Studying Alumina Flow Using DEM Numerical Simulation

Vanderlei Gusberti[1], Dagoberto Schubert Severo[2] and Jean Carlos Pardo[3]
1. PhD, Engineer, CAETE Engenharia Ltda, Porto Alegre, RS, Brazil
2. Director, CAETE Engenharia Ltda, Porto Alegre, RS, Brazil
3. Manager, CBA Companhia Brasileira de Aluminio, Aluminio, SP, Brazil
Corresponding author: vanderlei@caetebr.com

Abstract

A Discrete Element Method (DEM) model was developed by CAETE Engenharia in order to help understand and predict alumina flow. The DEM model is the adequate approach in order to simulate granular flows such as alumina. The simulation technique consists in a transient simulation which tracks the trajectory of the particles inside the studied system. It needs an intensive computational power to be performed. The numerical model was tested and validated by simulating the ISO902 angle of repose experiment of alumina.

Alumina flow DEM simulation can be quite useful to improve a variety of processes in the aluminium smelters. Some application examples are alumina silo's feeding, silo's discharge, cell alumina feeding and point feeding design improvement studies. In the alumina refinery, many other applications can also be found related to bauxite and alumina flows.

In this work, the DEM modelling was used to help the design improvement of a Søderberg point feeding system. CBA is in the process of installing point feeders in their Søderberg cells. For this purpose, a feeding chute was designed to receive the alumina from the hopper and to direct it to the anode gas skirt, close to the pneumatic crust breaker. In the initial design, the identified issue was the feeding hole being closed by the alumina. It was discovered that the feed chute was not feeding the alumina into the hole opened by the breaker, dropping the alumina in a wrong place instead. Then, an optimized feed chute was proposed. The new design was built and tested with success.

Keywords: Alumina flow simulation, Alumina angle of repose, Aluminium reduction cell point feeder, Granular flow, Discrete Element Method (DEM) simulation.

1. Introduction

Granular material is a set of a large number of discrete solid particles interacting with each other. It simultaneously presents characteristics of both solid and fluid materials. It can flow similar to a fluid, and also it can withstand a certain level of shear stresses, forming piles or stacks. Granular flows are quite common in mining activities and smelting industry. Alumina and bauxite flows are examples of such flows, as presented in Figure 1.

Figure 1. Examples of granular materials. Left: iron ore. Right: bauxite.

The dynamic behaviour of granular material is very complex, including particle-particle and particle-wall interactions.

2. Discrete Element Method

The Discrete Element Method (DEM) is a type of numerical model suitable for analysing granular flows. The method is essentially transient, and the state is calculated at the end of each small time step. It aims to track the movement of all particles of the system, requiring highly intensive computational effort. The basis of DEM can be found in literature [1]. Recently, granular flow simulation research has rapidly evolved worldwide, accompanying the increase in computational power [2].

Contrary to the traditional CFD models that consider the flow as a continuum discretized in mesh points/volumes, the DEM model simulates the motion of each individual particle. Motion equations are solved for each of these particles in the domain. Collisions of particles are also evaluated in DEM as well as the capillary forces.

A particle present in a granular flow can have two types of motion: translational and rotational. At every time step, a force balance according to Newton's second law of motion is carried out for each particle, considering its interaction with the contacting particles and a fluid in the case of a particle-fluid coupled model. In fine particle systems, non-contact forces such as the van der Waals and electrostatic forces are relevant, and they should also be included. DEM simulations can provide a variety of dynamic information results, such as the trajectories, forces acting on individual particles, and final configuration of particle packs in repose.

The forces present in DEM simulations are showed in Figure 2, where i, j, and k are particles. $\mathbf{F}^{c}$ is the contact force, $\mathbf{F}^{nc}$ is the non-contact force (van der Waals/electrostatic), f^{n} is the normal component of the contact force, $\mathbf{f}^{t}$ is the tangential component of the contact force, $\mathbf{m}^{r}$ is torque from rolling friction, $\mathbf{m}^{t}$ is torque from tangential forces, $\mathbf{v}$ is translational velocity, ω is angular velocity, m is the mass of the particle, $\mathbf{g}$ is the gravitational acceleration and h is the distance between spheres.

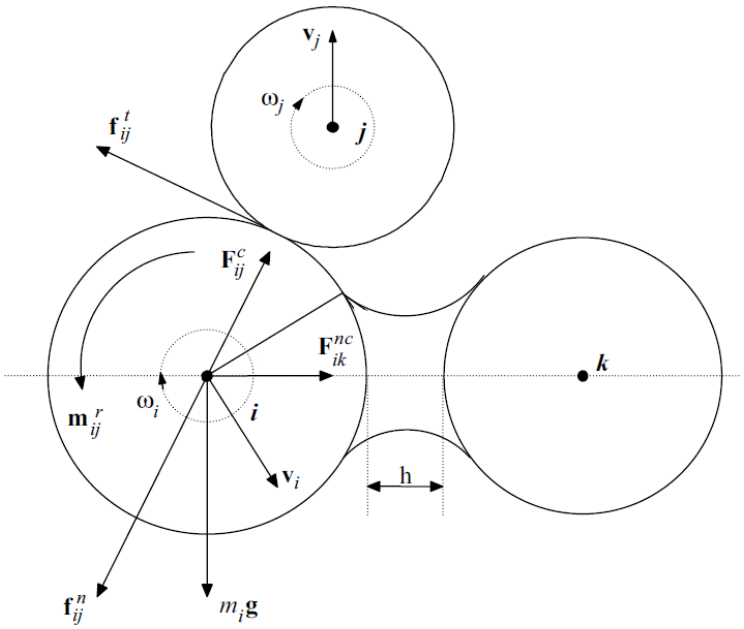

Figure 2. Possible acting forces on particles in a DEM simulation [3].

3. DEM Numerical Model of Alumina: Angle of Repose Experiment

The open-source code LIGGGHTS was chosen to perform the numerical DEM simulations. The most appropriate particulate contact model for this case according to its documentation is the Hertz contact model. More information can be found at the LIGGGHTS online resources [4].

The alumina properties necessary to run a Hertz DEM simulation are:

- Particle Young's modulus: $5x10^6$ Pa (usually lower than real Young's modulus to permit larger time steps, recommendations can be found in the literature [4]);
- Poisson ratio: 0.23;
- Restitution coefficient: 0.45;
- Friction coefficient (particle-particle): 0.625, obtained from a previous angle of repose experiment;
- Friction coefficient (particle-wall): 0.45, adjusted from experimental comparisons;
- "Coarse-graining": the diameter of particles are scaled to permit the result to be obtained in a reasonable timeframe.

The DEM simulation is computationally very intensive. A case where 500 000 particles are being inserted in the domain takes several days of calculation on an 8-processor core computer. In the case of alumina flow simulation in refinery equipment, the DEM method is only feasible if the particle is scaled because the alumina particles are quite small (diameters of 40–100 μm). Scaling particles in DEM means using larger particles where each one represents a set of smaller particles. In the DEM simulation literature, this process is called "coarse-graining" [6, 7]. In the Hertz model coarse-graining, the sum of forces and momentum is preserved. The simulation neglects only the small-scale particle-particle interactions (in the order of the real particle scale). This is considered a reasonable simplification for the study presented here.

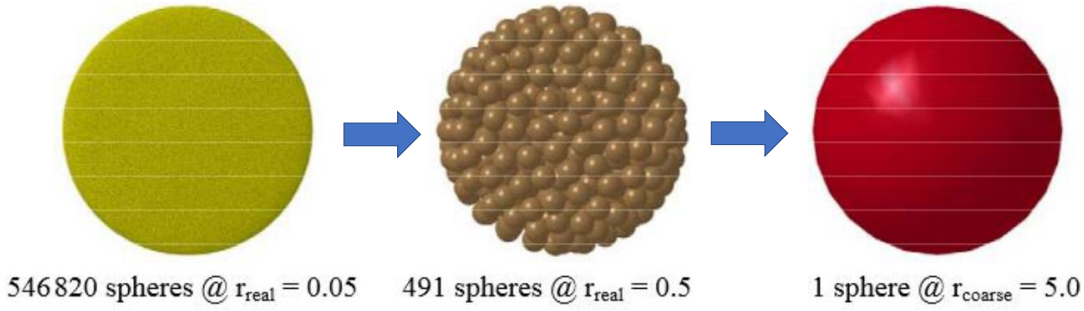

Figure 3. Coarse-graining procedure, sets of smaller particles represented by bigger particles without losing the macroscale physics.

At CAETE, the angle of repose essay was performed using alumina (Figure 4, right) according to the ISO902 standard. Afterwards, a DEM simulation was performed (Figure 4, left), and friction properties used in the simulation were adjusted in order to match with the experimental behavior.

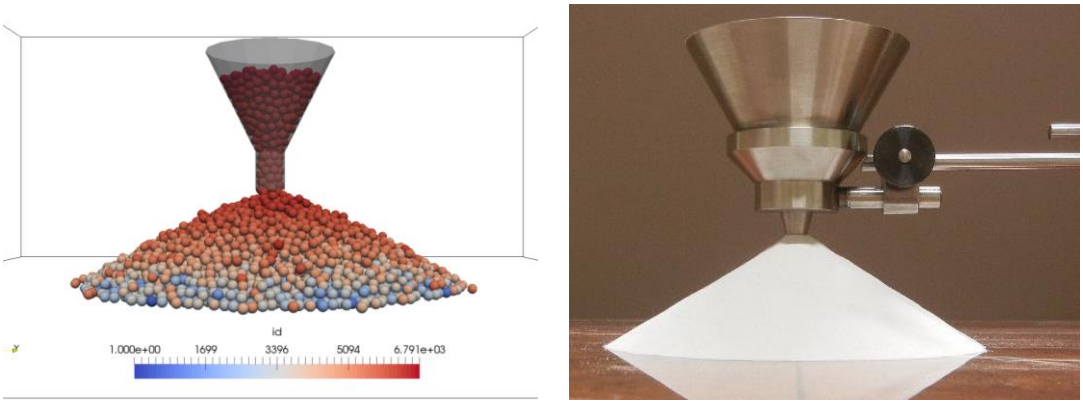

Figure 4. Left: DEM simulation of the angle of repose experiment. Right: ISO902 alumina angle of repose experiment.

4. Physical Scale Models of the Bottom Valve and DEM Simulations

The bottom valve study is another application case used for fine-tuning alumina flow parameters in the CAETE simulations, in addition to the previous ISO902 study. The bottom valve study can represent, for example, a conveyor belt system collecting alumina from the bottom of an alumina stack. At CAETE, a 1:20 physical scale model was built in order to compare the results with the predictions of DEM simulations for the same bottom valve case. In this experiment, a stack of alumina with the corresponding angle of repose was initially produced by the gravitational fall of material (Figure 5, left). The floor below the stack has a square gate. When the stacking was complete, this valve was released manually, and some of the alumina fell through it. It was then observed whether the final configuration of the alumina maintained the angle of repose or if the alumina was spread outwards the conic pile.

In Figure 5 (right), the shape of the final configuration of the alumina is shown after the gate valve was released.

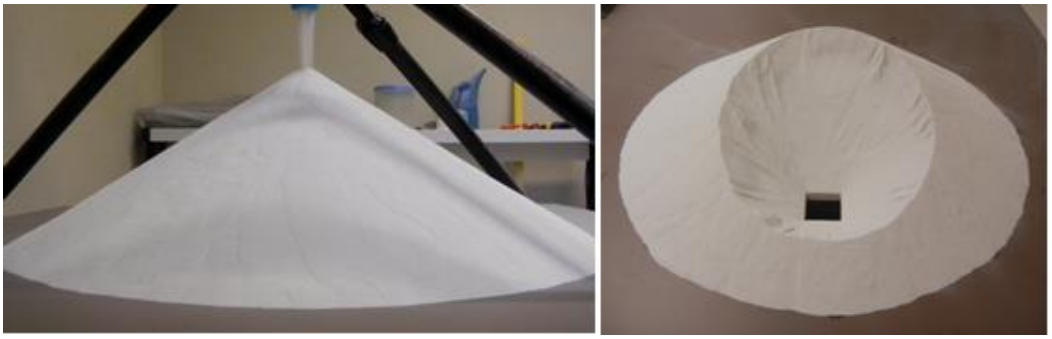

Figure 5. Left: Alumina being stacked at the angle of repose ~32°. Right: Aspect of alumina stack after the bottom valve was open.

In the experiments, it was observed that the repose angle is always maintained at the alumina stack, regardless of the position of the valve (central or lateral). The same results were obtained by DEM simulations as seen in Figure 6, where a DEM simulation is compared with the physical model.

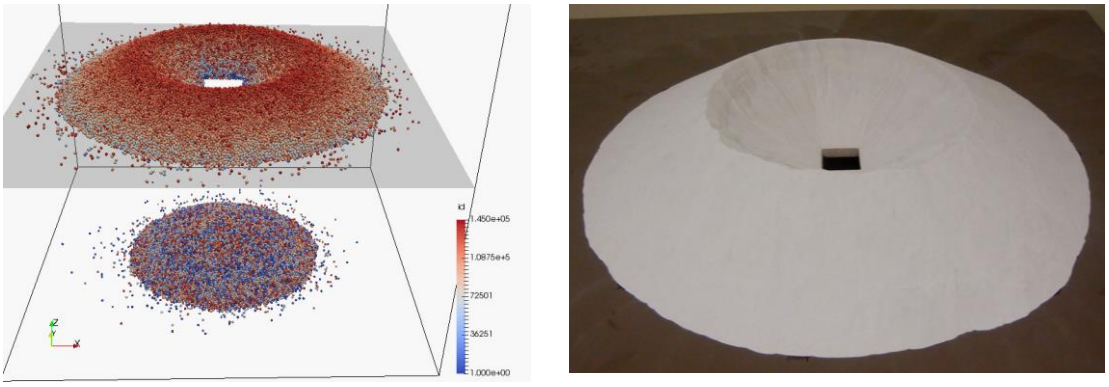

Figure 6. Comparison between DEM simulation and physical model. Final configuration of alumina pile, after bottom gate valve opening.

In DEM simulations, other situations can be easily tested without a real physical model, for example, the influence of multiple valves instead of a single valve as presented in Figure 7. The remaining alumina maintained the angle of repose again after releasing the two valves in the numerical experiment.

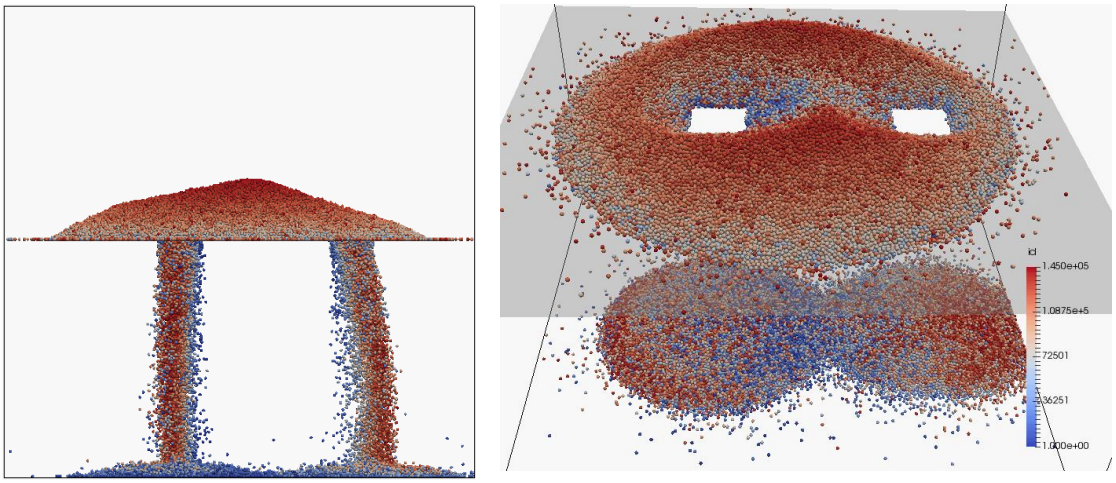

Figure 7. DEM simulation of 2 gate valves at the bottom of alumina pile.

Another aspect that can be studied in DEM simulations is the particle size segregation. It is possible to evaluate the distribution of the different particle sizes in the alumina stack in the DEM simulation. In Figure 8, the stacking of 3 different particle diameters is shown: the largest particles are represented in red (d = 10 mm), the mean particles (d = 6.5 mm) are represented in light blue, and the smallest particles (d = 4 mm) are represented in dark blue. Stacking is done by dropping the alumina from a certain height. In this simulation, there is a certain segregation of the larger particles towards the periphery of the pile. Also, the concentration of large particles is greater on the surface of the alumina stack.

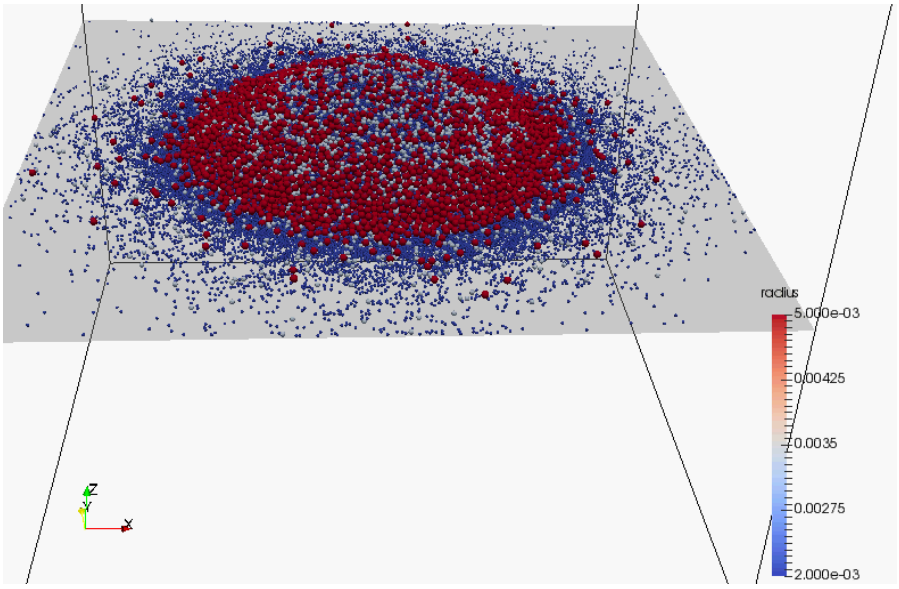

Figure 8. Model of a stacking with 3 different particle sizes.

In Figure 9, the configuration of the alumina stack is presented after opening the valve below the stack. The material collected by the valve appears to be quite homogeneous in terms of diameter, perhaps because the falling height below the valve is much smaller than the falling height of the initial pile formation.

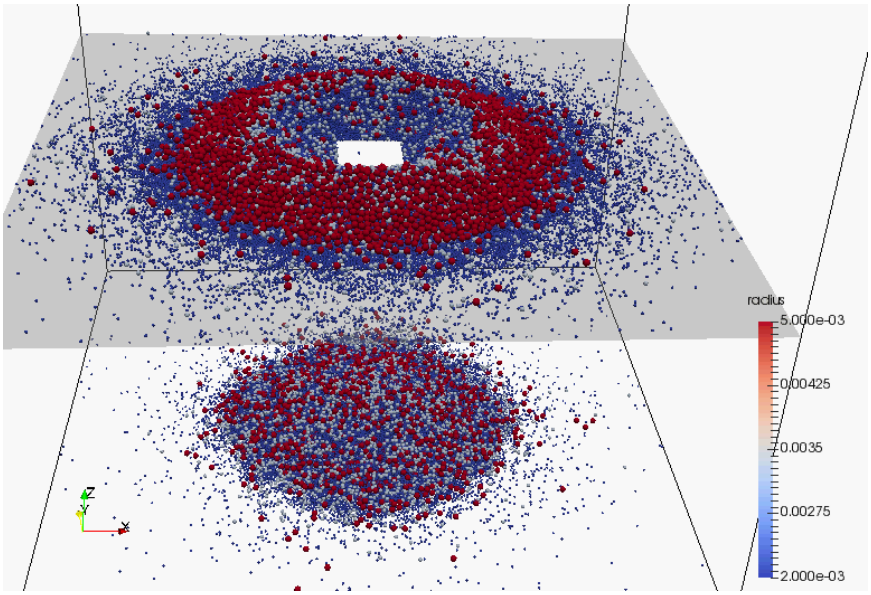

Figure 9. Model of silo discharge, with 3 different particle sizes.

5. Point Feeder Improvement at CBA

The CBA smelter (Companhia Brasileira de Alumínio) is retrofitting the Søderberg cells towards the "Green Søderberg" point feeding system [5]. The feeding improvement consists of replacing the sidewall side-break system by a new point-feeding system as shown in Figure 10. The point feeder provides a more continuous alumina addition, stabilizing the bath alumina concentration and bath chemistry over time. In addition, it also improves the environmental conditions of the potroom, avoiding a massive crust break that generates dust and liquid bath exposure.

Figure 10. Point feeder at CBA Søderberg cells, alumina duct, and feeding chute [5].

The DEM simulation method was used to improve the geometry and positioning of the alumina duct and the feeding chute of the point-feeder system (Figure 10). The initial project implemented by the smelter resulted in alumina accumulation on the crust and clogging problems. In the simulation, it was possible to identify the cause of the problem: alumina was falling from the chute outside the hole radius maintained by the breaker and accumulating on the top of the crust (Figure 11).

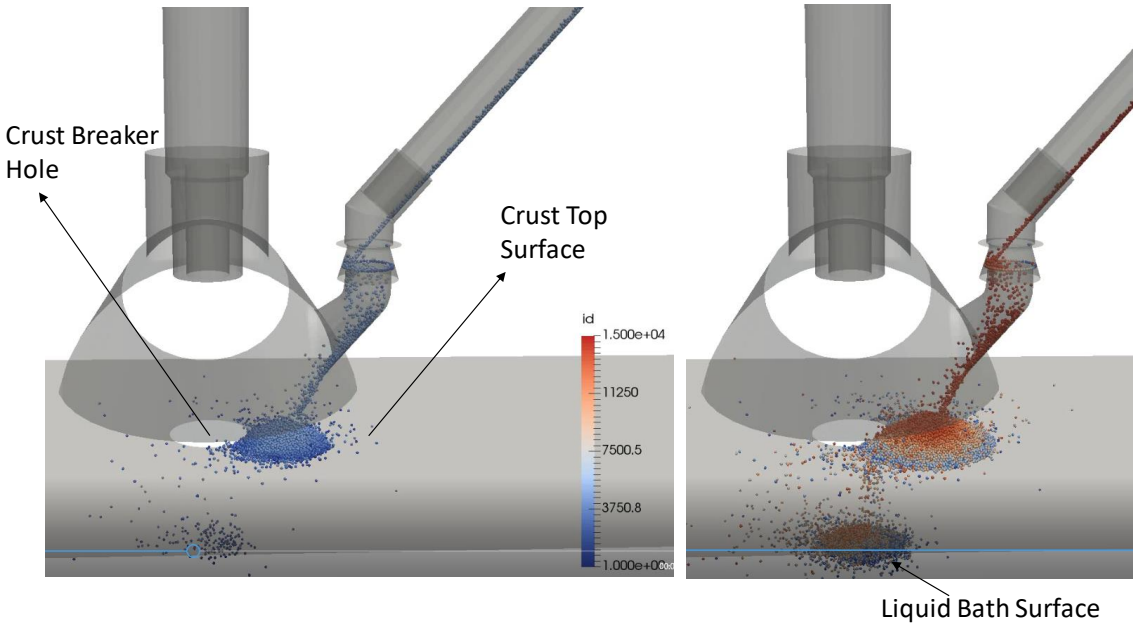

Figure 11. Point-feeder at CBA Soderberg cells, alumina duct and feeding chute (two sequential timeframes). Initial proposition.

Afterwards, the project was revised and a new geometry was proposed with the help of DEM simulations. In the revised case, a larger share of alumina falls directly onto the bath top while some minor share of alumina continues to fall outside the hole (Figure 12). The revised chute design is being implemented in all Green Søderberg cells at CBA, with reported success (Figure 13).

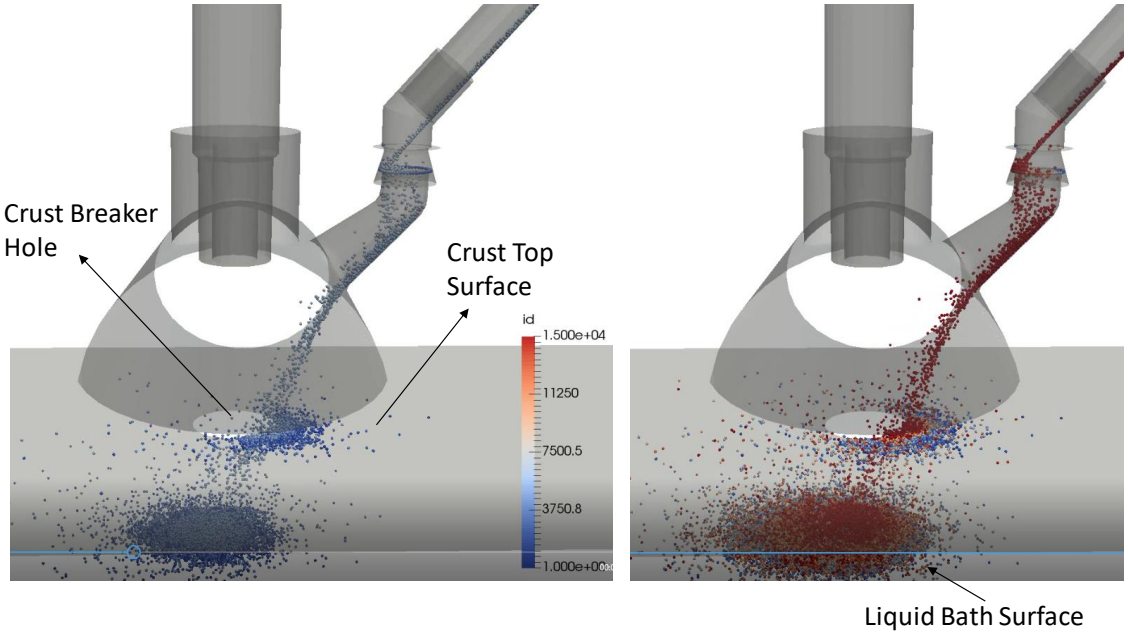

Figure 12. Point-feeder at CBA Soderberg cells, alumina duct and feeding chute (two sequential timeframes). Final revised configuration.

Figure 13. Final revised alumina chute implemented at CBA Soderberg cells.

6. Conclusions and Future Work

Both physical models and DEM simulations proved to be excellent tools to understand the granular flow present in many processes in aluminium production chain. Properties can be obtained from physical models and be used in DEM simulation. On the other hand, many tests can be done virtually via the simulation that otherwise would be difficult or practically impossible to test physically.

In this work, the alumina DEM modelling procedure was set up and validated against two physical experiments: the ISO902 angle of repose experiment and the bottom valve experiment. Physical properties of alumina such as restitution and friction coefficients were obtained in the validation process. In the bottom valve experiment, opening the valves at the bottom of the silo does not

cause the alumina to destabilize the repose angle. The position of the bottom valves is not relevant for the stack behaviour, neither the number of valves, according to the results of the DEM simulations.

The Green Søderberg point feeding system was improved with the help of DEM simulations. Initially, in the first prototypes, the alumina was accumulating on the crust top. This occurred because the alumina was falling outside the radius of the hole provided by the crust breaker. A revised project was proposed where the position of the tube in the chute was improved and the majority of the alumina now falls inside the crust hole directly on the bath. According to the recent reports, the new feeding system has been operating quite successfully [5].

The segregation of different-diameter particles can be studied in DEM simulations as shown in simulation results. Another possibility is to combine CFD models with DEM simulations, for example, in the case of particles in suspension. In such numerical simulations, the fluid flow drag forces are recalculated and applied to the particles at each time step. CFD/DEM coupling is being studied in CFDEM project, which aims to combine open-source software OPENFOAM with LIGGGHTS [4].

7. References

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