Development of a Solver for CFD-DEM Simulations of Suspensions Containing Arbitrarily Shaped Particles

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Abstract

This research focuses on the pivotal role of suspension flow and its rheological properties in diverse scientific and industrial applications, such as blood cell flow, pneumatic transport, fluidized beds, and catalytic material coating on porous substrates. The study aims to develop a numerical approach using computational fluid dynamics and the discrete element method (CFD-DEM) to investigate suspension behavior under different conditions. A hybrid fictitious domain-immersed boundary method is employed to account for the solid phase, with a unique virtual mesh method designed to enhance contact precision while minimizing computational costs. The developed solver is validated through a suspension rheology case study and applied to simulate the washcoating of a catalytic material into a porous substrate. To comprehensively understand particulate suspensions at the microscopic level, the CFD-DEM model is extended to include interactions between individual particles, considering van der Waals forces, electrostatic interactions, and short-range repulsive forces. The resulting extended CFD-DEM model, accommodating arbitrarily shaped particles and intricate microscopic interactions, offers a comprehensive framework for understanding suspension rheological properties.

**Keywords**: CFD-DEM, HFDIB, suspension rheology, OpenFOAM.

* 1. Introduction

Particle suspensions play vital roles in real-life and industrial processes, such as sediment transport, blood cell motion, fluidized beds, and catalytic coating of porous substrates. Numerous experimental and numerical efforts have been dedicated to understanding their behavior (Blazek et al., 2021). While the commonly used Eulerian-Eulerian approach is computationally efficient, it lacks the ability to capture local fluid-solid interactions and relies on empirical parameters. To address this, the computational fluid dynamics (CFD) coupled with the discrete element method (DEM) in a CFD-DEM approach offers a first-principles-based simulation of suspensions (Sourek and Isoz, 2021).

This paper employs an in-house developed solver based on the hybrid fictitious domain-immersed boundary (HFDIB) method and a level-set-like DEM to study suspension flows. Simulations explore rheological properties with variations in solid phase volume fraction and particle shape. The setup is validated through viscosity estimation for spherical particle suspensions, followed by investigations into non-spherical particles, where experimental data by Mueller et al. (2011) is used for comparison. The solver is also applied to simulate suspension flow through a porous medium, illustrating its potential for studying processes like the washcoating process. Finally, we extended the CFD-DEM model to account for electrostatic interactions between individual particles, providing a more comprehensive understanding of suspension behavior at the microscopic level. This extension enhances the model's accuracy by incorporating additional forces such as van der Waals forces and short-range repulsive forces, bridging the gap between macroscopic rheological properties and microscale phenomena.

* 1. HFDIB method

At each time step (t), the solid phase distribution is introduced into the computational domain using a discrete indicator function λ, defined as follows:

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| --- | --- |
| $$λ=\left\{\begin{array}{c}0 in Ω\_{f}\\1 in Ω\_{s}\\\left(0, 1\right) in Γ\_{sf}\end{array}\right.$$ | (1) |

Here, $Ω\_{f}$ represents the portion of the computational domain $Ω$ occupied by the fluid,

$Ω\_{s}$ is the portion occupied by the solid phase, and $Γ\_{sf}$ is the fluid-solid interface. It's essential to note that this projection may not preserve the sharp edges of particles. The governing equations for the considered flow are based on the standard variant of laminar Navier-Stokes equations for an incompressible Newtonian fluid, including an additional forcing term $s$:

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| --- | --- |
| $$\frac{∂u}{∂t}+∇∙\left(u⊗u\right)-∇∙\left(ν∇u\right)=-∇\tilde{p}+g+s$$$$∇∙u=0$$ | (2) |

Here, $u$ is the fluid velocity, $ν$ is the kinematic viscosity, $\tilde{p}$ is the kinematic pressure, $g$ is the gravitational acceleration, and $s$ is the forcing term constructed to generate a fictitious representation of the solid phase in the computational domain. This modeling approach is commonly known as the hybrid fictitious domain-immersed boundary method, building upon the works of Blais et al. (2016) and Municchi et al. (2017).

* 1. DEM method

The Discrete Element Method (DEM) serves as a finite difference numerical technique for predicting the motion of independently moving objects within the Lagrangian framework, treating each solid body individually. At any given time $t$, the position and angular velocity of each body are described by Newton's second law of motion:

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| --- | --- |
| $$m\_{i}\frac{d^{2}x\_{i}}{dt^{2}}=\sum\_{j=1}^{N}f\_{i}^{j}, I\_{i}\frac{dω\_{i}}{dt}=\sum\_{j=1}^{N}t\_{i}^{j}$$ | (3) |

Here, $m\_{i}$ is the mass of body $i$, $x\_{i}$ is its centroid position at time $t$, $ω\_{i}$ is the angular velocity, $I\_{i}$ and is the matrix of inertial moments. The sums on the right-hand sides encompass all the forces $f$ and torques $t$ acting on body $i$, respectively.

These equations are numerically solved using the finite difference method, assuming constant translational ($a\_{i}$) and angular ($α\_{i}$) accelerations during each time step. Subsequently, $a\_{i} $and $α\_{i}$ are employed to calculate incremental changes in the position and rotation of body $i$.

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| --- | --- |
| $$a\_{i}=\frac{1}{m\_{i}}\sum\_{j=1}^{N}f\_{i}^{j}, α\_{i}=I\_{i}^{-1}\sum\_{j=1}^{N}t\_{i}^{j}$$ | (4) |

For a more in-depth understanding of the DEM implementation, readers are directed to Sourek and Isoz (2021). It is crucial to note that our solver accommodates arbitrarily-shaped particles, allowing for the exploration of particle shape effects on the flow. A comprehensive description of the DEM extension for arbitrarily-shaped solids can be found in Studenik et al. (2022).

* 1. Simulation results

In our study, we concentrated on simulating the measurement of suspension viscosity, utilizing a computational domain designed to emulate rheometric equipment. The domain comprises a three-dimensional box with two parallel solid plates. In the absence of solid particles, the simulation setup mimics laminar Couette flow. Consequently, we defined a linear velocity profile as an initial condition to facilitate the development of the final velocity profile within the domain. The viscosity estimation itself is based on Newton's law of viscosity:

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| --- | --- |
| $$τ=ν\frac{du}{dz}$$ | (5) |

here, $τ$ represents shear stress and $\frac{du}{dz}$ is shear rate. The shear stress acting on the moving wall is obtained using the wallShearStress postprocessing function in OpenFOAM. The suspension composed of spherical particles was specifically chosen for validation purposes. The obtained results were rigorously compared not only against available experimental data but also against widely utilized correlations, specifically Batchelor's (1977), and Krieger's and Dougherty's correlations (1959).

Figure 1: Results of the viscosity study for suspensions made of spherical particles. Trinagles represents experimental data, squares simulation data, dashed line stands for Batchelor´s correlation and dashed-dotted line for correlation by Krieger and Dougherty

In addition to simulating a suspension containing spherical particles, we delved into exploring the influence of particle shape on the apparent viscosity of the suspension. To ensure comparability between our findings and experimental data, we selected particle shapes based on the work of Mueller et al. (2011). This strategic choice allows for a meaningful comparison between the outcomes of our simulations and the corresponding experimental observations.

Figure 2: Results for suspensions made of glitter and rod shaped particles. Crosses represents experimental data for rod particles and circles results of the simulations. Triangles stand for experimental data for glitter particles and squares represents results of the corresponding simulations.

The results obtained for suspensions composed of spherical particles exhibit a commendable agreement with both the available experimental data and widely employed correlations. Notably, it is important to highlight that these correlations are typically valid up to a volume fraction of 0.2. However, our simulations extend this scope, showing consistent agreement with experimental data even at higher volume fractions, specifically up to 0.4. The observed consistency between our numerical estimates and existing data underscores the applicability of our method for conducting numerical investigations on suspensions containing arbitrarily-shaped particles—an area often reliant on experimental approaches.

To demonstrate our solver's real-world applicability, we numerically studied the washcoating process—a crucial step in depositing catalytic material within the porous walls of automotive exhaust gas filters. Following the experimental work by Blazek et al. (2021), we simulated the deposition of catalyst in two different filter sections. Utilizing our CFD-DEM solver, we recreated the washcoating process involving a water-based slurry.



Figure 3: Comparison of the washcoating simulations (a,b,d,e) to the experimental data (c,f) for two different sections of the filter wall: a section with a large pore on (a,b,c) and a closed structure (d,e,f). Color code for the numerical results: grey = wall, red = catalyst. Color code for the experimental data: white = wall, black = void space, grey = catalyst.

The results presented in Fig. 7 offer a qualitative comparison between simulated and experimentally obtained distributions of catalytic particles. Fig. 7a and Fig. 7d provide an overall view of the resulting distributions for structures with a large open pore and a closed structure, respectively. Further insight is gained from a single slice through the structure in Fig. 7b, c and Fig. 7e, f, respectively.

Comparing images (b) and (e) in Fig. 7 highlights the impact of different filter wall morphologies on the final coating distribution. In the section with a large pore, the catalytic material is primarily deposited inside the wall, whereas, in the relatively closed section, the coating is concentrated predominantly on the wall. This observed trend aligns with experimental observations shown in Fig. 7c and Fig. 7f. However, it is noteworthy that a notable difference exists in the spatial arrangement of particles between the simulation and the real sample, with particles in the real sample appearing much more closely packed.

To address this discrepancy, we are incorporating an electrostatic force into our model. This addition aims to simulate the particle interactions more realistically, accounting for the increased proximity observed in the real sample. This enhancement in the model should contribute to more accurate predictions in future washcoating simulations.

* 1. Conclusions

In conclusion, our study showcases the CFD-DEM solver's versatility in simulating complex particulate suspension behaviors, as demonstrated through successful washcoating process simulations. The qualitative agreement with experiments supports its potential for understanding irregularly-shaped particle systems. Extending simulations beyond typical limits and introducing an electrostatic force enhance the solver's robustness.

Our work establishes a foundation for advancing numerical investigations in suspension dynamics, particularly in applications like the washcoating process. The CFD-DEM solver offers a valuable tool for optimizing particulate processes in diverse industrial and scientific contexts.

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