High-Fidelity DEM-CFD Simulation for Optimized Dental Powder Delivery

Luca Antonini[1]

[1]Parametric Design Suisse Sagl, Chiasso (CH), Switzerland

1 Introduction

Air polishing treatments have become a widely used methodology in modern dental prophylaxis. These techniques leverage a high-pressure jet of air to propel abrasive powder particles from a mixing reservoir toward the tooth surface [1]. The efficacy of such treatments is critically dependent on two key parameters: the selection of the powder and its delivery rate. Regarding this second aspect, the accurate quantification of powder consumption by dental hygiene devices has become a fundamental aspect to determine the clinical outcome of these tools [2]. Although experimental methods have been proposed to assess powder consumption, these approaches can be adopted only in the later development stages of a new product. Indeed, building *ad hoc* prototypes to be characterized via experimental testing is both resource-intensive and time-consuming and not compatible with the early design and optimization phases.
In this context, a computational approach is highly advantageous. Indeed, recent technological advancements have enabled the execution of increasingly complex analyses and highly multiphysical phenomena can now be addressed with dedicated software, such as LS-DYNA.
Predictive estimations can be obtained through *in silico* analyses, enabling the investigation of how device modifications impact performance without the need for experimental trials. Moreover, a design methodology that incorporates simulations not only provides predictive data but also offers the possibility to investigate powder's dynamics within the reservoir, a phenomenon that might be challenging to quantify using conventional experimental techniques. In this framework, such computational insight would allow designers to make data-driven decisions for the development and optimization of the new product.
Therefore, the present study aims to develop a computational model to represent the complex particle-particle and air-particle interactions within a powder mixing reservoir. The simulation was built in LS-DYNA by coupling the Discrete Element Method (DEM) for describing the powder with Computational Fluid Dynamics (CFD) for analyzing the airflow. The proposed numerical strategy was validated by comparing its results with experimental data of powder consumption rate.

2 Multiphysics simulation

2.1 Powder model development

A foundational step in developing a computational model to represent powder mixing and recruitment within the reservoir caused by air movement, is to create a particle model that accurately replicates its behavior. For this purpose, the Discrete Element Method was employed. This method allows for the representation of granular or particle-based materials using rigid, spherical particles. Such methodology enables a precise analysis of interactions between particles, as well as between particles and the structures that compose the computational domain.
Directly measuring the properties of individual powder particles is often complex. Therefore, it is generally preferable to base the model's calibration on indirect measurements. This approach involves experimentally evaluating the bulk behavior and then calibrating the particle model until the simulation accurately reproduces the experimental results [3].
After a preliminary analysis aimed at estimating the particle size range and density, the actual calibration phase was undertaken. For this study, the calibration was based on the experimental measurement of the angle of repose. Specifically, this test involves accumulating powder on a circular base until the heap height remains constant despite the continuous addition of material. At this point, the angle of repose can be measured as the arctangent of the ratio between powder height and base radius. Such experimental test was replicated using LS-DYNA adopting the following computational strategy: an initial quantity of particles representing the powder is generated above the circular base (Fig. 1 – left side). These particles are then subjected to the gravitational field and to a continuous flux which simulates the ongoing addition of particles to the top of the heap (Fig. 1 – right side). By calibrating the powder's elastic modulus and the parameters of the keyword **`*CONTROL_DISCRETE_ELEMENT,`** it was possible to tune

the computational result until it aligned with the experimental observations. The simulation output was considered acceptable when an angle of repose value within the experimental variability range was obtained.

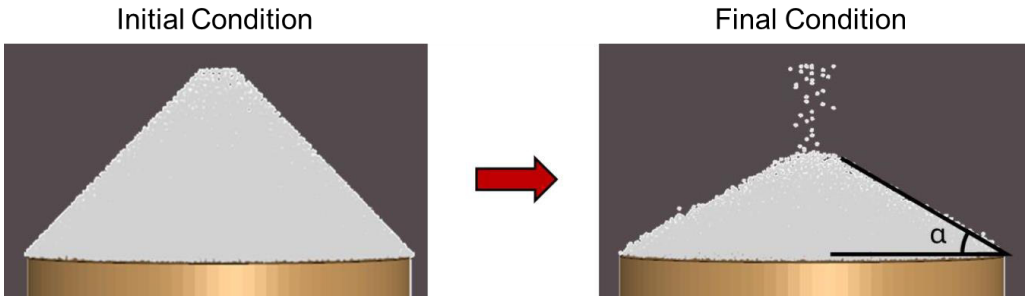

Fig.1: Representation of initial and final conditions of the simulation adopted to calibrate the powder model. The angle of repose, α, was measured once the heap height was constant despite the continuous addition of particles.

2.2 DEM-CFD simulation

The phenomenon to be computationally replicated is the motion of powder within the reservoir, which is agitated by a high-velocity air flow, and then collected toward the outlet conduit leading to the patient's teeth. Consequently, the domain analyzed in the simulation, which couples the previously developed powder model with a fluid dynamics simulation, is the powder mixing reservoir itself. The reservoir walls are included in the analysis as both rigid structural elements against which powder particles can impact and as mesh elements used to generate the tetrahedral mesh for the fluid dynamics analysis. The reservoir walls were discretized into triangular elements of varying sizes. A preliminary sensitivity analysis led to a discretized structure of approximately 10'000 elements. The initial condition of the simulation is represented by the discrete element model suspended in the lower part of the reservoir, with no airflow inside the mixing chamber. This condition is then perturbed at the start of the calculation by applying a gravitational field and progressively increasing the air velocity at the domain's inlet. Using the previously calibrated powder model and considering an initial condition with 20 grams of powder in the reservoir, it was necessary to represent approximately 1'000'000 powder particles (Fig.1 – a).
The computational analysis was divided into two distinct phases: an initial transient phase, where the velocity of the incoming air reaches the target value from zero, and a steady-state phase where the air velocity remains constant.

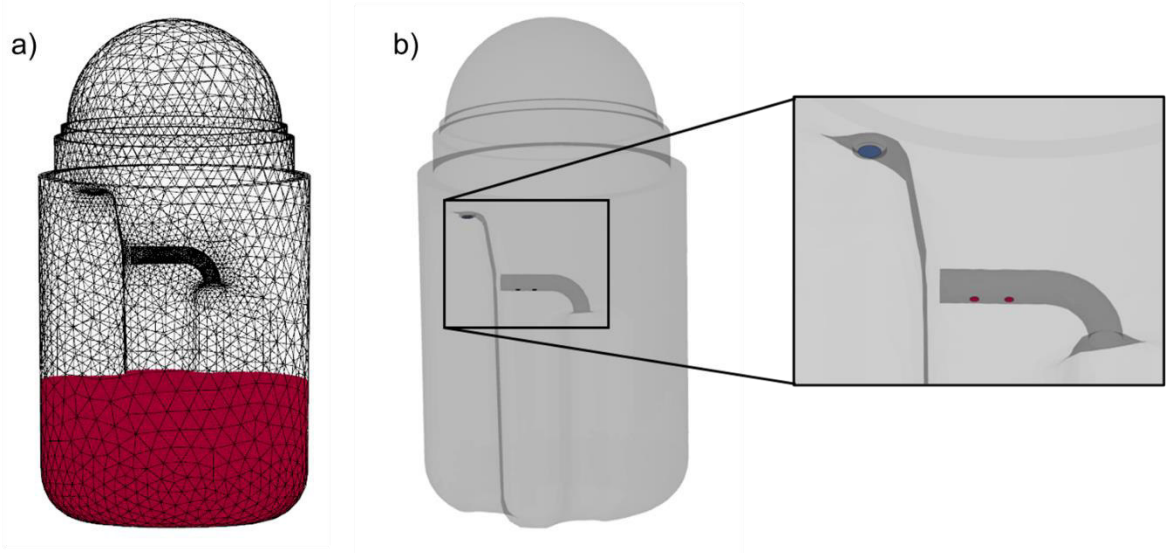

Fig.2: a) Triangular discretization of the reservoir and representation of an initial condition with 20 grams of powder. b) Fluid dynamic domain with detail of the inlet (red) and outlet (blue) surfaces.

For the fluid dynamic environment of the analysis, a no-slip condition was applied to the reservoir walls (**`*ICFD_BOUNDARY_NONSLIP`**), while the inlet and outlet surfaces (Fig. 2 - b) were controlled by imposing air velocity and pressure, respectively (**`*ICFD_BOUNDARY_PRESCRIBED_VEL`** and **`*ICFD_BOUNDARY_PRESCRIBED_PRE)`**. The target values for these boundary conditions were

determined by running preliminary CFD analyses, whose credibility was established through the comparison with experimental tests that evaluated the pressure drop upstream and downstream of the powder reservoir. A RANS k-epsilon approach was selected to manage turbulence.
As previously mentioned, for the structural part of the simulation, the reservoir walls were described as rigid, fixed shell elements, and their contact with the particles was managed using the keyword **`*DEFINE_DE_TO_SURFACE_COUPLING`**. To estimate the powder mass flow rate at the reservoir's outlet, the keyword **`*DEFINE_DE_MASSFLOW_PLANE`** was used, referencing a surface generated in correspondence to the system's outlet. This allowed the simulation output files to record the mass of powder that passed through this surface.
The coupling between the fluid dynamic and structural environments for this type of analysis consists in managing the interaction between the fluid (air) and discrete elements (powder) through the keyword **`*ICFD_CONTROL_DEM_COUPLING`**. Although the phenomenon intuitively requires a two-way interaction, preliminary analyses led to the decision to use a one-way coupling where the air's motion is not influenced by the powder's presence. Indeed, it was observed that this strategy sacrifices a bit of accuracy only in the initial phase of the calculation, when a jet of increasing air velocity begins to impact the stationary powder, without significantly affecting the rest of the simulation, offering the major advantage of reducing computational cost. Considering that the primary objective is to develop an accurate computational model suitable to be used for performance analysis and optimization studies of the device, the entire numerical environment was developed with a parametric approach. This allows a future user to conveniently modify key simulation variables, such as the analysis duration, the initial quantity of powder in the reservoir, and the boundary conditions of the fluid dynamic environment.

3 Simulation results

The computational outputs indicated that during the initial transient phase, the air impacts the powder with increasing velocity, progressively setting it into motion. As clearly visible in Fig. 3, this generates a wave-like movement that leads the powder from the area beneath the two inlet surfaces towards the reservoir's dome and then into the outlet region.

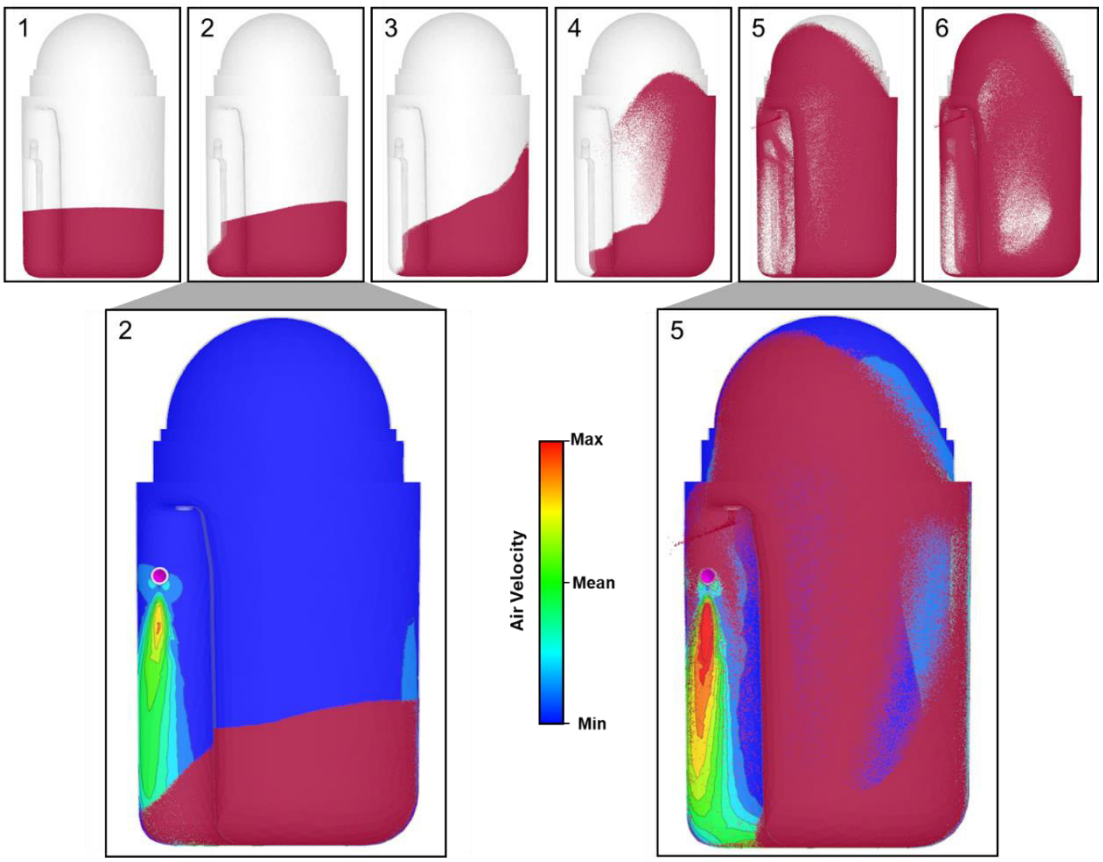

Fig.3: Simulation of powder consumption: initial agitation phase. Pictures in the upper part of the figure represent particle progressive motion due to the increase in air velocity at the inlet. Two details regarding air velocity profiles are also reported.

At the end of this phase, when the air has reached its target velocity, the powder's motion is observed to closely track the agitating airflow. As reported in Fig. 4, throughout the steady-state phase, the representation of particle velocities reflected the airflow streamlines, with high-velocity zones noted beneath the inlet surfaces and near the outlet surface. The numerical analysis also confirmed the absence of powder stagnation zones. While some areas of the reservoir show moderate powder velocities, particle residence in these zones is temporary, as the air motion continuously remixes and recruits them toward the system's outlet.

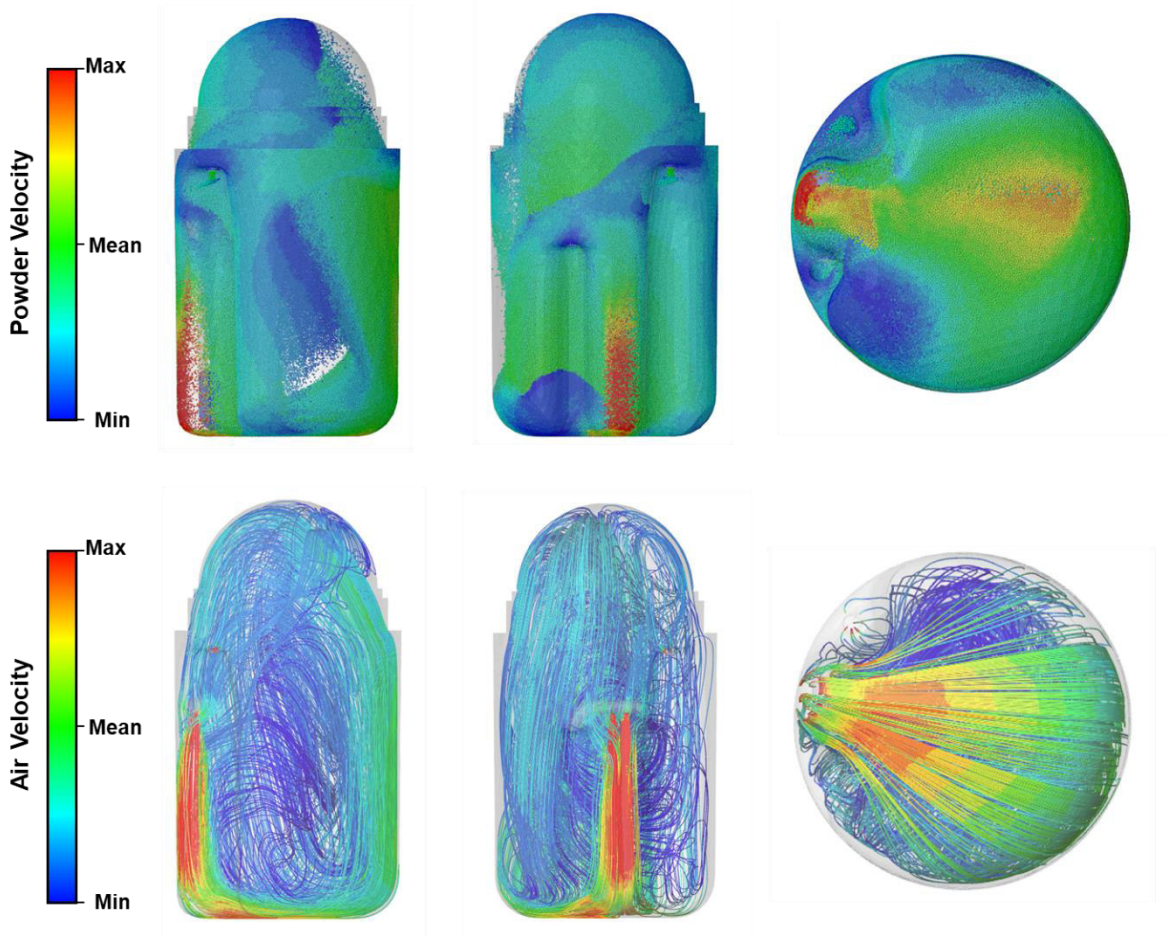

Fig.4: Lateral and inferior views of particle velocities (top) and air flow lines (bottom) during the steady-state phase of the simulation.

The initial transient phase and subsequent steady-state phase were also easily identifiable by observing the graph representing the progressive mass of powder exiting the reservoir (Fig. 5). Following an initial phase with zero powder consumption, the cumulative mass of discharged powder exhibits a linear trend over time. The results were consistent with experimentally collected data on powder consumption: as highlighted in Fig. 5, the linear trend representing powder flow rate falls within the experimental variability range.

Moreover, a comparative analysis of two simulations, differing in the duration of the initial transient phase (2 and 4 seconds), revealed that this duration has no impact on the steady-state powder flow rate from the reservoir. The obtained powder mass curves for both simulations are parallel, indicating that extending the initial transient step just delays the onset of the constant consumption phase (Fig. 6).

Furthermore, observing the graphs it is possible to notice that the constant powder consumption phase begins in both cases before the start of the steady-state phase. The phenomenon is particularly evident with a 4-second transient step, where the linear consumption phase starts approximately after 3 seconds. This finding indicates that the system's outlet saturates its capacity to recruit powder even when the inlet air velocity is below its steady-state value.

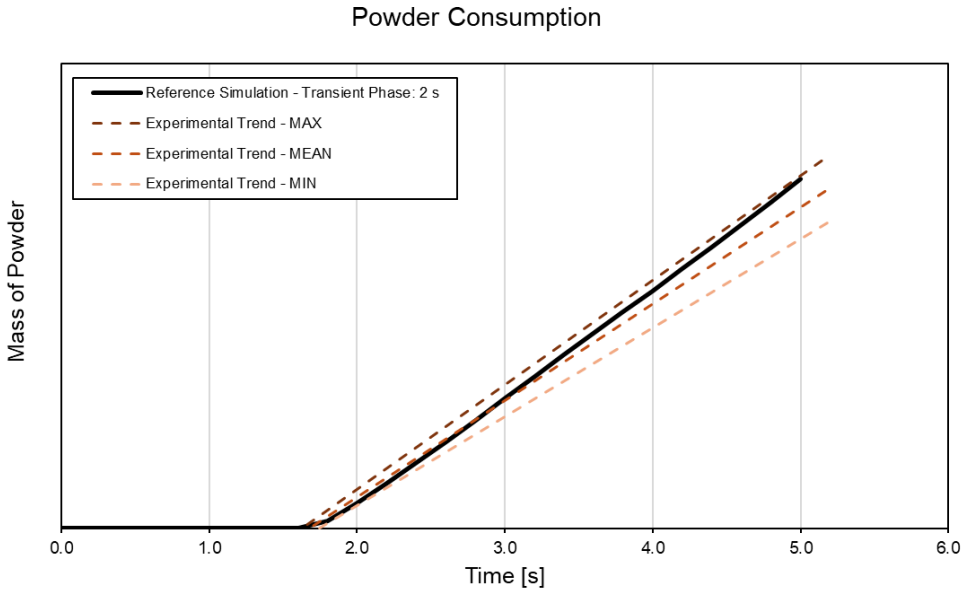

Fig.5: Comparison between the results obtained considering 2 seconds of initial transient phase. A complete superposition was observed between the values derived from the numerical analysis and the range of measurements acquired experimentally.

The device is designed to deliver a constant powder flow rate during operation until the powder level in the reservoir drops below a certain control threshold, at which point this performance can no longer be guaranteed. To confirm the computational model's accuracy, a simulation was also run with an initial powder level below the threshold that ensures constant consumption. In this case, the results showed that after the initial transient phase, the mass of powder passing through the outlet of the system no longer follows a linear trend (Fig. 6). In agreement with experimental expectations, the gradient of this trend is decreasing, indicating a reduction in the outlet powder flow rate over time.

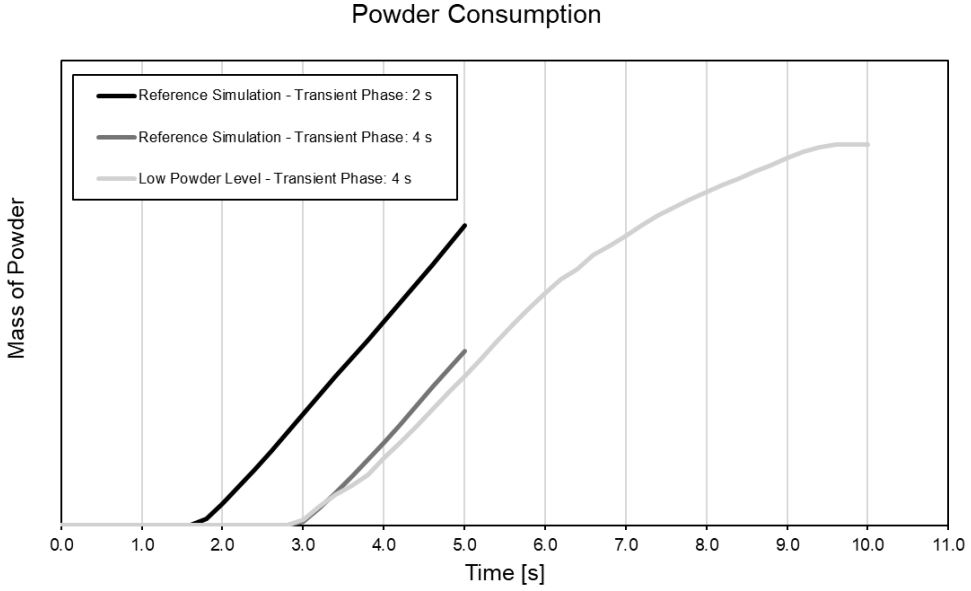

Fig.6: Comparison between simulations differing in terms of transient phase duration (2 or 4 seconds) and initial powder quantity (above or below the control threshold). The reference simulations were carried out considering only 5 s due to the significant amount of computational time needed to perform the analysis with a significant number of particles. On the other hand, the Low Powder Level analysis considered 10 s of simulation. In this case, during the last second the air velocity value drops to zero from the steady-state value).

4 Summary

In this study, a comprehensive multiphysics simulation framework was developed to model the complex phenomena of dental powder mixing and recruitment within the reservoir. By coupling DEM and CFD to represent the particulate phase interacting with the air flow dynamics, the simulation provided a high-fidelity representation of the system's behavior under operational conditions.

The results of the simulation showed excellent agreement with experimental data in terms of powder consumption over time, thereby assessing the model’s predictive capabilities. Furthermore, the numerical approach enabled detailed visualization and quantification of local phenomena that are inherently challenging to observe using conventional experimental techniques. Specifically, the simulation allowed for the analysis of particle velocity, identifying high- and low-velocity zones and confirming the effective absence of stagnant zones within the reservoir, a crucial aspect for ensuring optimal device performance.

The simulation was designed to be fully parametric, allowing for flexible adaptation to a wide range of operating conditions, such as varying powder initial quantities and airflow velocities. This adaptability makes the tool particularly valuable for predictive analysis and optimization tasks.

Additionally, the study demonstrated the robustness and versatility of LS-DYNA in modeling such complex, multiphase interactions, highlighting its potential to be integrated into the design and development workflow of new dental devices. Indeed, the adoption of this simulation-based approach can significantly enhance the efficiency of the development process by reducing reliance on physical prototyping and enabling a broader exploration of design spaces, offering a competitive advantage over traditional methods based solely on an experimental approach.

5 Literature

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[3] Jenkins, B.D. et al.: "The sensitivity of powder characterization tool measurements to particle properties", Powder Technology 448, 2024, 120231.