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Perspective article

Stochastic modelling for capturing the behaviour of irregular-shaped non-spherical particles in confined turbulent flows

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ABSTRACT

For calculating dispersed particle-laden flows in confined systems, the well-known Euler/Lagrange approach is most suitable. Lagrangian tracking of non-spherical particles with certain shapes is mostly performed by additionally solving for the orientation of particles in the flow and using resistance coefficients (i.e. drag, lift and torque) which depend on this orientation. For that in many cases theoretical results for Stokes flow around such particles are used. In practical situations where very often irregular shaped non-spherical particles are transported in a flow, such an approach cannot be adopted since the particles have mostly a statistical distribution of shape and hence it is difficult to define a major and minor axis of the particles. The novel approach developed here is based on a statistical treatment of the fluid forces and moments acting on irregular-shaped particles as well as the wall collision process in order to mimic their stochastic behaviour. The required probability distribution functions (PDF's) for the resistance coefficients were derived by applying direct numerical simulations (DNS) based on the Lattice-Boltzmann method (LBM). The PDF's for the wall normal and parallel restitution ratios were developed based on an experimental analysis of the wall collision of irregular-shaped particles using stereoscopic high-speed imaging. Preliminary Euler/Lagrange calculations applying these statistical models were conducted for a horizontal channel flow laden with irregular-shaped particles and compared to measurements. The results revealed that the calculation of the particle phase assuming the standard models for spherical particles yields completely wrong cross-stream profiles of particle mass flux, an under-prediction of the streamwise particle mean velocity and an over-prediction of the associated fluctuating component. The stochastic models for the flow resistance coefficients and the wall collision process on the other hand provided much better agreement with the measurements.

1. Introduction

The handling or treatment of powders though transportation by fluids (i.e. gas or liquid) is an important process in numerous industrial and technical areas. These flows are mainly confined flows as for example hydraulic or pneumatic conveying, particle separation devices, e.g. cyclones, particle dispersion in stirred vessels and fluidized beds. Hence, particle motion is strongly governed by fluid dynamic transport, including turbulence [1] as well as wall collisions [2]. For denser situations or if inertial segregation occurs, also inter-particle collisions have an important influence [3]. Numerical calculation of such large-scale industrial processes becomes of increasing importance for industry in order to support process design, lay-out and optimisation. However, even with the today available computational power not all scales can be resolved in such simulations (i.e. particles and apparatus), wherefore the dispersed phase elements are treated as point-particles or point-masses using appropriate correlations for describing their fluid dynamic transport as for example drag or lift coefficients. In most technical cases, the particle Reynolds number is larger than unity so that a theoretical derivation of such correlations is not possible and therefore experimentally-based correlations are mostly used assuming that the particles are spherical [4,5].

In addition, a large number of other particle-scale phenomena influence dispersed two-phase flows, such as, inter-particle collisions, wall collisions, deposition and agglomeration, to name only a few. In a point-particle approach, all these elementary processes need additional modelling and closures [6]. This is the most important task in the development of macro-scale numerical methods for industrial and technical processes.

The numerical computation of dispersed particle-laden flow systems may be done on the basis of two modelling approaches, namely the two-fluid or Euler/Euler and the Euler/Lagrange approach [1,4,6]. In the two-fluid approach, both phases are considered as interacting continua using appropriate averaging procedures and closures whereas in the Lagrangian approach the discrete nature of the dispersed phase, at

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least partly, is respected by tracking a large number of particles (i.e. point-masses) through the flow field in order to obtain statistical information on the dispersed phase properties. Mostly, in both approaches, the particles are considered to be spherical using appropriate closures and models for the resistance coefficients in the relevant fluid dynamic forces [5]. Only in a few cases the drag coefficient of non-spherical particles is considered using trajectory-averaged correlations for certain particle shapes as for example provided by Haider and Levenspiel [7]. These correlations for the drag coefficient are however only valid for certain orientations of non-spherical particles (i.e. horizontally aligned disc during sedimentation) and cannot resolve a continuous change of particle orientation with respect to the relative flow occurring in complex or turbulent flows [8].

In technical applications the particles are mostly non-spherical having either a regular shape (e.g. fibres, cylinders, granulates or disc-like particles) or are completely irregular in shape such as quartz sand and coal particles (see Fig. 1). Numerical calculations conducted for such systems are even today mostly done assuming spherical particles and using the respective correlations for the resistance coefficients. This is associated with the fact that fluid forces acting on non-spherical particles, especially for larger particle Reynolds numbers, are to a large extent unknown. Only in a few studies direct numerical simulations (DNS) are being used for deriving correlations for the resistance coefficients (i.e. drag, lift and torque) of regularly shaped non-spherical particles [9–11]. However, such simulations are very time consuming due to the large parameter space which has to be considered, i.e. resistance coefficients and moment coefficients in dependence of particle orientation. Having this information, Euler/Lagrange calculations may be conducted by additionally solving for the angular orientation of the particles in the flow (see e.g. van Wachem et al. [8], Njobuenwu and Fairweather [12]) and using correlations for orientation-dependent resistance coefficients (Table 1). Knowing the particle orientation, the wall collision process may be also calculated in more detail by solving the impulse equations in connection with Coulomb's law of friction, see e.g. Sommerfeld [13] and Quintero et al. [14].

However, if the particles are irregular in shape, as illustrated in Fig. 1 for quartz sand (number mean diameter of 185 μm) and Duroplast particles (number mean diameter of 240 μm), they generally have a distribution of shapes and it is difficult to define any specific major and minor axis of the particles [15]. Hence, the tracking of particle orientation for such particles is not very meaningful.

Consequently, in this work a statistical approach is suggested (Table 1) in order to model the behaviour of irregular-shaped particles in confined turbulent flows [16]. This includes modelling of the stochastic nature of fluid dynamic forces acting on the particles and of the wall collision process in a gas flow where any lubrication effects can be neglected. The following paragraph describes the Lattice-Boltzmann (LBM) simulations conducted and the resistance coefficients obtained therefrom. Following that, the experiments for analysing irregular particle wall collisions are described and the results are summarised. Finally the new correlations for the random treatment of fluid dynamic forces and the wall rebound of irregular-shaped particles are implemented into an in-house Euler/Lagrange code and the results are validated based on experiments for irregular particle motion in a turbulent horizontal channel flow as introduced by Kussin [15].

Table 1
Summary of deterministic and stochastic modelling approaches for simulating non-spherical particles in the frame of a Lagrangian approach.

Lagrangian treatment of non-spherical particles	
Regularly shaped non-spherical particles	Irregular non-spherical particles
Deterministic tracking of particles, new location, orientation, rotational and translational velocities	Stochastic tracking of particles, new location, translational and angular velocities
Requires additionally tracking of the particle orientation using Euler Parameters or quaternions for coordinate transformation	Determine the instantaneous values of the resistance coefficients from a-priory determined distribution functions (random process), e.g. by Lattice-Boltzmann simulations
Particle orientation-dependent resistance coefficients are required, may be obtained from simulations [9]	Apply these random resistance coefficients in the equation of motion each time step
Solving the impulse equations for non-spherical particle wall considering particle orientation (see Sommerfeld [13])	Calculate the particle velocity change during a wall collision process from measured distribution functions of the restitution ratios or the velocity ratios

2. Fluid forces on irregular particles

Regarding the flow resistance coefficients, first direct numerical simulation (DNS) based on the Lattice-Boltzmann method (LBM) were conducted for irregular particles placed fixed into a laminar plug flow. The applied in-house code allows for a local grid refinement around complex particle structures. Moreover, curved wall boundary conditions are used for the bounce-back condition at solid surfaces and in order to obtain the momentum exchange between fluid and particles [17]. More details about the LBM applied in this work are found in Sommerfeld and Qadir [18].

In general LBM solves for the change of a probability distribution function, which describes the number of fluid elements having a velocity v at location x and time t, to simulate the flow of Newtonian fluids. Hence, besides the spatial discretization realised by the numerical grid (in this case with local refinements), the fluid element velocities and the time are discretized as well. Hence, information is allowed to propagate to a neighboring lattice node in one of the discrete lattice directions at one time step only, followed by a collision step. In the

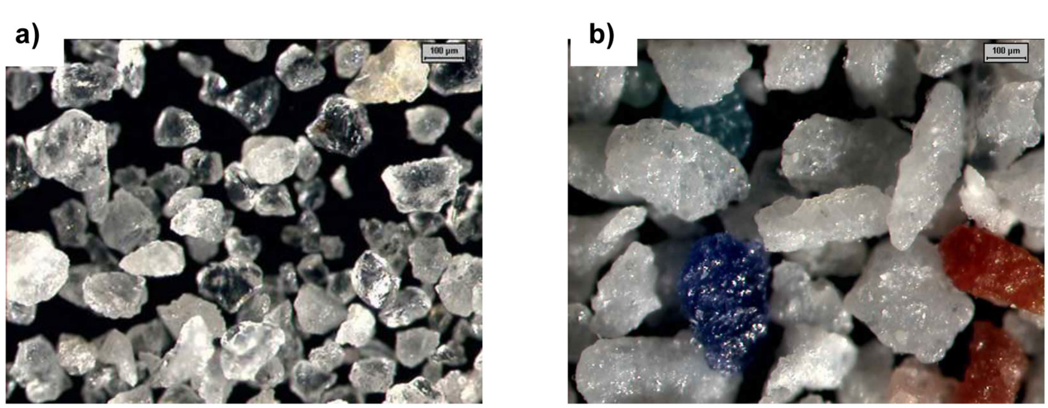

Fig. 1. Photographs of irregular-shaped particles; a) quartz sand with volume equivalent mean diameter 185 μm and sphericity 0.88; b) Duroplast particles with volume equivalent mean diameter 240 μm and sphericity 0.71 [15].