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CALIBRATION OF AM POWDERS FOR OPTIMIZATION OF RECOATING PROCESS USING DEM

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Abstract: Additive Manufacturing (AM) has been a subject of significant attention from both industrial manufacturers and research communities. However, several challenges hinder the widespread implementation of this technology in the industry. Powder recoating is a crucial step in powder-bed AM process that involves achieving a uniformly packed bed of powder particles that are later melted by an energy source, such as a laser or electron beam. One of the main challenges is calibrating the contact model parameters accurately to match the flowability and spreadability of specific powder alloys. This paper proposes a Discrete Element Method (DEM) model calibration framework based on surrogate model optimisation. The study utilises a Revolution Powder Analyser (RPA) as the experimental reference system. The proposed method is demonstrated with two AM powder samples, Ti64 and Inconel 718. The results indicate that particle-particle friction, rolling resistance, and van der Waals (vdW) surface energy significantly affect the system responses. Furthermore, the validation results show good correspondence between the simulation with calibrated parameters and experimental data. Overall, proposed calibration framework has the potential to optimise powder recoating and to improve the accuracy and effectiveness of the additive manufacturing.

Keywords. Additive Manufacturing (AM), Discrete Element Method (DEM), Revolution Powder Analyzer (RPA), Model calibration, Powder characterization

1 INTRODUCTION

Additive manufacturing (AM) is rapidly gaining recognition and interest among both industrial manufacturers and research communities. The technology offers several remarkable benefits such as the ability to produce intricate geometries with fine details, as well

as economic advantages and flexibility in both design and production. Nevertheless, there are several challenges hindering wide implementation of the technology in the industry, for example, process control, reliability and repeatability [1]. The main reason for this is relatively low maturity of the technology, which implies that the essential protocols and methods for process control and material and product characterization are still being developed.

A large portion of metal AM systems are powder bed based [2,3]. In powder bed based technologies, parts are built up by depositing powder layers and solidifying them by an energy source, such as laser or electron beam, progressively. Powder layer deposition or recoating is the process where a new layer of powder is spread over the powder bed with a recoater. This is a crucial step determining the profile of the powder layer such as packing and thickness and consequently the properties of the solidified layer and the final product [4]. Process parameters should be optimised to obtain the desired recoated layer profile. However, the optimum point is dependent on the powder properties and must be identified for each powder separately. A pure experiment based method to determine the process parameters can be time and cost extensive, therefore, simulation is a more efficient way for investigating the effect of process parameters.

The most common method for simulation of granular material is discrete element method (DEM). In DEM the granular material is modelled as individual particles interacting with each other and the objects in the environment. The simulation is divided to time steps where the forces applied to the particles at each step are integrated to obtain their velocity, position and orientation in the subsequent step. The models used in DEM are mostly based on a theory developed by Hertz in 1881 [5]. Mindlin and later Mindlin and Deresiewicz modified the theory by adding an elastic tangential force to establish the Hertz-Mindlin-Deresiewicz (HMD) model [6, 7]. HMD model is adopted since to enable different types of interaction such as adhesion and rolling resistance [8]. The bottleneck in DEM simulation is the computational cost that is mainly determined by simulation time-step and the number of particles in the simulation setup. The usual approach to run the simulations within a reasonable cost is reducing the number of particles compared to the realistic systems by scaling up the particle size [9, 10]. This results in an unrealistic estimate of the the model parameters since critical forces in the particle interaction, such as adhesion, are strongly size dependent [11].

Here we have implemented a GPU based DEM solver to simulate the behaviour of the powder in an RPA setup with the actual size distribution of the powder that falls within 45-130 μm [12]. The RPA consist of a drum with transparent walls which is set to rotate with a certain angular velocity after being partially filled by the powder under study. Our DEM model includes both rolling resistance and adhesion. An approach is presented to identify and calibrate the parameters in the model that have a significant effect on the behavior of the powder (i.e. active factors). The model is then calibrated with an experimental data set to find the values of the active factors. The process is applied to calibrate the DEM model for two commonly used AM powders, namely Inconel 718 and Ti64.

2 METHOD

The rheological behavior of the powders is studied by a Revolution Powder Analyzer (RPA) (Mercury Scientific Inc, Newtown, CT, USA). Equal sample size of 66 g in case of Ti64 and 110 g in case of Inconel 718 powder materials are freely loaded in the drum. For the flowability measurements, a constant speed of 0.6 RPM is selected in which 150 powder avalanches were analysed. In an avalanche motion regime as the drum rotates, the powder is carried up along the side of the drum, causing it to collapse or avalanche due to its weight. The test is aimed to extract powder energy as a time series and identify the avalanche events. The energy before and after the avalanche event and the difference between them are called break, rest and avalanche energy, respectively.

The AM powders used in the calibration process are Inconel 718 and Ti64, typically employed in Powder Bed Fusion - Laser Beam (PBF-LB), often referred to as Electron Beam Melting (EBM). The particle size distribution is measured by laser diffraction using a Mastersizer 3000 instrument (Malvern Panalytical, UK). The size distributions of powders are stated in Table 1.

Table 1: Particle size distribution for Inconel 718 and Ti64

Powder	D10 (μm)	D50 (μm)	D90 (μm)
Inconel 718	51.73	78.32	113.9
Ti64	50.1	69.8	97.1

DEM simulations are performed via the Python API of the GPU DEM solver Demify® [12]. Within the scale of this work simulations involving over 100,000 particles have been run, however Demify® is able to handle quantities reaching several millions of particles.

3 CONTACT MODEL

The DEM model is based on step wise identification of the position and orientation of the particles according to their properties and interactions with each other. For particle i interacting with particle j the following classical physics equations apply:

$$(m\ddot{\mathbf{r}})^i = m^i\mathbf{g} + \sum_j \mathbf{f}_{tot}^{ij} \ , \tag{1}$$

$$(I\dot{\omega})^i = \sum_j \mathbf{m}_{tot}^{ij} \ , \tag{2}$$

where m, I, $\mathbf{r}$ and ω are particle mass, momentum, position and angular velocity, respectively. $\mathbf{g}$ is the gravitational acceleration and $\mathbf{f}$ and $\mathbf{m}$ are force and momentum. ($\dot{}$) and ($\ddot{}$) denote first and second derivatives. The total force $\mathbf{f}_{tot}^{ij}$ is the sum of the normal and tangential contact forces ($\mathbf{f}_{CN}^{ij}$ and $\mathbf{f}_{CT}^{ij}$) and the normal adhesion component ($\mathbf{f}_{AN}^{ij}$). The

total momentum is the sum of particle momentum as the effect of the tangential force and rolling resistance ($\mathbf{m}_R^{ij}$):

$$\mathbf{f}_{tot}^{ij} = \mathbf{f}_{CN}^{ij} + \mathbf{f}_{CT}^{ij} + \mathbf{f}_{AN}^{ij} \ , \tag{3}$$

$$\mathbf{m}_{tot}^{ij} = \mathbf{m}_R^{ij} + \mathbf{r}_{CG}^{ij} \times \mathbf{f}_{CT}^{ij} \ . \tag{4}$$

Normal and tangential forces are calculated based on the HMD contact model and include elastic and dissipative components. The contact model implementation in Demify® that is utilised in this work is thoroughly explained by Ullrich [13].

3.1 Rolling resistance

The dissipative tangential force in the original HMD model does not account for the energy dissipated during the rolling motion, mainly due to surface roughness and satellite particles. The rolling resistance component in eq. (4) is added to encounter for this phenomenon. Rolling resistance torque in the DEM model is derived according to the momentum of the interacting particles through [11, 14]:

$$\mathbf{m}_R^{ij} = d_R \left\| \mathbf{f}_{CN}^{ij} \right\| r_{eff} \Delta\omega_\perp \quad \text{with} \quad \Delta\omega_\perp = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}^T)(\omega_i - \omega_j) \ , \tag{5}$$

where d_R is rolling resistance coefficient and r_{eff} is a value calculated based on the radius of the two colliding particles (r_1 and r_2) through $1/r_{eff} = 1/r_1 + 1/r_2$. An approach to determine the rolling resistance coefficient based on the particle properties is suggested by Brilliantov et al. [11, 15]:

$$d_R \approx \frac{1 - C_{COR}}{1.153} \left(\frac{1 - \nu^2}{V_{ref} E \sqrt{r_{eff}/2}} \right)^{1/5} \ , \tag{6}$$

where C_{COR} is the restitution coefficient, V_{ref} is the reference velocity, E is the Young's modulus, ν is the Poisson's ratio.

3.2 Adhesion

The adhesion force between the surfaces can be safely neglected in many cases with large and dense particles where other forces such as gravity are orders of magnitude larger. However, for particles with the size in range of tens of microns, adhesion remains a significant factor, even in case of metallic particles [11]. The most important source of adhesion in AM powders is vdW interaction. The vdW force is strongly dependent on the distance between the surfaces in the contact area. For two surfaces separated by the distance δ the surface energy can be written as [8]:

$$\gamma = \frac{A}{24\pi\delta^2} \ , \tag{7}$$

where A is the Hamaker constant. The normal adhesion force ($\mathbf{f}_{AN}^{ij}$) is the vdW interaction force between the particles in normal direction ($F_S(g_N)\mathbf{n}$) and is obtained through [11]:

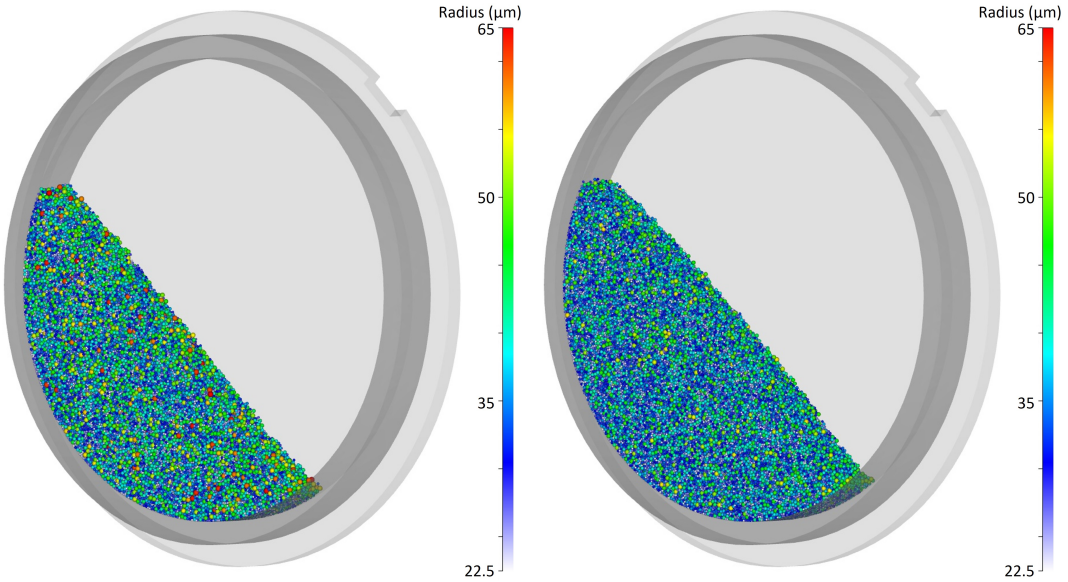
$$F_S(g_N) = \begin{cases} F_{S0} = -4\pi\gamma r_{eff}, & g_N \leq g_0 \\ \frac{Ar_{eff}}{6g_N^2}, & g_0 < g_N < g^* \\ 0, & g_N > g^* \end{cases}, \tag{8}$$

$$\text{with} \qquad g_0 := \sqrt{\frac{Ar_{eff}}{6F_{S0}}} \qquad \text{and} \qquad g^* := \frac{g_0}{\sqrt{C_{FS0}}},$$

where g_N is the normal gap between the two surfaces. C_{FS0} determines the transition area between adhesion force in short range (F_{S0}) and long range (0) and is considered to be 1%.

4 SCALING

One solution to reduce the computational cost of running DEM simulation is to scale up the particle size to lower the number of particles while having the same volume of material. This leads to an unrealistic estimate of the the model parameters since critical forces in the particle interaction, such as adhesion, are strongly size dependent [11].



(a) (b)

Figure 1: Down-scaled geometry of the RPA drum in the simulation filled with (a) Inconel 718 and (b) Ti64 powders.

Here a size distribution similar to the real powder is used. To ensure a feasible computational cost for the simulation, the number of particles is reduced by scaling down the geometry of the RPA, while preserving a substantially large ratio between the RPA

dimensions and the largest particle size. The drum width and radius are reduced from 35 mm and 25 mm in the experimental setup to 1 mm and 5 mm, respectively, in simulation. These dimensions are still considerably larger than the maximum particle size ($\text{diameter}_{\text{max}} = 65\,\mu$m in case of Inconel 718 and 55 μm in case of Ti64) as shown in Fig. 1.

Behavior of the powder in a rotating drum is strongly dependent on two dimensionless parameters; filling degree (f) and Froude number (Fr). Filling degree is the fraction of the cross-sectional area of the cylinder that is filled by the powder and Froude number is the ratio between the centrifugal and gravitational forces [16]:

$$Fr = \frac{\omega^2 R}{g} \,, \tag{9}$$

where ω and R are the angular velocity and radius of the drum respectively and g is the gravitational acceleration. The bulk weight of the powder and the angular velocity in the simulation setup are tuned to achieve matching Fr and f values with the experimental setup.

5 CALIBRATION STRATEGY

The contact models in DEM include a set of parameters determined by the properties of the materials and the types of interactions. A number of methods are suggested to extract the values of these parameters via the physical models. These values are also often measured or predicted and tabulated [9]. However, for most of these parameters there is a range of suggested values in the literature and a universally accepted constant value does not exist. The process of determining parameter values within the DEM model to achieve simulation results that closely represent experimental outcomes is referred to as calibration. A variety of calibration methods are developed among which the surrogate model based method is widely accepted in DEM [17]. The surrogate model is a function of the model parameters that estimates the simulation responses. It is developed by running a set of simulations using different values for the model parameters to investigate how each parameter affects the responses.

In this study a response surface methodology is applied to calibrate the parameters within the surrogate models. The simulation results used in objective functions during calibration, also referred to as responses, are the break, rest and avalanche energy and avalanche period. A schematic representation of the calibration approach is shown in Fig. 2. The process starts with finding the active factors i.e. the parameters that significantly affect the responses through Analysis of Variances (ANOVA). A set of simulations are run with parameter combinations drafted by Design of Experiment (DOE) with the fractional factorial design method. The DOE includes combinations of 6 variable simulation parameters i.e. friction and rolling friction coefficients and surface energy in particle-particle as well as particle-tool interaction. Once the active factors are determined another DOE is generated with Central Composite Design (CCD) involving only the active factors. The results of this set of simulations lead to development of a surrogate model for each response via ANOVA analysis followed by a response surface modeling and evaluation.

With a surrogate model in hand, that predicts the simulation results, the final step is to run an optimisation to find the set of parameters that produces the responses obtained in the experimental setup. The results of the optimisation are evaluated by running a simulation with the obtained optimum parameters and comparing the responses with the expected values. If the simulation responses lay within the margins of the standard deviation of the corresponding experimental values, the optimisation is terminated successfully. Obtaining results that significantly diverge from the expected values often indicates that the surrogate model has not been able to predict the results of the simulation accurately. Therefore, the surrogate model development step is repeated starting with generating a new DOE.

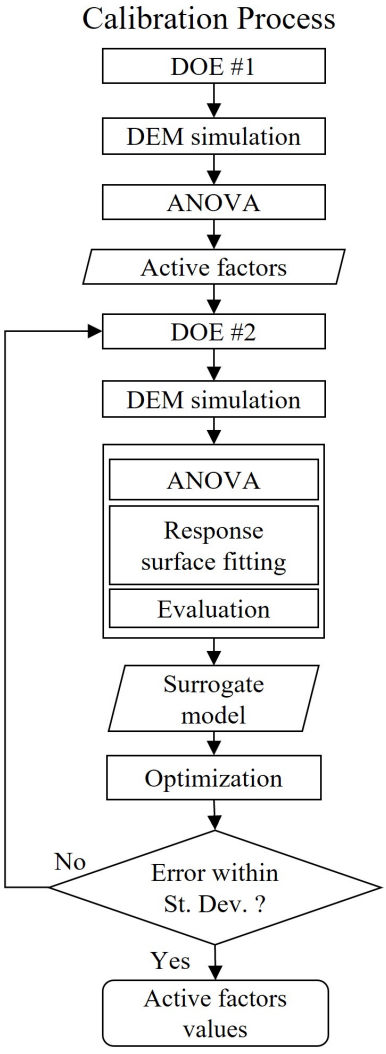


Figure 2: Calibration process steps to obtain the values of the active factors within the DEM model.

6 RESULTS AND DISCUSSION

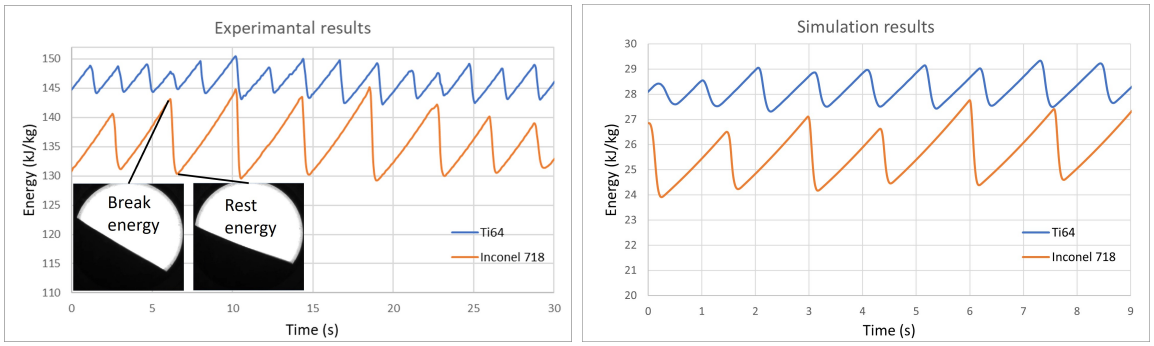
A set of simulations are performed according to the DOE #1 (see Fig. 2), as the first step in the calibration, to identify the active factors in the model. The ANOVA analysis of the results show that particle-particle friction, rolling resistance and surface energy are the active factors, and that variation of the particle-tool interaction parameters does not significantly affect the results. The values of the particle-tool interaction parameters are selected according to the literature while the active factors are obtained through the calibration process. The values for the surface energy and friction coefficient in particle-particle interaction model are expected to be around 0.1 mJ/m^2 and 0.4, respectively, as suggested by Meier et al. [11]. A theoretical expected value for the particle-particle rolling resistance coefficient is calculated according to eq. (6). V_{ref} is selected to be in the range of the highest impact velocities and r_{eff} is set to half of the mean particle radius assuming $r_1 = r_2 = r_{mean}$. The calculated rolling resistance coefficient is about 4.8×10^{-2} for both Inconel 718 and Ti64. The stated theoretical expected values are used to set the upper and lower limits of the calibration parameters during optimisation.

The experimental data from RPA for energy of both Ti64 and Inconel 718 is shown in Fig. 3(a). The inset of Fig. 3(a) illustrates images captured from the Inconel 718 powder during experiment just before and after an avalanche event. Since the energy is normalised by the material weight, its average throughout the experiment is mainly determined by the filling factor, which is slightly higher for the Ti64 compared to Inconel 718. However, the energy upper and lower peaks and avalanche period are strongly dependent on powder properties including particle size distribution, shape, density and particle-particle and particle-tool interactions. Therefore, they are used as the reference in the objective function in the optimisation to extract the values of the active factors. The values of the active factors achieved through the calibration process are listed in Table 2.

Table 2: Values of the active factors in the DEM model obtained via the calibration process.

	P-P Friction coefficient	P-P Rolling resistance coefficient	P-P Surface energy (mJ/m^2)
Inconel 718	0.465	1.35×10^{-2}	0.1918
Ti 64	0.651	7.26×10^{-2}	0.0557

The simulation results are shown in Fig. 3(b). Similar to the experimental results in Fig. 3(a), the Ti64 has a slightly higher average energy compared to Inconel 718. However, the average energy and avalanche period for both powders are significantly lower in simulation compared to the experimental results. This is due to down-scaling of the RPA geometry in the simulation. With a constant filling factor, the center of mass, which determines the energy, is lower in the simulation compared to the experiment. As mentioned in section 4, angular velocity of the RPA is increased to keep the Froude number

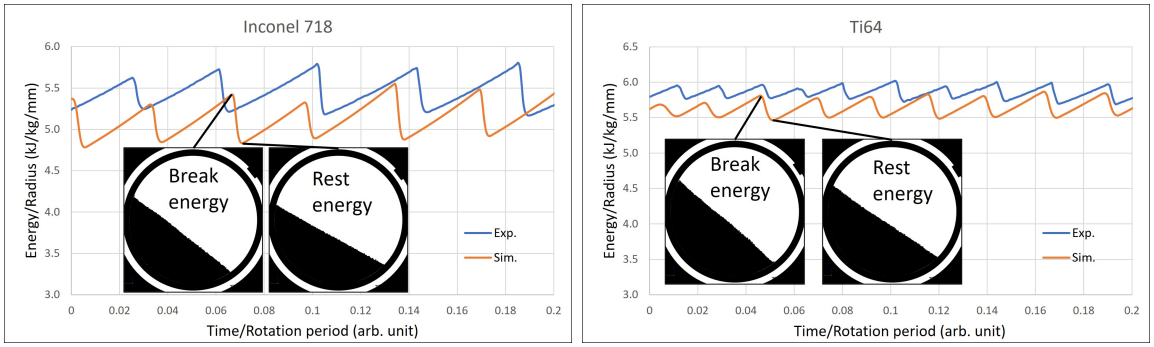


(a) (b)

Figure 3: The plots of energy time series of the Inconel 718 and Ti64 powders in RPA in (a) experimental and (b) simulation setup.

constant, which leads to a shorter avalanche period.

Fig. 4 illustrates a better comparison between the simulation and experimental results where the energy is normalised by the RPA device radius, and time is normalised by the period of the rotation of the RPA drum. The simulation results show a good agreement with experiment. The slight offset between the simulation and experiment is probably due to the implementation of the size distribution in the simulation which leads to a small variation from the packing density and consequently volume of the powder compared to the experiment.



(a) (b)

Figure 4: Comparison between the measured and simulated response of (a) Inconel 718 and (b) Ti64 powder in RPA. The time in x-axis is normalised by the rotation period and the energy in y-axis is normalised by drum radius for simplicity of comparison.

7 CONCLUSIONS

A method is developed to calibrate a complementary DEM model including adhesion and rolling resistance. The method is implemented to calibrate Inconel 718 and Ti64 AM powders using RPA as characterization tool. The calibration process starts with

identification of the model active factors and proceeds with development of surrogate models for system responses. The surrogate models are optimised with response surface fitting based on the experimental data to determine the values of the active factors.

A geometry scaling approach is presented to reduce the computational cost of the simulations with the original powder size distribution. The simulations are performed by the GPU based DEM solver Demify®.

The results of the simulation with the calibrated model show a good correspondence with the experimental data.

8 ACKNOWLEDGEMENT

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