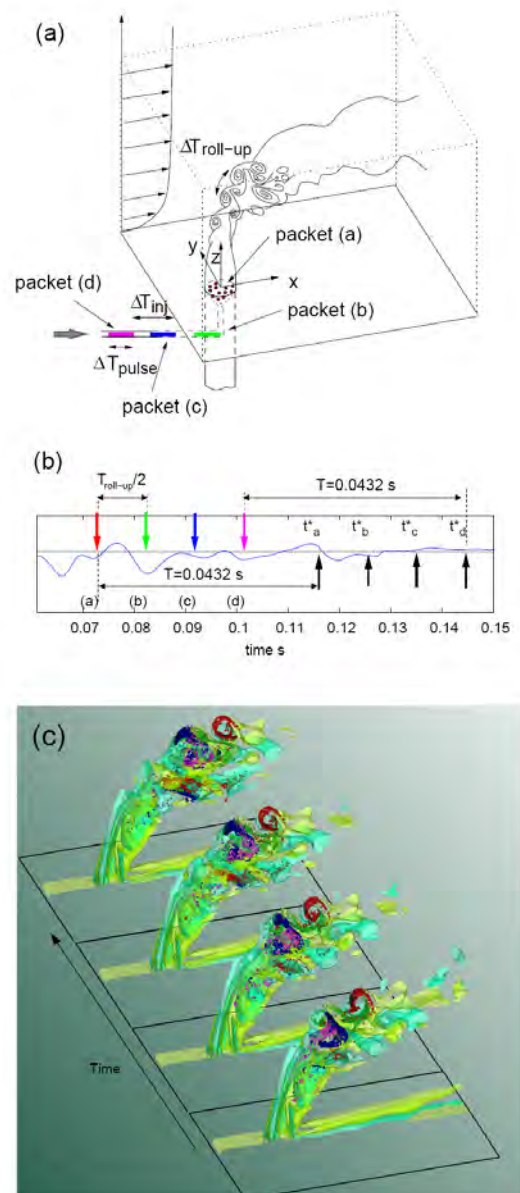


Figure 3: *Particle dispersion control by synchronized injection in transverse jet. Panels: a) b) Injection time of four particle packets (top-down grayscale arrows) and time of visualization (black arrows). The oscillating line represents the variation of spanwise vorticity sampled near the jet exit. Packets are injected $\Delta T_{roll-up}/2$ one after the other. c) Time evolution of dispersion patterns for the different packets.*

Figure 4 shows the time evolution of D for packets (a)-(d). Initially the value of D is large for all packets indicating that the preferential segregation of particles in the issuing volume is imposed by injection conditions. This value decreases over time as particles move and disperse into the flow. When the time of flight becomes larger than 0.02 s, particles start to interact with SLVs inducing fast decrease of D , the rate of decrease being larger for particle packets (a) and (c) than for particle packets (b) and (d). For all packets, the value of D remains very large for airborne particles, indicating that they do not disperse in the entire volume. Interestingly, after the interaction with SLVs, the value of D for particle packets (a) and (c) becomes lower than for particle packets (b) and (d). This indicates that for packets (a) and (c), the vortical structures are more effective in destroying the initial clustering, dispersing particles more homogeneously in space, whereas for packets (b) and (d), the interaction with the same structures at a different stage of their evolution is not strong enough to promote effective dispersion.

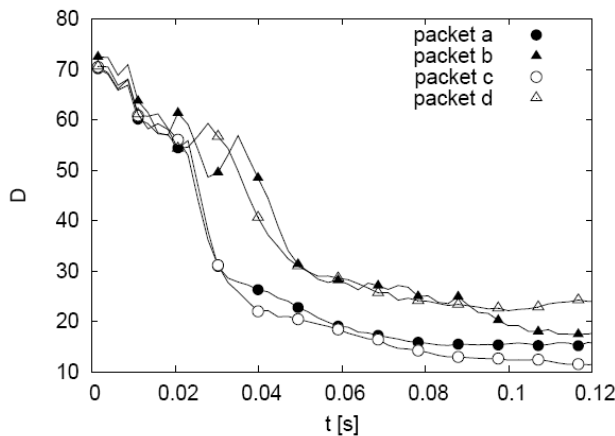


Figure 4: Variation over time of the segregation parameter for packets injected $T_{roll-up}/2$ one after the other.

3 Conclusions and Outlook

A statistical characterization of particle preferential segregation is important to provide a sound physical picture of the dispersion mechanisms and to develop accurate predictive models. In this paper, the possibility to measure and control local particle segregation in a turbulent flow is analyzed by means of two statistical tools: the segregation parameter and the correlation dimension. The analysis is performed considering two simple yet fully relevant case studies: particle-laden turbulent channel flow and particle-laden transverse jet. The segregation parameter can be used to compare the distribution of particle resulting from the actual concentration field to the expected distribution for the same number of particles randomly distributed throughout the flow domain. Results for particle dispersion in turbulent channel flow indicate that significant departures from randomness occur and that the differences are strongly dependent on the response time of the particles. Also, the length scale of the particle clusters is found to change with the particle size. To avoid such dependence, the correlation dimension can be used to produce a single parameter describing the degree of concentration regardless of the scale on which it occurs. Results for particle dispersion

in transverse jet demonstrate that the dispersion of particles changes if particles are injected at different times, indicating a potential route to particle dispersion control through synchronized pulsed injection of species.

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INVESTIGATION OF THE LANGEVIN MODEL PARAMETERS IN NON-HOMOGENEOUS TURBULENT SHEAR FLOWS

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1 Introduction

In the framework of dispersed two-phase flow prediction coupled with Reynolds-averaged Navier-Stokes (RANS) modelling for the fluid phase, the improvement of stochastic models aimed at predicting the fluid velocity along a discrete particle trajectory is a challenging issue. Actually, such models are of interest not only for Eulerian-Lagrangian techniques, but also for closure of Eulerian-Eulerian PDF (Probability Density Function) approaches based on the joint fluid-particle velocity distribution (Simonin et al., 1993; Minier and Peirano, 2001), in which a stochastic differential equation for the velocity of the fluid seen by a discrete particle is used to close the PDF transport equation. As this stochastic differential equation is generally built by analogy with the Langevin type equations used in the PDF approaches for one-phase turbulence modelling, in a way that ensures consistency in case of dispersed flow with low inertia particles, it is of special interest to investigate the parameters entering the Langevin model in non homogeneous turbulent shear flows.

Here we focus on the so-called “Generalized Langevin Model” (GLM, Haworth and Pope, 1986), which is consistent with Kolmogorov’s inertial range scaling and with second-order closure models (Pope, 1994a,b). Provided the time interval belongs to the inertial range, the increment of the instantaneous velocity of a fluid particle is modelled by:

$$du_i = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} dt + G_{ij} (u_j - \langle u_j \rangle) dt + B_{ij} dW_j, \quad (1)$$

where $\langle p \rangle$ and $\langle u \rangle$ are the mean terms (ensemble average) of pressure and velocity respectively, W_i is a Wiener process, G_{ij} and B_{ij} are the parameters of the GLM, called drift and diffusion tensors, respectively. This generalized Langevin model PDF equation is completely determined as soon as G_{ij} and B_{ij} are specified. The purpose of this paper is to present a route to derive G_{ij} and B_{ij} in some class of non homogeneous turbulent flows, namely channel or pipe flows.

A wide variety of turbulent flows can be modelled due to the flexibility in the functional form of G_{ij} and B_{ij} offered by the GLM equation (Minier and Pozorski, 1995; Das and Durbin, 2005). For instance, in isotropic turbulence, the functional form of these parameters is well established. The drift tensor is $G_{ij} = G\delta_{ij}$, where $-G$ exactly represents the inverse of the turbulence Lagrangian time scale. The consistency of the GLM with the Kolmogorov similarity theory for the second-order Lagrangian velocity structure function in the inertial subrange is usually invoked to determine B_{ij} . In this case B_{ij} is expressed as a function of Kolmogorov’s constant, C_0 , and the dissipation rate of the mean turbulent kinetic energy, ε , as $B_{ij} = \sqrt{C_0\varepsilon}\delta_{ij}$ (Pope, 1987). Yet, it has to be noted that this relation is generally used in more complex turbulent flows (Haworth and Pope, 1987). However, in such

cases there is a distinction between the Kolmogorov constant and the Langevin model constant (Pope, 2000).

In homogeneous turbulent shear flow, Pope (2002) showed the anisotropic character of the drift tensor G_{ij} and emphasized the strong anisotropic behavior of the diffusion tensor B_{ij} , contrary to conventional modelling assumptions. Moreover, Pope presented a guideline to determine the Langevin parameters using DNS data as a function of the Lagrangian time scale tensor and Reynolds stresses. More details about the identification procedure will be given in the next Section. This method was recently used by Walpot et al. (2007) in a pipe flow at two values of the Reynolds number based on pipe radius and friction velocity, i.e., $Re_\tau = 180$ and 323. From DNS and experimental data, Walpot et al. (2007) estimated partially the Langevin parameters appearing in the stochastic process. Similarly to Pope, they observed the anisotropic character of the drift term. To assess the diffusion term, they proposed to slightly generalize the usual isotropic model $\sqrt{C_0\varepsilon}\delta_{ij}$ to a diagonal diffusion matrix with $B_{ii} = \sqrt{C_0^{(i)}\varepsilon}$, where $C_0^{(i)}$ varies in the wall-normal direction.

In this work, we intend to specify the drift and diffusion matrices of the GLM from DNS data of a turbulent channel flow at $Re_\tau = 185$ (based on channel half-width). The layout of the paper is as follows. First, we describe the procedure used to identify the Langevin parameters from DNS data of a turbulent channel flow (Section 2). In Section 3, the results on Langevin parameters are presented and compared directly to those obtained by Walpot et al. (2007) for the drift tensor components in a turbulent pipe flow. The values of the diffusion tensor in the channel flow are also compared to those extracted from their DNS pipe flow results. Finally, a *posteriori* validation is carried out (Section 4) and some conclusions are drawn in Section 5.

2 Identification of the Langevin model parameters

The starting point of the study by Pope (2002) is the GLM written in terms of the fluctuating fluid velocity time increment, u'_i , as:

$$\begin{aligned} du'_i &= du_i - d\langle u_i \rangle \\ &= \tilde{G}_{ij} u'_j dt + B_{ij} dW_j + \frac{\partial \langle u'_i u'_j \rangle}{\partial x_j} dt, \end{aligned} \quad (2)$$

where $\tilde{G}_{ij} = G_{ij} - \frac{\partial \langle u_i \rangle}{\partial x_j}$. The analogy between our work and Pope’s analysis lies in the connection of $\tilde{G}_{ij}$ and B_{ij} to the Reynolds stress tensor $C_{ij} = \langle u'_i u'_j \rangle$ and the Lagrangian

time scale tensor $\mathcal{T}_{ij}$ defined by

$$\mathcal{T}_{ij} = \int_0^\infty C_{ik}^{-1} \langle u'_k(0) u'_j(\tau) \rangle d\tau, \quad (3)$$

where C_{ij}^{-1} denotes the i - j component of the inverse of the Reynolds stress tensor. The idea of Pope (2002) in a linear turbulent shear flow was to calculate the autocorrelation function of the stochastic process (2) in which $(\partial \langle u'_i u'_j \rangle / \partial x_j)$ vanishes due to the homogeneity of the turbulence. Such a pathway allowed him to obtain a simple relation between the drift and Lagrangian time scale ($\mathcal{T}$) tensors. In non homogeneous turbulence, the presence of the term $(\partial \langle u'_i u'_j \rangle / \partial x_j)$ in Eq. (2) complicates the situation. Therefore, we have to assume $\partial \langle u'_i u'_j \rangle / \partial x_j \approx 0$ in order to determine $\tilde{G}_{ij}$ and B_{ij} . The validity of this approximation will be checked in Section 4. Consequently, Eq. (2) reduces to:

$$du'_i = \tilde{G}_{ij} u'_j dt + B_{ij} dW_j. \quad (4)$$

It can be easily shown (Oesterlé and Zaichik, 2004) that the Lagrangian time scale tensor $\mathcal{T}$ and the drift matrix $\tilde{G}$ are connected by:

$$\mathcal{T} = (-\tilde{G}^{-1})^T. \quad (5)$$

In order to determine the diffusion tensor, B , the covariance of the stochastic process, Eq. (4), has to be calculated keeping in mind that the stochastic differential equation is defined in the Itô sense. Making use of Itô's formula to evaluate the differential of the product $u'_i u'_j$ and taking the average of the resulting expression yields:

$$\left\langle \frac{d(u'_i u'_j)}{dt} \right\rangle = \tilde{G}_{ik} C_{kj} + \tilde{G}_{jk} C_{ki} + B_{ik} B_{jk}. \quad (6)$$

The major difference between the study of Pope and ours lies in the non-homogeneous character of the turbulence. Actually, in a statistically homogeneous turbulence the left hand side of Eq. (6) can be expressed in terms of the Reynolds stress tensor as

$$\left\langle \frac{d(u'_i u'_j)}{dt} \right\rangle = \frac{d \langle u'_i u'_j \rangle}{dt}, \quad (7)$$

whereas in non homogenous turbulence the average of the time derivative of the product $u'_i u'_j$ is equal to:

$$\left\langle \frac{d(u'_i u'_j)}{dt} \right\rangle = \frac{\partial \langle u'_i u'_j \rangle}{\partial t} + \langle u'_k \rangle \frac{\partial \langle u'_i u'_j \rangle}{\partial x_k} + \frac{\partial \langle u'_i u'_j u'_k \rangle}{\partial x_k}. \quad (8)$$

Nevertheless, the present turbulent channel flow being statistically stationary and homogeneous in the streamwise and spanwise direction, Eq. (8) is reduced to:

$$\left\langle \frac{d(u'_i u'_j)}{dt} \right\rangle = \frac{\partial \langle u'_i u'_j u'_2 \rangle}{\partial x_2}, \quad (9)$$

where x_2 denotes the wall-normal direction. Invoking the local homogeneity assumption, the turbulent diffusion term $\partial \langle u'_i u'_j u'_2 \rangle / \partial x_2$ can be neglected, leading to the simplified relationship:

$$B_{ik} B_{jk} = -\tilde{G}_{ik} C_{kj} - \tilde{G}_{jk} C_{ki}. \quad (10)$$

In the next section, we present the estimated values of the Langevin parameters obtained using Eqs. (5) and (10) and data extracted from a channel flow DNS.

3 Results

As mentioned before, the definition of the fluid Lagrangian time scale tensor used by Pope (2002), see Eq. (3), is different from that used here. We have computed the Lagrangian time scales from the following relation:

$$T_{ij}^L = \int_0^\infty R_{ij}^L(\tau) d\tau, \quad (11)$$

where $R_{ij}^L(\tau)$ is defined by

$$R_{ij}^L(\tau) = \frac{\langle u'_i(0) u'_j(\tau) \rangle}{\sqrt{\langle u'^2_i(0) \rangle \langle u'^2_j(\tau) \rangle}}. \quad (12)$$

The major difference between Eq. (3) and Eq. (11) lies in the normalization of the covariance. Pope (2002) normalized it by the Reynolds stresses, $C_{ij} = \langle u'_i u'_j \rangle$, whereas we used the root mean square of the velocity fluctuations. Nonetheless, under the local homogeneity assumption, our definition of the Lagrangian time scales is equivalent to:

$$T_{ij}^L \simeq \frac{1}{\sqrt{\langle u'^2_i(0) \rangle \langle u'^2_j(0) \rangle}} \int_0^\infty \langle u'_i(0) u'_j(\tau) \rangle d\tau. \quad (13)$$

Consequently, our computed Lagrangian time scales are related to those defined by Pope (2002) by the following relationship:

$$\sqrt{\langle u'^2_i(0) \rangle \langle u'^2_j(0) \rangle} T_{ij}^L = \sum_k \langle u'_i u'_k \rangle \mathcal{T}_{kj}. \quad (14)$$

The Lagrangian time scales T_{ij}^L and the Reynolds stress tensor being known from our DNS computations, $\mathcal{T}_{ij}$ can be easily deduced from this system of linear equations.

To sum up, the Lagrangian time scale tensor, $\mathcal{T}_{ij}$, is computed from Eq. (14) using the data provided by a turbulent channel flow DNS. Then, the drift coefficients G_{ij} are deduced by Eq. (5). Finally, the diffusion tensor B_{ij} is estimated using Eq. (10).

A few details on the present DNS

The domain size in the streamwise, wall-normal, and spanwise direction is $2.5\pi\delta \times 2\delta \times 1.5\pi\delta$ and the corresponding grid $192 \times 128 \times 160$, respectively. Computations are operated at $Re_b = 2800$ and the flow rate is kept constant (the Reynolds number based on the wall shear velocity is 185). The channel flow is homogeneous in the streamwise and spanwise directions, and periodic boundary conditions are applied in these directions. The second order finite difference DNS solver is based on the model proposed by Orlandi (2000). The time discretisation is semi-implicit, *i.e.* the non-linear terms are written explicitly with a third-order Runge-Kutta scheme and the viscous terms are written implicitly using a Crank-Nicolson scheme. In the wall-normal direction, the mesh is stretched according to a hyperbolic tangent law, whereas a uniform mesh is applied in the streamwise and spanwise directions. The computational time step is $\Delta t^+ \approx 0.1$. This time step is smaller than the Kolmogorov time scale which is of the order of unity in wall units. The capability of second order finite difference solvers to predict realistic turbulent flow statistics has been shown in many papers, see for instance Choi et al. (1992) and Orlandi (2000).

The drift coefficients G_{ij} in channel and pipe flows

In Fig. 1, the components of G_{ij}^+ are plotted as a function of y^+ . Quantities in wall units (i.e., normalized using the friction velocity u_τ and the kinematic viscosity ν) are denoted by the superscript $+$. The results obtained by Walpot et al. (2007) are also reported. Concerning the diagonal components, similar results are obtained in the pipe and channel flows. The anisotropic character of the drift tensor is clearly noticed since the absolute values obtained for G_{11}^+ (streamwise direction) are lower than those of the wall-normal component G_{22}^+ , the latter being higher than those of the spanwise component G_{33}^+ . From the results plotted for the off-diagonal components, it is interesting to note that G_{21}^+ is zero across the channel and the pipe. The other non-diagonal component, G_{12}^+ , is seen to be similar to that obtained by Walpot et al. (2007) in a turbulent pipe flow. The present mean fluid velocity gradient as well as the one provided by Walpot et al. (2007) have also been plotted. The values of G_{12}^+ and of the mean fluid velocity gradient can be observed to be close to one another except in the near-wall region. These results about G_{ij} are important since they imply that $\tilde{G}_{ij}$ is a diagonal matrix (keeping in mind $\tilde{G}_{12} = G_{12} - \partial \langle u_1 \rangle / \partial x_2$). In the near-wall region, the results obtained at $y^+ < 10$ (Fig. 1) are questionable but not surprising for two major reasons. The first one lies in the use of the Langevin equation in the near-wall region, because such an equation does not take into account the viscous effects which are more important at low Reynolds number. The second reason is that the assumption of local homogeneity is violated in this region.

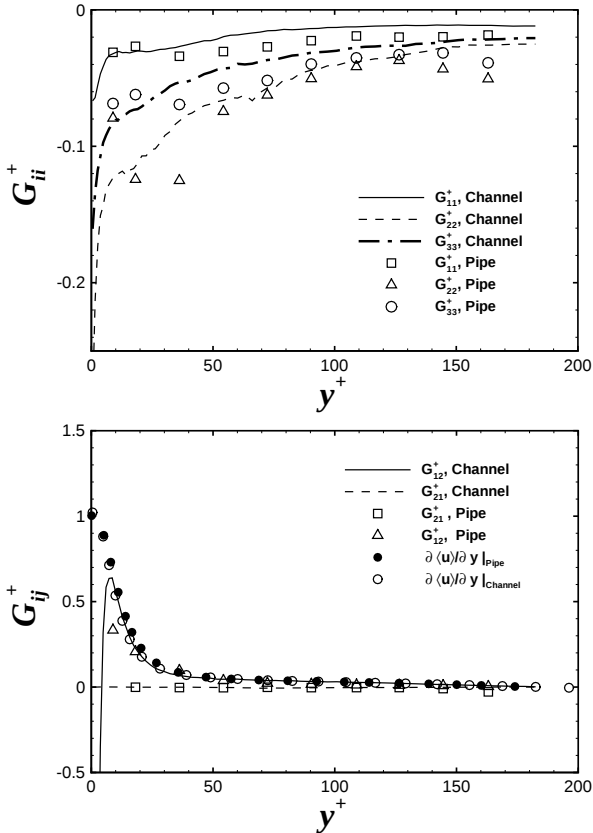


Figure 1: The diagonal and non-diagonal components of the drift tensor obtained in the present channel flow at $Re_\tau = 185$ and in a pipe flow at $Re_\tau = 180$ Walpot et al. (2007).

The diffusion tensor B_{ij} in channel and pipe flows

In Fig. 2, the components of the tensor $B_{ik}B_{jk}$ obtained from Eq. (10), normalized and denoted $(B^2)_{ij}^+$, are plotted as a function of y^+ . The components of the same tensor estimated in a similar way using the data on $\tilde{G}_{ij}$ and C_{ij} provided by Walpot et al. (2007) are also reported. Our procedure to obtain $(B^2)_{ij}^+$ is different from that used by Walpot et al. (2007), who assumed this term to be a diagonal diffusion matrix such as $(B^2)_{ij} = C_0^{(i)} \varepsilon \delta_{ij}$ in which $C_0^{(i)}$ was generally called “Kolmogorov constant” even if it depends on the considered velocity component. It is preferable to consider $C_0^{(i)}$ as a new parameter of the stochastic model since the Kolmogorov constant has a physical meaning only in high Reynolds number flows. The results confirm that the diffusion tensor is anisotropic, as previously observed by Pope (2002) in a turbulent homogeneous shear flow. According to Pope (2002), such a behavior is probably due to the low Reynolds number at which the flow is numerically simulated. For the diagonal and off-diagonal components, it can be noted that the results in the channel and pipe flows are very similar for $y^+ > 50$. Below this value, some significant discrepancies appear. The major one is found for the maximum of $(B^2)_{11}^+$ since the present value is more than twice as large as the one extracted from the pipe flow DNS of Walpot et al. (2007).

In the near-wall region, a zero value of $(B^2)_{ij}^+$ at $y^+ = 0$ is observed from the results provided by the channel flow DNS. In the pipe flow case, the results seem also to tend to zero at $y^+ = 0$. This value of the diffusion components at the wall cannot be assessed with the usual modelling of $(B^2)_{ij}^+$ since the dissipation rate of the turbulent kinetic energy, ε , is nonzero at the wall and the constant C_0 is a positive constant. Therefore, the diffusion tensor cannot be estimated from the usual relation $(B^2)_{ij} = C_0 \varepsilon \delta_{ij}$ in non homogeneous turbulent flow at low Reynolds number. On the whole, the results obtained for $\tilde{G}_{ij}$ and $(B^2)_{ij}^+$ in pipe or channel flows at Reynolds number of the same order of magnitude reveal similar trends.

To summarize, we would like to emphasize that $\tilde{G}_{ij}$ is found to be a diagonal matrix whereas $(B^2)_{ij}^+$ is non diagonal (therefore the diffusion tensor $\mathbf{B}$ is also non diagonal) and its components tend to zero at the wall.

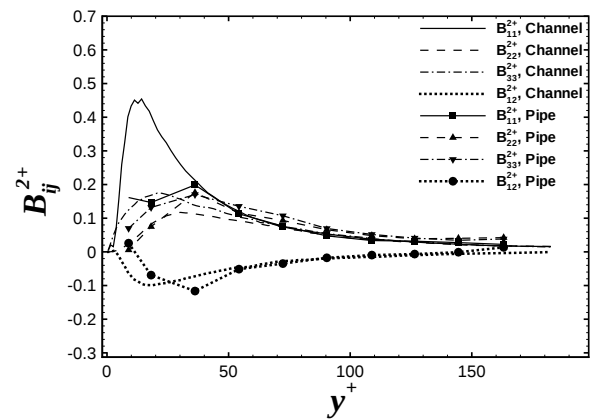


Figure 2: The diagonal and non-diagonal components of $(B^2)_{ij}^+$ obtained in the present channel flow at $Re_\tau = 185$ and in a pipe flow at $Re_\tau = 180$ Walpot et al. (2007).

4 A posteriori validation

In this section, we present some results obtained by tracking fluid particles using Eq. (2) to generate their fluctuating ve-

locity, with the drift and diffusion coefficients estimated by means of our DNS data. Two test cases have been performed. The first one is intended to check from the instantaneous fluid particle distribution if the basic law of mass conservation can be satisfied, while the second test has been performed to assess the validity of our parameter identification and its ability to produce the correct time decorrelation of the fluid particle velocity. Moreover, in these two test cases, the influence of the presence of the divergence of the Reynolds stresses in the stochastic equation has been studied, recalling that this term has been neglected in our estimation of the stochastic equation parameters.

Fluid particle concentration profile

The first test has been conducted to check the mass conservation law, taking the divergence of the Reynolds stress tensor $[(\partial \langle u'_i u'_j \rangle / \partial x_j) dt]$ into account or not in Eq. (2). It has to be noted that Legg and Raupach (1982) demonstrated that the absence of this term in a Markov chain model introduces a spurious drift effect, i.e., an unphysical preferential concentration of fluid-like particles near the wall. In other words, the concentration profile of fluid-tracer particles uniformly introduced should remain uniform when this term is present. To perform this test, we have tracked fluid particles according to the equation :

$$\frac{dX_{f,i}}{dt} = \langle u_i \rangle + u'_i, \quad (15)$$

where $X_{f,i}$ are the coordinates of the fluid particle, the data for $\langle u_i \rangle$ are extracted from the present DNS while u'_i is directly obtained from the integration of Eq. (2). It should also be noted that all the mean properties of the fluid motion ($\partial \langle u_i \rangle / \partial x_j$ and $\partial \langle u'_i u'_j \rangle / \partial x_j$) appearing in the stochastic differential equation are also issued from DNS data. The domain was divided into 40 slabs in the wall-normal direction. Initially, 10 000 particles were introduced in each slabs. During the simulations, fluid particles impacting the wall were eliminated.

In Fig. 3 the concentration profile normalized by the bulk concentration is plotted as a function of y^+ . We have reported the initial concentration profile of the fluid particles, C_i and the final stationary profiles obtained with and without neglecting the term $(\partial \langle u'_i u'_j \rangle / \partial x_j) dt$ in the integration of Eq. (2). As can be seen, the computed concentration remains uniform if the term $(\partial \langle u'_i u'_j \rangle / \partial x_j) dt$ is taken into consideration while without this term the concentration is seen to increase in the viscous sub-layer and near the channel center. Consequently, the mass conservation of the fluid is shown to be satisfied by the formulation of Eq. (2) as soon as the term $(\partial \langle u'_i u'_j \rangle / \partial x_j) dt$ is introduced in the stochastic differential equation.

Fluid Lagrangian time scales

In the second test case, the fluid Lagrangian time scales obtained by tracking fluid particles using the stochastic differential equation (2) have been compared with the results extracted from the DNS, in order to verify that our identification of the drift and diffusion coefficients produces the correct time decorrelation of the fluid particle velocity.

For this stochastic simulation, 100 000 fluid particles were tracked by means of Eq. (15). As for the previous test, the required Eulerian statistics are taken from the DNS and Eq. (2) is used to predict the fluctuating fluid velocity at particle location. The Lagrangian velocity correlations were computed during the simulation and post-processed in order to obtain the associated time scales. The simulations have been conducted in taking or not the divergence of the Reynolds stress

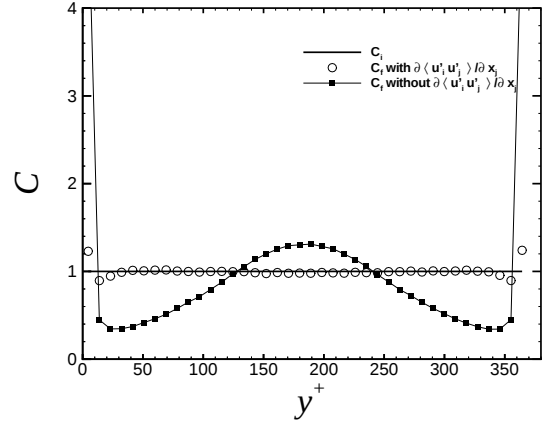


Figure 3: Concentration of fluid particles across the channel.

tensor into account in the differential stochastic equation. We have observed that the results were nearly identical, which means that this term does not influence the time decorrelation of the fluid particle velocity. Therefore, only the results obtained in taking the Reynolds stress tensor divergence into account are presented hereafter.

In Fig. 4, the fluid Lagrangian time scales T_{ij}^+ issuing from both the DNS and the stochastic computations are presented in wall units as a function of y^+ . Good agreement between the DNS results and those provided by the stochastic equation (2) is observed for the three diagonal components of the Lagrangian time scales. Concerning the off-diagonal components, which are also plotted in Fig. 4, the results obtained from the stochastic simulation are qualitatively in good accordance with the DNS data since T_{21}^+ is correctly found to be lower than T_{12}^+ whatever the position in the channel. However, the absolute values obtained from the stochastic computation for T_{12}^+ and T_{21}^+ are slightly lower than those provided by DNS when $50 < y^+ < 150$. Nevertheless, even if the results for the non-diagonal components are less satisfactory than those obtained for the diagonal components, the results are still in acceptable agreement with the DNS data.

Finally, we would like to emphasize the fact that this *a posteriori* test is not a complete self-consistent validation. In order to really check the pertinence of the present estimation of the drift and diffusion coefficients, $\tilde{G}_{ij}$ and B_{ij} , it would be necessary to incorporate them in a purely Lagrangian PDF method, i.e., a stand-alone PDF method for the turbulence. From this numerical simulation, the Eulerian statistics (such as the mean fluid velocity, the Reynolds stress tensor, the skewness and the flatness of the velocity, etc.) could be extracted and compared to DNS results as done in the study by ?. Even if the large number of particles required for robust and accurate simulations would make the simulations very time-consuming, such tests should be considered as a next step of the present study.

5 Conclusion

The main goal of the present work was to provide, for a non homogeneous turbulent flow, estimates of the drift and diffusion coefficients appearing in a Langevin-type stochastic equation used to predict the fluctuating velocity of fluid particles. By mimicking the approach derived by Pope (2002) for homogeneous turbulent shear flows, these parameters have been identified by means of DNS data.

The present results show that the drift tensor matrix $\tilde{G}_{ij}$ can

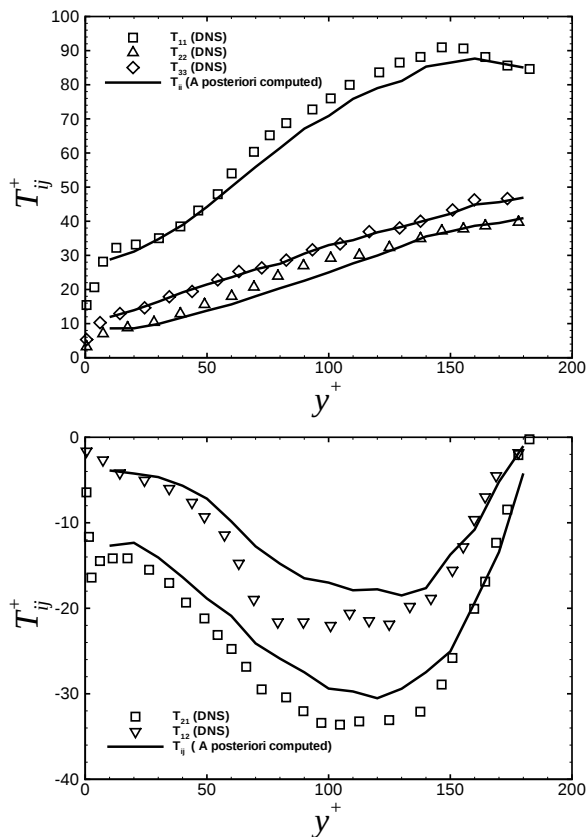


Figure 4: Comparison of the diagonal and non-diagonal components of the decorrelation time scales extracted from DNS and those a posteriori computed.

reasonably be assumed to be diagonal, but not spherical, both for channel and pipe flows at low Reynolds number. The diffusion tensor has been found to be anisotropic, in line with the observation made by Pope (2002) for a homogeneous turbulent shear flow. Moreover, a zero value at the wall was found whatever the components of B_{ij} and similar results were also obtained using the data extracted from the turbulent pipe flow DNS by Walpot et al. (2007).

In order to validate our estimation of the drift and diffusion coefficients, we have computed fluid particle trajectories using the generalized Langevin equation (2). We have verified from the concentration profiles that the model does not induce any spurious drift provided that the divergence of the Reynolds stress tensor is included in the stochastic differential equation. The fluid Lagrangian time scales have also been extracted from the stochastic simulation, showing satisfactory agreement with the DNS data. This means that the time decorrelation of the fluctuating velocity is correctly reproduced using the estimated drift and diffusion coefficients in the stochastic differential equation (2). Finally, it should be noted that the divergence of the Reynolds stresses has to be taken into account in the stochastic simulation to avoid the effect of spurious drift, even if it has been neglected in the procedure used to estimate the stochastic equation parameters. Nevertheless, as shown by the *a posteriori* simulations, this approximation does not have any consequences on the time decorrelation of fluid particle's fluctuating velocity.

To conclude, we have shown that it is possible to use a Langevin-type equation to properly predict the time increment of the fluctuating velocity of a fluid particle in a non homogeneous flow provided that its parameters are correctly specified. Anisotropic models of the drift and diffusion tensors remain an open question but it is hoped that the present

study will help to the improvement of PDF models, including the Lagrangian stochastic approaches for dispersed two-phase flows.

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VALIDATION PROCEDURE FOR DISCRETE PARTICLE SIMULATION OF TURBULENT TWO-PHASE FLOWS WITH DROPLET COALESCENCE

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Abstract

Discrete Particle Simulation (DPS) can be used in order to understand the physical mechanisms fluid turbulence exerts on particle dispersion or on particle-particle collisions and at the same time to provide a reliable reference data base for the development of statistical modelling approaches. A correct prediction of these deterministic simulations is therefore fundamental for the understanding and modelling of these complex phenomena. In this work a validation procedure for DPS is proposed focusing on both the correct prediction of fluid properties at the particle position and a correct prediction of collision handling. The strategy to validate the collision algorithm is based on dry granular flows, which allow testing the algorithm performance without the disturbing influence of the fluid phase. Finally it is shown how a correct handling of droplet coalescence can be assured.

1 Introduction

Particle laden turbulent flows are found in many industrial and practical applications like pneumatic conveying, circulating fluidized bed, liquid-fuel injection in internal combustion engines or rain drop formation. These flows involve a variety of complex phenomena, such as turbulent dispersion, particle-particle collisions, droplet coalescence, particle-wall interactions, turbulence modulation by the particles or heat and mass transfer.

The numerical simulation of turbulent two-phase flows has been extensively improved for the last decades. Nowadays the development of numerical methods and the parallel computing allow performing a Direct Numerical Simulation (DNS) of the interstitial fluid between moving particles [Prosperetti & Oguz 2001]. This approach is the most physical as it requires a minimum of closure models. However, even for the simulation of low-scale particle-liquid fluidized beds [Corre et al. 2009], the computational cost restricts this method to a quite low number of particles (roughly 5000 particles). Hence, this method is usually employed to investigate the momentum or heat transfer at the particle diameter scale [Masol 2004], but it is impossible to investigate collective phenomena taking place, such as particle accumulation.

An alternative approach considers each particle as a material point and the trajectory of each individual particle is computed in a Lagrangian frame. This approach, called Discrete Particle Simulation (DPS), can be applied for several millions of particles and can be coupled either with DNS or Large Eddy Simulation (LES) of the carrier phase. The DPS needs models for the momentum or heat transfer from the fluid to the particles. The turbulence

modulation by the particles (the so-called two-way coupling) is questionable especially when the DPS is coupled with a LES.

The DPS can be used in order to understand the physical mechanisms fluid turbulence exerts on particle dispersion or on particle-particle collisions and at the same time to provide a reliable reference data base for the development of statistical modelling approaches. A correct prediction of these deterministic simulations is therefore fundamental for the understanding and modelling of these complex phenomena.

In this paper we propose a step-by-step validation procedure for DPS of inertial droplets suspended in turbulent flows and undergoing droplet coalescence. This work proposes a methodology that ensures an accurate treatment of particle dispersion (section 3) and particle-particle collisions or droplet coalescence handling (section 4). As particles transported by a turbulent flow are considered, section 2 briefly introduces the numerical predictions of turbulent flows, while focusing on the problems related to the coupling of DPS with the numerical simulation of single-phase turbulent flows.

2 Particle path computation & validation

2.1 Particle trajectory

A dispersed phase of N_p spherical particles with diameter d_p and density ρ_p is considered in this work. Turbulence modulation by the dispersed phase (two-way coupling) is neglected, as the solid mass loading is small. Assuming that the particle to fluid density ratio ($\rho_p \gg \rho_f$) is large, the forces acting on a single particle are reduced to the drag force and gravity only. Thus, the governing equations of a single particle is written as [Maxey & Riley 1983, Gatignol 1983]

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \quad (1)$$

$$\frac{d\mathbf{v}_p}{dt} = -\frac{\mathbf{v}_p - \mathbf{u}_{f@p}}{\tau_p} + \mathbf{g}, \quad (2)$$

where $\mathbf{x}_p$ and $\mathbf{v}_p$ are the position and velocity vector of the p -particles. The particle response time τ_p is given by

$$\tau_p = \frac{4}{3} \frac{\rho_p}{\rho_f} \frac{d_p}{C_D} \frac{1}{|\mathbf{v}_p - \mathbf{u}_{f@p}|}. \quad (3)$$

According to Schiller & Naumann [1935], for particle Reynolds number smaller than 1000 the drag coefficient C_D is written as

$$C_D = \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}), \quad (4)$$

with $Re = d_p |\mathbf{v}_p - \mathbf{u}_{f@p}| / \nu_f$ and ν_f the kinematic viscosity of the fluid.

2.2 Fluid flow prediction

The computation of particle paths in a turbulent flow needs the knowledge of the exact instantaneous fluid velocity. From a theoretical point of view, Direct Numerical Simulation (DNS) of the Navier-Stokes equations is the most accurate approach. It is well known that the DNS is restricted by the Reynolds number and the consequently required grid. However, the development of the parallel computing permits to perform DNS of quite large Reynolds number by using with a huge number of grid points [Kaneda 1996]. The Large Eddy Simulation (LES) consists in solving the large scales of turbulence and in modelling the small scales (subgrid scales). The coupling of DPS with a LES is questionable, as in order to compute the particle trajectory the instantaneous fluid velocity is required, but LES gives the instantaneous filtered fluid velocity only. In the literature many papers are found analyzing the effects of the subgrid fluid velocity [Armenio et al. 1996, Yamamoto et al. 2001, Kuerten 2006, Fede & Simonin 2006] and proposing stochastic or deconvolution models [Fede et al. 2006, Pozorski & Apte 2009, Mashayek & Randya 2003]. For a very large number of particles, more than 10 millions, the coupling of DPS with an evolving DNS becomes unrealizable due to the computational cost. However, it is possible to couple the DPS with a frozen turbulent velocity field extracted from an evolving DNS [Wang et al. 2000]. In such a numerical simulation some spurious effect may appear leading to unphysical phenomena. Figure 1 shows the particle kinetic energy with respect to the inverse of the Stokes number with

$$q_p^2 = \frac{1}{2} \langle v'_{p,i} v'_{p,i} \rangle, \quad q_{f@p}^2 = \frac{1}{2} \langle u'_{f@p,i} u'_{f@p,i} \rangle, \quad \frac{\tau_{f@p}^t}{\tau_{fp}^F} = \frac{1}{St},$$

where $1/\tau_{fp}^F = \langle 1/\tau_p \rangle$ and $\tau_{f@p}^t$ is the Lagrangian integral time scale given by

$$\tau_{f@p}^t = \int_0^{+\infty} R_{f@p}(\tau) d\tau, \quad (5)$$

with

$$R_{f@p}(\tau) = \frac{\langle u'_{f@p,i}(t) u'_{f@p,i}(t + \tau) \rangle}{2/3 q_{f@p}^2}. \quad (6)$$

Figure 1 shows that the particle kinetic energy measured in DPS coupled with evolving DNS is the same as the one in DPS coupled with a frozen flow for a wide range of Stokes numbers.

In contrast, fig. 2 shows that the Lagrangian fluid integral time scale seen by the particle measured in a frozen flow deviates from the one in evolving DNS for large Stokes number. The particles with a large Stokes number experience the turbulent field as a motionless observer. Then the time scale seen by the particles goes to the Eulerian time scale which is nearly identical to the eddy-life time that is infinite in frozen flows. This effect is clearly shown in fig. 2 and it is seen that frozen flow simulation (empty symbols) clearly overestimates the Lagrangian fluid integral time scale seen by large Stokes number particles.

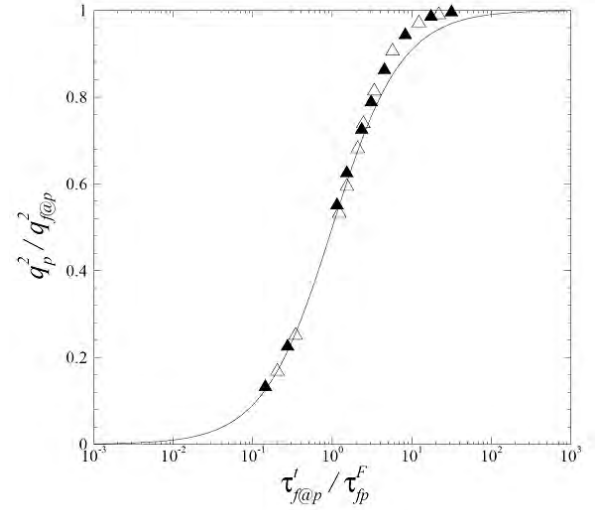


Figure 1: Particle kinetic energy normalized by the fluid kinetic energy measured at the particle position with respect to the inverse of Stokes number measured along inertial particle suspended in Homogeneous Isotropic Turbulent flows. The black filled symbols are the evolving DNS, the empty symbols the frozen flow and the solid line the relations based on the theory of Tchen & Hinze [1947].

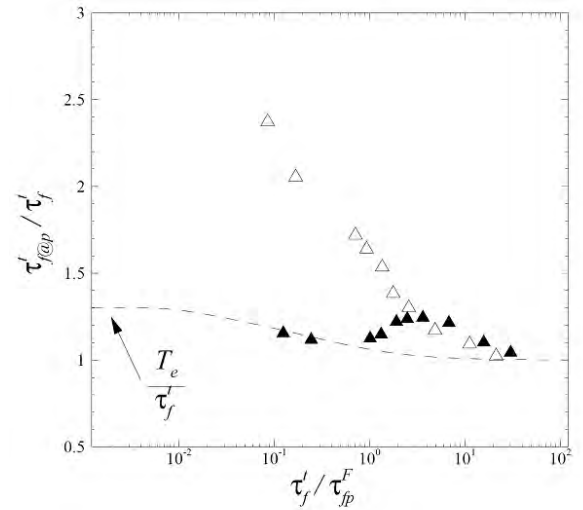


Figure 2: Lagrangian fluid integral time scale seen by the particle with respect to the inverse of Stokes number measured along the path of inertial particles suspended in Homogeneous Isotropic Turbulent flows. The black filled symbols are the evolving DNS and the empty symbols the frozen flow. The dashed line represents the semi-empirical model by Wang & Stock [1993].

Therefore, frozen flows can be coupled with DPS, if particle dispersion is investigated. However, care should be taken for particles with larger Stokes numbers, as the particle distribution could be modified and consequently have an effect on the collision kernels or coalescence rates.

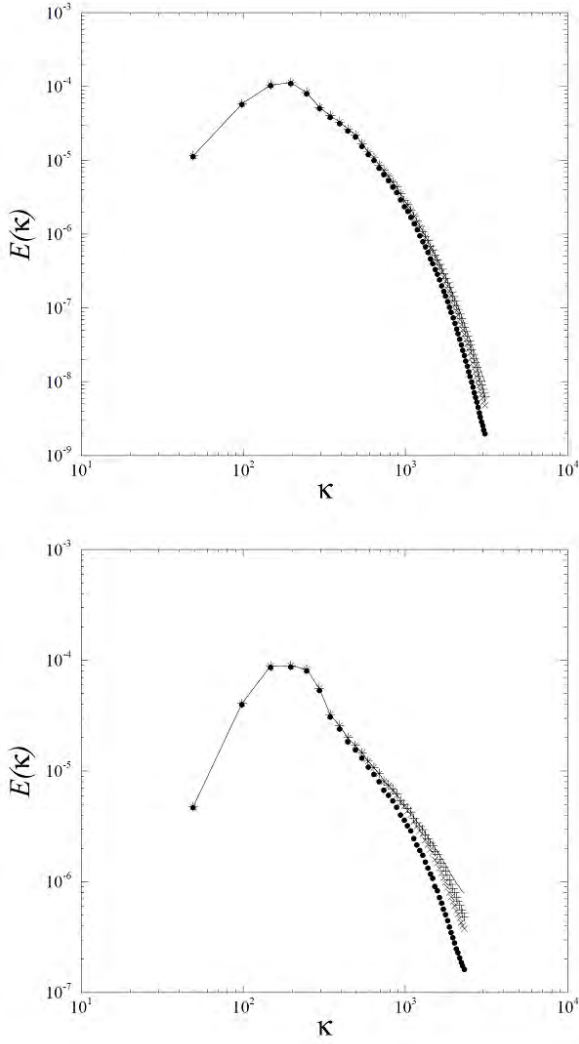


Figure 3: *Turbulent spectrum computed on staggered grid. Top: DNS with $Re=60$ (128^3 grid points) and bottom: LES with $Re=819$ (96^3 grid points). Solid lines are the spectrum computed on fluid grid, $\bullet$: linear scheme, $\times$: SFM and $+$: cubic splines.*

2.3 Validation of particle trajectory computation

The key element for solving system (1) is the computation of the undisturbed fluid velocity at the particle position $u_f@p$. As two-way coupling is neglected the fluid velocity at the position of the particle is computed by interpolating the turbulent fluid flow predictions obtained by means of DNS [Balachandar & Maxey 1989]. As an interpolation scheme is a filter, an inaccurate interpolation scheme may change the physics of the two-phase flow. The validation of the interpolation scheme is done using a staggered grid. Therefore, the fluid flow is predicted by DNS (or LES) on a given uniform grid with N^3 grid points. Then the interpolation scheme is used to compute the velocity field on a second uniform grid staggered from the first one. For illustration, three interpolation schemes are used here: linear, Shape Function Method (SFM) and cubic splines.

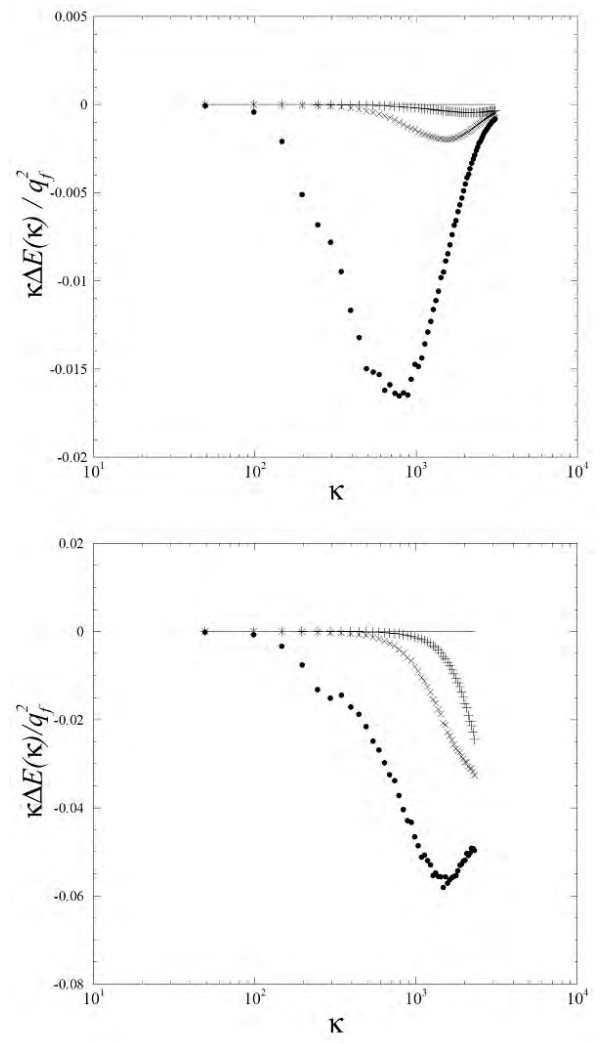


Figure 4: *Error evaluation of the interpolation scheme. Top: DNS with $Re=60$ (128^3 grid points) and bottom: LES with $Re=819$ (96^3 grid points). Solid lines are the spectrum computed on fluid grid, $\bullet$: linear scheme, $\times$: SFM and $+$: cubic splines.*

Two turbulent velocity fields are considered: first, a flow field predicted by means of DNS on a grid with 128^3 grid points and a turbulent Reynolds number $Re=60$. Second, a flow field predicted by LES with 96^3 grid points and turbulent Reynolds number $Re=819$. The first-order evaluation of the interpolation scheme consists of comparing the moments of the fluid velocity computed for both grids, the original and staggered one. The error of the interpolation scheme is quantified by

$$\frac{\Delta q_f^2}{q_f^2} = 100 \frac{[q_f^2]_{DNS} - [q_f^2]_{Stag}}{[q_f^2]_{DNS}} \quad (7)$$

The error produced by the linear scheme is much more important than the error given using by the SFM or cubic spline scheme, as expected and seen in Tab. 1. Following the results given in tab. 1, the question about the

real value of a cubic spline scheme instead of SFM might arise, as SFM already gives an error of the order of 0.05% and is much more computational cost efficient compared to the cubic spline scheme. To answer this question, fig. 3 compares the energy spectrum computed on the DNS grid and on the staggered grid. It is observed that all interpolation schemes modify the turbulent spectrum as a filter. However the cubic spline gives a better representation of the small scales of turbulence. Fig. 4 shows the difference between the spectra normalized by the integral of the DNS spectrum given as

$$\frac{[\kappa \Delta E(\kappa)]_{DNS} - [\kappa \Delta E(\kappa)]_{Stag}}{[\int \kappa \Delta E(\kappa) d\kappa]_{DNS}} = \frac{\kappa \Delta E(\kappa)}{q_f^2}. \quad (8)$$

Figure 4 clearly shows that the cubic splines interpolation scheme predicts better for the small scales of fluid turbulence. This is a very important point. If only particle dispersion is studied, the SFM interpolation scheme is probably sufficiently accurate. However, if particle-particle collisions in homogeneous isotropic turbulence are studied, the collision frequency in the limit case of zero inertia but finite volume particles is controlled by the local fluid velocity gradients (see Saffman & Turner [1956]). In this case an inaccurate interpolation scheme may lead to erroneous collision rates.

		Linear	SFM	Cubic splines
$\Delta q_f^2/q_f^2$ (%)	$Re=60$	1.60	0.053	0.007
	$Re=819$	2.90	0.24	0.05

Table 1: Error of the interpolation scheme on turbulent kinetic energy.

2.4 Particle dispersion with mean slip

The settling of particles in a turbulent field is an important complex phenomenon in multiphase flows. DPS is a powerful tool to bring some answers about the physical mechanisms acting in particle-turbulence interaction [Fessler et al. 1994, Février et al. 2005] or preferential concentration [Squires & Eaton 1991]. However, Fede et al. [2007] show that the periodical boundary conditions may cause a statistical bias in DPS of inertial particles falling in a homogeneous turbulence. Indeed, in such a numerical simulation a particle that crosses an edge of the computational domain is re-injected at the opposite side.

Fede et al. [2007] show that when the particle residence time in the box is smaller than the turbulent eddy-life time the particles may interact with nearly the same fluid velocity field. Consequently the fluid velocities seen by the particles are correlated with themselves inducing a statistical bias. To illustrate this phenomenon fig. 5 shows the Lagrangian fluid velocity correlation function measured along the solid particle path.

Figure 5 shows the fluid velocity correlation function measured for two kinds of particles differing by the residence time to Eddy-Life time ratio. The particle residence time can be defined as

$$\tau_{inbox} = \frac{L_b}{|V_{set}|} = \frac{L_b}{g\tau_p}, \quad (9)$$

where L_b is the computational box length and V_{set} is the settling velocity $V_{set} = \tau_p g$. As seen in fig. 5 peaks

appear in the Lagrangian correlation function for a small value of τ_{inbox}/τ_E . It corresponds to a re-correlation effect due to periodical boundary conditions. Fede et al. [2007] proposed the limiting value of $\tau_{inbox}/\tau_E > 4$ to ensure that this statistical bias does not change the particles behaviour.

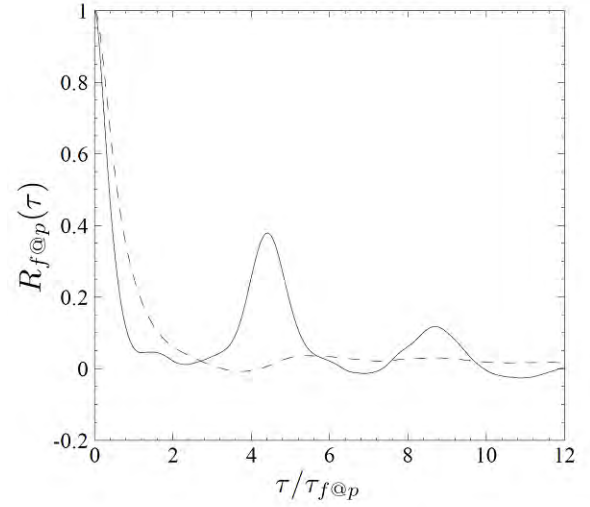


Figure 5: Fluid velocity correlation seen by settling particles for $\tau_{inbox}/\tau_E = 0.91$ (solid line) and $\tau_{inbox}/\tau_E = 4.34$ (dashed line). The fluid integral time scale $\tau_{f@p}$ is computed by integration of $R_{f@p}$ (6).

3 Collision/Coalescence validation

If collisions or coalescence are taken into account in DPS validation needs to be performed at two levels: first for the collision or coalescence model (in terms of momentum transfer) and second for the detection algorithm as both are independent.

The collision algorithm is validated performing dry granular flow simulations of mono- and bi-disperse particle mixtures. The results on a bi-disperse mixture, which are comparing the statistics obtained in dry granular flows with predictions originating from the kinetic theory of rarefied gases, can equally be considered as a validation of the collision detection algorithm in a poly-disperse particle mixture. As usually only binary collisions are treated, a bi-disperse simulation validates the case of a poly-disperse mixture. The validation is conducted in dry granular flows as the statistical properties that should represent the particulate system are known from the theory of rarefied gases. It is therefore possible to conduct simulation without the ‘disturbing influence’ of a fluid phase. All changes in the particle trajectories are exclusively related to particle-particle collisions. This configuration of dry granular flows offers therefore ideal conditions for the validation of the collision detection algorithm.

In this section we first introduce a detection algorithm and a collision model. Second we present criteria in order to validate the collision model and third the detection algorithm. The last part is dedicated to the validation of coalescence. It is emphasized that the validation criteria do not depend on the collision model or detection algorithm.

3.1 Particle detection and collision model

Several algorithms for the treatment of the dispersed phase are found in literature [Hopkins & Louge 1990, Sigurgeirsson et al. 2001, Sundaram & Collins 1997]. The simplest, but also an extremely inefficient way to detect particle-particle collisions is checking for collision between all possible particle pairs in the computation domain. This way the cost of checking for collision is $N_p(N_p - 1)/2$ and hence in the order of $O(N_p^2)$. The computation cost can be reduced by using a detection grid. In Wunsch et al. [2008] a collision detection algorithm for a polydisperse particulate phase is proposed. This algorithm has two collision detection criteria, the first is the standard overlap criterion, i.e. a collision between two particles is found by overlap of the particles at a given time step. This kind of algorithm demands a small time step in order to accurately predict the collision frequency. Wunsch et al. [2008] show that the introduction of a second criterion, which compares the relative position of the colliding particles in two consecutive time steps increases the time step significantly.

The detection algorithm provides a list of colliding particles for which a collision or coalescence model has to be applied. Assuming an instantaneous frictionless collision of spherical solid particles, the particle velocities after a collision are given by

$$\begin{aligned} \mathbf{v}_p^\bullet &= \mathbf{v}_p + \frac{m_q}{m_p + m_q} (1 + e_c) (\mathbf{w} \cdot \mathbf{k}) \mathbf{k}; \\ \mathbf{v}_q^\bullet &= \mathbf{v}_q - \frac{m_p}{m_p + m_q} (1 + e_c) (\mathbf{w} \cdot \mathbf{k}) \mathbf{k}, \end{aligned} \quad (10)$$

where $\mathbf{w}$ is the particle-particle relative velocity, $\mathbf{k}$ the normalized unit vector connecting both particle centres and m_p the p -particle mass. The particle restitution coefficient e_c represents the loss of particle energy during the collision.

3.2 Collision model validation

The validation of the collision model is handled by performing DPS of homogeneous granular flows. The particles are initially randomly distributed and the particle velocity distribution becomes Gaussian due to the redistribution effects of collisions as seen in fig. 6. In case of monodisperse elastic particles ($e_c=1$) the particle kinetic energy is perfectly conserved. So the particle kinetic energy must be constant.

One of the main differences with a system of a monodisperse mixture is the fact that in a bi-disperse particle mixture the energy levels for each particle class are not the same in the thermal equilibrium state. Heavier particles do not show the same particle agitation in the equilibrium state as lighter particles. This equilibrium state of the particle agitation can be expressed by the following relation

$$m_p q_p^2 = m_q q_q^2 \quad (11)$$

If the particle collisions are elastic, the particle agitation of the bi-disperse mixture q_m^2 can be written as

$$q_m^2 = \frac{n_p m_p q_p^2 + n_q m_q q_q^2}{n_p m_p + n_q m_q} \quad (12)$$

The relations (11) and (12) allow writing the particle agitation for each class in function of the particle agitation of the mixture

$$q_m^2 = \frac{n_p m_p q_p^2 + n_q m_q q_q^2}{n_p m_p + n_q m_q} \quad \text{and} \quad q_q^2 = \frac{n_p m_p + n_q m_q}{m_q (n_p + n_q)} q_m^2. \quad (13)$$

Now, it is possible to find an expression for the ratio of q_p^2/q_m^2 and q_q^2/q_m^2 , which only depends on the mass of the particle classes m_p and m_q as well as on their number densities n_q and n_p . The same values can be measured in the DPS simulations. A comparison of the measured values to the predictions of the equilibrium theory is given in fig.7. Figure 7 shows that the particle kinetic energies converge towards their respective theoretical values. This is due to the transfer of particle kinetic energy by collisions.

Note that the proposed validation of the collision model is independent of the collision detection algorithm. Indeed the detection algorithm gives the number of collision, in other word the collision frequency. Then even if the collision frequency is wrong the relation (13) remains correct. The difference is the time needed to reach the equilibrium (11).

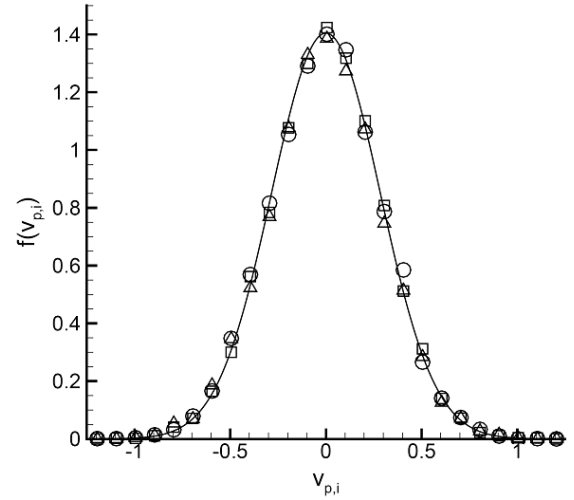


Figure 6: Particle velocity distribution. Gaussian distribution with mean $\mu = 0$ and $\sigma = 0.284$ (Solid line), $\square$: x-component, $\triangle$: y-component, $\circ$: z-component.

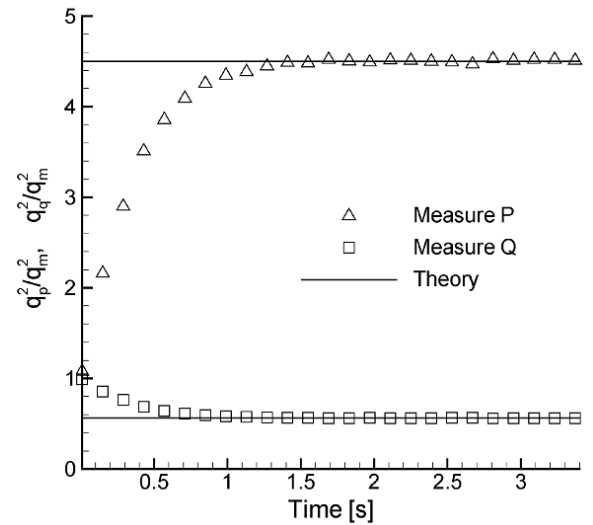


Figure 7: Comparison of particle kinetic energy ratios measured in DPS to predictions from the equilibrium theory (13).

3.3 Collision detection algorithm

The validation of the detection algorithm is mainly related to the collision frequency and consequently with the time step of the simulation. To evaluate the collision detection algorithm the relevant parameter is the mean particle displacement during a time step δl . For a mean displacement larger than the particle diameter collision missing is expected. In the frame of the kinetic theory of rarefied gases applied to granular media, the mean particle displacement during a time step normalized by the particle diameter is expressed as

$$\frac{\delta l}{d_p} = \frac{3}{2} \sqrt{\frac{2\pi}{3}} q_p^2 \frac{\Delta t}{d_p}. \quad (14)$$

Distributions of collision angle N_θ and relative velocity at the moment of collision $N_{\mathbf{w}_{pq}}$ are used to quantify the efficiency of the collision algorithm. The kinetic theory provides the following theoretical relations

$$f(\theta) = -4n_p^2 d_p^2 \sqrt{\frac{2\pi}{3}} q_p^2 \sin(2\theta) \quad (15)$$

and

$$f(\mathbf{w}_{pq}) = n_p^2 d_p^2 \sqrt{\frac{2\pi}{3}} q_p^2 \frac{9}{8q_p^2} \mathbf{w}_{pq}^3 \exp\left(-\frac{3\mathbf{w}_{pq}^2}{8q_p^2}\right) \quad (16)$$

The accuracy of the predictions with respect to the time step criterion $\delta l/d_p$ is shown in fig.8 and fig.9.

As clearly seen in fig.8 and fig.9 a sufficient algorithm performance is achieved when the particle propagation is limited to about 13% of a particle diameter, thus for a ratio $\delta l/d_p = 0.13$. Similar results are obtained by Sakiz [1999]. For ratios $\delta l/d_p$ larger than this value the simulation results deviate from the prediction based on the kinetic theory of rarefied gases and especially grazing collision are missed. In dependence of the flow configuration in DNS/DPS simulations of turbulent two-phase flows the criterion $\delta l/d_p$ can be more stringent than the CFL number of the DNS, which is disadvantageous as the DNS of the continuous phase then needs to be solved applying a time step which is not optimal. In fig.9 it is seen that with an increasing ratio of $\delta l/d_p$ more and more particle-particle collisions are missed between particles with a high relative velocity. This appears logic as faster particles cover a larger distance during a fixed time step than slower ones. Consequently fig.8 shows that the grazing collisions are more sensitive to a higher ratio of $\delta l/d_p$. To remedy this restriction in the time step criterion a second particle pair detection criterion is introduced in the algorithm developed in Wunsch et al. [2008]. In practice, this criterion is a significant advantage as the time step criterion on the dispersed phase is still more stringent than the one on the fluid phase and therefore corresponds to a net increase of the time step by a factor of ten.

Representing correctly the relative velocity and collision angle distributions is not sufficient for the validation of the detection algorithm. If for example a systematic error in the detection algorithm persists that affects random particles, the distribution PDF's exhibit a correct behaviour, but the collision frequency is not correctly represented. A correct prediction of the collision frequency is crucial. It is the most important statistic of the dispersed phase. The influence of collisions on any quantity is written as the change in the quantity by the collision multiplied with the collision frequency. Therefore, the collision frequency measured is compared to the

predictions of the theoretical collision frequency. For a binary mixture of particles the kinetic theory gives the following relation for the collision frequency

$$f_{pq}^\kappa = g_0 n_p n_q \pi \left(\frac{d_p + d_q}{2} \right)^2 \sqrt{\frac{16}{3\pi} (q_p^2 + q_q^2)}, \quad (17)$$

where g_0 is radial distribution function introduced to take into account the increase of collision frequency due to particle packing. In diluted granular flows the radial distribution function is nearly equal to 1 but for dense flows g_0 depends on the particle volume fraction α_p [Carnahan & Starling 1969, Lun & Savage 1986].

As can be seen in fig.10 the DPS results correspond very well with the theoretical predictions for the collision frequency corrected by the model for the radial distribution function of Carnahan & Starling [1969]. Thus, it is verified that the collision frequency is correctly predicted.

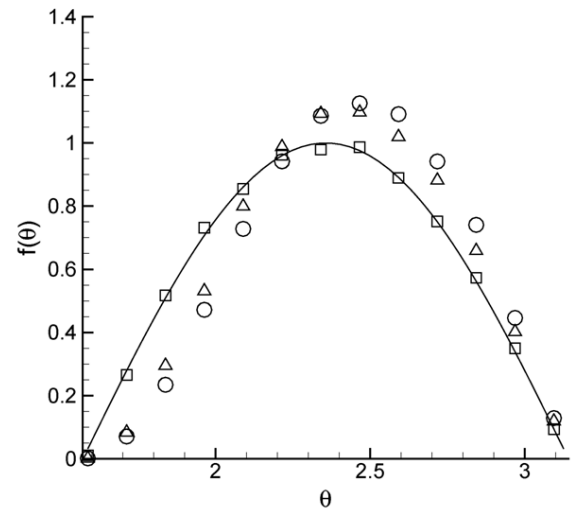


Figure 8: Collision angle PDF in dependence on ratio $\delta l/d_p$ using a pure overlap detection algorithm. The symbols stand for $\square:0.13$, $\triangle:1.3$, $\circ:1.9$ and the solid line the prediction given by (11).

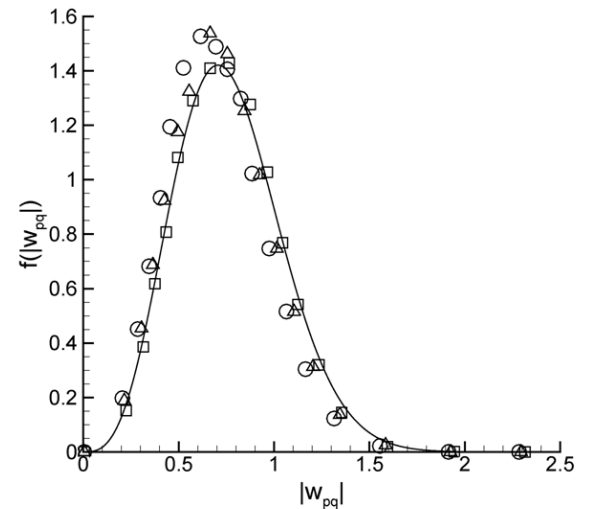


Figure 9: Impact relative velocity PDF dependence on ratio $\delta l/d_p$ using a pure overlap detection algorithm. The symbols stand for $\square:0.13$, $\triangle:1.3$, $\circ:1.9$ and the solid line the prediction given by (11).

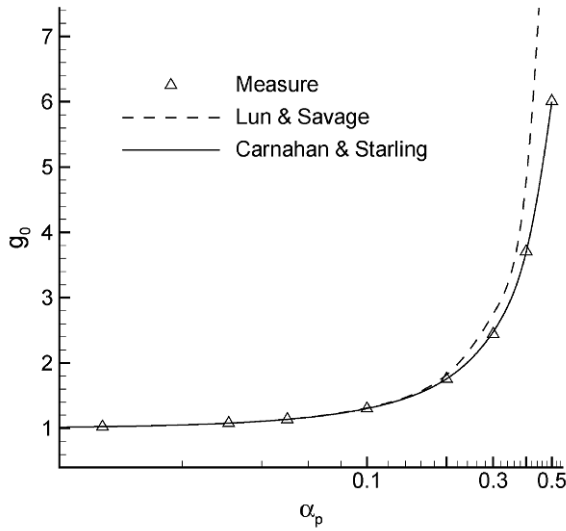


Figure 10: Comparison of radial distribution function g_0 measured in DPS to theoretical predictions with respect to the particle volume fraction α_p .

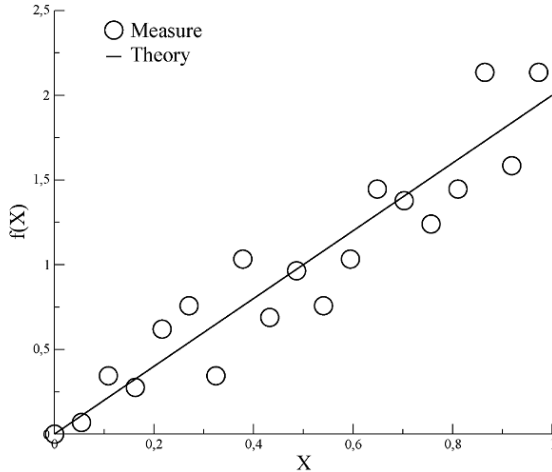


Figure 11: Comparison of measured impact parameter X in dry coalescence to predictions from theory.

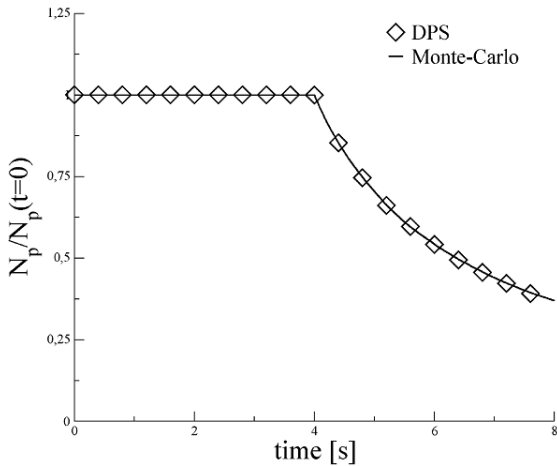


Figure 12: Particle number measured in DPS in comparison with Monte-Carlo simulations in dry coalescence.

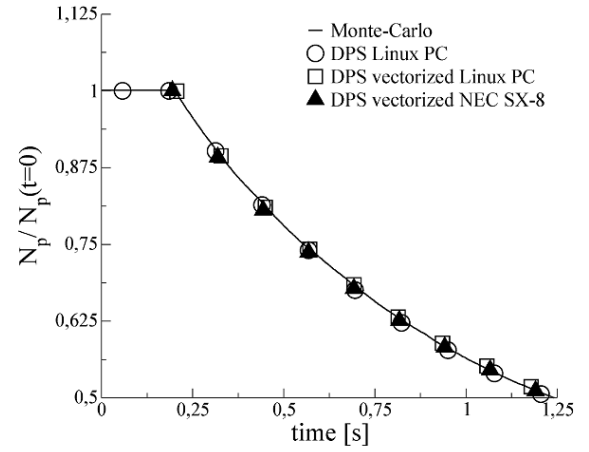


Figure 13: Droplet number N_p measured in DPS in comparison with predictions from Monte-Carlo simulations comparing vectorized and non-vectorized versions of the code on different platforms.

3.4 Coalescence

The collision of liquid droplets can lead to different collision outcomes, such as droplet rebound, permanent coalescence, reflexive or stretching separation. These collisions regimes can be described in terms of the Weber number We , which is the ratio of droplet inertia to surface tension, and the impact parameter X , which is a geometrical quantity. $X-We$ diagrams are known from experimental studies [Ashgriz & Poo 1990; Qian & Law 1997]. The droplet pair detection in case of other collision outcomes than rebounds, such as the above mentioned, remains the same and only the droplet collision handling is altered.

Coalescence phenomena are modelled representing a pure coalescence regime only for the sake of distinctness. This means that each collision leads to permanent coalescence and no other collision outcomes exist. Moreover, the coalescence handling is validated in a dry coalescence regime, which means that only the disperse phase is present, such that there is no influence of a fluid on the droplet interaction. Permanent coalescence is modelled applying mass and momentum conservation

$$m^* = m_p + m_q, \quad m^* \mathbf{v}^* = m_p \mathbf{v}_p + m_q \mathbf{v}_q \quad (18)$$

with m_p and m_q the mass of the particles before coalescence and m^* after. Analogous for the particle velocities $\mathbf{v}_p$, $\mathbf{v}_q$ and $\mathbf{v}^*$. The corresponding particle diameter is directly deductible from the mass conservation equations as the particle density is constant and the particles are modelled as rigid spheres. The position of the new particle that arises from coalescence is given as

$$\mathbf{x}^* = \frac{d_p^3 \mathbf{x}_p + d_q^3 \mathbf{x}_q}{d^*{}^3} \quad (19)$$

with $\mathbf{x}^*$ the position of the new particle and d_p , d_q and d^* the particle diameters.

It is possible to determine a theoretical probability density function (PDF) for both the Weber number and the impact parameter. For the purposes of this article, only the PDF of the impact parameter is regarded. A correct prediction of the Weber number and impact parameter is necessary for the determination of the droplet

collision regime, if more than a pure coalescence regime is taken into account. The prediction of the collision regime is crucial to the correct prediction of droplet size distribution and coalescence rate, especially if the formation of satellite droplets is accounted for. A distribution function is derived for the impact parameter X [Wunsch 2009], which is a purely geometrical quantity and can be calculated as a function of the collision angle PDF given in (11). It can be written as

$$N(X) dX = N_\theta(\theta) d\theta. \quad (20)$$

This leads to

$$N_X(X) = \frac{N_\theta(\theta)}{\left| \frac{dX}{d\theta} \right|}. \quad (21)$$

With some manipulations, respecting the relation between the collision angle and impact parameter, this equation can be transformed applying trigonometric rules in the interval $\theta \in [\frac{\pi}{2}; \pi]$, which is the interval of collision angles as it is defined here. It writes then

$$N_X(\theta) = 2 \sin(\theta), \quad (22)$$

which, expressed in terms of the impact parameter and applying $\theta = \pi - \arcsin(X)$, gives the final form for the PDF of the impact parameter as

$$N_X(\theta) = 2X. \quad (23)$$

The PDF of the impact parameter therefore describes a straight line through the origin. A comparison with measurements from DPS on a dry permanent coalescence flow is given in fig.11. The statistics verify this theoretical prediction of the impact parameter, although the statistics are moderate, which is due to the lack of events that can be taken into consideration.

The number of particles finds its maximum at the beginning of the simulation and decreases then with each single collision in the simulations performed here. Therefore, collisions are limited in number.

Measures of the coalescence rate in DPS simulations of dry coalescence, where permanent coalescence is the only possible collision outcome, are compared to predictions of Monte-Carlo simulations. These simulations are considered to be exact in dry granular flows and a correct measure of the coalescence rate and particle kinetic energy in the system is qualified by agreement with the Monte-Carlo predictions. The algorithm used is of Babovsky type [Babovsky 1986], where numerical particles represent a given number of real particles. These numerical particles are first grouped in $N_p/2$ pairs ($(N_p - 1)/2$ in case N_p is odd). Second, the collision probability for each pair is calculated, based on the particle properties and third, a random number is created and compared with the collision probability in order to decide, whether a collision takes place or not. The coalescence rate is presented in the following and then, the algorithm is validated on different platforms, using the DPS predictions in comparison with predictions of Monte-Carlo simulations.

The initialization of the Monte-Carlo simulations is done with an underlying fluid flow field which brings the particulate phase into a stationary state. At the moment coalescence is started the fluid flow is turned off and thus the configuration of dry granular flows is produced. Figure 12 shows that the particle number (and therefore the coalescence rate) is correctly represented.

The collision detection algorithm and collision treatment is integrated into the DNS solver and adapted to

its structure. Then, the algorithm is vectorized due to the vectorial structure of the NEC-SX-8 on which the DNS/DPS simulations were performed. Obviously a re-validation is necessary in order to assure not to introduce errors by these modifications. Besides the validations presented above, while validating the collision algorithm, also the coalescence rate and particle kinetic energy on different platforms are compared. The results are presented in fig.13. It is seen that the particle number as well as the particle kinetic energy are well represented and coincide with predictions on other platforms.

4 Conclusions

Several validation procedures for Discrete Particle Simulation of turbulent two-phase flows with droplet coalescence are proposed. First, restrictions of the coupling of DPS with DNS or LES are discussed, showing first limits for turbulent Reynolds number, in respect of computational cost for DNS and in terms of accuracy for LES and second for the high number of droplets for which a frozen DNS needs to be applied. Then a validation procedure for particle-particle collisions or droplet coalescence is presented. First discussing the correct prediction of fluid properties at the particle position and then validating the collision handling. The collision handling consists of first, validating the collision model and second the collision detection algorithm. The particle energies and PDFs of collision statistics are used to verify a correct collision handling. Finally, the modelling of droplet coalescence is validated in comparison with Monte-Carlo type simulations which are considered as accurate in dry granular flows.

Acknowledgements

This work was granted access to the HPC resources of IDRIS under the allocation 2009- i2009021066 made by GENCI (Grand Equipement National de Calcul Intensif).

This research project has been supported by a Marie Curie Early Stage Research Training Fellowship of the European Community's Sixth Framework Programme under contract number 'MEST-CT-2005-020426'.

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STOCHASTIC DISPERSION MODELLING BASED ON THE RANS APPROACH FOR A PARTICLE-LADEN SHEAR FLOW

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1 Introduction

The prediction of turbulent particle dispersion is important for many technical and natural processes. However, an accurate and generally accepted model has not been developed yet and different model predictions of particle dispersion in complex non-isotropic and non-homogeneous flows may differ substantially. Hence, models which are based on physically correct assumptions for the flow turbulence and still can be implemented with reasonable effort are needed.

This paper describes calculations of particle dispersion in a turbulent two-phase free shear layer based on the Euler/Lagrange approach using a standard $k-\varepsilon$ turbulence model for closure of the gas phase. The purpose of this work is to test a generalized Langevin equation model (GLE) for the turbulent carrier fluid velocities seen by the particles, which accounts for anisotropy by considering Reynolds stress gradients, local velocity gradients and time scale differences for different directions (see Minier & Peirano, 2001). Melheim et al. (2005) presented calculations of particle dispersion in a shear layer using this GLE model and focussed on the discussion of the particle concentration profile, particle velocity profile and shear stress profiles of particles and fluid seen by the particles at one stream-wise position and for one particle size. The current paper extends this work and discusses in more detail the particle dispersion mechanism and its implication on particle concentration profiles and their velocities.

2 The test case

As a test case, a shear layer flow was chosen, since it is well understood for the single-phase case while being a non-homogeneous and non-isotropic turbulent flow. Measurements of particle dispersion of this type of flow are available in Hishida et al. (1992), where gravity was in flow direction, Wen et al. (1992) with gravity pointing from the high speed side towards the low speed side, and Chang et al. (1993) with gravity in stream-wise direction. Lazaro & Lasheras (1992), Hardalupas & Horender (2003) and Horender & Hardalupas (2009) measured particle characteristics in a shear layer where gravity pointed from the low speed to the high speed side. The origin of the coordinate system was chosen so that the end of the splitter plate was at stream-wise position $x=0$ and cross-stream position $y=0$. The fluid velocity was 0.8m/s on the low speed side and 5.5m/s on the high speed side. The inlet conditions were the velocity profile as measured at the end of the splitter plate. Fig. 1 shows a vector plot of the velocity field and the different spacing

between velocity vectors shows the non-uniform resolution of the computational grid, which was necessary to resolve properly the inlet profile.

Nearly mono-dispersed glass beads of density 2590kg/m^3 with mean diameters of 90 microns were injected through a pipe with inner diameter 5mm just above the splitter plate. The particles had a free fall velocity of 0.058m/s. The particle feeding rate was 0.55g/s leading to a local maximum mean mass loading of approximately 12% and the air flow velocity through the injection pipe was approximately 3m/s. The particles were injected with a mean velocity of 2.7m/s. The rms velocity for the stream-wise particle velocity component was 0.3m/s and the cross-stream velocity fluctuations were set to 0.25m/s with a Gaussian distribution according to the experiment. The flow developed large scale vortex structures which grow with stream-wise development (Horender & Hardalupas, 2009). The Stokes numbers, defined as the ratio of particle relaxation time scale to vortex time scale (obtained with the shear layer thickness,) is 2.3 at stream-wise position $x=300\text{mm}$. Hence, particle centrifuging by the large scale fluid eddies was the main dispersion mechanism.

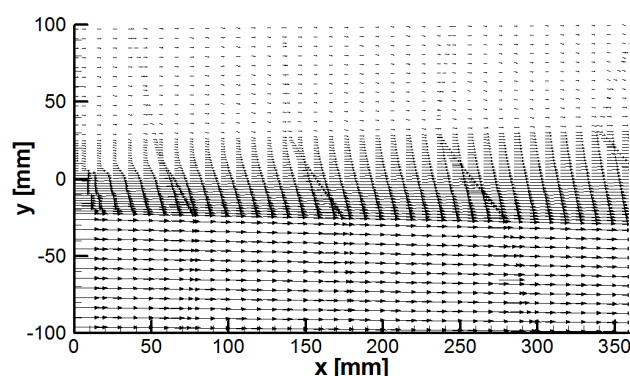


Figure 1: *Vector plot of the fluid velocity field.*

3 Flow computation and dispersion model

The steady fluid flow was computed by a standard 3D finite volume code (FASTEST4.0) using a $k-\varepsilon$ model for turbulence closure. Details can be found in Melheim et al. (2005) and therefore are not reported here. However,

it should be noted that the Reynolds stresses and their gradients were reconstructed from the flow field by the eddy viscosity hypothesis. The particles were tracked with the Lagrangian approach using the software Lag3D considering only drag force and gravity. Two-way coupling has been neglected here. It should be noted that the fluid velocity is denoted by u and the particle velocities by v and capital letters are mean quantities, small letters are the instantaneous velocities and dashed letters the rms values of the fluctuating quantities. Index 1 denotes the x -axis which is pointing in stream-wise direction and index 2 is the cross-stream component.

For the GLE model, the instantaneous fluctuating fluid velocity seen by the particles is modelled in terms of its acceleration as:

$$du_i = \left(-u_j \frac{\partial U_i}{\partial x_j} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} + (\bar{V}_j - \bar{U}_j) \frac{\partial \bar{U}_i}{\partial x_j} - \frac{1}{T_L} H_{ij} u_i \right) dt + B_{ij} \xi_i \quad (1)$$

Here, H_{ij} is a generalisation of the drift matrix for arbitrary mean slip between the flow phases, B_{ij} is the diffusion matrix and ξ_i is a Gaussian random process. It should be noted that the mean particle velocity appears in the third term on the r.h.s. of this model equation. Therefore, 100.000 parcels were tracked through the flow, representing many identical real particles to achieve the actual particle number density in the flow, for 8 iterations. The mean particle velocity in eq. (1) always was derived from the previous run and updated for the subsequent calculation.

The Lagrangian time scale is defined as:

$$T_L = \frac{1}{\left(\frac{1}{2} + \frac{3}{4} C_0\right) \frac{\varepsilon}{k}} \quad (2)$$

The constant $C_0=2.1$ and b_i are the Csanady factors, defined in Minier & Peirano (2001) and Melheim et al. (2005):

$$b_i = b_{\perp} + (b_{=} - b_{\perp}) \frac{(V_i - U_i)^2}{|\vec{V} - \vec{U}|^2} \quad (3)$$

$$b_{=} = \left(1 + \beta^2 \frac{|\vec{V} - \vec{U}|}{2k/3} \right)^{0.5} \quad (4)$$

$$b_{\perp} = \left(1 + 4\beta^2 \frac{|\vec{V} - \vec{U}|}{2k/3} \right)^{0.5} \quad (5)$$

Here, β is the ratio of Lagrangian to Eulerian time scale with $\beta = 1/C_L$ and with $C_L = 1.1$. This choice is applied for the current work since it is commonly used, however it deviates from eq. (12) and will be discussed below.

The matrix H_{ij} in the drift term of eq. (1) is defined as:

$$H_{i,j} = b_{\perp} \delta_{ij} + (b_{=} - b_{\perp}) r_i r_j \quad (6)$$

With r_i being the unit vector in direction of the mean slip between fluid and particles. The diffusion matrix B_{ij} is defined as:

$$(BB^T)_{ij} = D_{ij} \quad (7)$$

With

$$D_{ij} = \varepsilon \left(C_0 \lambda H_{ij} + \frac{2}{3} (\lambda H_{ij} - \delta_{ij}) \right) \quad (8)$$

and λ defined as:

$$\lambda = 3Tr(H_{ij}R_{ij}) / (2kTr(H_{ij})) \quad (9)$$

Here, Tr denotes the trace of the matrix and R_{ij} is the Reynolds stress tensor of the fluid.

With the above equations the model for the fluid velocity seen by the particles is closed and the change of particle velocity due to aerodynamic drag was then calculated according to:

$$\frac{d\vec{V}}{dt} = \frac{3\rho_f}{4\rho_p d_p} \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) \cdot (\vec{V} - \vec{U}) |\vec{V} - \vec{U}| + \vec{g} \quad (10)$$

Re_p is the Reynolds number defined based in the particle diameter d_p and the gas viscosity. ρ_p is the particle density and ρ_f the fluid density.

Particle collisions were model according to the stochastic iterative scheme of Sommerfeld (2001). Therefore, as described above, 8 iterations with 100.000 parcel tracks each were performed and the particle properties for the collisions, which are number density and mean as well as fluctuating velocities, were deduced from the previous run. However, it should be noted that for stream-wise positions larger 100mm only 15% of the particles experienced collisions. Only close to the injection collisions were relevant for particles dispersion, and hence, collisions will not be further discussed in this manuscript.

4 Results

Figure 2 presents the calculated mean and fluctuating carrier gas velocities as cross-stream profiles for stream-wise positions 10, 100 and 300mm. The measured values are also presented. Regarding the smallest stream-wise position it should be noted that in the simulations the air flow trough the particle injection pipe was considered, while for the experiments at that position it had been switched off. The larger positions were with air jet for both simulations and experiments. Some deviations exist on the high speed (lower) side, which may be attributed to the fact that the boundary layer below the splitter plate has not been properly resolved by the numeric grid. For the larger stream-wise positions, fig. 2 (b) and (c) this deviation is reduced. However, some discrepancies remained, especially the deviation from a clean shear layer profile for stream-wise position $x=100$ mm and cross-stream position $y=10$ mm was found in the experiments. The reason might be that the injecting pipe diameter was only resolved by three computational cells and hence the developing jet disappeared faster in the simulations due to numerical diffusion compared to the experiment. Hence, for highly accurate simulations the grid must be finer at the particle injection pipe. However, it is expected that the effect on the particles is small, since they have Stokes number much larger than one at the injection position and, as a consequence, are unable to be accelerated noticeably close to the injection position. The main influence of the gas flow on the particles occurred further down-stream, when their Stokes number becomes of the order of unity and the large scale fluid vortices mainly influence the particles. The predicted velocity fluctuations (Fig. 2 - dashed line) agree well on the high speed side ($y<0$) but show too small values for cross-stream positions $y>0$ for stream-wise position $x=100$ mm and for cross-stream positions $y>20$ mm

for $x=300$ mm. This again might be an effect due to the air flow through the particle injection pipe.

The integral time scale is an important parameter in the equation for the velocity seen by the particles. It has been deduced from the $k-\varepsilon$ turbulence model as

$$T_L = 0.24 \frac{2/3k}{\varepsilon} \quad (11)$$

and compared with measurements of the Eulerian autocorrelation function of the fluctuating stream-wise velocity. The simulations resulted in T_L on the centre line ($y=0$) for stream-wise positions 100, 300 and 500mm of 4.8ms, 7.8ms and 10.7ms. The measured Eulerian autocorrelation functions at the same stream-wise positions, see Horender (2002) fig. 11, have their first zero crossings at $t=6, 11$ and 26 ms. The deduced Eulerian integral time scale are then approximately 1.5, 3.0 and 6.0ms. McComb (1999, p. 445) reviewed earlier work and suggested the ratio of Lagrangian to Eulerian integral time scale as:

$$\beta = \frac{0.44\bar{U}}{u'} \quad (12)$$

For a shear layer this leads to $\beta \approx 1.9$ on the centre line, which is in approximate agreement with the above estimates.

Fig. 3 shows the measured and predicted mean particle concentrations at different stream-wise positions. It should be noted that the concentrations are all normalized by their maximum cross-stream value and that a calculation with the particles seeing only the mean gas flow was performed and is denoted as ‘laminar’ simulation. The figure shows that for the smallest stream-wise position the simulated particle concentrations agree well with the measurements. For the larger positions $x=300$ and 380 mm some deviations exist on the upper low speed side. Here the model predicts a too large dispersion against gravity towards the low speed side, while the simulations agree well with the measurements on the high speed side ($y<0$). The laminar calculations were performed to clarify the influence of the velocity distribution of the particles at the injection position on the downstream dispersion pattern. Clearly, the particles disperse much less upward with stream-wise development compared to the turbulent simulation. Additionally, there is a stronger downward drift when turbulence is not considered. This becomes most pronounced for cross-stream positions $y<-30$ mm. For the largest stream-wise position $x=380$ mm, the laminar simulations predicts well the measured values, however this is believed to happen to due neglecting several effects, which may cancel each other at exactly this position. Hence, in the following we will focus on the predictions of the turbulent dispersion model and try to identify reasons for the deviation from the measured profiles.

An explanation for the predicted too large dispersion of the turbulent calculations on the upper low speed side of the flow may be as follows. First, as shown in Fig. 2, the fluid velocity fluctuations for $y>20$ mm are predicted too small by the calculations, which might, however, lead to smaller dispersion. This might not be so important for the current flow situation, since the particle concentration at that cross-stream position was small due to gravity. The reason for the over-prediction of dispersion on the upper side of the shear flow may be related to particle clustering due to the fluid vortex structure. Horender & Hardalupas (2010) used a point vortex method to simulate the large scale vortex structure in a two-dimensional shear layer, which was similar to the current one, and

tracked particles, also with 90 μ m in diameter, through the flow field. They obtained probability density functions of the fluctuating carrier fluid velocities as seen by the particles and compared them with the Eulerian ones. They found that the particles on the lower (high) speed side viewed fluid velocity PDFs which were only slightly less broad compared to the Eulerian ones. However, on the centre line of the flow and on the low speed side ($y>0$), the viewed velocity fluctuations at stream-wise position $x=300$ mm were reduced by approximately 30% compared to the Eulerian value for the 90 micron particles, which had Stokes number between 2.6 and 4.5 based on the larger scale fluid vortices (not on the integral time scales). On the high speed side this effect was also present, however the reduction of the seen fluid velocity fluctuations were less than approximately 10%. Additionally, Horender & Hardalupas (2010) tracked 55 micron particles, with Stokes numbers ranging from 1.0 to 1.7, for which a stronger degree of preferential concentration was observed. These smaller particles showed even stronger reduced seen velocity fluctuations of the carrier fluid. Although the simulations by Horender & Hardalupas (2010) were two-dimensional, they should capture the main dispersion mechanism in a developing shear layer, which is pairing of the fluid vortices. Hence, considering their results on the reduction of the carrier fluid velocity fluctuations viewed by the particles due to particle clustering may be the reason that in the experiment dispersion towards the low speed side is reduced. This must be clarified by future calculations taking particle clustering effects into account. To further investigate the ability of the suggested model for the fluid velocity seen by the particle we will discuss the resulting particle mean velocities and compare them with measurements of Hardalupas & Horender (2003) and Horender & Hardalupas (2009).

Figure 4 shows the predicted mean particle velocities in stream-wise and cross-stream directions again for stream-wise positions $x=220, 300$ and 380 mm for the laminar and turbulent case and the experiments. It is observed that the mean cross-stream velocity V_2 generally is predicted well, only for the smallest stream-wise position it is slightly over predicted. This is in agreement with the over prediction of mean particle concentration on the upper low speed side, since particle moving towards positive y values must have a positive mean velocity. The possible reason for that was explained above. The mean stream-wise particle velocity V_1 also is over-predicted on the upper low speed side. The reason for that cannot be the small differences in the predicted mean fluid velocity (see Fig. 2), since they were predicted too small, which should lead to smaller predicted particle mean velocities compared to the measurements. The reason, however, might again be the dispersion, which was predicted too large towards the upper part of low speed side, resulting in particles being present on the low speed side originating from the high speed side with large stream-wise velocity. However, this may not explain why the particles move faster in the simulations also on the high speed side ($y=-30$ to 0). Therefore, future research should clarify whether there are spurious effects present in the model equation (1). Also, it must be quantified how well the stochastic model can describe the role of the unsteady pairing fluid vortices on particle dispersion.

Since the particle fluctuating velocities are an important quantity resulting from the dispersion model, for example for the calculation of collision rates, Fig. 5 presents the calculated rms of the particle velocity fluctuations for the laminar and the turbulent tracking to-

gether with measurements. Generally, the laminar simulations show much smaller fluctuations of the particle velocities, especially for the cross-stream component these are nearly zero. The turbulent simulations capture the main trends of the measured particle velocity fluctuations. However, the absolute values of the fluctuations of particle velocities are larger in the simulations compared to the experiments by up to approximately 30-50%, depending on position. Two reasons could be responsible for that, first a PIV algorithm was used to measure the particle velocities, hence around 3 to 8 particle velocities were average in one interrogation window, which may suppress extreme velocity events of single particles leading to a smaller measured rms velocity. Second, due to preferential particle concentration the velocity fluctuations of the carrier fluid viewed by the particles were reduced as described before. This might also led to smaller particle velocity fluctuations and has not been taken into account. The simulation predicted larger fluctuations on the low speed side ($y > 0$) compared to the high speed side ($y < 0$) and the fluctuation levels are approximately a factor of two larger for the stream-wise compared to the cross-stream velocity component.

5 Conclusions

A particle-laden shear layer was calculated by using a standard $k-\varepsilon$ turbulence model for the gas flow phase. Lagrangian particle tracking with a Langevin equation model for turbulent dispersion was applied to simulate a particle flow dispersing in the shear flow. Two-way coupling was neglected. The results in terms of profile of mean particle concentration and mean and rms of fluctuations of particle velocities in stream-wise and cross-stream direction were compared with measured values. The following conclusions could be drawn from the performed simulations:

- For the particles with a mean diameter of 90 micron and a Stokes number of 2.3 the dispersion model agreed well with the experiments on the high speed side. On the top side with the low fluid velocity, dispersion was over-predicted at the larger stream-wise positions investigated. This could be related to the enhanced clustering of the particles, since their Stokes number was close to unity. As a consequence they might ‘see’ reduced fluid velocity fluctuations in the real flow (Horender & Hardalupas, 2010).
- The mean cross-stream velocity agreed satisfactorily with the experiments, however, the mean particle velocity in stream-wise direction showed deviations from the experiments. This point needs to be addressed in future research dealing with improved diffusion and drift coefficients for the Langevin equation model of Eq. (1).
- The trends of the fluctuating particle velocities were captured well by the dispersion model, however their levels were over-predicted by approximately 30%. The particle velocity fluctuations were larger on the low speed side compared to the high speed side and the fluctuations of the stream-wise component were approximately twice as large as the fluctuations of the cross-stream component.

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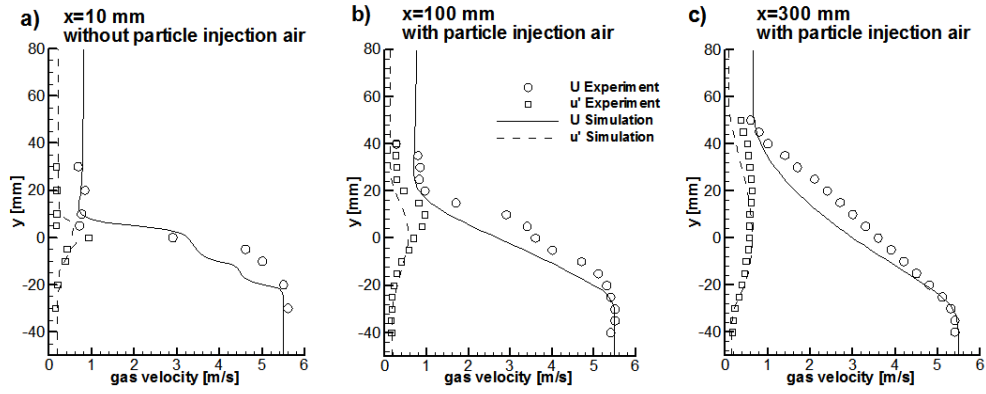


Figure 2: Simulated and measured mean and fluctuating gas velocities in the shear layer flow for stream-wise distance (a) 10mm, (b) 100mm and (c) 300mm.

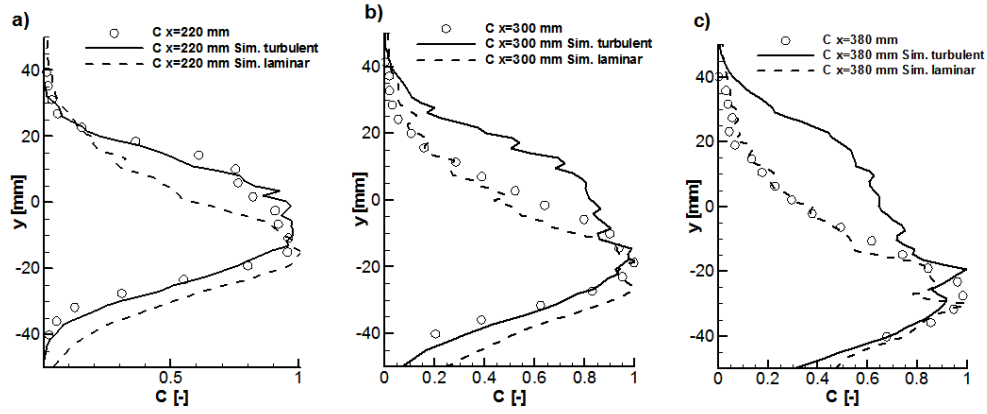


Figure 3: Simulated and measured mean particle concentration profiles for stream-wise positions (a) 220mm, (b) 300mm and (c) 380mm. (open circle: experiment, closed line: turbulent particle tracking, dashed line: laminar particle tracking).

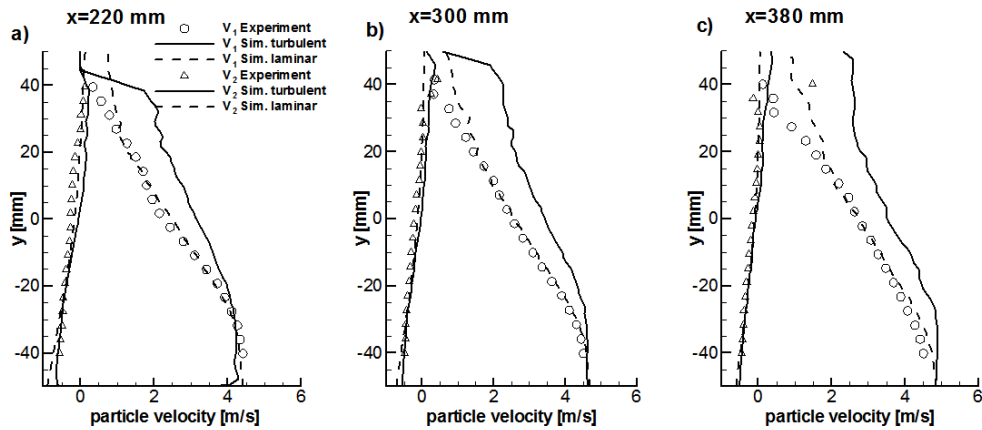


Figure 4: Mean of stream-wise and cross-stream particle velocities for positions (a) 220mm, (b) 300mm and (c) 380mm. (open circle: experiment, closed line: turbulent particle tracking, dashed line: laminar particle tracking).

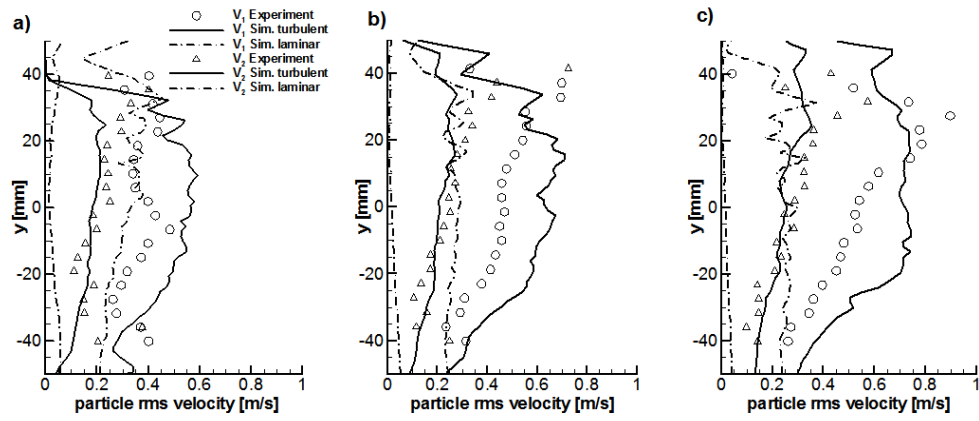


Figure 5: *RMS values of the stream-wise and cross-stream particle velocities for stream-wise positions (a) 220mm, (b) 300mm and (c) 380mm. (open circle: experiment, closed line: turbulent particle tracking, dashed line: laminar particle tracking).*

AERODYNAMICS OF LARGE NON-SPHERICAL PARTICLES

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1 Introduction

Non-spherical particles are found in most industrial particulate flows. However, the vast majority of scientific investigations of particulate flows assume particles to be perfect spheres. For irregular, near spherical particles modification to the drag coefficient using shape factors can be applied, but these becomes increasingly inaccurate at increasing aspect ratios. Non-spherical particles at $Re > 100$ are associated with significant secondary motion which also can affect the primary motion of the particle. This entitles an altogether different methodology, where also the orientation of the particle should be considered. This paper attempts to give an account of the present state of modeling the motion of large non-spherical particles. The relevance of this paper also becomes evident considering the increasing efforts towards the replacement of pulverized coal with biomass in existing and new power plants. Whereas pulverized coal particles are small and the spherical ideal is considered a good approximation, pulverized biomass particles can be characterized as being large and with high aspect ratios due to their fibrous nature. This investigation is limited to the Eulerian-Lagrangian methodology and to solid non-deforming particles in Newtonian fluids.

2 Equations of motion

Whether spherical or non-spherical, regular or irregular, the motion of particles is derived by considering the conservation of linear and angular momentum. In differential form the equations can be stated as:

$$\frac{d\vec{x}}{dt} = \vec{u}_p, \quad m_p \frac{d\vec{u}_p}{dt} = \sum_i \vec{F}_i \quad (1)$$

$$\frac{d\vec{\theta}}{dt} = \vec{\omega}_p, \quad \vec{I}_p \frac{d\vec{\omega}_p}{dt} = \sum_i \vec{T}_i \quad (2)$$

where x is the position vector, u_p is the particle linear velocity, m_p is the particle mass, F is the force acting on the particle, θ is the angle between the principle axis of the particle and the inertial coordinate system, ω_p is the angular velocity, I_p is the moment of inertia and T is the torque acting on the particle. Where eq. (1) deals with the location and linear velocity of the particle, eq. (2) is responsible for the orientation and the angular velocity. Eq. (1) and (2) nicely demonstrate the similarity between translational and rotational motion. However, these equations are only strictly correct for a particle which is symmetric around the center of mass (a sphere). For a generic non-spherical particle it is necessary to include additional terms which address the difference of the moment of inertia in the different directions:

$$\begin{aligned} I_{x'} \frac{d\omega_{x'}}{dt} &= \sum T_{x',i} + \omega_{y'} \omega_{z'} (I_{y'} - I_{z'}) \\ I_{y'} \frac{d\omega_{y'}}{dt} &= \sum T_{y',i} + \omega_{z'} \omega_{x'} (I_{z'} - I_{x'}) \\ I_{z'} \frac{d\omega_{z'}}{dt} &= \sum T_{z',i} + \omega_{x'} \omega_{y'} (I_{x'} - I_{y'}) \end{aligned} \quad (3)$$

Generally, the particle translation is evaluated in the inertial coordinate system whereas the particle rotation is evaluated in the co-rotational coordinate system as seen in Figure 1.

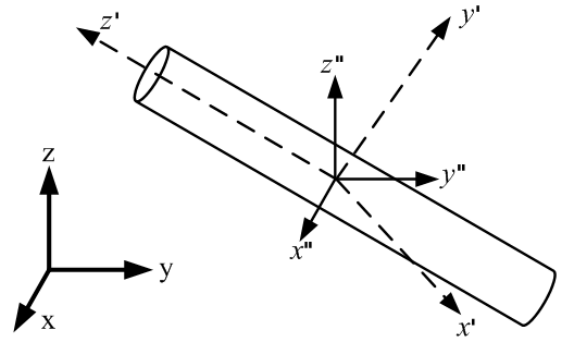


Figure 1: The inertial (x, y, z) , the co-rotational (x', y', z') and the co-moving (x'', y'', z'') coordinate systems.

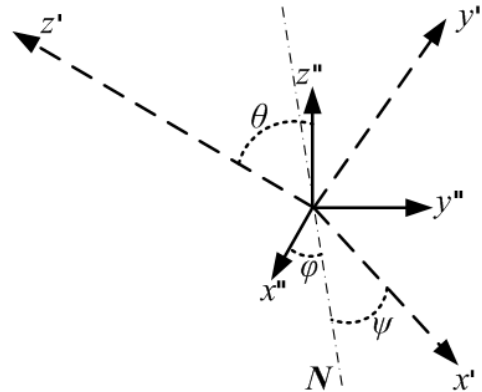


Figure 2: Euler angles: $N = \text{plane}(x', y') \cap \text{plane}(x'', y'')$.

The transformation between the co-moving and the co-rotational coordinates is accomplished by means of a transformation matrix, $\mathbf{A}$ [1]:

$$\vec{x}' = \mathbf{A} \vec{x}'' \quad (4)$$

where the elements in $\mathbf{A}$ represent the directional cosines of the angles $[\theta, \phi, \psi]$ between the principle axis of the co-rotational and the co-moving coordinate system as seen in Figure 2. These angles are also known as the Euler angles. However, these angles are not suitable for particles which undergo full rotation due to a singularity which occurs when they are used in relation to the angular velocities of the particle. Instead Euler's four parameters $[\varepsilon_1, \varepsilon_2, \varepsilon_3, \eta]$, which are also known as quaternions, are used. The four Euler parameters represent an expansion of the three Euler angles to eliminate the singularity. The transformation matrix, $\mathbf{A}$, using the Euler parameters is given as [2]:

$$\begin{bmatrix} 1 - 2(\varepsilon_2^2 + \varepsilon_3^2) & 2(\varepsilon_2\varepsilon_1 + \varepsilon_3\eta) & 2(\varepsilon_1\varepsilon_3 - \varepsilon_2\eta) \\ 2(\varepsilon_2\varepsilon_1 - \varepsilon_3\eta) & 1 - 2(\varepsilon_3^2 + \varepsilon_1^2) & 2(\varepsilon_3\varepsilon_2 + \varepsilon_1\eta) \\ 2(\varepsilon_1\varepsilon_3 + \varepsilon_2\eta) & 2(\varepsilon_3\varepsilon_2 - \varepsilon_1\eta) & 1 - 2(\varepsilon_1^2 + \varepsilon_2^2) \end{bmatrix} \quad (5)$$

Where the Euler parameters are related to the Euler angles by the following relations:

$$\begin{aligned} \varepsilon_1 &= \cos \frac{\phi-\psi}{2} \sin \frac{\theta}{2}, & \varepsilon_2 &= \sin \frac{\phi-\psi}{2} \sin \frac{\theta}{2}, \\ \varepsilon_3 &= \sin \frac{\phi-\psi}{2} \cos \frac{\theta}{2}, & \eta &= \cos \frac{\phi-\psi}{2} \cos \frac{\theta}{2} \end{aligned} \quad (6)$$

and the time rate of change of the Euler parameters is calculated by:

$$\begin{bmatrix} \frac{d\varepsilon_1}{dt} \\ \frac{d\varepsilon_2}{dt} \\ \frac{d\varepsilon_3}{dt} \\ \frac{d\eta}{dt} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \eta\omega_{x'} - \varepsilon_1\omega_{y'} + \varepsilon_2\omega_{z'} \\ \varepsilon_3\omega_{x'} + \eta\omega_{y'} - \varepsilon_1\omega_{z'} \\ -\varepsilon_2\omega_{x'} + \varepsilon_1\omega_{y'} + \eta\omega_{z'} \\ -\varepsilon_1\omega_{x'} - \varepsilon_2\omega_{y'} - \varepsilon_3\omega_{z'} \end{bmatrix} \quad (7)$$

Similar to that most studies involving particles assume a spherical shape, most studies involving non-spherical particles assumes Stokes flow. For a non-spherical particle in Stokes flow it is possible to derive the steady states resistance force and torque which act on the particle on a theoretical basis [3]. However, unsteady forces, such as virtual mass and Basset history force remain to be formulated for non-spherical particles. The main difficulty seems to be the coupling of the unsteady terms with the orientation of the particle. One study tried to derive the full equated motion for creeping flow by simplifying the problem. As such, Lawrence and Weinbaum [4],[5] conducted a study on a slightly eccentric ellipsoid of revolution with major semi-axis $b = a(1 + \varepsilon)$, in oscillatory cross flow, where only translational motion was considered. In addition to relevant expansions of the steady state, virtual mass and Basset force a new time dependent term emerged related to the eccentricity. This shows the magnitude of the awaiting challenge and suggests that BBO-equation perhaps only is an asymptotic solution for a more general formulation as the shape goes towards complete symmetry around the center of geometry. When considering non-spherical particles in Stokes flow especially the work by Fan and Ahmadi [6],[7] should be accentuated. There a complete formulation of the resistance forces as well as shear induced lift can be found along with a discussion of the importance of the individual terms.

For non-spherical particles at higher Reynolds numbers, appropriate expansions could be obtained by including empirical coefficients in front of the force and torques. However, it is also necessary to account for the offset of the center of pressure in relation to the center of geometry, x_{cp} , as seen in Figure 3.

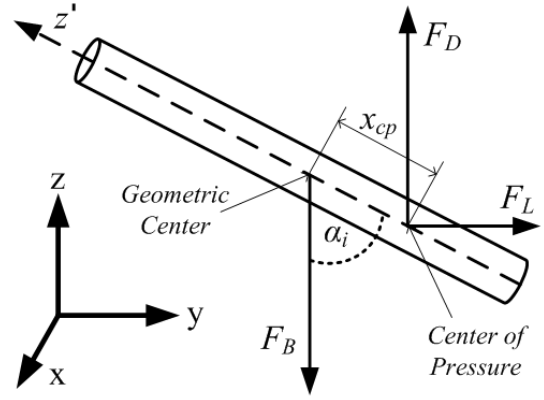


Figure 3: The location of the center of pressure, the inclination angle α and the resulting forces acting on a falling non-spherical particle.

The pressure distribution on the surface of a particle inclined to the flow direction does no longer follow the symmetry of that particle. This gives rise to an additional lift force as well as an addition torque due to the displacement of the center of pressure. Besides this, the main complication when considering non-spherical particles is the endless variations of the shape of the particle. To combat this, most investigations include some sort of parameter variation in the formulation of forces and torques. The most popular being the ellipsoid of revolution which can be used to resemble a large array of different shapes including flake-like particles and rod-like particles. A distinctive advantage of the ellipsoid of revolution is that it has no sharp edges which in a mathematical analysis would be seen as discontinuities.

3 Orientation dependent drag

With regards to the drag force the main advantage for an orientation dependent calculation method is that the drag is calculated on basis of the projected area, evaluated at the present orientation of the particle:

$$\vec{F}_{Drag} = \frac{1}{2} C_D \rho A_p |\vec{u} - \vec{u}_p| (\vec{u} - \vec{u}_p) \quad (8)$$

The challenge, with regards to the drag force, is the proper formulation of the drag coefficient which is applicable for a large range of Reynolds numbers, shapes and orientations. It has become common practice to procure empirical fits at a range of Reynolds number for a specific shape. Some fits also includes a parametric variation of the shape e.g. the aspect ratio of a cylinder or a spheroid. However, these expressions are usually based on either a fixed orientation or a freely falling particle. Thus, correlations of the drag coefficient, which consider the inclination angle, are not widely available. Two approaches have been proposed to address this predicament: The work of Rosendahl [8] suggests using a 'blending' function between the drag coefficient for flow normal and parallel to the major axis of the particle:

$$C_D(\alpha) = C_{D,\alpha=0} + (C_{D,\alpha=90} - C_{D,\alpha=0}) \sin^3 \alpha \quad (9)$$

where α is the angle between the major axis of the particle and the flow direction. Here the projected area at the evaluated orientation is used in the calculation of the drag force. Secondly, the work by Yin et al. [9] suggests using available drag correlations expressed by the

sphericity and thus solely accounting for the dependence of orientation by using the projected area in the calculation of the drag force. Recently, a third option has been presented. Based on a plethora of empirical data for fixed and freely falling particles Hölzer and Sommerfeld [10] came up with an expression which uses a cross-wise, $\psi_{\perp}$, and lengthwise sphericity, $\psi_{\parallel}$, to account for the drag coefficient of different shapes at different orientations:

$$C_D = \frac{8}{Re} \frac{1}{\sqrt{\psi_{\parallel}}} + \frac{16}{Re} \frac{1}{\sqrt{\psi}} + \frac{3}{Re} \frac{1}{\sqrt{\psi^{3/4}}} + 0.4210^{0.4(-\log \psi)^{0.2}} \frac{1}{\psi_{\perp}} \quad (10)$$

Here the cross-wise sphericity is the ratio between the cross-sectional area of the volume equivalent sphere and the projected area of the actual particle. The lengthwise sphericity is the ratio between the cross-sectional area of the volume equivalent sphere and the difference between half of the surface area and the mean projected area. The cross-wise sphericity should thus aid in the correlation of the form drag while the lengthwise sphericity is expressive of the friction drag. Note that here the Reynolds number and the drag coefficient are based on the volume equivalent sphere.

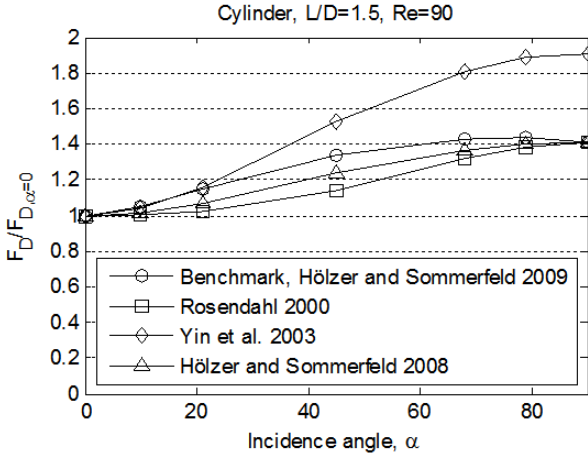


Figure 4: Evaluation of the different approaches to correlate the drag coefficient with the incidence angle.

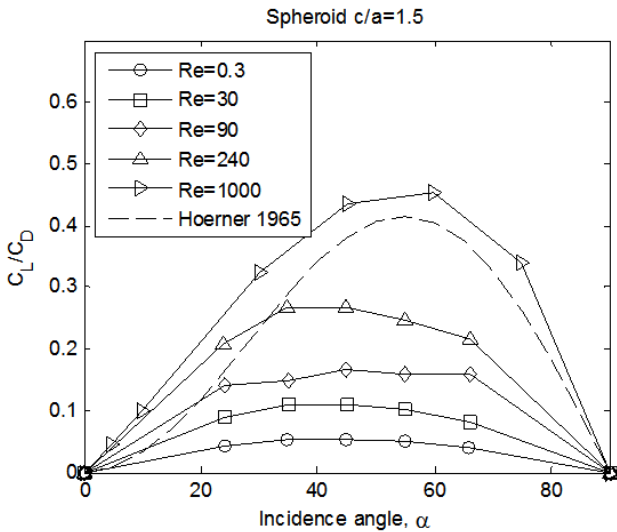


Figure 5: Lift/drag ratio at different Reynolds numbers [11], [15].

Figure 4 shows the drag force for a cylinder at different orientations, normalized with the drag force at zero incidence angle, calculated using the three suggested methods and compared to the benchmark (lattice-Boltzmann simulations) by Hölzer and Sommerfeld [11]. Overall, it may be noted that the drag force increases with increasing incidence angles due to the increase in projected area. However, this alone is not sufficient to properly account for the observed results.

The method by Rosendahl [8] provides a pragmatic way to calculate the drag force at different incidence angles but also relies upon the availability of experimental data. For regular shapes these can typically be found for particles at 90 degree incidence angle whereas empirical fits for particles at zero incidence angle are not widely available. In this regard it might be useful to refer to the studies by Militzer et al. [12] which provide a parametric fit for spheroids as a function of the Reynolds number and the aspect ratio as well as Isaacs and Thodos [13] which provide the same for disks and cylinders at 90 degrees incidence angle. For the present benchmark data it may be noted that a ‘blending’ function using $\sin(\alpha)$ instead of $\sin^3(\alpha)$ provides a superior fit. Hölzer and Sommerfeld [10] constitute a good fit of the present benchmark data and attractively addresses all possible shapes at all Reynolds numbers in a single expression. However, this also indicates that for some specific shapes such a correlation, similar to the one by Yin et al. [9], might be associated with relatively large errors compared to correlations developed for that specific shape.

4 Orientation dependent lift

The lift force accounts for the sideward motion and is present whenever the particles principle axis is inclined to the main flow direction. With a concept taken from aerodynamics this can be explained as ‘profile’ lift. The theoretical and empirical basis of predicting the profile lift relies at much more scant information compared to that available for drag. For symmetric particles the lift is zero at both $\alpha=0^\circ$ and $\alpha=90^\circ$ and it assumes a maximum somewhere in between, depending on the shape and Reynolds number. The usual assumption has been to assume that the lift is proportional to the drag and that the dependence with the orientation is given by the so-called ‘cross-flow principle’ [14]:

$$\frac{C_L}{C_D} = \sin^2 \alpha \cdot \cos \alpha \quad (11)$$

This relationship was developed for infinite cylinders at Reynolds numbers in the Newtons law regime. Figure 5 shows data for a spheroid with small aspect ratio together with the cross-flow principle from eq. (11).

It can be seen that the cross-flow principle provides a fair fit to the present data at Reynolds numbers in the Newtons law regime whereas the maximum lift/drag ratio diminishes as the Reynolds number decreases. This is related to the relative importance of the friction and pressure drag at these intermediate Reynolds numbers. Here we provide the following fit to the present data set ($30 < Re < 1500$) to correlate the influence of the Reynolds for the cross-flow principle:

$$\frac{C_L}{C_D} = \frac{\sin^2 \alpha \cdot \cos \alpha}{0.65 + 40Re^{0.72}} \quad (12)$$

This expression gives correct asymptotic values for large and small Reynolds numbers but is based on a narrow dataset with resulting low accuracy. It should also

be noted that data shown in Figure 5 is for a spheroid with relatively low aspect ratio. It seems like the better the shape approximates an infinite long cylinder the clearer the resemblance with the cross-flow principle becomes. Once the lift coefficient is specified the lift force can be found using an expression equivalent to eq. (8).

5 Offset of the center of pressure

In order to correctly predict the incidence angle for estimating the forces and torques, it is of prime importance to locate the center of pressure. As previously stated a non-spherical particle tends to fall with its largest cross-sectional area normal to the flow direction i.e. $\alpha=90^\circ$. Here the center of pressure is coincidental with the geometric center and lift force and torque are zero. Hence this can be described as the state of stable equilibrium of the particle. A non-spherical particle inclined to the flow direction with $\alpha=0^\circ$ will also experience no lift or torque but this can instinctively be perceived as an unstable equilibrium. At this extreme, the center of pressure must therefore be no-coincidental with the geometric center to match observed behavior. Using concepts from airfoil theory the center of pressure at this extreme inclination is placed at the ‘quarter chord point’ which is equivalent to half the distance from the geometric center to the end of the particle being oriented towards the flow [8],[9]. Please refer to Figure 3 for visual illustration. Marchildon et al. [16] provides a linear approximation to the derivation by Rayleigh [17] for the pressure distribution on an infinite flat plate to predict the center of pressure of a cylinder. This is reported by Marchildon et al. [16] to be valid for inclinations above $\alpha=15^\circ$ due to the uniformity of the pressure distribution above this angle. Both Rosendahl [8] and Yin et al. [9] present expressions which close the gap with regards to the location of the center of pressure between the two extremes.

Rayleigh [17]	$x_{cp}/L = (3/4) (\sin \alpha_i) / (4 + \pi \cos \alpha_i)$
Marchildon et al.[16]	$x_{cp}/L = (90 - \alpha_i)/480$
Rosendahl [8]	$x_{cp}/L = 0.25 (1 - \sin^3 \alpha_i)$
Yin [9]	$x_{cp}/L = 0.25 \cos^3 \alpha_i$

Table 1: Expressions to find the center of pressure.

Figure 6 shows an illustration of the different expressions and it can be seen there is some discrepancy in the prediction of the center of pressure. More unfortunately, there seems not to be any guidelines towards which expression is the most appropriate to use. A freely falling non-spherical particle will spend most of the time close to $\alpha=90^\circ$ and effort should thus be directed towards finding the best fit close to this point.

Assuming that Rayleigh’s derivation is valid for general non-spherical particles at intermediate Reynolds numbers it seems attractive to use the simple linear fit by Marchildon et al. [16]. Once the lift and drag forces are found as well as the location of their point of attack, i.e. the center of pressure, it is a small matter of calculating the resulting torque which is due to the offset from the geometric center, T_{offset} .

$$\vec{T}_{offset} = x_{cp} (\vec{F}_{Lift} + \vec{F}_{Drag} + \vec{F}_{Other}) \quad (13)$$

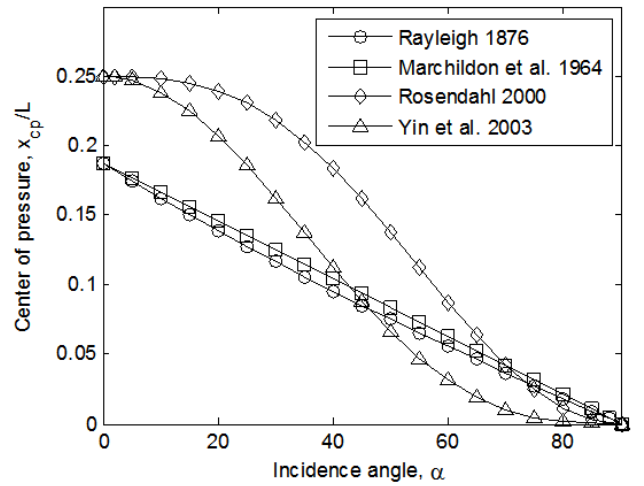


Figure 6: Location of the center of pressure for a cylinder with length L , using the different expressions.

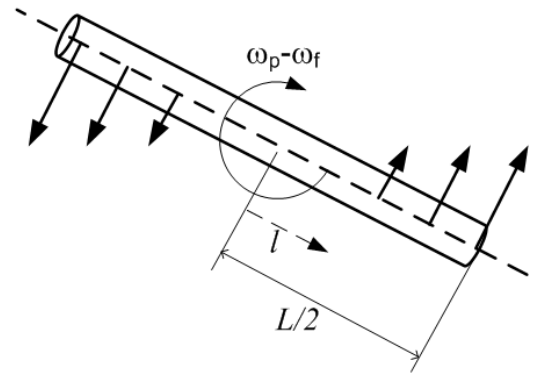


Figure 7: Resistance towards rotation.

6 Rotational resistance

The torque due to resistance can be directly derived by integration of the friction, caused by rotation, over the length of the particle. For spheroids subject to the Stokes conditions, solutions have been known since Jeffery [3] and have since been expanded to other shapes [18]. Relevant expansions for higher Reynolds number can be found by incorporating appropriate fits for the drag coefficient in the definition of the drag force before the integration is performed.

$$\begin{aligned} \vec{T}_{resist} &= 2 \int_0^{L/2} \vec{F}_{resist} dl \\ &= \int_0^{L/2} C_{D,cyl} \rho (\omega_f - \omega_p)^2 l^2 A_p dl \end{aligned} \quad (14)$$

This integral can be evaluated with increasing degree of sophistication. Note that if the particles aspect ratio is sufficiently large the angular velocity will tend to be low and an assumption of creeping flow may suffice.

7 Other forces and torques

The unraveling of orientation dependent models up to now constitutes a description of the minimum number of forces and torques which are required for the modeling of non-spherical particles. For specific problems it may be necessary to address additional forces and torques. For general fluid flow, these other forces are primary those

caused by pressure and velocity gradients as well as unsteady forces such as virtual mass and Basset history force. Some of these forces may be evaluated by simple expansions of the equivalent expressions derived for a sphere whereas others, such as the Basset force, are utterly hopeless to be evaluated for non-spherical particles even in creeping flow. As a general guideline these forces may be accounted for by using the projected area or an equivalent diameter as is suggested in the approach by Rosendahl [15]. Clearly, order-of-magnitude estimates may be performed for the unsteady forces acting on non-spherical particles similar to those which are custom to be performed for spheres and thus for most gas-solid flows it is justified to neglect the unsteady forces. For a freely falling cylinder in water it is not possible to neglect the unsteady forces. By the nature of this process these non-spherical particles are oscillating. As such Sorensen et al. [19] found that the terminal velocity of a steady falling cylinder slightly oscillated in tune with the larger oscillations of the angular velocity. For that investigation an intricate expansion of the drag force, depending on the angular acceleration was developed to account for the unsteady forces. However, the general application of this expression in the calculation procedure presented here is not possible. For small non-spherical particles it might be necessary to model non-continuum effects. This is addressed in the study by Fan and Ahmadi [6] which introduces both an additional Brownian force and a Brownian torque in the equations of motion to supplement the fluid dynamic forces. At the same time the fluid dynamic forces are modified by introducing approximations of the translational and rotational slip factors. There, in an Eulerian-Lagrangian framework, the nature of Brownian motion is modeled as a Gaussian random process. Considering the similarities between Brownian and turbulent motion such an approach also indicates possible approaches for non-spherical particles in turbulent flow. Also note that the effect of velocity gradients has already been incorporated into the expression for rotational resistance, eq.(14), though the vorticity of the flow field.

8 Conclusion

This outline on the motion of large non-spherical particles is made to give an overview of the present status of this topic. The additional consideration of orientation and angular velocity gives a number of decisive advantages. Firstly, by modeling the orientation dependent forces and torques it is possible to predict the secondary motion caused by the non-spherical shape. Secondly, the modeling of non-spherical particles in the Lagrangian reference frame, without the severe restriction of creeping flow allows for the possibility to use this methodology on a variety of engineering flows which contain large non-spherical particles. Thirdly, it should be noted that the solution procedure is only around twice as computational intensive compared to the present implementation in commercial codes.

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SEGREGATION OF INERTIAL PARTICLES IN TURBULENT FLOWS: THE APPLICATION OF THE FULL LAGRANGIAN METHOD

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1 Introduction

Turbulent structures play a crucial role in many particle/fluid processes in the environment and industry: examples include combustion, the production of powder, the motion of droplets in gas/liquid separators and the formation and growth of PM10 particulates in the atmosphere. An area of much investigation is the mechanism for warm-rain initiation and in particular the way droplet interaction with the small scales of turbulence in clouds influence the droplet size distribution ([16]).

It is by now well known that turbulence, contrary to traditionally held views, can demix a suspension of particles (see e.g. [8]). The process of segregation depends upon the ratio of the particle response time to the timescale of the turbulent structures in the flow (i.e. the Stokes number, St). Early experiments and simulations (e.g. [6]) have shown that the demixing reaches a maximum when the particle response time is approximately equal to the timescale of the turbulent structure (i.e. the particle Stokes number ~ 1), the suspended particles being observed to segregate into regions of high strain rate in between the regions of vorticity. In addition Maxey and his co-workers ([12, 19]) showed that the gravitational settling of particles in homogeneous turbulence was enhanced due to preferential sweeping in the direction of gravity as particles interweave through turbulent structures in the flow. Since then there have been numerous studies to understand and quantify this segregation process. Of particular note have been the seminal studies by [18] and [20] to quantify the influence of segregation on two-particle dispersion and the process of particle agglomeration.

Intrinsically related to the motion of inertial particles is the presence of random uncorrelated motion in flow fields that are spatially random but smoothly varying. RUM refers to the possibility that particle trajectories may cross, and relates to the sling effect (see e.g. [22] and [7]) and to the occurrence of caustics in the particle motion (see [21]). [9] have observed that the spatial velocity field resulting from the motion of suspended particles in a direct numerical simulation (DNS) of homogeneous isotropic turbulence consists of two components: a smoothly (continuous) velocity field that accounts for all particle-particle and fluid-particle two point spatial correlations (they referred to this component as the mesoscopic Eulerian particle velocity field (MEPVF)); and a spatially uncorrelated component which we will refer to here as RUM (the component of random uncorrelated motion) whose contribution to the particle kinetic energy increases as the particle inertia increases. [9] attribute this feature to the ability of the particles with inertia to retain the memory of their interaction with very distant, and statistically independent eddies in the flow field.

Segregation and RUM are related to the occurrence of inter-particle collisions as follows ([18], [20]): i) segregation enhances the particle concentration of certain regions of the flow, ii) RUM, i.e. the decorrelation of

velocity between particles, causes two nearby particles to collide and possibly to coagulate. Segregation is well-known to manifest itself especially for $St \sim 1$, whereas the effect of RUM is almost invisible for small particles and becomes increasingly important for larger St . Since the interplay between these two effects determines the collision rate in a turbulent flow, it is essential to quantify segregation and RUM as accurately as possible as a function of the Stokes number and some typical flow properties in order to correctly predict the rate of inter-particle collisions.

In recent years, the process of segregation of inertial particles has been studied from different viewpoints when the Stokes number is relatively small. On the one hand, [4] demonstrated a strong correlation between the positions of small inertial particles and the locations of zero-acceleration points in the carrier flow. On the other hand, [1] carried out a theoretical analysis based on the assumption that the velocity of inertial particles can be directly related to the carrier flow velocity. By doing so, they were able to show that the segregation of particles continues indefinitely in the course of time, and they showed that the concentration of inertial particles in a turbulent flow is highly intermittent, so the particles are distributed far from uniformly over space. A similar approach was chosen by [5] who demonstrated that the time-converged solution of the radial distribution function is of the form $g(r) \sim r^\beta$, where the negative number β is proportional to St^2 . In addition, they confirmed this by showing results from a DNS of statistically stationary homogeneous isotropic turbulence.

The understanding of dilute suspensions of inertial particles has been vastly extended by interpreting the motion of particles in terms of dynamical systems theory. The first approach in this direction was given by [17], and was later specifically applied to the motion of inertial particles in turbulent flows by [2] and [21]. [21] derived an analytical expression for the Lyapunov exponents associated with the motion of inertial particles in physical space. The derivation was based on the assumption that the typical correlation time of the carrier flow was very small, i.e. the Kubo number $Ku \ll 1$. Unfortunately, this assumption is not exactly valid in real turbulence where $Ku = \mathcal{O}(1)$, as [21] acknowledge themselves. [2] showed that if the particle clustering is fractal, the exponent in the radial distribution function is equal to $\beta = n_d - D_{corr}$, where D_{corr} is the correlation dimension introduced by [11], and n_d is the number of dimensions of the problem ($n_d = 2$ in a two-dimensional flow and $n_d = 3$ in a three-dimensional flow). [2] expressed the clustering of particle in terms of its fractal dimension in phase space and showed how this was related to the Lyapunov exponents of the $2n_d$ -dimensional dynamical system. [3] obtained a correlation dimension D_{corr} by calculating the Lyapunov exponents in a Direct Numerical Simulation of turbulence for a wide range of Stokes numbers, and found that $n_d - D_{corr}$ scales with St^2 , in agreement with the aforementioned results by [5].

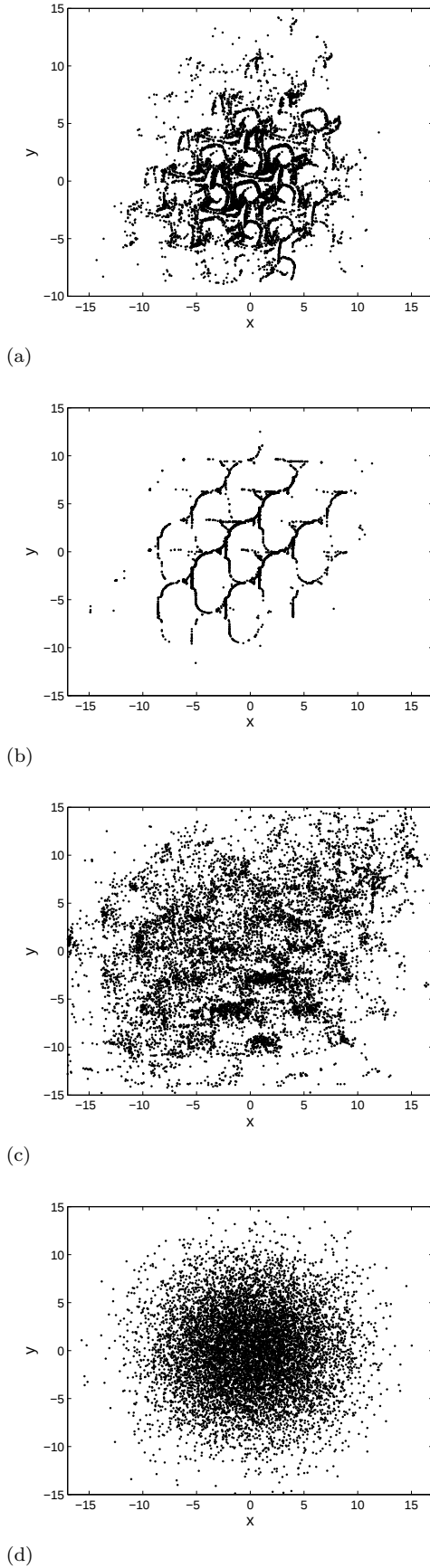


Figure 1: a)-c) Positions of 10^4 particles after time $t = 20$ in a non-isotropic random straining flow, for $St = 0.05$ (a), $St = 0.5$ (b) and $St = 5$ (c). d) Position of one single particle after $t = 20$ in 10^4 separate realisations of the non-isotropic random straining flow, for $St = 0.5$.

In the present paper we employ the Full Lagrangian Method (FLM) to investigate the segregation and preferential concentration of inertial particles in turbulence-like flows. This method, originally introduced by [13] but later also used by [15] and [10], consists of calculating the size of an infinitesimally small volume occupied by a group of particles, along the trajectory of one single particle. This immediately yields the concentration of particles along the trajectory, since the inverse of the volume occupied by a fixed number of particles corresponds to the particle concentration by definition. We show how the results from the FLM can be translated into statistics of the particle number density, thus providing a wealth of information on the segregation process. An important advantage of the FLM is that it provides meaningful results for the compressibility along the trajectory of a single particle in the course of time; Lyapunov exponents are, in contrast, only defined in the limit of time approaching infinity ([14]).

We describe here how the FLM can be used to quantify non-uniformities in the spatial distribution of particles, the singularities in the particle velocity field and the presence of RUM. What we show here, is that the FLM can be further developed and translated into higher-order statistics of the particle number density. In order to illustrate our application of the FLM and to understand some of the important underlying features of particle segregation, we first consider its application to the dispersion of particles in relatively simple random flows which share features of real turbulence. We later go on to show that the features we reveal in these simple flows are common in particle segregation in a DNS of homogeneous isotropic turbulence.

The Full Lagrangian Method

We consider small spherical particles with a density ρ_p and a radius a_p immersed in a carrier flow with a density ρ_f and kinematic viscosity ν_f . Upon assuming the density of the particle to be much higher than the density of the carrier flow, i.e. $\rho_p/\rho_f \gg 1$, the equation of motion of each particle can be derived from the expression given in Maxey & Riley (1983):

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \quad ; \quad \frac{d\mathbf{v}}{dt} = \frac{1}{St}(\mathbf{u} - \mathbf{v}) \quad (1)$$

where $\mathbf{x}$ and $\mathbf{v}$ denote the position and the velocity of the particle, respectively, and $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ is the velocity of the carrier flow at the position of the particle. All variables have been made dimensionless by a typical wave number k_0 and a typical velocity u_0 of the carrier flow. The dimensionless parameter $St \equiv \tau_p u_0 k_0$ denotes the Stokes number, where τ_p denotes the Stokes particle relaxation time defined as $\tau_p \equiv 2a_p^2 \rho_p / 9\nu\rho$. In all cases presented here we neglect gravity to isolate effects which occur purely due to the finite inertia of particles. The segregation in the course of time can be analysed by using the Full Lagrangian Method (see Osipov (2000), Reeks (2004) and Healy & Young (2005)). For this purpose, we investigate the volume occupied by a large number of particles, which are initially released inside a relatively small volume centered around $\mathbf{x}_0$. The deformation of such a volume is characterized by the temporal evolution of the unit deformation tensor $\mathbf{J}$, whose component J_{ij} are defined by:

$$J_{ij} \equiv \frac{\partial x_i(\mathbf{x}_0, t)}{\partial x_{0,j}}, \quad (2)$$

where $\mathbf{x}_0$ is the position of the particle at some initial time say $t = 0$. Differentiating Eq. 2 with respect to time gives:

$$\frac{d}{dt} J_{ij} = \frac{\partial v_i(\mathbf{x}_0, t)}{\partial x_{0,j}}. \quad (3)$$

The second derivative with respect to time is:

$$\begin{aligned} \frac{d^2}{dt^2} J_{ij} &= \frac{\partial}{\partial x_{0,j}} \left(\frac{dv_i(\mathbf{x}_0, t)}{dt} \right) = \\ &= \frac{1}{\tau_p} \left(\frac{\partial x_k}{\partial x_{0,j}} \right) \frac{\partial}{\partial x_k} u_i(\mathbf{x}, t) - \frac{1}{\tau_p} \frac{\partial v_i(\mathbf{x}_0, t)}{\partial x_{0,j}}. \end{aligned} \quad (4)$$

Inserting Eq. 2 and Eq. 3 into Eq. 4 results in the equations of motion of each component J_{ij} :

$$\frac{dJ_{ij}}{dt} = j_{ij}, \quad \frac{d}{dt} j_{ij} = \frac{1}{\tau_p} \left(J_{kj} \frac{\partial u_i}{\partial x_k} - j_{ij} \right), \quad (5)$$

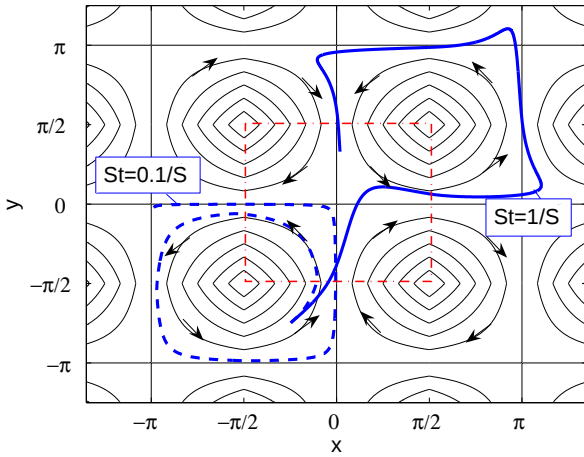


Figure 2: Particle trajectories in a frozen field of periodic vortices, for $St = 0.1/S$ (dashed blue line; heavily damped case) and $St = 1/S$ (thick solid line; lightly damped case), where S represents the strain rate in the flow. The two particles are released in $(x, y) = (-\pi/4, -3\pi/4)$ with a velocity equal to the local carrier flow velocity at time $t = 0$, and traced for a time $t = 20$. The highlighted area (grey dash-dotted line) designates the basic element out of which the entire flow field is constructed.

We choose as initial conditions $J_{ij}(0) = \delta_{ij}$ and $\dot{J}_{ij}(0) = \partial u_i(\mathbf{x}_0, 0)/\partial x_j$. The total deformation $J(t)$ is the determinant of the matrix J_{ij} : $J(t) = |\mathbf{J}|$. If the initial distribution of particles is uniform over a certain domain, the deformation in the course of time is inversely proportional to the particle number density measured along the trajectory of one reference particle $n(t)$:

$$J = n^{-1}(t) \quad (6)$$

where n is normalized so that it is equal to J^{-1} at time $t = 0$. Eq. (6) implies that $J^{-\alpha} = n^\alpha$ for any $\alpha \in \mathbb{R}$. The average over all particles, denoted by the brackets $\langle \rangle$, is

$$\langle J^\alpha \rangle = \langle n^{-\alpha}(t) \rangle \quad (7)$$

The spatially averaged value of any quantity Φ can be related to the particle averaged value as follows:

$$\langle \Phi \rangle = \frac{1}{\Omega} \int_{\Omega} \Phi(\mathbf{x}) n(\mathbf{x}) d^3 \mathbf{x} = \overline{n\Phi} \quad (8)$$

where the overbar $\overline{(\cdot)}$ denotes a spatial average over the domain of size Ω considered. Combination of Eq. 7 and Eq.8 yields:

$$\overline{n^\alpha} = \langle J^{1-\alpha} \rangle \quad (9)$$

Thus a spatially averaged moment of the particle number density, n , can be calculated directly from the deformation $\mathbf{J}$ along sufficiently many particle trajectories.

FLM in simple random flows

The Full Lagrangian Method can also be used to determine the compressibility of the particle phase, $\mathbb{C}$ which we define $J^{-1} dJ/dt = d \ln J / dt$. We can relate this to the divergence of the particle velocity field $\mathbf{v}_p(\mathbf{x}, t)$ providing that the velocity field is single valued and continuous, namely

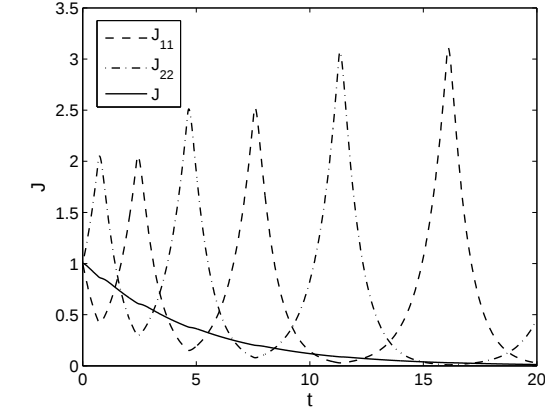
$$\mathbb{C} = d \ln J / dt = \nabla \cdot \mathbf{v}_p(\mathbf{x}, t)$$

Note that the calculation of $\mathbb{C}$ does not require the uniqueness and single valued ness of $\mathbf{v}_p(\mathbf{x}, t)$.

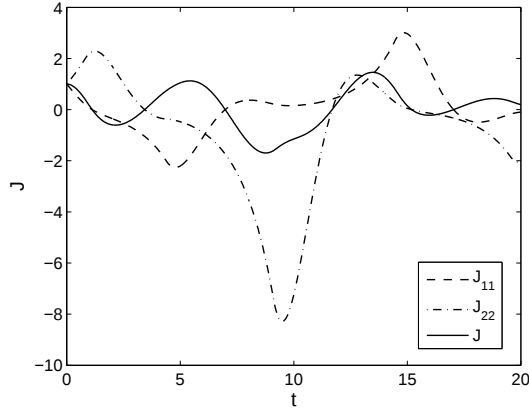
Figs. 3a) and 3b) show the values of $J(t)$ along the heavily damped and lightly damped particle trajectories plotted in Fig. 2. In both cases the value of J approaches zero as $t \rightarrow \infty$. However in the lightly damped case $J(t)$ passes through zero at intermediate times as the particle oscillates backwards and forwards across a stagnation line. In so doing the value of J oscillates from positive to negative, with the corresponding elemental volume rotating through 180° as it passes through zero volume. Each time $J(t)$ passes through zero, the corresponding particle concentration becomes infinite instantaneously. This raises the possibility that such events may occur in real turbulent flows and that the process of particle dispersion could be a highly intermittent process associated with large deviations in the particle concentrations (see also [10]). It also indicates the conditions under which particle trajectories cross and RUM becomes important.

Therefore the frequency at which J passes through zero, $\omega_{J=0}$, can be an important parameter characterising the spatial intermittency in the distribution of particles. The result is given in Fig. 4a), for a value of the strain rate $S = \sqrt{S^{2*}} = \sqrt{12}/\pi$. If $St < 0.25/S$, $\omega_{J=0} = 0$ and J never passes through zero. If $St > 0.25/S$, however, $\omega_{J=0}$ increases very rapidly with St and reaches a maximum at $St = 0.5/S$. Thus, the phenomenon of two particles at the same position with different velocities (caustics) is apparently completely absent for small Stokes numbers and increases rapidly as the Stokes number goes beyond a threshold value of $0.25/S$. These results are in correspondence with the observation of [21], who show that in real turbulence the collision rate (i.e. the probability that particle trajectories cross) has an activation dependence on the Stokes number.

The time-converged solution of $t^{-1} \langle \ln |J| \rangle$ is equal to the time-converged solution of $\langle \mathbb{C} \rangle = \langle \nabla \cdot \mathbf{v} \rangle$ and can thus obtain $\langle \mathbb{C} \rangle$ by calculating J along a particle trajectory at a given Stokes number in 10^5 different realisations of the flow and determine the time-converged value of $t^{-1} \langle \ln |J| \rangle$, i.e. of $\langle \nabla \cdot \mathbf{v} \rangle$. The result is shown in Fig. 4b) as a function of St , both for the isotropic random straining flow and for the non-isotropic random straining flow. If the Stokes number is smaller than a threshold value St_{cr} , $\langle \mathbb{C} \rangle$ is negative, which means that particles are continuously segregated: the segregation process continues indefinitely, and therefore the particles will distributed on a pattern that becomes ever stringier in the course of time. For large Stokes numbers, $\langle \mathbb{C} \rangle$ approaches a positive value.

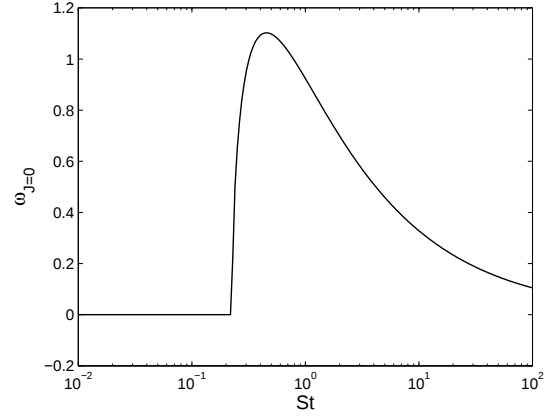


(a)

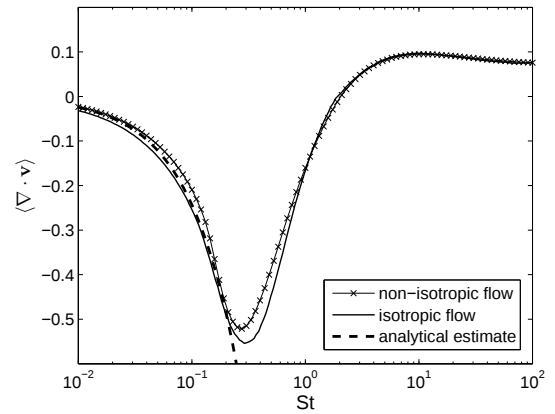


(b)

Figure 3: Values of the deformation J and the components of the deformation matrix J_{11} and J_{22} in the frozen field of periodic vortices depicted in Fig. 2, for (a) the heavily damped case $St = 0.1/S$, and (b) the lightly damped case $St = 1/S$. The strain rate is taken as $S = \sqrt{S^2}^* = \sqrt{12}/\pi$.



(a)



(b)

Figure 4: (a) The frequency at which the deformation J passes through zero, $\omega_{J=0}$, as a function of the Stokes number, St ; b) Time-converged solution for the compressibility $\langle \mathbb{C} \rangle = \langle \nabla \cdot \mathbf{v} \rangle$ as a function of the Stokes number St for both the isotropic random straining flow and the non-isotropic random straining flow. For the sake of comparison, the analytical estimate valid for small Stokes numbers is shown.

FLM in kinematic flow simulation (KS)

We present results based on the FLM for a ‘kinematic’ flow field composed of 200 random Fourier modes where we consider segregation in a similar manner to the analysis of segregation in the simple random straining flow discussed earlier. In addition we also calculate the statistics of the particle number density and analyse the occurrence of RUM. In all of the simulations, the initial velocity of a particle was taken equal to the local velocity of the carrier flow. Fig. 5 shows the results of $\lim_{t \rightarrow \infty} t^{-1} \langle \ln |J| \rangle$ for a wide range of values of Stokes numbers. It is noted that this value is equal to $\lim_{t \rightarrow \infty} \langle \mathbb{C} \rangle$, i.e. the time converged compressibility of the particle velocity field. Just like in case of Fig. 4b), a critical value of the Stokes number can be determined, St_{cr} ; in the present case, $St_{cr} \simeq 0.7$. If the particle Stokes number is lower than St_{cr} , then the particles are continuously compressed into smaller volumes in the course of time and the process of segregation continues indefinitely. If, on the other hand, the Stokes number is larger than St_{cr} , the particle volumes expands or alternatively if the particles are confined they become fully mixed.

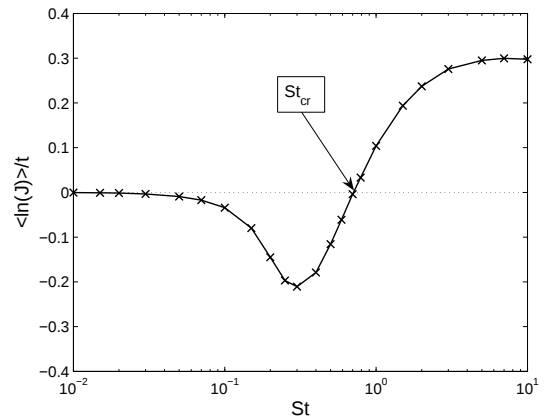


Figure 5: Long term net compressibility as a function of Stokes number, St in the KS flow field composed of 200 random Fourier modes.

Statistics of the particle number density

Now we investigate the statistics of the particle number density in the course of time. The moments of the particle number density can be determined from Eq. 9. The result for four values of α is presented in Fig. 6, for (a) $St = 0.05$ and (b) $St = 0.5$. In both cases the value of $\overline{n^0}$, which corresponds to $\langle |J| \rangle$, remains equal to unity for all time, as expected. In addition, it follows directly from Eq. 9 that $\overline{n^1} = \langle |J|^0 \rangle = 1$. The other moments of the particle number density are markedly higher than 1 and are associated with the non-uniformity in the spatial distribution of particles.

There is a qualitative distinction between the cases of small Stokes numbers such as $St = 0.05$ in Fig. 6a), and large Stokes numbers such as $St = 0.5$ in Fig. 6b). If the Stokes number is large, it may happen that $|J| = 0$ for a particle due to the crossing of trajectories. These intermittent events, which cause $n \rightarrow \infty$, dominate the statistics of higher-order moments of the eps at certain moments in time, as is reflected by the spikes in the curve for $St = 0.5$ in Fig. 6b). Hence, the spatial distribution of particles in a random turbulence-like flow may be highly intermittent.

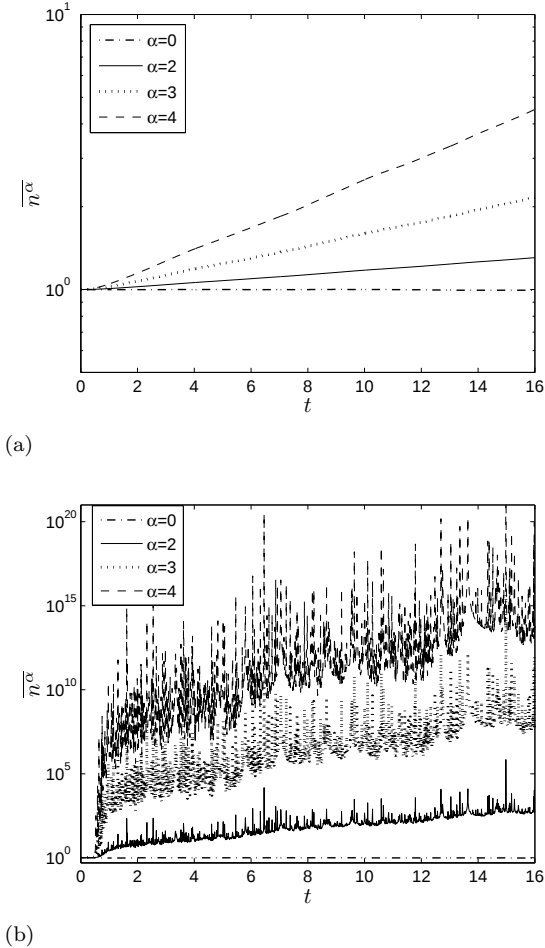


Figure 6: Spatially average of the α -th moment of the particle number density, $\overline{n^\alpha}$, for four values of α ; a) Stokes number, $St = 0.05$; b) $St = 0.5$.

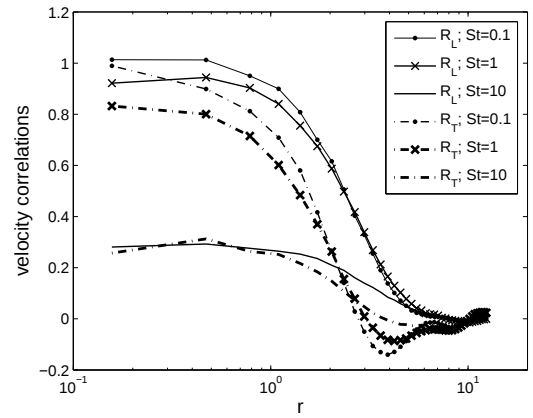
However, for sufficiently small Stokes numbers where RUM is not important (such as $St = 0.05$ in Fig. 6a)), we observe that $\overline{n^\alpha}$ depends exponentially on time and:

$$\overline{n^\alpha} \propto \exp(\gamma t), \quad (10)$$

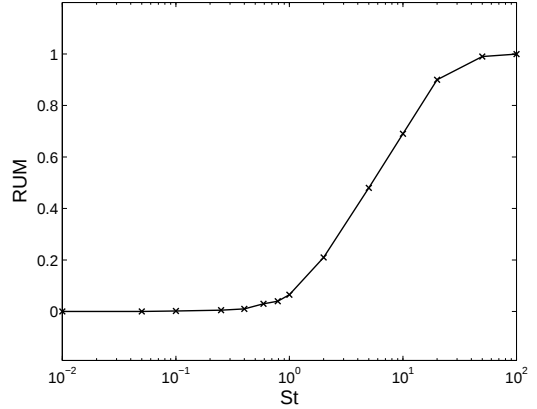
where γ is a function of α and St As can be seen in 6a), the higher-order moments grow faster than the lower-order moments. This demonstrates unambiguously that the segregation process continues indefinitely in this case where $St = 0.05$.

Random uncorrelated motion (RUM)

We present here the velocity correlations between particles in the flow composed of 200 random Fourier modes. Particular attention is paid to RUM, i.e. the random uncorrelated component of the kinetic energy of the particles. For this purpose, the correlation between the velocities of two inertial particles is calculated. We determine the longitudinal and transverse velocity correlations, R_L and R_T respectively, being normalized in such a way that they would become 1 at $r \downarrow 0$ if they were calculated for fluid particles in a homogeneous and isotropic flow.



(a)



(b)

Figure 7: a) Two-particle velocity correlation in longitudinal (R_L) and transverse (R_T) direction as a function of the inter-particle separation distance r , for three different values of the Stokes number, St b) RUM component as a function of the Stokes number, St . Both cases refer to the flow field composed of 200 random Fourier modes.

In Fig. 7a), results are shown for R_L and R_T as a function of the inter-particle distance r , for three different Stokes numbers: $St = 0.1$, $St = 1$ and $St = 10$. For a relatively small Stokes number such as $St = 0.1$, both the longitudinal and the transverse velocity correlations are close to unity as $r \downarrow 0$. This can be explained by the fact that the particles have relatively little iner-

tia, so that the velocities of two neighboring particles are almost the same. As r becomes larger, R_L and R_T decrease and eventually they approach zero as $r \rightarrow \infty$, as expected. For a larger Stokes number, such as $St = 1$, the particle inertia becomes more important which is reflected by deviations of R_L and R_T from unity for small separation distances. If the particles have a very large Stokes number like $St = 10$, then the velocities of two particles become to a large extent uncorrelated, even if the particles are close together in physical space. Therefore, both R_L and R_T are considerably lower than unity when $r \downarrow 0$. The typical decorrelation length, however, is not altered conceivably with respect to the cases of the lower Stokes numbers.

The RUM component, i.e. the random uncorrelated component of the kinetic energy of the particles, is defined as 1 minus the velocity correlation in the limit that particles are infinitesimally close together: In Fig. 7, we show the RUM-component of the particle pair velocity as a function of St . The value of RUM is approximately zero for small Stokes numbers, and it increases monotonically with the Stokes number, indicating that the velocities of inertial particles are more and more decorrelated. Eventually, $RUM \rightarrow 1$ for sufficiently large Stokes numbers, i.e. the velocities of these particles are entirely decorrelated, even when they are very close to each other.

The RUM component is non-zero for particles with e.g. $St \simeq 0.5$, although the long-time value of $t^{-1} \langle \ln |J| \rangle$ is clearly negative, see Fig. 5. Thus, the particle segregation may go on indefinitely despite the fact that RUM is present. This contradicts the claim made by [9] that RUM is responsible for a saturation of the segregation process.

The results presented here show that particle inertia can have major implications for the collision rates between particles. Two effects enhance the collision rate between particles: i) preferential concentration of particles in relatively few regions of the flow, ii) RUM, i.e. the decorrelation of velocities between neighboring particles so that particles are more likely to hit each other. From Fig. 5, we know that preferential concentration manifests itself especially for $0.1 < St < 1$. The effect of RUM is most visible for $St > 0.5$ and increasingly important for larger St . Collision rates are therefore expected to be highest in the Stokes number regime $St > 0.5$. Certainly more research is needed to confirm this statement, but the results presented in the seminal paper by [18] do point in that direction, since they found a maximum collision rate for a Stokes number St_k (based on the smallest scale of the flow, the Kolmogorov time scale) of $2 < St_k < 5$, with a collision rate vanishing for $St_k \downarrow 0$, and a collision rate decreasing only slowly with St_k if $St_k > 5$.

FLM in DNS of Homogeneous isotropic turbulence (HIT)

The DNS simulation of statistically stationary HIT is obtained using a pseudo spectral code using a grid size $128 \times 128 \times 128$ giving an $Re_\lambda = 65$. Forcing of the flow is applied at the lowest wave numbers. 100.000 inertial particles are randomly distributed initially in a box of $L=2$. Interpolation of the velocity fluid at the particle position is obtained with a 6th order Lagrangian polynomial. Particles trajectories and compressibilities are calculated by solving the equations of motion using an RK4 method. The initial conditions are set so that each elemental volume of particles is a cube. Validity of the simulation and the numerical calculation of the

compressibility were tested by comparing results for the compressibility with values obtained from an analytical expression for small Stokes numbers. Fig.8a) shows the value of $\langle \ln J \rangle / t$ for Stokes numbers $St = 0.1, 0.7, 1, 10$. The trend in behaviour is similar to that for KS and simple flows, exhibiting a transition from $-ve$ to $+ve$ compressibilities at a critical Stokes number St_{cr} though similar but not the same in each case. Fig 8b) shows the values for the density moments $\overline{n^\alpha}$ for $\alpha=0,2,3$, for a particle with Stokes number, $St = 1$. As with case of the density moments in KS for $St = 0.5$, the intermittent events, which cause $n \rightarrow \infty$, dominate the statistics of higher-order moments of the PDF at certain moments in time, as is reflected by the spikes in the curve.

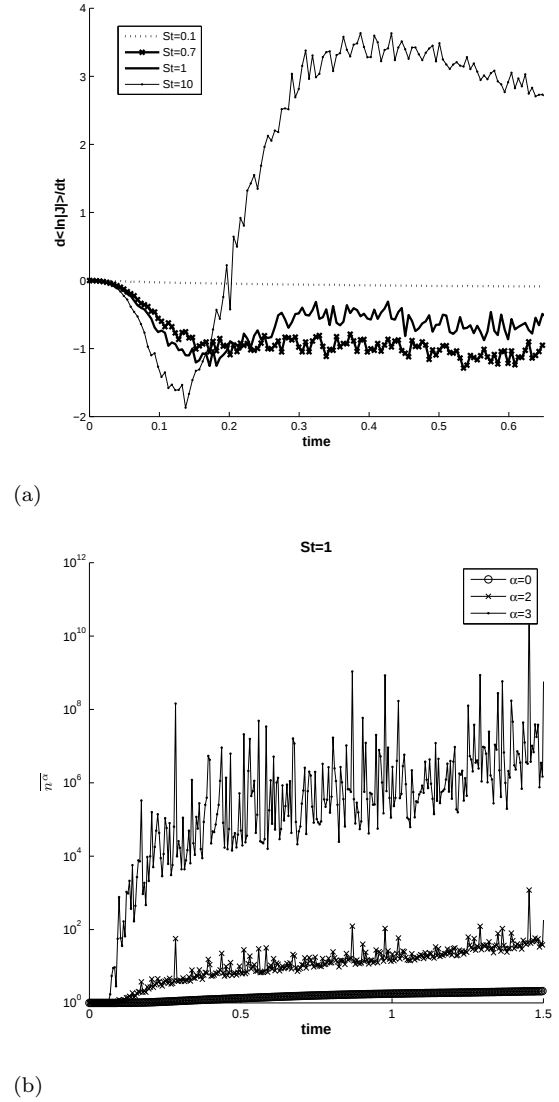


Figure 8: Segregation of inertial particles in DNS homogeneous isotropic stationary turbulence: a) compressibility $C = d/dt \langle \ln J \rangle$ for Stokes number, $St = 0.1, 0.7, 1, 10$; b) moments of the particle concentration $\overline{n^\alpha}$, $\alpha=0,2,3, St = 1$.

Summary and concluding remarks

We have shown how the Full Lagrangian Method (FLM) can be used to study the segregation of inertial particles in turbulent flows by calculating the deformation

of an initially infinitesimally small volume of particles along the trajectory of one particle. In particular we have demonstrated how this method can be used to determine the compressibility of the particle velocity field, and any spatially averaged moment of the particle number density. The FLM enables the detection of the very high intermittency in the spatial distribution of particles and the associated singularities in the particle velocity field. These features, which take place on infinitesimally small scales (in the commonly assumed approximation of point particles), can not be identified by box counting methods as they rely on finite box sizes by definition. We have applied the FLM to particle motion in three different random flows: a random straining flow field consisting of counter-rotating vortices, an incompressible flow field composed of 200 random Fourier modes and a homogeneous isotropic flow field generated by DNS. In all three cases the qualitative behaviors were very similar. In particular all three cases, the volume occupied by the particle phase as a continuum decreases continuously if $St < St_{cr}$, with $St_{cr} \sim 0.7$, indicating that the ongoing process of segregation is not limited to relatively simple flow fields. We also measured the component of random uncorrelated motion of the particles (RUM) which becomes important if $St \gtrsim 0.5$; for sufficiently large Stokes number, $RUM \rightarrow 1$, indicating that the particle velocities become virtually uncorrelated with the underlying carrier flow field. The presence of RUM is also visible in the spatially averaged higher-order moments of the particle number density, which show that the particle distribution may be highly intermittent.

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A DIFFUSION-INERTIA MODEL FOR SIMULATING DISPERSION OF AEROSOL PARTICLES IN TURBULENT FLOWS

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Introduction

The methods of modeling turbulent two-phase flows can be subdivided into two categories depending on the Lagrangian tracking and Eulerian continuum approaches for handling the particulate phase. In the framework of the Lagrangian method, the particles are assumed to encounter randomly a series of turbulent eddies, and the macroscopic particle properties are determined solving stochastic equations along separate trajectories. As a consequence, such a method requires tracking a very large number of particle trajectories to achieve statistically invariant solution. As the size of particles decreases, the representative number of realizations should increase because of the increasing contribution of particle interactions with turbulent eddies of smaller and smaller scale. Thus, this technique, especially when coupling with DNS or LES for the computation of fluid turbulence, provides a very useful research tool of investigating particle-laden flows, but it can be too expensive for engineering calculations. The Eulerian method deals with the particulate phase in much the same manner as with the carrier fluid phase. Therefore, the two-fluid modeling technique is computationally very efficient, as it allows us to use the governing equations of the same type for both phases. In addition, the description of fine particles does not cause great difficulties because the problem of the transport of particles with vanishing response times reduces to the turbulent diffusion of a passive impurity. Overall, the Lagrangian tracking and Eulerian continuum modeling methods complement each other. Each method has its advantages and, consequently, its own field of application. The Lagrangian method is more applicable for non-equilibrium flows (e.g., high-inertia particles, dilute dispersed media), while the Eulerian method is preferable for flows that are close to equilibrium (e.g., low-inertia particles, dense dispersed media).

To simulate the dispersion of low-inertia particles in turbulent flows, the Eulerian models of diffusion type appear to be very efficient. In [1-3], a simplified Eulerian model called the diffusion-inertia model (DIM) was developed. This model was based on a kinetic equation for the probability density function (PDF) of particle velocity distribution [4-6] and was coupled with fluid RANS in the frame of one-way coupling. The DIM was applied to simulate various turbulent flows laden with low-inertia particles and was incorporated in the CFD code SATURNE for modeling aerosol transport in ventilated rooms [7]. The advantage of the Eulerian diffusion-type models is that the particle velocity can be explicitly expressed in terms of the properties of the carrier fluid flow. By this means, one avoids the need to solve the momentum balance equations for the particulate phase, and the problem of modeling the dispersion of the particulate phase amounts to solving a sole equation for the particle concentration. Thus, computational times are

seriously shortened as compared to full two-fluid Eulerian models. The disadvantage is that these are applicable only to the two-phase flows laden with low-inertia particles. For example, the DIM is valid when the particle response time is less than the integral timescale of fluid turbulence. Nevertheless, these models are capable of predicting the main trends of particle distribution, including particle preferential concentration, over a fairly wide range of particle inertia.

In this paper, we extend the DIM to include the back-effect of particles on the fluid turbulence in the frame of two-coupling. Moreover, the so-called inertia and crossing-trajectory effects we incorporated into the model and the boundary condition for the particle concentration equation is refined. This extended model is applied to the three-dimensional simulation of aerosol deposition in straight ducts and circular bends.

Mathematical formulation

The theoretical background of the model is a transport kinetic equation for the one-particle PDF, P , that is the probability of observing a particle at a point $\mathbf{x}$, with a velocity $\mathbf{v}$, at time t . This kinetic equation has the form

$$\begin{aligned} \frac{\partial P}{\partial t} + v_i \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial v_i} \left[\left(\frac{U_i - v_i}{\tau_p} + F_i \right) P \right] \\ = \lambda_{ij} \frac{\partial P}{\partial v_j} + \mu_{ij} \frac{\partial P}{\partial x_j} + \frac{D_B}{\tau_p^2} \frac{\partial^2 P}{\partial v_i \partial v_i}, \\ \lambda_{ij} = \langle u'_i u'_j \rangle \left(\frac{f_{u \, kj}}{\tau_p} + l_{u \, kn} \frac{\partial U_j}{\partial x_n} \right) - \frac{D_p \langle u'_i u'_k \rangle f_{u1 \, kj}}{Dt}, \\ \mu_{ij} = \langle u'_i u'_k \rangle g_{u \, kj}, \quad f_{u \, ij} = \frac{1}{\tau_p} \int_0^\infty \Psi_{Lp \, ij}(\tau) \exp \left(-\frac{\tau}{\tau_p} \right) d\tau, \\ f_{u1 \, ij} = \frac{1}{\tau_p^2} \int_0^\infty \tau \Psi_{Lp \, ij}(\tau) \exp \left(-\frac{\tau}{\tau_p} \right) d\tau, \\ g_{u \, ij} = \frac{T_{Lp \, ij}}{\tau_p} - f_{u \, ij}, \quad l_{u \, ij} = g_{u \, ij} - f_{u1 \, ij}, \\ T_{Lp \, ij} = \int_0^\infty \Psi_{Lp \, ij}(\tau) d\tau, \\ \frac{D_p \langle u'_i u'_j \rangle}{Dt} = \frac{\partial \langle u'_i u'_j \rangle}{\partial t} + U_p k \frac{\partial \langle u'_i u'_j \rangle}{\partial x_k} + \frac{\partial \langle u'_i u'_j u'_k \rangle_p}{\partial x_k}, \\ U_p i = U_i - \tau_p \mu_{ij} \frac{\partial \ln \Phi}{\partial x_j}, \\ \langle u'_i u'_j u'_k \rangle_p = -\frac{\tau_p}{3} \left(\mu_{in} \frac{\partial \langle u'_j u'_k \rangle}{\partial x_n} + \mu_{jn} \frac{\partial \langle u'_i u'_k \rangle}{\partial x_n} + \mu_{kn} \frac{\partial \langle u'_i u'_j \rangle}{\partial x_n} \right), \end{aligned} \quad (1)$$

where τ_p is the particle response time, F_i is a body force acting on particles (e.g., gravity), U_i is the average fluid velocity, D_B is the Brownian diffusivity, $\langle u'_i u'_j \rangle$ is the fluid kinetic stresses, $\Psi_{Lp \, ij}(\tau)$ is the autocorrelation function of the fluid velocity seen by particles, $T_{Lp \, ij}$ are the Lagrangian timescales of the fluid velocity

seen by particles (the so-called eddy particle interaction timescales), and $f_{u\,ij}$, $f_{u1\,ij}$, $g_{u\,ij}$, $l_{u\,ij}$ are the tensor coefficients that measure a response of particles to the fluid turbulence, i.e., a coupling between the fluid and particulate phases. The first two terms on the right-hand side of (1) describe the interaction of particles with fluid turbulent eddies, and the second term quantifies the contribution of Brownian motion. To determine the particle turbulence interaction terms, we model the fluid turbulence by a Gaussian random process and use the functional formalism [4-6]. The modeling of the fluid velocity field by the Gaussian process is the key assumption that allows us to present the particle turbulence interaction in the form of a second-order differential operator. The quantities $U_{p\,i}$ and $\langle u'_i u'_j u'_k \rangle_p$ denote the fluid average velocity and third-order fluctuating correlation seen by particles [8].

By integrating Eq. (1) over the velocity subspace, we can obtain a set of governing conservation equations for the volume fraction, Φ , the average velocity, V_i , and the kinetic stresses, $\langle v'_i v'_j \rangle$, of the particulate phase

$$\frac{\partial \Phi}{\partial t} + \frac{\partial \Phi V_i}{\partial x_i} = 0 \quad (2)$$

$$\frac{\partial V_i}{\partial t} + V_j \frac{\partial V_i}{\partial x_j} = - \frac{\partial \Phi \langle v'_i v'_j \rangle}{\partial x_j} + \frac{U_i - V_i}{\tau_p} + F_i - \mu_{ij} \frac{\partial \ln \Phi}{\partial x_j} \quad (3)$$

$$\begin{aligned} \frac{\partial \langle v'_i v'_j \rangle}{\partial t} + V_k \frac{\partial \langle v'_i v'_j \rangle}{\partial x_k} + \frac{1}{\Phi} \frac{\partial \Phi \langle v'_i v'_j v'_k \rangle}{\partial x_k} = & - (\langle v'_i v'_k \rangle + \mu_{ik}) \frac{\partial V_j}{\partial x_k} \\ & - (\langle v'_j v'_k \rangle + \mu_{jk}) \frac{\partial V_i}{\partial x_k} + \lambda_{ij} + \lambda_{ji} + \frac{2D_B \delta_{ij}}{\tau_p^2} - \frac{2\langle v'_i v'_j \rangle}{\tau_p}. \end{aligned} \quad (4)$$

For the purpose of simplification, the Lagrangian timescale tensor of fluid turbulence, $T_{L\,ij}$, is assumed to be isotropic, $T_{L\,ij} = T_L \delta_{ij}$. And yet we shall still take into account the different timescales of particle interaction with turbulent eddies in different directions a phenomenon that arises as a consequence of the ‘crossing-trajectories effect’ [9]. As a result, we shall still observe the distinction between the longitudinal, T_{Lp}^l , and transverse, T_{Lp}^n , components of $T_{Lp\,ij}$. In this case, the tensor $T_{Lp\,ij}$ is given by $T_{Lp\,ij} = T_{Lp}^n \delta_{ij} + (T_{Lp}^l - T_{Lp}^n) e_i e_j$, $e_i = \frac{V_{r\,i}}{|\mathbf{V}_r|}$, $\mathbf{V}_r = \mathbf{V} - \mathbf{U}_p$, where the superscripts l and n symbolize, respectively, the longitudinal (parallel) and normal (perpendicular) directions to the relative velocity vector $\mathbf{V}_r$.

From Eqs. (3) and (4), one can express the velocity of low-inertia particles as an expansion in terms of the local characteristics of the turbulent fluid, with the particle response time as a small parameter. Truncating the velocity expansion to the first-order effect of particle inertia and substituting this into (2), we can obtain a diffusion-type equation for the particle concentration in a quasi-isotropic approximation

$$\begin{aligned} \frac{\partial \Phi}{\partial t} + \frac{\partial U_i \Phi}{\partial x_i} + \frac{\partial}{\partial x_i} \left[\tau_p (F_i - \frac{DU_i}{Dt}) \Phi \right] \\ = \frac{\partial}{\partial x_i} \left[(D_B + D_{Tp}^m) \frac{\partial \Phi}{\partial x_i} \right] + \frac{\partial}{\partial x_i} \left(\Phi \frac{\partial q_u^m D_{Tp}^m}{\partial x_i} \right), \end{aligned} \quad (5)$$

$$D_{Tp}^m = \frac{D_T T_{Lp}^m}{T_L}, \quad T_{Lp}^m = \frac{T_{Lp}^l + 2T_{Lp}^n}{3}, \quad q_u^m = \frac{\tau_p f_u^m}{T_{Lp}^m}$$

with D_T being the turbulent diffusivity of noninertial admixture.

By this means, for low-inertia particles, namely, when the particle response time is shorter than the turbulence

time macroscale, the conservation equation set can be reduced to the diffusion-type equation for the particle concentration, and hence one does not require solution to conservation equations for the momentum of the particulate phase. This approach was called the DIM. In the limit of zero-inertia particles, the concentration equation becomes the conventional diffusion equation. In comparison with the latter, the DIM allows us to take into account a number of effects caused by particle inertia: (i) the impact of gravity and other body forces, (ii) the so-called inertial bias effect, i.e., the transport by reason of the deviation of particle trajectories from the fluid streamlines, (iii) the turbulent migration (turbophoresis) due to the gradient of velocity fluctuations, and (iv) the inertia and crossing-trajectory effects on particle turbulent diffusivity.

To determine the response coefficients, we involve the two-scale bi-exponential autocorrelation function proposed by Sawford [10]. The eddy particle interaction timescales are determined using the model presented in [11]. The particle response time is given by

$$\tau_p = \frac{\rho_p d_p^2 \{1 + Kn[A_1 + A_2 \exp(-A_3/Kn)]\}}{18\rho_f \nu_f (1 + 0.15 Re_p^{0.687})}$$

where d_p is the particle diameter, ρ_p and ρ_f are the particle and fluid densities, ν_f is the fluid kinematic viscosity, Kn designates the Knudsen number, and according to [12] $A_1=1.2$, $A_2=0.41$, $A_3=0.88$.

In order to avoid the need to solve the particle concentration equation up to the wall, we use the method of wall-functions that has extensively employed in modeling single-phase turbulent flows. In accordance with this method, we invoke a relation between the flow rate of depositing particles, J_w , and the particle concentration in the near-wall region outside the viscous sub-layer, Φ_1 ,

$$\begin{aligned} J_w &= \frac{1-\chi}{1+\chi} (\gamma V_{DT} + V_{CF}) \Phi_1, \\ \gamma &= \frac{\exp(-b^2/\pi)}{1 + \text{erf}(b/\pi^{1/2})}, \quad b = \frac{V_{CF}}{V_{DT}}, \quad V_{DT} = V_{DF} + V_{TR}, \\ V_{CF} &= U_w + \tau_p (F_w - \frac{DU}{Dt}|_w), \quad V_{DF} = \frac{0.115 u_*}{Sc_B^{3/4}}, \\ V_{TR} &= \frac{2 \cdot 10^{-4} \tau_+^{2.5} (1 + 10^{-3} \tau_+^{2.5})^{-1} u_*}{\max[0.8, \min(1.32 - 0.27 \ln \tau_+, 1)]}. \end{aligned} \quad (6)$$

Here V_{DT} designates the ‘diffusion turbophoresis’ deposition rate defined as the sum of the diffusion V_{DF} and turbophoresis V_{TR} velocities, and V_{CF} designates the ‘convection force’ deposition rate where U_w , F_w , and $DU/Dt|_w$ are the wall-normal components of fluid velocity, body force acceleration, and fluid acceleration in the near-wall region. The quantity χ is the rebound coefficient that measures a probability of particle rebound from the wall and its return into the flow after collision. The surface is perfectly adsorbing if $\chi=0$, and the particle deposition is absent if $\chi=1$. The parameter b quantifies the ratio of the ‘convection force’ and ‘diffusion turbophoresis’ components of the deposition rate. Deposition is controlled by the ‘convection force’ mechanism when $b \rightarrow \infty$ ($\gamma \rightarrow 0$), and the deposition rate tends to zero when $b \rightarrow \infty$ ($\gamma \rightarrow -b$) because the action of this inhibits the motion of particles to the wall.

The coefficient γ is obtained assuming that the normal velocity PDF of particles in the near-wall region obeys a bi-normal distribution. The ‘diffusion’ component of the deposition rate, V_{DF} , is found as a result of solving the diffusion equation in the viscous sub-layer for the fourth-degree-law of rise in the turbulent diffusivity at high Schmidt numbers, where u_* is the wall

friction velocity, and $Sc_B \equiv D_B/\nu_f$ is the Schmidt number. The ‘turbophoresis’ component of the deposition rate, V_{TR} , is obtained as a result of approximating a numerical solution of Eqs. (2)–(4) in the near-wall region. The boundary condition (6) is valid for the particles with $\tau_+ \equiv \tau_p u_*^2/\nu_f \leq 100$ when the first grid node is chosen outside the viscous sub-layer ($y_+ \equiv y u_*/\nu \geq 30$) where Φ_1 changes weakly with variation in the normal distance from the wall.

The balance fluid momentum equation is given by $\frac{DU_i}{Dt} = -\frac{1}{\rho_f} \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\nu_f \frac{\partial U_i}{\partial x_j} - \langle u'_i u'_j \rangle \right) + \frac{M}{\tau_p} (V_i - U_p)_i$, where P is the average pressure, $M \equiv \rho_p \Phi/\rho_f$ is the mass particle loading of the fluid, and the last term quantifies the back-effect of particles on the fluid momentum.

Turbulent flow characteristics are simulated on the basis of a k - ε turbulence model modified due to the presence of particles in the flow

$$\begin{aligned} (1 + M f_{u1}^m) \frac{Dk}{Dt} &= \frac{\partial}{\partial x_i} \left\{ \left[\nu_f + (1 + M f_{u1}^m) \frac{\nu_T}{\sigma_k} \right] \frac{\partial k}{\partial x_i} \right\} \\ &\quad + (1 + M f_{u1}^m) \Pi - (\varepsilon + \varepsilon_p + G_p), \\ (1 + M f_{u1}^m) \frac{D\varepsilon}{Dt} &= \frac{\partial}{\partial x_i} \left\{ \left[\nu_f + (1 + M f_{u1}^m) \frac{\nu_T}{\sigma_\varepsilon} \right] \frac{\partial \varepsilon}{\partial x_i} \right\} \\ &\quad + \frac{\varepsilon}{k} [C_{\varepsilon 1} (1 + M f_{u1}^m) \Pi - C_{\varepsilon 2} (\varepsilon + \varepsilon_p + G_p)], \\ \langle u'_i u'_j \rangle &= \frac{2k\delta_{ij}}{3} - \nu_T \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right), \\ \nu_T &= \frac{C_\mu (1 + M f_{u1}^m) k^2}{\varepsilon + \varepsilon_p + [(1 + M f_{u1}^m) \Pi - (\varepsilon + \varepsilon_p)]/C_1}, \\ \Pi &= -\langle u'_i u'_j \rangle \frac{\partial U_i}{\partial x_j}, \quad \varepsilon_p = \frac{2M}{\tau_p} (1 - f_u^m) k, \\ G_p &= \frac{2\rho_p g_m k}{3\rho_f} V_{ri} \frac{\partial \Phi}{\partial x_i} \end{aligned} \quad (7)$$

with the values of constants being as follows: $C_\mu = 0.09$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $C_{\varepsilon 1} = 1.44$, $C_{\varepsilon 2} = 1.92$, and $C_1 = 1.1$.

Simulation results and discussion

The DIM, consisting of the particle concentration equation (5) and the boundary condition (6), is coupled with the fluid balance equations. The model advanced is evaluated against experiments and numerical simulations of aerosol deposition in vertical ducts and circular bends. The surface is assumed to be perfectly adsorbing, that is, the rebound coefficient, χ , is taken as zero in (6). Calculations have been performed using a three-dimensional finite-volume CFD code.

First we examine the performance of the model for the deposition of particles in a vertical duct flow, when the gravity force does not exert direct action on the deposition rate. It is a common convention to describe the deposition rate of particles from turbulent flow by the dependence of the deposition coefficient $j_+ \equiv J_w/\Phi_m u_*$, where Φ_m is the bulk volume particle fraction, on the particle inertia parameter τ_+ . In line with the primary mechanism governing the process of deposition, the entire range of particle inertia may be subdivided into three regimes: the diffusion regime ($\tau_+ < 1$), the turbophoresis regime ($1 \leq \tau_+ \leq 100$), and the inertia regime ($\tau_+ > 100$). The deposition process of the diffusion regime is mainly governed by Brownian and turbulent diffusion, and, in this situation, j_+ declines monotonously with τ_+ as a result of a decrease in the Brownian diffusivity with increasing aerosol size. The basis deposition mechanism of the turbophoresis regime is the turbulent migration of particles from the flow core,

which is characterized by high-level velocity fluctuation intensity, to the viscous sublayer adjacent the wall. This regime features a strong dependence of j_+ on τ_+ . High-inertia particles ($\tau_+ > 100$) are weakly involved in turbulent flow of the carrier fluid, which causes the deposition coefficient j_+ in a vertical duct to decrease with τ_+ .

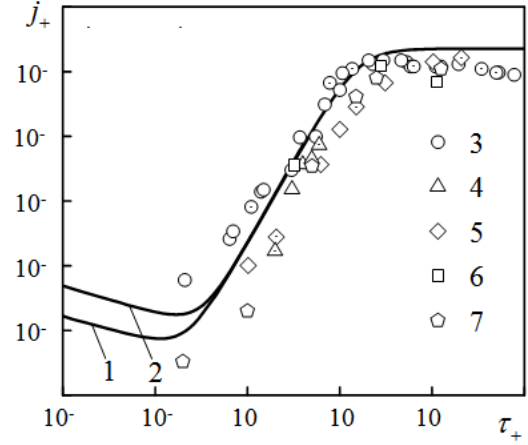


Figure 1: The deposition coefficient in vertical duct flows. (1) DIM $Re=10000$, (2) DIM $Re=50000$, (3) [13], (4) [14], (5) [17], (6) [15], (7) [16].

Figure 1 presents the predictions of the deposition coefficient for the pipe flow conditions which correspond to experiments [13]. To focus attention on the deposition mechanisms caused by the interaction of particles with turbulent eddies, the gravity and lift forces are neglected and hence $F_i = F_w = 0$. In Fig. 1, the deposition coefficients obtained for duct flows using DNS [14–16] and LES [17] are shown as well. Note that, in the diffusion and turbophoresis regimes, the deposition process is mainly governed by the interaction of particles with near-wall turbulent eddies. Therefore, the deposition rates determined in round pipe and flat channel flows are hardly distinguishable. As is clear from Fig. 1, the DIM properly captures the dependence of j_+ on τ_+ at $\tau_+ < 100$. The deposition coefficient predicted for high-inertia particles is found to systematically deviate from the measurements, because the model does not predict a decrease in j_+ with τ_+ . Thus, to predict the deposition rate, the DIM can be successfully employed only in the diffusion and turbophoresis regimes.

In what follows we focus our attention on the dispersion and deposition of aerosol particles in 90° bends. Hydrodynamic structure of these flows is complex. It is characterized by the existence of curved streamlines and recirculating regions. The key nondimensional parameters that govern the flow are the Reynolds number defined as $Re = DU_m/\nu_f$ and the Dean number defined as $De = Re/R_0^{1/2}$ where $R_0 \equiv 2R_b/D$ is the curvature ratio, D is the duct diameter, U_m is the mean axial fluid velocity, and R_b is the bend curvature radius. For high Dean numbers, the flow in the bend is mainly governed by the centrifugal force which changes cardinally the flow pattern as compared to that in the straight duct. The main features of the flow in the bend consist in separating the mean flow from the inner side, displacing it to the outer side, and generating the secondary flow in the form of a symmetric pair of counter-rotating helical vortices.

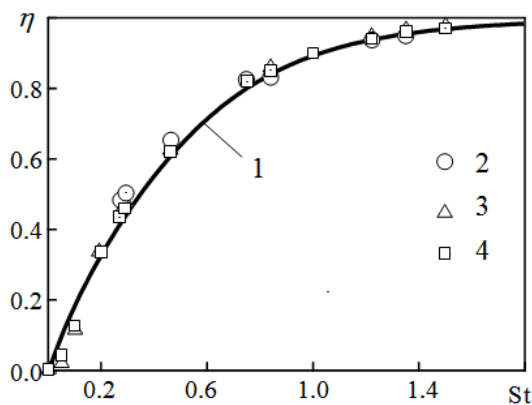


Figure 2: The effect of Stokes number on the deposition efficiency. (1) DIM, (2) [18], (3) [19], (4) [20].

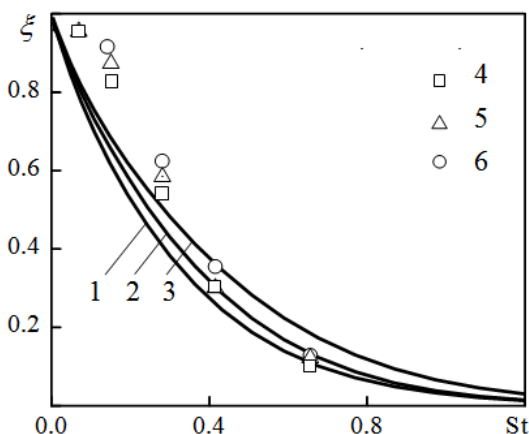


Figure 3: The effects of curvature ratio and Stokes number on the penetration. (1 3) DIM, (4 6) [21]: (1, 4) $R_O=4$, (2, 5) 10; (3, 6) 20.

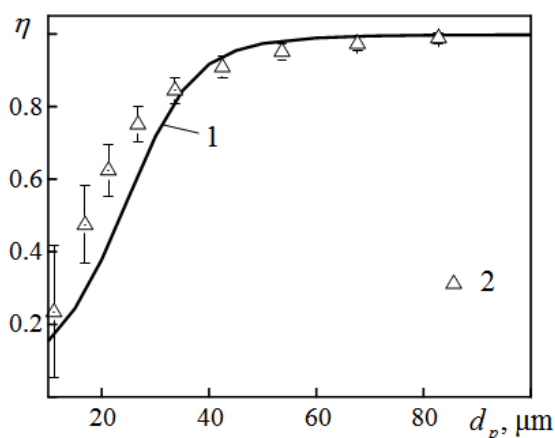


Figure 4: The effect of particle size on the deposition efficiency in the bend. (1) DIM, (2) [22].

The total process of aerosol deposition can be measured by the penetration of particles which is defined as

the ratio of the particle flow rates in the outlet and inlet sections of the bend, $\xi = G_{outlet}/G_{inlet}$, or by the deposition efficiency, $\eta = 1 - \xi$. Figure 2 presents the deposition efficiency predicted in the bend under the conditions corresponding to experiments [18] for $Re=10000$, $De=4225$, and $R_O=5.6$. The inertia of particles is quantified by the Stokes number defined as $St = 2\tau_p U_m/D$. In these circumstances, the deposition of particles is caused by the simultaneous action of diffusion, thermophoresis, gravity, and centrifugal force. However, the dominating mechanism is the centrifugal force due to the bend of the main flow and the formation of the secondary flow. As is clear from Fig. 2, the effect of the Stokes number predicted by the DIM is in good agreement with both experimental data [18] and simulations [19, 20].

Figure 3 demonstrates the effects of the curvature ratio and the Stokes number on the penetration of particles in the bend at $Re=10000$. Predictions are compared with experiments performed in [21] over a wide range of curvature ratios. It is obvious that the centrifugal effect increases as the curvature ratio decreases. Therefore, the penetration falls with both increasing St and decreasing R_O . As is clear, the DIM reasonably reproduces these effects. Some distinction between the predictions and the measurements is observed at small Stokes numbers, when the DIM overestimates the deposition rate.

Figure 4 compares the deposition efficiency with experimental data [22] in the bend at $Re=203000$ and $R_O=5$. These experiments were carried out in a bend of $D=0.152$ m at a mean velocity of 20 m/s, and hence they were the first to be directly applicable to industrial bends. It is clear that the DIM can adequately predict the deposition of aerosols at such high Reynolds numbers which are typical of industrial applications.

Summary

The paper is focused on development and application of the DIM for the simulation of dispersion and deposition of aerosol particles in two-phase turbulent flows. The model stems from a kinetic equation for the probability density function of velocity distribution of particles whose response times do not exceed the integral timescale of fluid turbulence. The salient feature of the DIM consists in expressing the particle velocity as an expansion in terms of the properties of the carrier fluid, with the particle response time as a small parameter. By this means, the problem of modelling the dispersion of the particulate phase reduces to solving a sole equation for the particle concentration. Thus, computational times are seriously shortened as compared to full two-fluid Eulerian models. The model presented is capable of predicting the main trends of particle distribution including the effect of preferential accumulation due to turbophoresis. The DIM has been incorporated in a CFD code and coupled with fluid RANS in the frame of two-way coupling. Simulations of aerosol deposition in vertical pipes and circular bends have been performed. The results of deposition efficiency obtained using the DIM are found to be in encouraging agreement with both experimental data and Lagrangian tracking simulations coupled with fluid DNS or LES.

Acknowledgements

This work was supported by the Russian Foundation for Basic Research (Grants No. 09-08-00084 and 10-08-00210).

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Best Practice Guidelines for Computational Fluid Dynamics of Dispersed Multi-Phase Flows

Editors

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The simultaneous presence of several different phases in external or internal flows such as gas, liquid and solid is found in daily life, environment and numerous industrial processes. These types of flows are termed multiphase flows, which may exist in different forms depending on the phase distribution. Examples are gas-liquid transportation, crude oil recovery, circulating fluidized beds, sediment transport in rivers, pollutant transport in the atmosphere, cloud formation, fuel injection in engines, bubble column reactors and spray driers for food processing, to name only a few. As a result of the interaction between the different phases such flows are rather complicated and very difficult to describe theoretically. For the design and optimisation of such multiphase systems a detailed understanding of the interfacial transport phenomena is essential. For single-phase flows Computational Fluid Dynamics (CFD) has already a long history and it is nowadays standard in the development of air-planes and cars using different commercially available CFD-tools.

Due to the complex physics involved in multiphase flow the application of CFD in this area is rather young. These guidelines give a survey of the different methods being used for the numerical calculation of turbulent dispersed multiphase flows. The Best Practice Guideline (BPG) on Computational Dispersed Multiphase Flows is a follow-up of the previous ERCOFTAC BPG for Industrial CFD and should be used in combination with it. The potential users are researchers and engineers involved in projects requiring CFD of (wall-bounded) turbulent dispersed multiphase flows with bubbles, drops or particles.

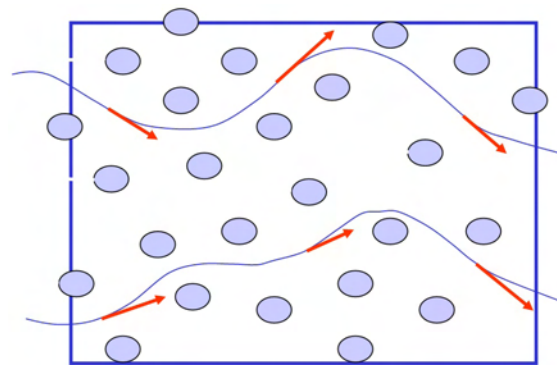


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* * *

Copies of the Best Practice Guidelines can be acquired electronically from the website:

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