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Coarse Graining in Discrete Element Modelling (DEM-CFD) of High Solids Loading Cyclones

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Cyclones are often used in the separation of solid particles from gas inside recirculating fluidized beds. Design, scale-up and operation remain essentially based on simplified models and experience. Recent developments in simulations allow the complex gas swirl inside reverse flow cyclones to be obtained with reasonable accuracy. For coupled gas-particle flow in medium-large systems, as in industrial applications, numerical models based on the DEM-CFD approach, despite its recognized reliability, remain prohibitive due to the high number of particles involved and the corresponding computational cost. In recent years, methods have been proposed to reduce the number of particles by grouping them into representative particles, called *parcels* or grains, to reduce the number of simulated elements and possibly increase the time step. This technique proved to be efficient in simple systems, but much remains to be understood and characterized, such as the extent to which the predictive capability of the model is preserved also in complex flows and geometries. In the present work, coarse-grained DEM-CFD methods are investigated to simulate two-phase flow in solid-gas cyclones at different solid and gas loads. A standard Stairmand high-efficiency design is simulated using an extended version of the open-source MFIX-DEM code. Attention has been paid on the effect that the strategy and the degree of coarse grain have on the replicability of the results compared to pure DEM-CFD simulations. Property scaling is examined in both macroscopic performance indicators and local distribution of gas and solid flows within the cyclone, including vortex formation, solid flow, number of revolutions and collection efficiency, with the aim of quantifying, on the one hand, the computational saving and, on the other one, the acceptable level of coarse graining and its expected impact on the quality of results.

1. Introduction

The separation of solid from a gas stream is an operation often required by industrial processes, to recover product or for environmental control. The cyclone separator is a reliable device designed and used for this purpose (Nakhaei et al. 2020). Its geometry combined with the flow rates that pass through it define its overall properties, such as the pressure drop and the capture efficiency (Hoffmann and Stein, 2008).
The complexity of two-phase flow contributed to the development of semi-empirical models with significant simplifications (Muschelknautz and Greif 1997). However, some performance improvement had been achieved through experimental methods (Hoffmannc et al. 1992). The computational simulation offered possibilities to describe the solid-gas to improve design and scale-up of process. Simulation approaches differ mainly in the ways in which solids are described. Extensive studies have been performed on the single gas phase, neglecting the particles (Gronald and Derksen 2011). A first approach for the study of particle motion was based on Lagrangian particle tracking in combination with Computational Fluid Dynamics (CFD), which excludes the particle-particle interaction (Wan et al. 2008). The use of Euler-Lagrange methods using commercial codes (Kozołub et al. 2017) showed that the presence of high solid load yields significant changes in the gas velocity field; the adoption of DEM-CFD approach with full four-way coupling have been used for medium dense hydrocyclones (Chu et al. 2009). In order to reduce the computational cost of DEM simulations, in terms of amount of resources required to perform them, the coarse-grained technique appear as an alternative. For simulations of medium dense cyclones (Chu et al. 2015), this technique was quantitatively effective. However,

the computational savings and physical accuracy have scarce quantitatively information. This work aims to investigate the effect of the coarse-grain technique on the main macroscopic for cyclone performance and, on the two-phase flow local dynamics. In the absence of sufficient detail of the experimental data, it is assumed that the base case is the pure CFD-DEM case.

2. Coarse-Grain DEM-CFD Numerical Model

The modelling approach adopted in the simulations combines the Discrete Element Method (DEM) to describe the particle (solid phase) motion field and a locally averaged Computational Fluid Dynamics (CFD) approach for the fluid (gas phase). Two-way coupling is ensured by the presence of a source term that balances the drag force and the force of the pressure gradient on the particles in the locally averaged equations of continuity and momentum balance. Taking into consideration particle-particle interactions, such as particle-particle collision/dissipation, particle rotation and sliding with walls, the four-way coupled model is adopted. (Di Renzo and Di Maio 2007). The main basic equations for the description of the two phase motion are available in the documentation of MFIX-DEM, the used software (Garg 2013). Turbulence is not considered due the presence of particles sliding along the walls, which profoundly changes the eddy generation and dissipation, typically accounted for single phase flow, as well as the need for relatively coarse grids to apply the particle-fluid interactions averaging. It has to be considered that the most significant information achievable by the DEM-CFD is the highly realistic description of particle dynamics, fully coupled to gas flow. The adaption of the cyclone geometry was obtained by the Cartesian grid cut-cell method (Dietiker et al. 2013). Several in-house implementations were added to the MFIX-DEM code: the coarse-grain methodology is similar to the proposed by Bierwisch et al. (2009); the drag model was implemented Di Felice’s formula (Eq. 1), some modifications guaranteed a constant solid mass inlet at different particle/grain dimension and minor numerical optimizations. Contact forces between the particles were considered using the Hertzian non-linear elastic-frictional model with dissipation based on a constant coefficient of restitution.

$$F_d = F_{d0}\varepsilon^{-\chi} \tag{1}$$

$$\chi = 3.7 - 0.65 \cdot e^{-0.5\left[1.5-\log_{10} Re_p\right]} \tag{2}$$

Where F_d is the drag force for multi-particle systems and F_{d0} is the drag force on isolated particle defined as:

$$F_{d0} = C_d \, \frac{\pi}{4} d^2 \, \frac{1}{2} \rho_f \varepsilon^2 |u-v|(u-v) \tag{3}$$

with $C_d = \left(0.63 + \frac{4.8}{\sqrt{Re_p}}\right)^2$ as the drag coefficient, where $Re_p = \frac{\rho_f d\varepsilon|u-v|}{\mu_f}$ is the particle Reynolds number with u as the average fluid velocity, v the particle velocity, d the particle diameter, ε the gas volume fraction, ρ_f the fluid density, μ_f the fluid viscosity. The pressure gradient force is $F_b = V_p \nabla p$ where V_p is the particle volume and ∇p is the gradient of the average pressure.

2.1 Coarse Grain Method (CGM)

The coarse-grained method allows the correlation of single particles with entities called "grains", properly adjusting properties to represent the original particles. This concept is illustrated in Figure 1.

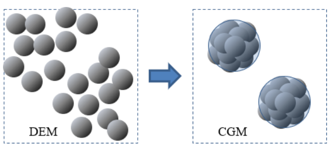


Figure 1 - Concept of DEM-CGM: original particles (left), representative grains (right).

The volume of the grain (V_g) is equal to the sum of the original respective particles (V_p), considering the same density to ensure the mass conservation of the system. According to the number of particles per grain (NPG), it is possible to calculate:

$$V_g = NPG \cdot V_p \tag{4}$$

The diameter of grain (d_g) is deductible from the original particle one (d_p):

$$d_g = NPG^{\frac{1}{3}} \cdot d_p \tag{5}$$

The scale correlation for the drag and buoyancy forces between the grains ($F_{d,g}$, $F_{b,g}$) and particles ($F_{d,p}$, $F_{b,p}$) are, respectively:

$$F_{d,g} = NPG \cdot F_{d,p} \tag{6}$$

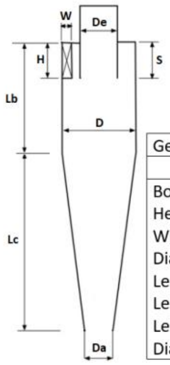
$$F_{b,g} = NPG \cdot F_{b,p} = V_g \nabla p \tag{7}$$

The correct way to estimate the collision properties of the grain starting from those of the particles have studied. Such study assumes that the collisional grain properties are equal to the real particle, including the material stiffness, friction and damping coefficients.

3. Simulated System

3.1 Geometry

In this study the Stairmand high-efficiency cyclone has been adopted as the separator system (Figure 2).



Geometry Dimensions Legend			
		Diameter ratio	Length [cm]
Body Diameter	D	1.0	9
Height of Inlet	H	0.5	4.5
Width of Inlet	W	0.2	1.8
Diameter of Gas Exit	De	0.5	4.5
Length of Vortex Finder	S	0.5	4.5
Length of Body	Lb	1.5	13.5
Length of Cone	Lc	2.5	22.5
Diameter of Dust Outlet	Da	0.375	3.375

Figure 2 - Stairmand configuration high-efficiency cyclone with geometrical dimension ratios

3.2 Boundary Conditions (BCs)

No-slip wall condition was assumed. The two phases enter the cyclone with the same fixed velocity u_{in}. Particles are randomly generated at the inlet boundary. The constant pressure BC was used for both outlets, setting 0 and 50 Pa as the differential pressure with respect to atmospheric pressure for the upper and lower outlet, respectively. The adoption of a constant pressure at the lower outlet is representative of cyclones in loop reactors, without imposing constraints on the velocity field.

3.3 Simulation Set-Up

A simulation has been performed with the conditions to analyze the effect of the coarse-grained degree passing from NPG=1 (i.e. no CGM) to 8, as reported in Table 1. Relatively large particles were considered having in mind a cyclone used in polymerization loop reactors. Similarly, solids loading as high as 0.5% in volume have been considered. With the increase of NPG, the number of simulated entities decreases and simultaneously the time-step increases, which leads to a considerable simulation speed-up. The process quickly reaches its steady-state, making one second of simulation long enough.

Table 1 - Summary table of the variables and parameters used in the simulation set-up

Particle properties	$D =$ 500 µm, $\rho =$ 2500 kg m^{-3}	
Contact model	Hertz, $E =$ 5·10^{7} Pa, $e_n =$ 0.9	
Solids loading (%vol)	0.1%, 0.2%, 0.5%	
Inlet velocities	10, 14, 20 m/s	
	Condition 1	**Condition 2**
Particle or grain size, d [mm]	500	1000
Particles per grain, NPG [-]	1 (DEM)	8
Grain-to-particle size ratio	1	2
Holdup in number of grains, [-]	136k–717k	11k–94k
Solid-phase time-step, D_{ts} [10^{-6} s]	0.6	1.9
Fluid-phase (typical) time-step	5·10^{-4} s	

4. Results and Discussion

4.1 Computational Savings

One of the most impressive and attractive features of the coarse graining technique is the computational advantage over pure DEM and DEM-CFD. A quick estimation of the theoretical savings can be made based on the system data (Table 1). In terms of numerical elements to track, the solids hold-up in the cyclone shows a decrease factor between 7 and 12 while the integration time-step increased by a factor of 3. Assuming a reasonable linear scaling, this means that by simply considering grains twice as large as the original particles (NPG=8), an overall speed-up of about 20 times over pure DEM is expected. In actual runs, wall clock time for the simulations scaled by about 10 times for ε=0.5% and u_{in}=10. This is based on parallel simulations on 32/16 cores of a HPC cluster available at Unical and includes the negligible influence on the CFD part of the code.

4.2 Hydrodynamics and Gas Flow

As can be seen in Figure 3, the gas phase exhibits the typical flow field: it tangentially enters in the body of the cyclone, descends along the walls and from the lower part of the conical section rises into the internal vortex. From the comparison of the gas flow fields it appears that the coarse grain has minimal effect in the flow behavior.

In order to have a quantitative measure of the impact of the NPG value on the fundamental macroscopic proprieties of cyclonic flow, the overall pressure drop and the length of the internal vortex cone were evaluated (Figure 4).

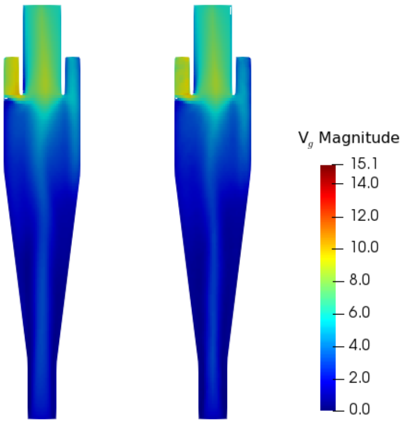


Figure 3 - Comparison of the velocity magnitude at u_{in} = 10 m/s and ε = 0.2%. for NPG 1 (left) and 8 (right).

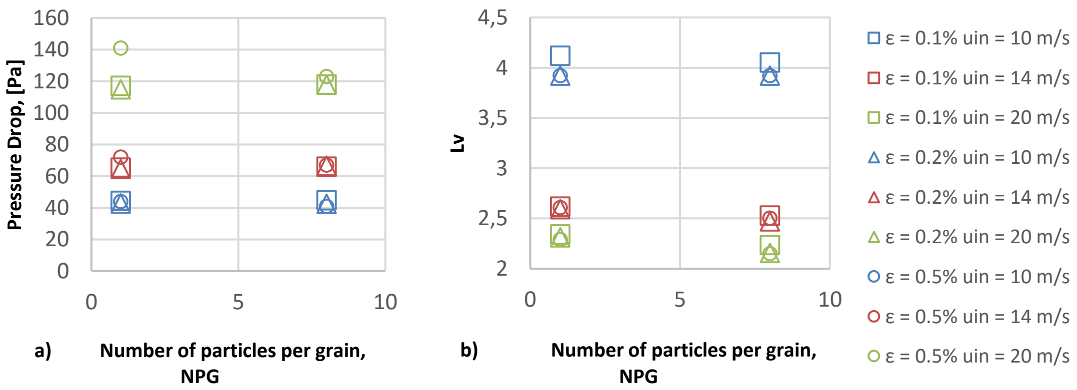


Figure 4 - Pressure drop (a) and vortex length (L_v) (b) vs. NPG for solids volume loadings (ε) for gas velocities (u_{in}).

The dependence of the overall pressure on the coarse graining degree (NPG) is depicted in **Errore. L'origine riferimento non è stata trovata.**a. It shows a correlation with the inlet velocity, while the influence of the solids

loading manifests only at the highest value. The increase of NPG value does not reveal a significant effect at the overall pressure, with variations limited to within 10% maximum.
The vortex length represents maximum vertical extension of the iso-surface with zero axial velocity. This surface initiating from the vortex finder until it develops down following the cyclone shape, closing on itself. Such length measure is divided by the barrel diameter to have a dimensionless variable indicated as Lv. This variable is related to the inlet velocity, but has not influence of the solids. Consequently, the coarse grain introduced variations limited to within 7%. A particular case has been observed for the lowest velocity, where the inner vortex often reaches the bottom exit, making its length not well defined.

4.3 Solid Flow and Efficiency

In all the cases explored, the solid phase presents its typical motion field descending / rolling on the walls of the cyclone and reach the bottom outlet. At high loadings, the classic "strips" of solids appear descending along the walls. As expected, only a small fraction of the particles avoids the correct separation, being entrained by the gas flow and escaping from the vortex finder, eventually causing a small but measurable loss of efficiency.
To better understood the solids load role on the cyclone separation process efficiency it was evaluated the system at a fixed particle velocity (u_{in} = 20 m / s) and with solids load increments (ε = 0.1, 0.2, 0.5%) after 1 s of simulation (Figure 5). From the observation of the instantaneous positions of the particles it is possible to appreciate how much the degree of coarse grain affects the results.

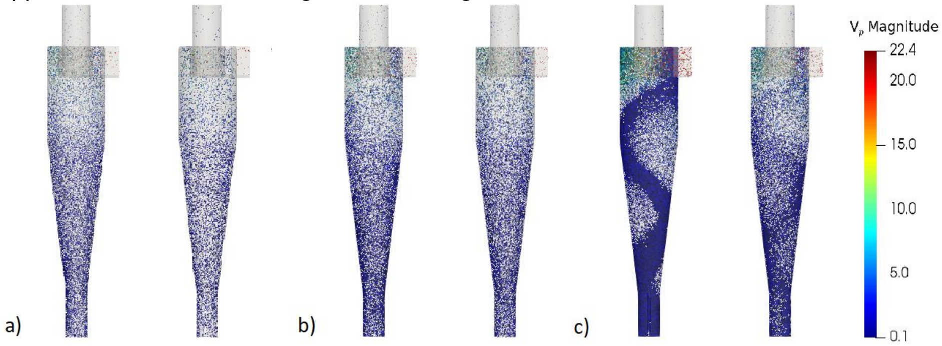


Figure 5 - Solid flow at time = 1 s, u_{in} = 20 m/s and ε = 0.1% (a), ε = 0.2% (b), and ε = 0.5% (c). For every ε, NPG takes the values 1 and 8 from left to right, respectively.

In fact, although the particle size scales only by a factor of 2 by increasing the NPG from 1 to 8, the description of the solid flow loses detail. This is readily apparent for the case at ε = 0.5%, where the descending solid strips are evident for NPG = 1 but turn out to be somewhat diffused for NPG = 8 (Figure 5c).
Keeping in mind that this technique keeps constant the mass of the system, acting on dimension and number of simulated entities reducing about 717 k (NPG = 1) to 94 k (NPG = 8) probable causing the discrepancies.
To quantify the effect of the addition of the coarse-grained technique on the solid flow, the separation efficiency was evaluated (Figure 6). This parameter is chosen as a macroscopic variable capable of defining cyclonic behavior. Its represents the ratio between the outlet and inlet solids flow rate, being calculated as the average of the last 0.3 s of the simulation.
It is apparent that NPG produces a limited effect on the overall efficiency, implying that the discrepancies are caused by the scattering of the occasional passage of particles (or grains).

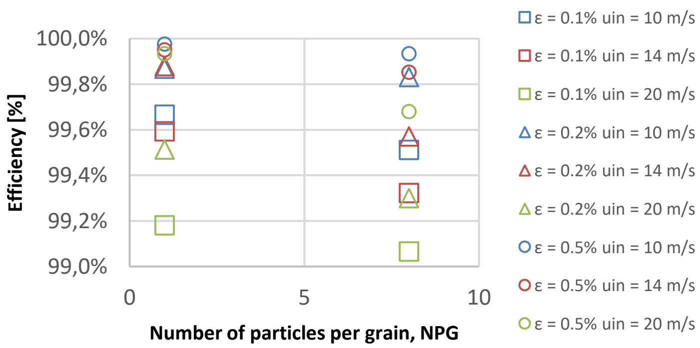


Figure 6 - Efficiency vs. coarse graining degrees (NPG) for different inlet velocities (u_{in}) and solids loadings (ε).

5. Conclusions

The use of DEM-CFD models to perform cyclone simulation in the most common industrial applications is impractical due to the huge number of particles involved and the small-time step required. In this work, the CGM technique was utilized to simulate a small-scale Stairmand cyclone, to evaluate its ability to describe this type of system compared to conventional DEM-CFD.

The CGM allows computational gains of the order of six, even for NPG as low as 8 (grain size ratio = 2), with reasonable accuracy of the macroscopic variables at this scaling correlation.

Quantities such as overall pressure drop; internal vortex length and separation efficiency are marginally affected by the NPG values. However, focusing on the local solid motion, some differences appear, suggesting that possible deteriorations of the accuracy, even affecting macroscopic quantities, are plausible at higher coarse graining degrees. This implies that the significant advantage in terms of computational savings of the CGM has to be carefully assessed against its approximations.

The CGM appears as a useful resource to perform simulations of complex systems also with a strong computational saving. Unfortunately, the maximum degree of coarse grain that can be used until the discrepancies become too heavy depends on the system being considered. An useful good estimation parameter is the number of grains, it is indicated to avoid low number, while high NPG numbers should be more investigated. Considering the flow in cyclone separators, it is expected that the wall-grain interaction can have a positive impact on the simulation, for example by considering correctly scaled rolling friction. Downsizing of this type of mechanism within the coarse grain method is currently under development.

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