A Novel HGD-CFD Framework for Efficient Simulation of Granular Flow Dynamics

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Abstract

Computational modelling of granular flows is vital for optimising and controlling material handling in the alumina industry. Moreover, understanding how particle size distributions evolve over time provides key insights for enhancing process performance. However, existing discrete particle methods are limited by the number of particles that can be simulated. To address this gap, we introduce a novel numerical method that couples the stochastic Heterarchical Granular Dynamics (HGD) model with Computational Fluid Dynamics (CFD). The HGD component tracks the particles and their interactions, while the CFD component models the fluid flow. Coupling the two components allows to capture particle-fluid interactions. This coupled approach overcomes the computational limitations of traditional discrete particle methods while accurately tracking the population of particle sizes in space and time. Validation against benchmark cases demonstrates the method's effectiveness in capturing the dynamic behaviour of granular flows in fluids, offering a promising tool for advancing process design and optimisation.

Keywords: Granular flow, Size distribution evolution, Computational fluid dynamics.

1. Introduction

Bulk solids handling is a common and persistent challenge in alumina operations. Irregular discharge from storage silos often causes variations in particle size, which leads to uneven feed quality and affects downstream processing [1]. For example, size segregation in precipitators can produce slurries that are either too fine to filter efficiently or too coarse to dissolve properly in the smelter. When flow problems occur, operators often rely on basic measures, such as hitting equipment, using aeration without a clear strategy, or lowering conveyor speeds, to keep things moving, even if it reduces productivity. Even short periods of unplanned downtime in alumina refining can result in significant financial losses and reduced energy efficiency in the smelter. As a result, plant managers demand tools that reduce guesswork, improve consistency, and help make better use of the equipment they already have.

In practice, engineers often rely on two main types of models:

- **Continuum models** use empirical formulas or simplified equations, such as the Beverloo equation for discharge or the Ergun equation for pressure drop. Some advanced versions apply probability balance equations to describe bulk flow behaviour. These models are fast and convenient but overlook important details like changes in particle size, buildup on equipment walls, or shifting flow regimes. As a result, they struggle to predict how a small change in particle size distribution (PSD) will affect mass flow or stability [2].

- **Particle-based models** simulate every particle and its interactions with others and with walls. This approach captures fine-scale physics but is extremely computationally intensive. Simulating large-scale industrial systems with these methods often requires significant computational resources and time. To reduce this burden, engineers sometimes simplify the problem setup, but such approximations can eliminate the very size effects that are critical to the process [3].

The objective of this paper is to present the developed HGD-CFD framework and validate its accuracy and robustness using two lab-scale scenarios. The validation results aim to establish confidence in the framework as a reliable and efficient tool for simulating granular flow dynamics in fluid environments.

2. A Middle Path: The Novel HGD-CFD Framework

To bridge the gap between overly simple models and overly detailed ones, we introduce a new simulation approach called the heterarchical granular dynamics/computational fluid dynamics (HGD-CFD) framework. This method, further developed from the original HGD formulation [4], combines fluid simulation with a stochastic model of particle movement, offering a balance between speed and accuracy. The approach is built on two main ideas:

- **Probabilistic particle transport on a grid:** Instead of tracking every particle, the HGD model divides the domain into grid cells. Within each cell, particles are treated as groups that move based on stochastic rules informed by kinetic theory. Each cell keeps track of key information like how much solid is present, the average particle size, and how much size variation there is.
- **Coupled fluid-solid interaction:** A CFD solver calculates the fluid forces, such as drag, buoyancy, and lift, acting on each cell. These forces influence particle motion, and, in return, the moving solids affect the fluid flow. This two-way exchange captures important effects like how particles expand when flowing or how fluid helps promote flow.

The result is a solver that runs much faster than particle-based models while still capturing accuracy at the outlet level. A typical alumina silo may contain on the order of 10^{17} particles, which is far beyond the limits of discrete simulations, where current high-performance computing resources typically allow simulations of up to 10^7–10^9 particles. In contrast, the HGD-CFD framework can simulate a full 1000 t silo overnight (8–10 hours) on a standard 32-core workstation, delivering next-morning results that support real-time decision-making in plant operations. This corresponds to approximately 10^{17} particles, depending on particle size, which is several orders of magnitude beyond the practical limits of Discrete Element Method (DEM) -based models.

2.1 Delivering Value in Alumina Flow Management

The developed model offers practical value across several aspects of alumina flow management, including improving flow consistency, supporting product quality, and guiding infrastructure decisions.

- **Reducing discharge variability:** At the refinery, small variations in feed rate to the calciner were known to impact downstream process stability and overall efficiency, including fuel consumption and product quality consistency. Our developed model was used to explore how different aeration ring placements might influence flow variability, supporting decision-making for potential operational improvements.
- **Improving smelter product quality:** Fluctuations in particle size distribution can influence smelter chemistry and energy efficiency. Our developed model was used to simulate particle transport through precipitation tanks and silos, helping to understand

how PSD evolves over time. These insights can support better control strategies that reduce variability in the material reaching the smelter and contribute to more consistent process performance. For example, if the model predicts fines segregation during discharge, operators may adjust the drawdown rate or sequence the discharge from multiple silos to improve blending.

- **Delaying capital spending:** Silo blockages and pipeline choking can limit throughput and lead to expensive upgrades. Our developed model can be used to explore whether design changes such as adjusting the cone angle or adding internal inserts could improve flow reliability. In addition, if coupled with online data, the model could support real-time operational decisions. For example, if the simulation indicates a developing risk of blockage due to fines accumulation, operators could respond by adjusting the discharge rate, altering the sequence of silo usage, or temporarily reducing feed to downstream equipment to relieve buildup. By identifying and responding to these issues early, operators may be able to maintain stable flow, extend the life of existing infrastructure, and delay major capital investments.

Together, these examples show how the model can provide useful insights into complex flow behaviour across alumina storage and handling systems. While not a replacement for plant trials or detailed particle simulations, it offers a practical tool to support operational decision-making, reduce uncertainty, and explore low-cost improvements before committing to physical changes.

2.2 HGD-CFD Framework Design and Coupling Strategy

Building on the concepts introduced earlier, this section outlines the implementation of our HGD-CFD framework and its role in simulating coupled fluid-particle systems. Rather than tracking each particle individually, the model represents local particle behaviour statistically within a discretised grid, allowing for efficient simulation of large-scale granular flows. The CFD and HGD components exchange information at every time step, ensuring momentum consistency and capturing key interactions between the fluid and solid phases. A schematic representation of this two-way coupling mechanism is shown in Figure 1, highlighting the iterative data exchange between the fluid and particle modules.

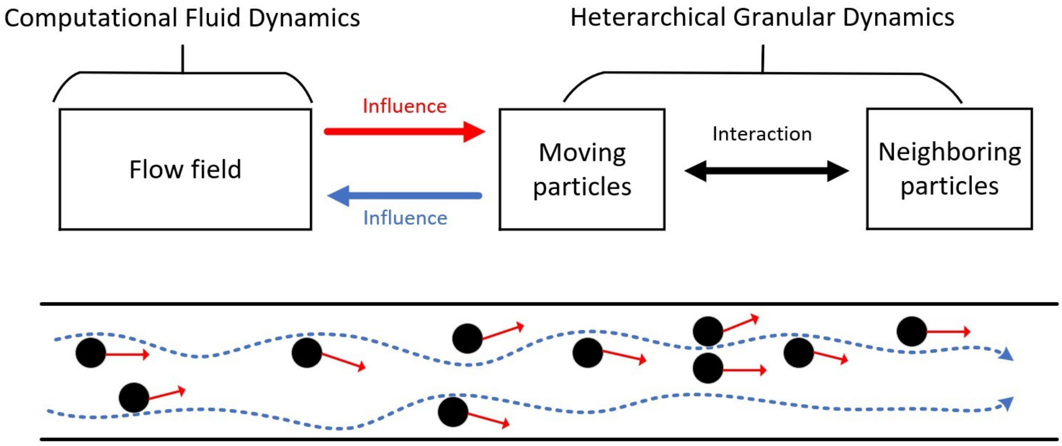

Figure 1. Schematic representation of the two-way coupling framework.

The model captures several important physical phenomena that govern granular flow in fluid environments:

- **Interphase drag:** Accounts for the resistance between the fluid and moving particles, central to momentum exchange.

- **Particle inertia:** Enables the framework to represent delayed particle response and acceleration under fluid forces.
- **Size segregation:** Models how particles of different sizes separate during transport or discharge.
- **Diffusion:** Captures particle spreading due to local concentration gradients and stochastic effects.

This approach enables rapid and robust simulations that retain essential physical detail while remaining computationally tractable, making it well-suited for analysing complex flow behaviour in industrial systems.

3. Benchmark Validation

This section presents two validation tests designed to confirm the accuracy of the HGD-CFD model under controlled conditions. The first test verifies fundamental force balance in a single-particle settling scenario, while the second assesses the model's ability to reproduce size segregation in dense suspension discharge, using a lab-scale experiment as a reference.

The first benchmark test validates the correct implementation of fluid-solid coupling in the model, particularly the balance between gravity, buoyancy, and drag forces acting on a particle settling in a stationary fluid. Figure 2 illustrates the physical forces involved.

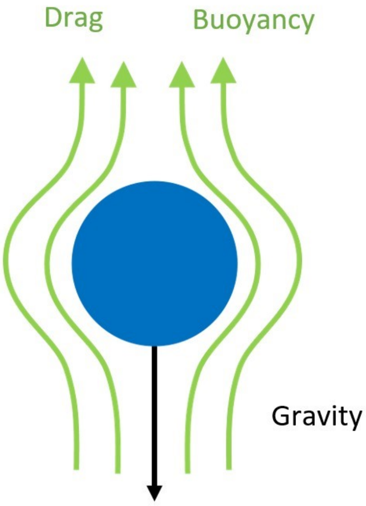

Figure 2. Schematic of the forces acting on a settling particle in a quiescent fluid: gravitational force (F_g), buoyancy force (F_b), and drag force (F_d).

In the simulation, a single particle is released into a stationary fluid and allowed to settle under gravity. The goal is to confirm that the model accurately captures how the particle slows down and reaches a steady speed due to the opposing effects of buoyancy and drag forces. The computational domain is tall enough to let the particle settle naturally without interference from the boundaries, no-slip boundary conditions are applied at the side and bottom walls to represent solid confinement, while an open boundary is applied at the top to allow fluid displacement and prevent artificial pressure buildup.

To further evaluate the model, we simulated the discharge of a bi-dispersed alumina mixture from a lab-scale silo setup. The experimental configuration, illustrated in Figure 3, consists of a quasi-two-dimensional (2D) cell filled with a homogeneous mixture of alumina particles of two distinct sizes: 150 μm and 53 μm, submerged in propanol. The cell is 8 cm wide with a fill height of 5 cm above the outlet and is constructed from transparent plates with a narrow internal gap to allow visualisation of the flow. To replicate the flow conditions and particle-fluid interaction regimes observed in full-scale silos operating in air, the experiment uses propanol as the interstitial fluid. This choice allows the laboratory system to match the Stokes number of industrial-scale flows, ensuring that the dominant balance of drag, inertia, and buoyancy is similar despite the difference in physical scale.

The particles are initially well mixed to ensure a uniform starting condition. This validation focuses on the model's ability to capture key features of dense suspension flows, including particle-fluid momentum exchange and the size segregation effects that often arise during discharge. The corresponding simulation was conducted under identical conditions using the HGD-CFD model.

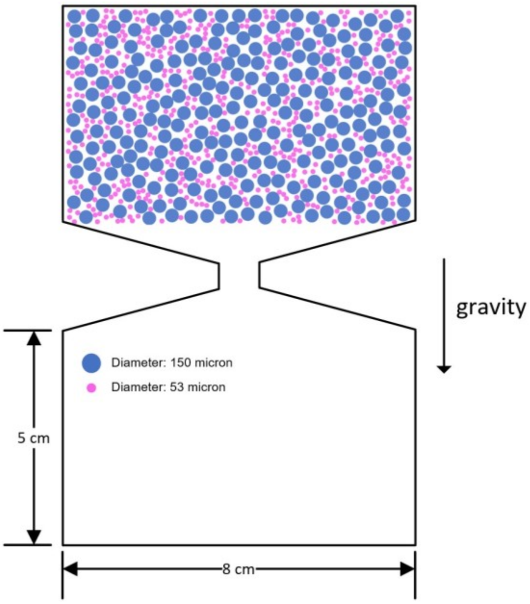

Figure 3. Schematic of the experimental setup and forces acting on particles in a bi-dispersed alumina suspension undergoing hourglass discharge.

3.1 Single Particle Settling in Quiescent Fluid

Figure 4 compares the particle settling velocity over time for three particle diameters (0.1, 0.5, and 1 mm), showing results from both the analytical solution and the HGD-CFD simulation. The model accurately reproduces the expected exponential decay in particle velocity as drag and buoyancy counteract gravity. In all cases, the simulated velocity closely follows the analytical curve, confirming that the fluid-solid coupling is correctly implemented across a range of particle sizes. The good agreement, particularly at low Reynolds numbers, demonstrates that the model captures the transient and terminal settling behaviour consistent with Stokes flow conditions.

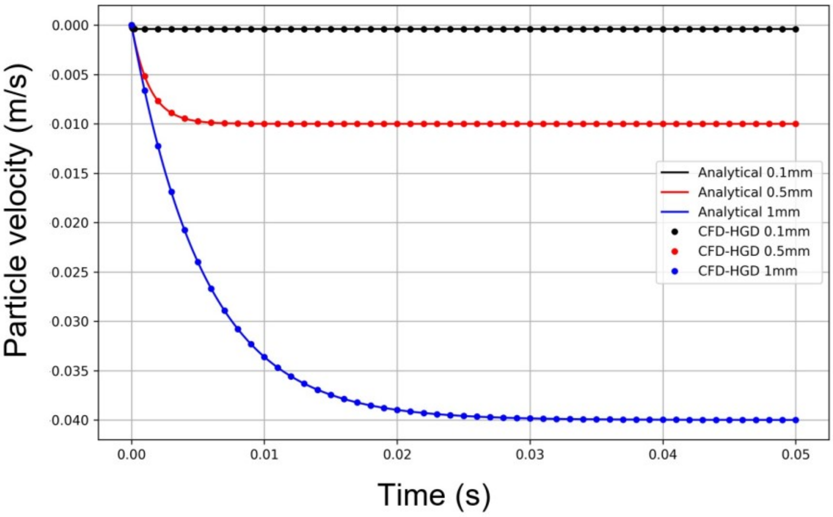

Figure 4. Validation of the drag and buoyancy implementation by comparing the simulated settling velocity of a single particle with Stokes' analytical solution.

3.2 Bi-Dispersed Particle Discharge from a Lab-Scale Silo

Figure 5 presents a comparison between experimental observations and simulation results at different discharge times. The simulation successfully reproduces key flow features observed in the experiment, including the formation of a central pile enriched with coarse particles and the lateral accumulation of fine particles near the side walls. It also captures the upward transport of fine particles into suspension, driven by fluid drag, highlighting the model's ability to resolve coupled fluid-particle dynamics.

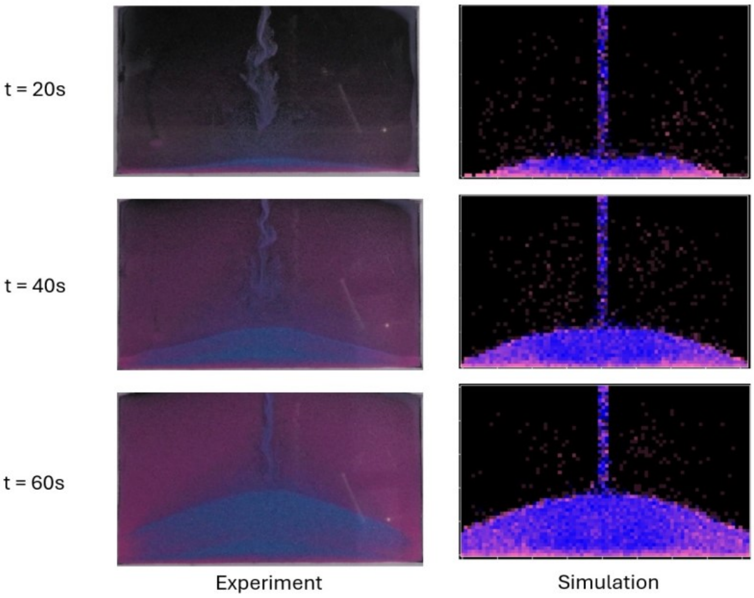

Figure 5. Comparison between experimental observations and simulation results of bi-dispersed particle discharge in propanol at different times (t = 20 s, 40 s, and 60 s).

These validation cases demonstrate that the proposed HGD-CFD framework can accurately reproduce both simple and complex fluid-particle interactions. The agreement with analytical and experimental benchmarks confirms the reliability of the model and its suitability for studying dense granular suspensions in fluid environments. The insights gained here provide a foundation for more advanced simulations and practical applications for industrial-scale scenarios.

4. Conclusion

This study introduces and validates a coupled HGD-CFD framework for simulating granular flows in fluid environments, with a particular focus on scenarios relevant to alumina storage and handling. The model captures key interphase interactions, including drag and buoyancy, while avoiding the computational demands of fully particle resolved simulations.

Two validation cases were presented to build confidence in the model's implementation. The first involved a single particle settling under gravity, confirming the correct treatment of basic fluid-solid coupling in a low Reynolds-number regime. The second used a lab-scale silo filled with a bi-dispersed particle mixture to test the model's ability to reproduce complex behaviours such as segregation and fluid-assisted particle transport in dense suspensions.

Although this work is limited to lab-scale validation, the results suggest that the framework has strong potential to support industrial decision-making. For example, it may be used to evaluate how design changes influence flow consistency, assess the impact of particle size distribution on discharge behaviour, or test operational strategies before implementation. Its computational efficiency makes it suitable for running large parameter sweeps or exploring multiple scenarios rapidly, providing engineers with actionable insights without the need for costly or time-consuming trials.

Future developments may extend the model's capabilities to include additional physics such as frictional rheology, particle breakage, or cohesive forces. Moreover, as the current validation is limited to lab-scale scenarios, future work will focus on demonstrating the model's performance in full-scale industrial systems. This would further enhance its value as a practical simulation tool for optimising granular material processing in real plant environments.

5. References

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