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A Study on Powder Spreading Quality in Powder Bed Fusion Processes Using Discrete Element Method Simulation

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Abstract: Powder deposition is a very important aspect of PBF-based additive manufacturing processes. Discrete Element Method (DEM) is commonly utilized by researchers to examine the physically complex aspects of powder-spreading methods. This work focuses on vibration-assisted doctor blade powder recoating. The aim of this work is to use experiment-verified DEM simulations in combination with Taguchi Design of Experiments (DoE) to identify optimum spreading parameters based on robust layer quality criteria. The verification of the used powder model is performed via angle of repose and angle of avalanche simulation–experiment cross-checking. Then, four criteria, namely layer thickness deviation, surface coverage ratio, surface root-mean-square roughness and true packing density, are defined. It has been proven that the doctor blade’s translational speed plays the most important role in defining the quality of the deposited layer. The true packing density was found to be unaffected by the spreading parameters. The vertical vibration of the doctor blade recoater was found to have a beneficial effect on the quality of the deposited layer. Ultimately, a weighted mean quality criteria analysis is mapped out. Skewness and kurtosis were proven to function as effective indicators of layer quality, showing a linear relation to the weighted means of the defined quality criteria. The specific weights that optimize this linearity were identified.

Keywords: powder spreading; additive manufacturing; doctor blade; recoater; layer thickness; surface roughness; packing density; surface coverage; skewness; kurtosis; Taguchi DoE; recoating speed; vibration; frequency; amplitude



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1. Introduction

Selective Laser Sintering/Melting (SLS/SLM) is a Powder Bed Fusion-based (PBF) additive manufacturing (AM) process. During this process, a three-dimensional object is manufactured by sequentially sintering or melting powder layers via a focused laser beam at the predefined points. By the superposition of the successive layers, an object is formed [1,2].

Most commercial SLS/SLM machines feature a built-in powder deposition system (PDS) that is responsible for performing the task of spreading even, homogeneous layers of powder one above the other. The most widespread PDSs use a simple, compliant doctor blade which, as it translates parallel to the fabrication piston, evens out the top surface of the powder, creating a layer of the desired theoretical layer thickness. The recoater works in conjunction with a dual powder piston, one of which, the feeding piston, moves upwards to provide the necessary amount of powder, and the other one, the fabrication piston, moves downwards in order for the powder to be deposited on its surface, where it will then be sintered or melted. Alternate methods of powder deposition have been examined [2]. However, it has been found via Analytical Hierarchy Process (AHP) analysis that the most beneficial is the purely mechanical powder deposition, i.e., the one that utilizes a simple mechanical recoater, such as a doctor blade or a roller [2]. It has been proven via DEM simulations that the counter-rotating roller is more beneficial compared to the simple doctor

blade since it promotes a higher packing density of the deposited layer [3]. Furthermore, researchers have used DEM simulations to examine the most important powder deposition aspects in terms of the translational speed of the recoater [4], blade shape [5,6], roller rotational speed [4], roller diameter [7], etc.

It is a fact that powder spreading greatly affects the finished part's quality, as has been proven by many works, e.g., [8–10]. More specifically, Ziegelmeier et al. proved that low powder bed volume fraction is connected to the high porosity of the finished part, while low surface roughness of the un-sintered powder layer leads to poor surface quality of the finished part [11]. Despite that, not many works focus on the powder kinematics that govern the process. Some works utilize DEM simulations to reach conclusions about the powder spreading process; however, not many works systematically identify layer quality criteria, strictly define them and follow statistical analysis or DoE to reach safe, universal conclusions. Haeri et al. examined the performance of roller and doctor blade recoaters on the spreading of elongated particles with various aspect ratios based on the packing fraction and the surface roughness of the powder bed. However, they did not provide a robust statistical analysis to identify possible interactions of the spreading parameters. They also omitted to adequately define the volume fraction of the powder bed [3]. Tan et al. studied a composite powder made of elongated polymer and glass fiber. They calibrated the powder via angle of repose checks and only examined roller recoaters. However, they only examined layer thickness, spreading velocity and powder mixture composition without providing enough data on possible interactions between the examined parameters [12]. Wang et al. examined the possible connection between various recoater shapes to the surface coverage and packing density of the powder bed; however, they did not adequately examine recoating translational velocity. Instead, they focused more on the theoretical layer thickness, i.e., the gap between the bottom of the recoater and the fabrication surface [13]. In all these works, the common point is a lack of a robust statistical analysis that would provide a quantification of the qualitative results and observations provided by the DEM simulations.

To the authors' knowledge, the present work is the only one that provides a systematic method of tackling the complex aspect of powder bed characterization and optimization via DEM simulations, by simultaneously focusing in five different aspects, namely the following: (i) thorough examination of minimizing computation time methods without hampering the validity of the simulations; (ii) calculation of particle size distribution as long as adhesive and cohesive forces and established contact model selection; (iii) accurate definition of six powder layer quality criteria (layer thickness deviation, surface coverage ratio, surface root mean square roughness, true packing density, skewness and kurtosis); (iv) Taguchi DoE with subsequent ANOVA for all the quality criteria to identify optimum parameter sets and develop regression equations of the criteria, as long as identifying possible interactions between the spreading parameters with possible ways to compensate for, e.g., higher spreading speed; (v) statistical analysis that proves skewness and kurtosis as equivalent powder bed quality criteria based on weighted means of the predefined four with least-squares analysis for best fit.

In this work, in order to evaluate mechanical powder spreading via a doctor blade, a Taguchi Design of Experiments (DoE) is implemented. The tests were carried out via Discrete Element Method simulations in the EDEM (version 2022.2) software package, which was kindly provided by Altair™. Firstly, the authors present the reasoning behind the selection of the particle size distribution and the particle contact model selection for computational time economy without damaging the reliability of the simulations. Secondly, the simulation geometry and bodies, as well as the simulation steps, are presented. Thirdly, the authors define the deposited layer quality criteria and present the ways in which they are calculated. Then, the Taguchi DoE is presented, with its selected L27 orthogonal array and the ANOVA and regression equations, as calculated by the statistical analysis. Afterward, the authors approach the quality criteria via their weighted means and connect

them to surface skewness and kurtosis for a novel method of equivalent surface quality evaluation. Finally, conclusions are presented, along with suggestions for future work.

2. Materials and Methods

2.1. State-of-the-Art in Modelling of Powder Spreading

2.1.1. Critical Timestep and Simulation Time

In order for the DEM simulation to keep a low computational time while running in a stable manner, the critical time step Δt_c is calculated using the Rayleigh equation [14],

$$\Delta t_c = \frac{\pi \cdot r_{min}}{\beta} \sqrt{\frac{\rho}{G}} \quad (1)$$

where r_{min} is the minimum particle radius in the simulation's domain [15,16], ρ is the powder bulk density, G is the powder material's shear modulus, and β can be approximated by Equation (2) [17,18], with ν being the powder material's Poisson ratio.

$$\beta = 0.8766 + 0.163\nu \quad (2)$$

It is common practice to use lower G values for particle materials compared to the real-world value, granted that preliminary checks ensure small deviations in terms of results and powder behavior.

Zhang et al. (2020) selected a value of 3 GPa [7], outside the suggested range (1 MPa–1 GPa). However, this value is still two orders of magnitude below its actual value (150 GPa) [19–21]. After running shear cell tests to define the interparticle as well as the particle/wall coefficients of restitution, static and rolling friction, they ran cross-checking simulations/experiments of the angle of avalanche and angle of repose tests, finding deviations of +1.1% and +1.6%, respectively, validating the realistic behavior of the powder within the simulation. However, Chen et al. (2017) [22] examined how many orders of magnitude can decrease E without affecting the simulation's results for an angle of avalanche test. If ν is constant, then E and G are linearly related: $E = 2G \cdot (1 + 2\nu)$.

Chen et al. proved that when E varied between the real-world value, E_0 , and the value, $0.001E_0$, the simulation was in agreement with the real experiment in terms of avalanche angle, powder mixing mechanics and behavior. However, when E was set to any value below $0.0007E_0$, the angle of avalanche was reduced by approximately 15% (from 33° to 28°), and, due to the reduction in shearing forces, the mixing rate was decreased [22]. However, drum powder mixing relies more on shear forces than doctor blade powder recoating. Fouda et al. (2019) studied doctor blade spreading of a mono-sized Ti6Al4V powder. They calibrated the simulation via cross-checking simulation and experimental results of an angle of repose test. They also studied the shear modulus range of 1 MPa to 100 MPa, i.e., $2.2 \cdot 10^{-5}G_0$ to $2.2 \cdot 10^{-3}G_0$, with G_0 being the real-world value (42.5 GPa). Only minimal powder kinematics differences were observed; hence the smallest value was selected.

2.1.2. Particle Cohesion/Adhesion Models

"Cohesive" forces refer to those that are applied between particles of the same material, while "adhesive forces" refer to those that are applied between different materials, e.g., between the particles and the doctor blade, the deposition plate, or any other bodies of the simulation. The motion of very fine powders ($D \leq 100 \mu\text{m}$) is not solely governed by gravity but also by attractive Van der Waals forces [23].

There are four different models that describe auto-adhesive particle behavior due to Van der Waals forces; the JKR (Johnson–Kendall–Roberts) model [24], the DMT (Derjaguin–Muller–Toporov) model [25], the BD (Bradley–Derjaguin) model [26] and the MD (Maugis–Dugdale) analytical model [27].

Hertz–Mindlin with JKR Model

The general relationship between normalized normal force and normalized relative particle approach in the JKR model is given by Equation (3). Figure 1 depicts the contact stages of two particles as described via the JKR model.

$$\frac{\delta_n}{\delta_{to}} = \frac{3 \left(\frac{F_n^{JKR}}{F_{po}^{JKR}} \right) + 2 + 2 \left(1 + \frac{F_n^{JKR}}{F_{po}^{JKR}} \right)^{\frac{1}{2}}}{3^{2/3} \left[\frac{F_n^{JKR}}{F_{po}^{JKR}} + 2 + 2 \left(1 + \frac{F_n^{JKR}}{F_{po}^{JKR}} \right)^{\frac{1}{2}} \right]^{1/3}}, \frac{F_n^{JKR}}{F_{po}^{JKR}} \geq -1 \quad (3)$$

where F_{po} is the maximum tensile force required to break the contact among the two particles (i.e., the “pull-off force”) (see Equation (4)):

$$F_{po}^{JKR} = \frac{3}{2} \pi R^* \Gamma \quad (4)$$

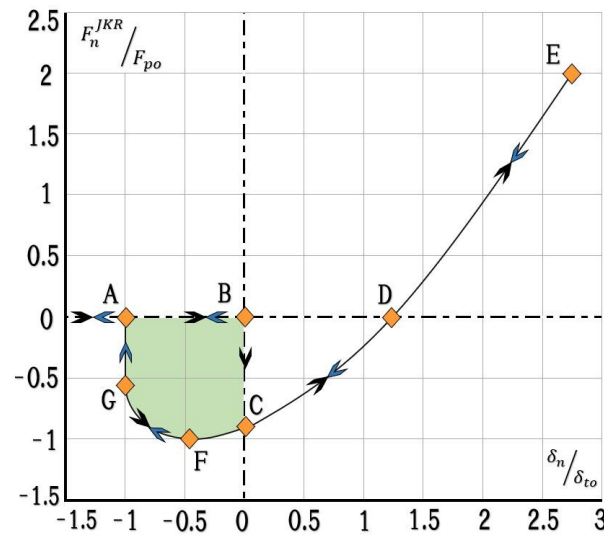


Figure 1. Visual depiction of the work of adhesion between the two surfaces and order of contact evolution [28].

And δ_{to} is the relative approach at the tear-off moment (see Equation (5)):

$$\delta_{to} = \left(\frac{3F_{po}^2}{16R^*E^*2} \right)^{1/3} \quad (5)$$

JKR model gives the Equations (6) and (7) for the normal force F_n^{JKR} and relative approach δ_n , respectively, as functions of the contact patch radius, a .

$$F_n^{JKR} = \frac{4E^*a^3}{3R^*} - \left(8\pi E^* \Gamma a^3 \right)^{1/2} \quad (6)$$

$$\delta_n = \frac{a^2}{R^*} - \left(\frac{2\pi \Gamma a}{E^*} \right)^{1/2} \quad (7)$$

Tabor Parameter and Model Applicability

JKR and DMT initially appeared to be competitive with each other. However, they soon appeared to be limited to a range of solutions governed by the non-dimensional Tabor parameter μ (see Equation (8)) [23]. Grierson et al. (2005) [29] state that “Tabor’s parameter

is physically equivalent to the ratio between the normal elastic deformation caused by adhesion (i.e., in the absence of applied load) and the spatial range of the adhesion forces themselves”.

$$\mu = \left(\frac{R^* \Gamma^2}{E^* z_0^3} \right)^{1/3} \tag{8}$$

where z_0 is the equilibrium separation in the Lennard–Jones potential, Γ is the work of adhesion (see Equation (9)):

$$\Gamma = \gamma_1 + \gamma_2 - \gamma_{12} \tag{9}$$

where γ_1 and γ_2 are the surface energies of the two contacting bodies and γ_{12} is the interface energy. For the same material contacting particles, $\gamma_{12} = 0$, and Equation (9) gives $\Gamma = 2\gamma$, since $\gamma_1 = \gamma_2 = \gamma$.

Opinions on contact adhesion model applicability within the areas of the Tabor parameter vary. Thornton [23] suggests that, for $\mu < 0.1$, the DMT model is suitable, while for $\mu > 5$, the JKR theory is preferable. For the values that lay in between, Maugis (1992) developed the analytic Maugis–Dugdale (MD) approach [27]; however, its analytic nature renders it more complicated than DMT and JKR. Nevertheless, it has been proven that MD is accurate in all μ areas [30], while JKR and DMT are the MD approximations at high and low μ values, respectively. Greenwood (1997) states that, for $\mu \geq 3$, JKR theory accurately approximates the actual radius of contact, the shapes and pressure distributions [26]. Greenwood also proves that DMT theory is “wrong in theory and in practice” (Greenwood, 2017) [26]. Instead, the Bradley–Derjaguin Equation (10) describes accurately how the tensile load varies with regard to the separation. Equation (10) is accurate for all values of μ for large positive separations and for negative separations for small values of μ [26].

$$T(\delta_n) = 2\pi R^* \Gamma \left[\frac{4}{3} \left(\frac{z_0}{\delta_n} \right)^2 - \frac{1}{3} \left(\frac{z_0}{\delta_n} \right)^8 \right] \tag{10}$$

MD model implementation in a DEM simulation would drastically increase the simulation time since it is analytic. In general, the JKR model is applied for large-diameter and more compliant materials (smaller E), while the DMT model is preferable for smaller bodies of more rigid materials (larger E) [30]. Table 1 summarizes the particle contact model range applicability.

Table 1. Particle contact model applicability based on Tabor parameter range.

	JKR [24]	DMT [25]	BD [26]	MD [27]
Thornton [23]	$\mu > 5$	$\mu < 0.1$	Not mentioned	$0.1 \leq \mu \leq 5$
Shi [30]	$\mu \geq 5$	$\mu \leq 0.1$	Not mentioned	Any μ
Greenwood [26]	$\mu \geq 3$	Wrong in theory and in practice	Any μ	Any μ

2.2. Simulation Setup

2.2.1. The Simulation Software Platform

The simulation platform used was the EDEM™, version 2022.2, provided by Altair™. EDEM™ is a Discrete Element Method simulation platform that provides the capability of handling particles of various sizes, shapes and materials. EDEM™ provides the capability of importing physical bodies designed in 3D CAD environments, such as SolidWorks™, and populating certain virtual geometrical shapes with particles of predefined physical properties and particle size distribution. EDEM™ offers a wide range of contact models from which the users can select the most suitable model combinations for the simulation they desire to run. These models include friction, electrostatic or Van der Waals adhesion and cohesion, air drag, restitution and others, covering a wide range of physical phenomena. Finally, EDEM™ offers the capability of NVIDIA™ CUDA computing. Graphics card

programming drastically decreases the simulation time for problems that are compatible with parallel computing.

2.2.2. Powder Modelling

The powder selected for the experiments was the SA-ZL-20 spherical alumina (Al₂O₃) powder provided by the manufacturing company Sinoenergy GroupTM (Beijing, China). The powder specifications can be seen in Table 2.

Table 2. Specifications of the powder used in the simulations.

	Item	Unit	Typical Value
Particle size	D ₁₀	μm	8.2
	D ₅₀	μm	21
	D ₉₀	μm	47.5
Specific Surface Area (S.S.A.)		m ² /g	0.19
Electrical Conductivity (E.C.)		μS/cm	300
pH		-	8.5
Moisture		%	0.05
True Density		g/cm ³	3.8
Spheroidization		%	96
Chemical Composition	Al ₂ O ₃	%	99.5
	Fe ₂ O ₃	ppm	300
	Na ₂ O	ppm	3500
Ion content	Na ⁺	ppm	400

Material Properties Modelling

The following values were used in the simulation: Poisson’s ratio (ν) of alumina equal to 0.3 [7], the solid’s bulk density (ρ) equal to 3820 kg/m³ [7], the shear modulus (G) equal to 1·10⁷ Pa. Furthermore, the alumina–alumina and alumina–SAE 304 stainless steel restitution (c_r), static friction (c_{sf}) and rolling friction (c_{rf}) coefficients were used [7], and the values were as follows: $c_{r,al-al} = 0.5$, $c_{sf,al-al} = 0.34$, $c_{rf,al-al} = 0.05$, $c_{r,al-304} = 0.52$, $c_{sf,al-304} = 0.2$ and $c_{rf,al-304} = 0.05$.

The minimum particle radius is set at $r_{min} = 2.5 \mu\text{m}$, in order to not allow very small particles to enforce a very small timestep and to prevent the powder from displaying an extremely cohesive behavior. Similarly, the maximum particle diameter is set at $D_{max} = 75 \mu\text{m}$, 25% smaller than the theoretical layer thickness $h_{l,th}$ (100 μm), in order to prevent quality deterioration of the surface [8]. Finally, as explained in Section 2.1.1, the shear modulus is set at a low value (10 MPa) after checking that this value minimizes the simulation time without affecting the validity of the results (see Section 3.2).

Particle Size Distribution

The powder selected was spherical alumina; hence, a uniform spherical shape was selected for all particles. Spreadsheet calculations were carried out in order to examine which kind of distribution best fits the three PSD numbers (D₁₀, D₅₀ and D₉₀) provided by the powder manufacturer.

In many studies, a lognormal distribution is used to approximate the particle size distribution of a given powder; however, no method of defining the lognormal distribution parameters based on the aforementioned powder PSD specifications has been documented.

Let Z be a standard normal variable; then, the variable $X = e^{\mu + \sigma Z}$ follows the log-normal distribution with parameters μ and σ , $\mu \in (-\infty, +\infty)$, $\sigma > 0$ are real numbers.

The mean and the standard deviation of the variable X and the cumulative distribution function are given by Equations (11), (12) and (13), respectively; erf is the error function.

$$\mu_X = \sqrt{e^{2\mu + \sigma^2}} \tag{11}$$

$$\sigma_X = \sqrt{\mu_X^2 (e^{\sigma^2} - 1)} \tag{12}$$

$$F_X(x) = \frac{1}{2} \left[1 + erf \left(\frac{\ln x - \mu}{\sigma \sqrt{2}} \right) \right] \tag{13}$$

The following equations characterize the particular powder employed:

$$\left\{ \begin{array}{l} D_{90} = 47.5 \\ D_{50} = 21 \\ D_{10} = 8.2 \end{array} \right\} \Leftrightarrow \left\{ \begin{array}{l} F_X(47.5) = 0.9 \\ F_X(21) = 0.5 \\ F_X(8.2) = 0.1 \end{array} \right\} \tag{14}$$

$$\tag{15}$$

$$\tag{16}$$

Equations (15) and (16) are used to calculate μ and σ , using Equation (13): $\mu = 3.0445$ and $\sigma = 0.7338$. If Equation (14) is used for validation, it yields $F_X(47.5) = 0.867 \approx 0.9$. If Equation (13) is used to calculate D_{90} , it gives $x = 53.78 \cong 47.5$ with a deviation of 13.2%, which is deemed acceptable. Thus, using Equations (11) and (12), the values of μ_X and σ_X result as $\mu_X = 27.488$ and $\sigma_X = 23.216$, and the values of their normalized counterparts (by the particle diameter $D_{ave} = 50 \mu\text{m}$): 0.549758 and 0.464323. Furthermore, the user sets the maximum and minimum particle size caps, namely 0.1 and 0.5, as a number to be multiplied by the average particle size (“Physical Radius”).

Contact Model Selection

The model requires a value for “contact radius”, which has to be greater than the physical radius, and it is only used in the case where cohesive and adhesive attractive forces are to be taken into consideration.

There is a multitude of mechanisms by which microscopic particles may adhere to each other. In the case of relatively strong bonds, it may be solid, cemented or glued by a viscous liquid. Weaker bonds may be provided by pendular liquid bridges, Van der Waals forces, electrostatics or electro-magnetic fields [23]. In this work, however, there is no presence of viscous liquid or moisture that could create liquid bonds. Electrostatic charge is ignored since the minimum particle diameter is at 5 microns, which is not at the nanoscale, where the forces due to electrostatic charges begin to surpass gravitational forces. Even though some electrostatic charge can be developed, either via contact between the insulator (aluminum oxide) and the substrate (stainless steel plate) or via contact of particles of alumina with each other, granted they are of dissimilar size [31], they would be negligible due to the rather large average size of the powder sample used. Furthermore, even in the case of a fluidized bed of alumina particles, the charge of alumina dust is relatively neutral [32]. Hence, during powder deposition, where particle excitation is weaker, even more insignificant charges will develop. Similarly, no electro-magnetic fields exist, so only Van der Waals forces are to be considered. Furthermore, no plastic deformation was taken into consideration in this work since the materials are of very high hardness, and the low-speed collisions result in no permanent deformations.

For contact model selection, μ is calculated for a-alumina particles as follows:

The surface energy of amorphous alumina (a- Al_2O_3) is $\gamma_{a-\text{Al}_2\text{O}_3} = 0.97 \pm 0.04 \frac{\text{J}}{\text{m}^2}$ [33]. However, this value refers to nanoparticles of diameters between 2 and 5 nm and is valid for surface areas greater than $370 \text{ m}^2/\text{g}$. The diagram of Figure 2 shows how the surface area of spherical alumina particles changes with the change in the particle’s diameter. The surface energy depends on particle size, the general consensus being that it decreases with the decrease in particle size [34]. This is justified since the number of next neighbors of surface atoms reduces with decreasing particle size [34]. Tepesch et al. (2000) calculated the surface energy of stoichiometric (1-Al-terminated) amorphous alumina (a- Al_2O_3) as $\gamma_{a-\text{Al}_2\text{O}_3} = 2.13 \frac{\text{J}}{\text{m}^2}$ [35]. This surface is the most stable expression of a-alumina. Indeed,

this value comes in accordance with the rule of thumb that as the particle size increases, the surface energy also increases. Hence, for two contacting particles of a-alumina, $\Gamma \cong 4.26 \frac{J}{m^2}$.

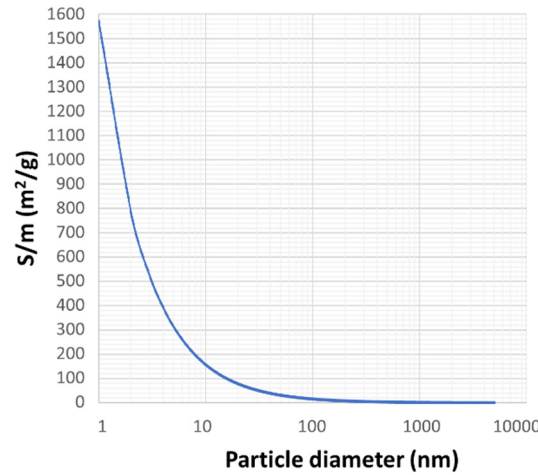


Figure 2. Surface area vs. particle diameter plot for spherical a-alumina particles.

R^* and E^* are calculated by the Equations (17) and (18)

$$R^* = \frac{R_1 R_2}{R_1 + R_2} \tag{17}$$

$$E^* = \frac{E}{2(1 - \nu^2)} \tag{18}$$

Finally, the equilibrium separation in the Lennard–Jones potential for a- Al_2O_3 is $z_{0a-Al_2O_3} = 5.1 = 5.1 \cdot 10^{-10}$ m [36]. Figure 3 shows how μ varies with the diameter of the two contacting particles. G is adjusted to $1.29 \cdot 10^{11}$ Pa, so that, combined with a ν of 0.3, E is the maximum within the limit provided in [21], i.e., 413 GPa.

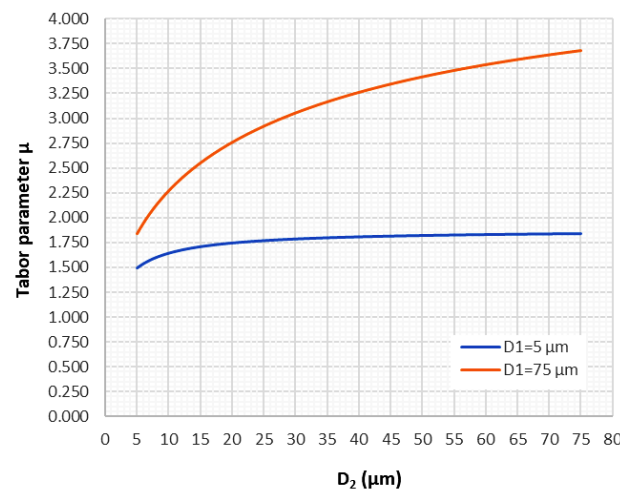


Figure 3. Tabor parameter curve vs. the second particle’s diameter for two extreme diameters of the first particle.

The Tabor parameter μ increases with the increase in the particle size (see Equation (8)). If the first among the two particles in contact has a diameter of 5 μm , then μ ranges between 1.492 and 1.840 for the second particle’s diameter of 5 and 75 μm , respectively. If the first particle’s diameter is 75 μm , however, μ ranges between 1.840 and 3.681 for the second particle’s diameter of 5 and 75 μm , respectively.

Judging by Figure 3, it can be deduced that, for the real-world material, almost all contacts of the larger particles (around 60–75 μm diameter) could be modeled via JKR or at least hybrid JKR-BD, as Greenwood suggests for $2 \leq \mu \leq 3$ values [26]. However, for smaller particles (around 5–15 μm diameter), the BD model (see Equation (10)) or even the analytic MD approach would be better. The MD approach would render the simulation much slower; however, the BD and hybrid JKR-BD models would be beneficial in areas where the JKR seems to deviate significantly from the analytical solution of the adhesive elastic contact problem.

In the trial runs that were performed in this study, in order to determine which shear modulus value should be used in the simulations, the shear modulus and, thus, Young’s modulus was varied from its actual value to a value 4 orders of magnitude smaller. The Tabor parameter’s value increases with the decrease in the relative modulus of elasticity (E^*) taking it to larger values by 3 orders of magnitude. Hence, the selection of the “Hertz–Mindlin with JKR v2” model in the EDEM software is perfectly justified.

Parametrization of Cohesive Forces

“Contact radius” (see Section 2.2.2, Sub-Section: “Contact Model Selection”) will, from this point on, be called $R_{c,EDEM}$, and is given by the Equation (19).

$$R_{c,EDEM} \geq R_{particle} + |\delta_{to}| \tag{19}$$

where $R_{particle}$ refers to the “Physical Radius”, and δ_{to} is the relative approach of the two particles in contact (both of $R_{particle}$ radius) at which the contact breaks, with “to” standing for “tear-off” (see Equation (5)).

F_{po} is the maximum tensile force required to break the contact among the two particles (i.e., the “pull-off force”), given by Equations (4) and (20) for the JKR and Bradley (or DMT) model, respectively [23]

$$F_{po}^{Bradley} = 2\pi R^* \Gamma \tag{20}$$

Finally, Equation (5), after replacing by Equations (4), (17) and (18), takes the form of Equation (21):

$$\delta_{to} = \sqrt[3]{\frac{16.655R_1R_2\Gamma^2(1-\nu^2)^2}{(R_1 + R_2)E^2}} \tag{21}$$

So, Table 3 is created by taking $R_1 = R_2 = R_{ave} = 25 \mu\text{m}$.

Table 3. Calculated relative approach and Tabor parameter for different shear modulus values.

CASE	G (Pa)	ν	E (Pa)	E^* (Pa)	R_{ave} (μm)	R^* (μm)	$\Gamma \left(\frac{\text{J}}{\text{m}^2} \right)$	z_0 (Å)	δ_{to} (μm)	μ
SIM – 1	1×10^7	0.3	3.2×10^7	1.76×10^7	25	12.5	4.26	5.1	1.451	1768.56
SIM – 2	1.5×10^8	0.3	4.8×10^8	2.64×10^8	25	12.5	4.26	5.1	0.239	290.78
RW – 3	1.29×10^{11}	0.3	4.13×10^{11}	2.27×10^{11}	25	12.5	4.26	5.1	0.003	3.22

It remains, to the authors’ knowledge, untested whether the contact radius setting has to be chosen based on the real-world G value or based on the G value that is set within the simulation environment in order to increase the timestep. Table 3 compares three different cases. By examining μ for each case, it is noticeable that the higher the particle’s stiffness, the smaller its relative approach at bond breakage. Indeed, when the material becomes less compliant and elastic, μ decreases by 3 orders of magnitude, from 1768.56 to 3.22, while the respective approach at bond breakage also decreases from around 1.5 μm to around 3 nm.

In order for adhesive/cohesive forces to facilitate, two particles or a particle and a body need to come into physical contact first. This check happens via the physical radii of the two bodies. However, the contact radius creates a zone around each particle where a negative

approach is possible. As the two particles collide, they simultaneously demonstrate their compliance/elasticity and their cohesion. Upon collision, they behave like springs, initially with a positive approach, where they decelerate as they deform more and more. However, this collision is less “violent”, and they decelerate slower than they would if the cohesive forces had not been present since they are now attracted to each other due to Van der Waals forces. Eventually, the approach will stop increasing, and it will decrease again; however, when it becomes zero, the particles will not separate, but the “bottleneck effect” will develop since the particles will remain in contact due to the cohesive forces, and further work is required in order to create two new, separated surfaces. Figure 1 explains the stages of contact between two particles. The larger EDEM’s contact radius is, the larger the negative approach it will allow, hence the larger the “zone of influence” each particle will create around it, within which attracting adhesive forces will act. Hence, the larger the EDEM’s contact radius, the more cohesive the behavior the powder will exhibit. The real-world material is much stiffer and less cohesive compared to the one in the simulations. For the simulations, the value of the contact radius is 26 μm, which would be valid in the case where the relative approach at bond breakage would be 1 μm. By setting the difference between the physical and contact radii of the average particle at 1 μm, the simulation is easily scalable, while the increased cohesion makes this a study “on the safe side”, since, if the suggested system can counter the simulation material’s cohesion, the real-world material will be much easier to spread evenly.

It is of some interest to examine the fluctuation of the particles’ behavior in the simulation with regard to their real-world behavior (see Table 4).

Table 4. The relation of parameter values between the real world and the simulation-defined material. In parentheses, it is stated how this parameter affects the powder’s behavior compared to its counterpart.

	<i>REAL-WORLD PARTICLES</i>	<i>SIMULATION PARTICLES</i>
<i>Young’s modulus</i>	↑ (less elasticity)	↓ (more elasticity)
<i>Tabor’s parameter</i>	<5 (less elasticity)	>100 (more elasticity)
<i>Suitable model for F_{p0}</i>	Bradley ($2\pi R^*\Gamma$) (more cohesion)	JKR ($3/2\pi R^*\Gamma$) (less cohesion)
<i>Relative approach to bond breakage δ_{to} (μm)</i>	3 nm (less cohesion)	1451 nm (more cohesion)

Table 4 shows that the real-world material is stiffer and less compliant, which is also reflected in the calculated μ . The most suitable model for the real-world particles would be the BD, while the simulation implements a JKR pull-off force, which is 25% lower. Despite their higher rigidity, which is translated to shorter collisions of smaller deformations and sharper force profiles during contact with real-world particles, these demand a 25% larger pull-off force in order to escape from cohesive forces by their neighboring particles, which slightly compensates for the less cohesive behavior they demonstrate and is also visible by examining the relative approach at bond breakage.

2.2.3. Experimental Validation

In order to ensure that the modeled powder behaves realistically in terms of flowability and kinematics in any possible situation, a cross-check between simulation and experiment is necessary. It has been proven in the literature that a simulation–experimental cross-check for the combination of angle of avalanche and angle of repose tests is enough to ensure whether the powder model is adequate and whether its rheological characteristics approach the real powder [7,8]. This is explained since “the avalanche angle experiment suggests the powder to gravitational, cohesive and shear forces inflicted by the wall of the cylinder till a dynamic equilibrium state is reached (if possible), whereas the repose angle experiment only examines the powder’s cohesion in respect with the gravitational forces, letting the powder reach a static equilibrium state.” (Avrampos et al., (2022)) [8].

The powder material properties, particle–particle and particle–body interaction coefficients, and contact model implemented in this work were the same as in the work of Zhang et al. (2020) [7] (see Section 2.2.2. Zhang et al. (2020)); in their work, they initially ran a Jenike shear test (ASTM D6773 [37]) to define the static friction coefficients. The rolling friction coefficients were set to a low value due to the brittleness of alumina, while the restitution coefficients were referenced by the literature [38]. The interparticle and particle–wall interfacial surface energies were calibrated according to the cross-check for the angle of repose test.

They found the experimental values for the angle of repose and angle of avalanche to be 25.8° and 36.7° , respectively, while the simulation values were 26.2° and 37.1° , respectively, showing a deviation of only +1.6% and +1.1%, respectively; hence, proving the realistic behavior of the powder model that was used [7].

2.2.4. Simulation Geometry and Kinematics

The powder spreading simulation features 6 physical bodies and a virtual shape necessary to use as a powder factory. The 6 physical bodies are the substrate onto which the powder is deposited; the doctor blade, which performs the powder spreading; and 4 metal plates that serve as the left, right, back and front border of the powder layer. These geometrical borders create a square sample area with a side of 1 mm. The height of the back and front border plates is equal to the theoretical layer thickness, i.e., $100\ \mu\text{m}$, while that of the right and left border plates is equal to 1 mm (see Figure 4a).

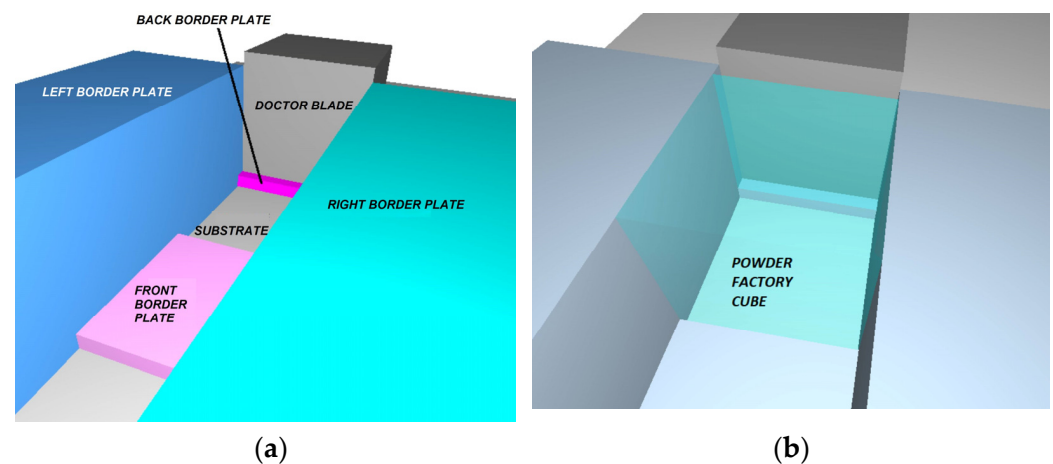


Figure 4. (a) The physical bodies of the powder spreading simulation; (b) semi-transparent cyan cube, which functions as a powder factory.

Above the sample square, there is a virtual cube with a 1 mm side, which functions as the powder factory (see Figure 4b). The simulation populates the area inside this virtual cube with spherical powder particles of a diameter that follows the lognormal distribution that was described in previous sections. This area is simultaneously populated for all particles at the start of the simulation, ensuring that no particles are in physical contact with each other at the moment of their generation.

Then, the particles free-fall vertically onto the sample square under the influence of gravity, creating a slope in front of the doctor blade that performs the deposition (see Figure 5).

The smaller particles fall slower compared to larger ones due to the effect of air drag. The simulation enables natural gravity and Schiller–Naumann drag model [39,40]; the air’s characteristics are as follows: $\rho_{air} = 1.225\text{kg}/\text{m}^3$, $\nu_{air} = 1.81 \cdot 10^{-5}\text{Pa}\cdot\text{s}$, $\vec{u}_{air} = 0\hat{i} + 0\hat{j} + 0\hat{k}$, $scale = 1$, where ν_{air} is the kinematic viscosity of the air; \vec{u}_{air} is the velocity of the air, indicating that the simulation features no air flow; and “scale = 1” means that the amount of drag applied to each particle is the full amount with regard to its size and not a fraction of it.

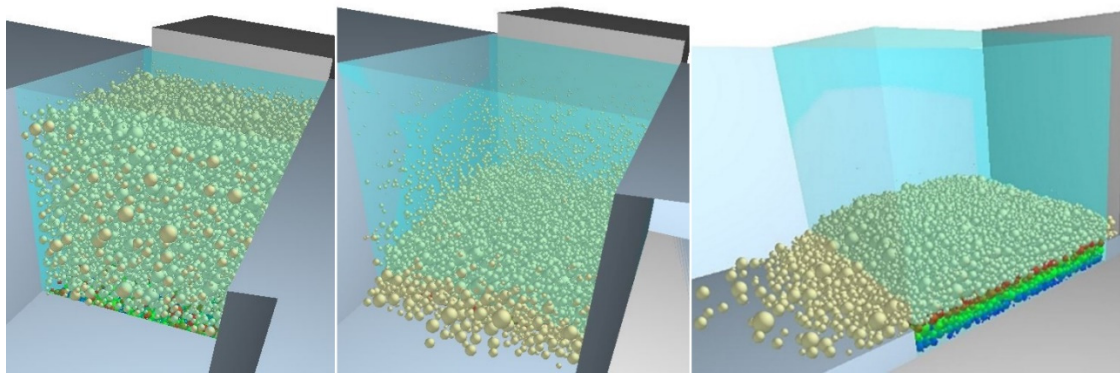


Figure 5. (Left) The initial moment of powder generation; (Middle) particles’ free-fall onto the substrate, over the sample square; (Right) particles’ free-fall complete. The slope has been created/deposition is ready to begin.

The material of the physical geometry is stainless steel 304; its properties are as follows [41]: $\rho_{St.304} = 8000 \text{ kg/m}^3$, $\nu_{St.304} = 0.275$, $G_{St.304} = 62.3 \text{ GPa}$, $E_{St.304} = 193 \text{ GPa}$.

The powder material properties and the powder–powder and powder–body interaction coefficients were set as described in Section 2.2.2, Sub-section “Material Properties Modelling”.

After the slope was created and the particles were all “frozen”, i.e., at a status of negligible kinetic energy, the doctor blade performed the spreading process. The spreading consists of a superposition of a linear translational motion with a constant speed along the axis of deposition (x-axis) and a vertical (along z-axis) vibrational motion, i.e., a sinusoidal oscillation of constant frequency and amplitude throughout the deposition process. In this example, the frequency was set to $f_{vib} = 2000 \text{ Hz}$ and the amplitude to $A_{vib} = 5 \text{ }\mu\text{m}$. Similarly, the spreading speed was set to $u_{tr} = 0.01 \text{ m/s}$.

2.3. Surface Evaluation and Quality Criteria

The result of each powder-spreading simulation is a square layer of (1 mm × 1 mm), with a theoretical thickness of 0.1 mm. Then, a file containing the coordinates of the centers of the spherical particles, the particles’ diameter and the particles’ ID is exported. Particle ID is a unique number for each particle assigned to them at the moment of their generation. The same file contains the timestamp of the moment, which corresponds to the extracted data, and the total mass of the particles that comprise the layer. Table 5 shows the format of the exported data.

Table 5. Structure of the exported EDEM file for the particles constituting the layer of the simulation trials.

Particle ID	Diameter	X_{centre}	Y_{centre}	Z_{centre}
1	1.39×10^{-5}	−0.0001	−0.00017	0.000507
3	1.98×10^{-5}	−0.00038	−0.0002	0.000531
⋮	⋮	⋮	⋮	⋮
20,609	3.51×10^{-5}	−0.00013	−0.00035	0.000531

Figure 6 is a top view of the finished deposited powder layer. The particle coloring happens either via their centers’ Z-coordinate (see Figure 6a) or via their diameter (see Figure 6b). Particles that are positioned higher or have a larger diameter are assigned red colors, and the ones that are positioned lower or have a smaller diameter are assigned blue colors. The exported file (see Table 5) includes the data of every particle that constitutes the layer. To calculate the actual layer thickness, only the points that constitute the top of the exported layer are mathematically defined via the following methodology.

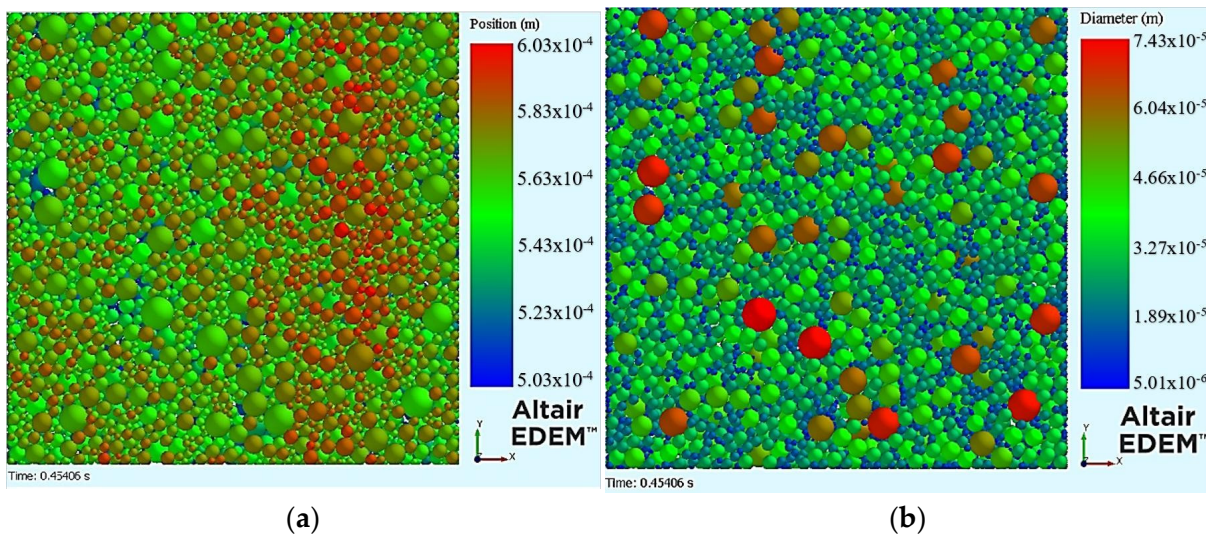


Figure 6. Sample top view of the deposited powder layer, with the coloring of the particles via (a) vertical position and (b) diameter.

Initially, a grid is defined within the $1\text{ mm} \times 1\text{ mm}$ square within which the powder is located. The grid has x-step $\Delta x = 1\text{ }\mu\text{m}$ and y-step $\Delta y = 1\text{ }\mu\text{m}$. The grid size is 5 times smaller than the smallest particle’s diameter ($5\text{ }\mu\text{m}$). An even finer grid was proved to not increase the results’ accuracy; contrariwise, it increases the computational time and even causes an overflow in some cases. Hence, the square has 1001 x-values and 1001 y-values, the respective lines intersecting each other, developing a grid of $n_{nodes} = 1,002,001$ “nodes”. The start of the coordinate system is positioned at the center of the square. From each node, a vertical linear “ray” is cast. This vertical line intersects some particles of the layer. To calculate the layer points, a script in C language, which uses the exported data (see Table 5) as input, compares the z-coordinates of all the intersection points of each “ray” with the particles and keeps the one with the highest z-coordinate. If a “ray” has no intersections with any particles, then the layer point that refers to this node is the node itself. The code is explained via the flowchart in Figure 7.

The point cloud of the layer’s top surface is then used to quantify the layer’s quality by four quality criteria, namely the layer thickness deviation (LTD), surface coverage ratio (SCR), root-mean-square surface roughness (S_q -RMS) and true packing density (PD or PD_{tr}), which will be defined in Sections 2.3.1–2.3.4.

2.3.1. Actual to Theoretical Layer Thickness Deviation

It is necessary to examine how closely the actual layer thickness approaches the theoretical layer thickness, which corresponds to the vertical distance between the substrate’s surface and the plane that the lower edge of the doctor blade creates as it moves horizontally along the x-axis. The vertical displacement of the fabrication piston is commonly assumed to be equal to the layer height, which is inaccurate. The actual layer thickness is slightly smaller due to interparticle cohesive and particle-recoater adhesive phenomena, where the impact varies with basic spreading parameters such as the recoater’s translational speed or the layer height.

Based on the calculated point cloud of the layer’s top surface, the actual layer thickness deviation is given by Equation (22):

$$(LTD) = (h_l - h_{l,th}) = \left(\frac{1}{n_{nodes}} \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} z_{LAYER_{i,j}} \right) - h_{l,th} \tag{22}$$

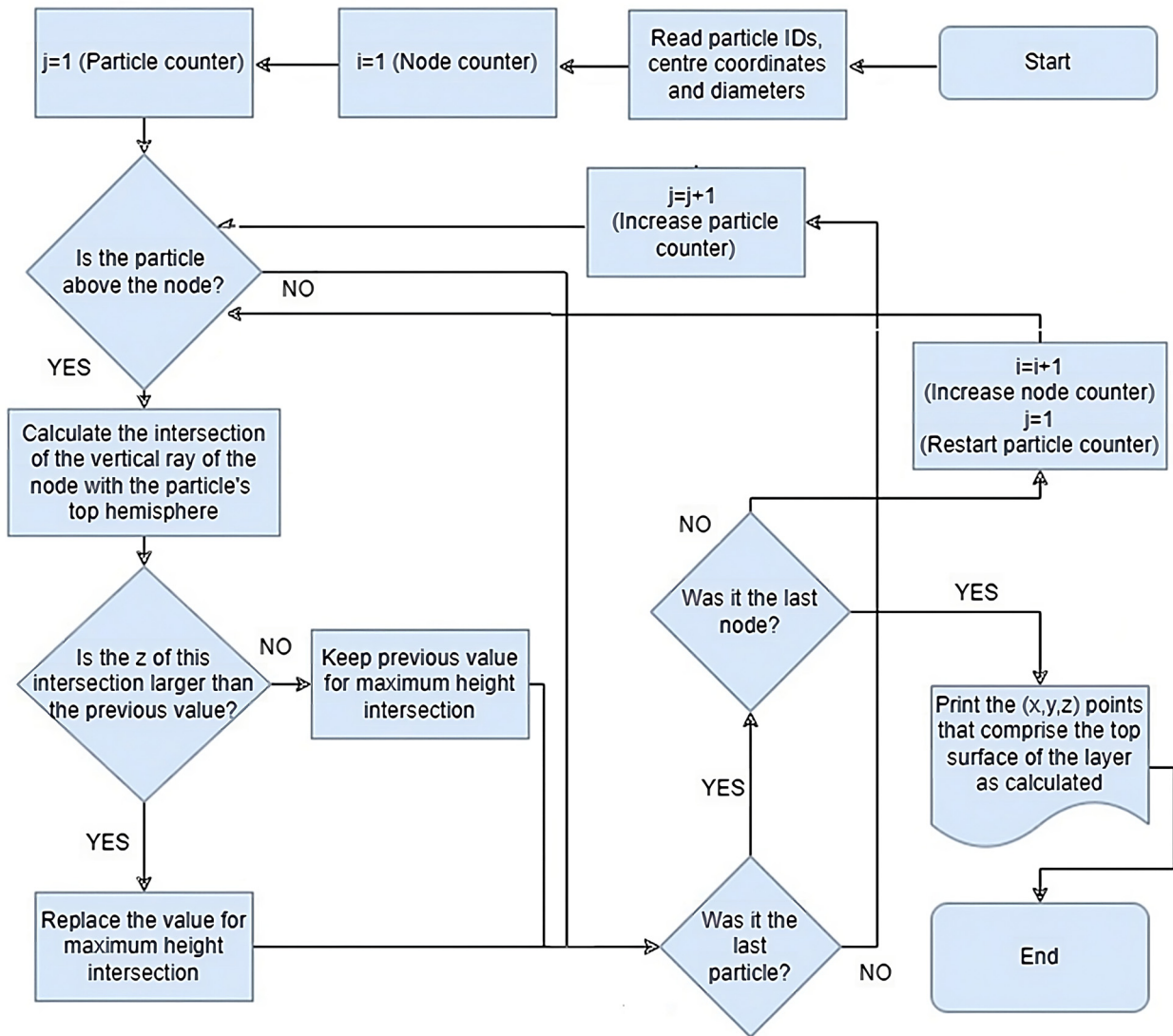


Figure 7. Flowchart of the top-surface layer calculation code.

The actual layer thickness corresponds to the mean plane of the powder layer surface, i.e., the plane $z = h_l$. In order to calculate surficial parameters (see Section 2.3.3), a “capital- z ” (Z) height variable is defined, which corresponds to the plane $z = h_l$, instead of the reference plane $z = 0$; see Equation (23) as follows:

$$Z_{i,j} = z_{LAYER_{i,j}} - h_l \tag{23}$$

2.3.2. Surface Coverage Ratio

By examination of the layer’s top view, uncovered areas might be spotted, i.e., areas where the substrate is visible (see Figure 8). In optimum deposition, the gaps are filled with smaller-sized particles, completely eradicating such defects.

These uncovered areas might be caused by a larger particle/particle cluster being dragged along the surface or being pushed at such a high speed that its inertia enables it to keep moving for a longer than the desirable distance after losing contact with the recoater, causing a gap behind it. To create high-quality layers, it is of paramount importance to minimize the uncovered nodes, i.e., the nodes for which the c -code (see Figure 7) has returned no “ray”–particle intersections; hence, it has zero particles above it. The surface

coverage ratio (SCR) is calculated by dividing the number of uncovered nodes by the total number of nodes within the sample square (Equation (24)).

$$SCR(\%) = \left(\frac{n_{uncovered}}{n_{nodes}} \right) \cdot 100\% \tag{24}$$

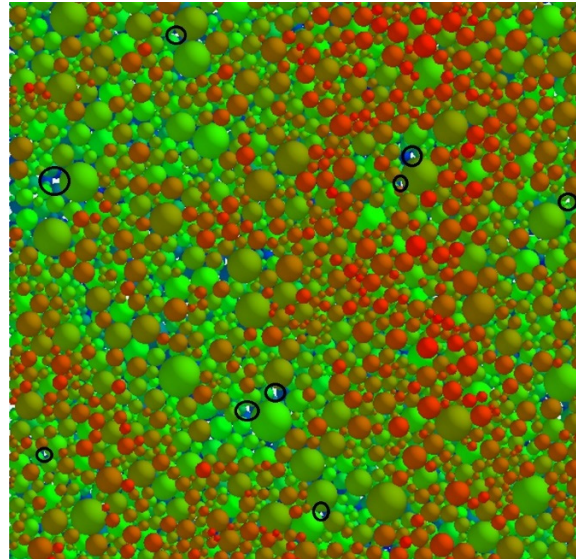


Figure 8. Black circles are uncovered areas where the substrate is visible, denoting coverage defects.

The maximum SCR value is 100% by definition, corresponding to perfect coverage. It was estimated by examining the 27 layer samples developed for the Taguchi DoE (see Table 6) that layers with SCR below 98.5% are considered to be unacceptable for PBF processes since the surface quality deteriorates drastically below that SCR value.

Table 6. L27 Taguchi orthogonal array for powder spreading.

#	$u_{tr} (\frac{m}{s})$	$f_{vib} (Hz)$	$A_{vib} (\mu m)$	$\theta_{rel} (deg.)$	(LTD) (μm)	LTD (μm)	SCR (%)	$S_q (\mu m)$	$PD_{tr} (%)$	$S_a (\mu m)$	Ssk	Sku
1	0.01	500	1.0	0	−29.0	29.0	98.9	19.9	68.4	15.5	−0.672	3.889
2	0.01	500	2.5	5	−26.0	26.0	99.1	17.9	68.0	13.6	−0.906	4.852
3	0.01	500	5.0	10	−21.2	21.2	99.3	17.4	67.1	13.0	−1.179	5.572
4	0.01	1000	1.0	5	−26.7	26.7	99.1	18.1	67.6	13.8	−0.956	4.741
5	0.01	1000	2.5	10	−24.3	24.3	99.0	18.0	67.4	13.5	−1.351	5.626
6	0.01	1000	5.0	0	−22.2	22.2	99.3	16.1	68.0	12.1	−1.515	6.403
7	0.01	2000	1.0	10	−23.8	23.8	99.0	17.9	67.0	13.6	−1.338	5.570
8	0.01	2000	2.5	0	−23.0	23.0	99.1	17.0	67.8	12.8	−1.503	6.075
9	0.01	2000	5.0	5	−21.5	21.5	99.3	16.4	67.8	12.3	−1.431	6.232
10	0.05	500	1.0	5	−36.6	36.6	97.7	21.6	67.2	17.0	−0.685	3.347
11	0.05	500	2.5	10	−34.9	34.9	97.7	22.4	66.8	17.6	−0.577	3.362
12	0.05	500	5.0	0	−31.7	31.7	98.6	18.8	67.5	14.6	−1.042	4.358
13	0.05	1000	1.0	10	−36.9	36.9	97.9	20.4	66.8	16.1	−0.811	3.602
14	0.05	1000	2.5	0	−33.8	33.8	98.5	19.2	67.0	15.0	−0.926	3.993
15	0.05	1000	5.0	5	−32.1	32.1	98.4	19.9	67.1	15.5	−0.898	3.993

Table 6. Cont.

#	u_{tr} (m/s)	f_{vib} (Hz)	A_{vib} (μm)	θ_{rel} (deg.)	(LTD) (μm)	LTD (μm)	SCR (%)	S_q (μm)	PD _{tr} (%)	S_a (μm)	Ssk	Sku
16	0.05	2000	1.0	0	−35.0	35.0	98.1	20.2	67.1	15.9	−0.869	3.698
17	0.05	2000	2.5	5	−32.4	32.4	98.6	19.2	67.1	14.9	−0.962	4.116
18	0.05	2000	5.0	10	−32.2	32.2	98.5	20.0	67.1	15.5	−0.815	3.956
19	0.10	500	1.0	10	−40.8	40.8	97.0	22.8	67.3	18.2	−0.399	3.051
20	0.10	500	2.5	0	−41.2	41.2	96.9	21.8	67.9	17.4	−0.597	3.059
21	0.10	500	5.0	5	−36.9	36.9	97.5	22.0	67.0	17.3	−0.596	3.310
22	0.10	1000	1.0	0	−41.4	41.4	97.0	21.7	67.6	17.3	−0.633	3.063
23	0.10	1000	2.5	5	−40.7	40.7	96.1	24.9	67.4	20.1	−0.323	2.732
24	0.10	1000	5.0	10	−37.0	37.0	94.9	28.7	66.9	22.9	−0.224	2.753
25	0.10	2000	1.0	5	−40.2	40.2	97.3	21.3	67.3	17.0	−0.622	3.169
26	0.10	2000	2.5	10	−41.1	41.1	97.3	22.5	67.5	18.0	−0.335	2.940
27	0.10	2000	5.0	0	−40.2	40.2	97.2	21.3	67.5	16.8	−0.558	3.604

2.3.3. Root-Mean-Square Surface Roughness

The importance of the deposited layer’s surface roughness to the finished product’s quality has already been stressed in the literature [8]. Deep valleys or high peaks are detrimental to the quality since they can be inherited by the next layers, affecting the surface quality or even the part’s dimensional accuracy. It is common practice to extract powder layer profiles via methods such as white light scanning [42] to evaluate the two-dimensional surface roughness. This method’s disadvantage is the possible omission of profiles where significant defects are present, falsely leading to a higher layer quality estimation. To address this issue, the areal method is implemented in this work to calculate the surficial root-mean-square (RMS) roughness.

S_q (see Equation (25)) is among the most widely used parameters. It corresponds to the standard deviation of the height distribution, generates reliable statistics and enables stable results since it is not significantly influenced by scratches, contamination, and measurement noise.

$$S_q = \sqrt{\frac{1}{A} \iint_A Z^2(x, y) dx dy} \tag{25}$$

where A is the sample area (in this work $A = 1 \mu\text{m}^2$), and $Z(x, y)$ is given by Equation (23). As noted in Section 2.3.1, in order to calculate any surficial parameters, the height $Z(x, y)$ that denotes the top surface of the layer refers to the mean plane of the surface, $z = h_l$ (see Equation (23)). Hence, from now on, the term Z refers to $(z_{LAYER} - h_l)$. Since it is not possible to formulate an analytical equation to describe the top surface of the powder layer, Equation (25) must be solved numerically.

The integral in Equation (25) is the volume between the surface $Z^2(x, y)$ and the plane $Z = 0$. The calculation happens via a column of points with coordinates $P_{i,j}(x_{i,j}, y_{i,j}, Z_{i,j}^2)$. This volume is divided into many infinitesimal volumes shaped like truncated right rectangular prisms with square bases of $\Delta x = \Delta y = 1 \mu\text{m}$. More specifically, they are prisms with square bases; however, the four vertical edges of each prism are of various lengths (or heights) (see Figure 9). These volumes are calculated via the trapezoid rule.

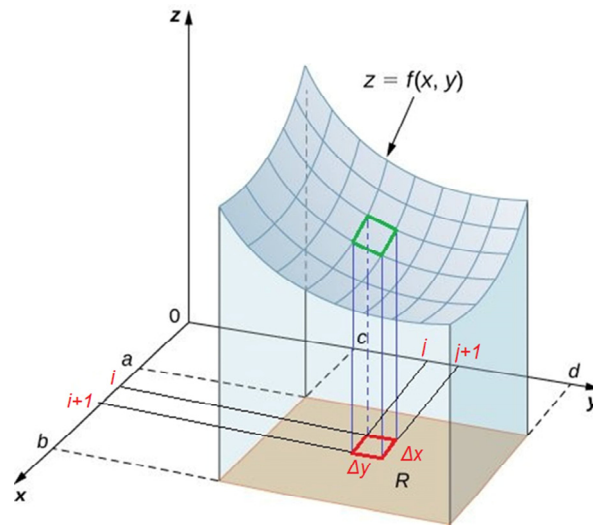


Figure 9. Infinitesimal prism visualization.

The volume secluded between the nodes ($N_{i,j}, N_{i+1,j}, N_{i+1,j+1}, N_{i,j+1}$) and the points ($P_{i,j}, P_{i+1,j}, P_{i+1,j+1}, P_{i,j+1}$) is given by Equation (26):

$$\Delta V_{Z^2} = \frac{\Delta x \cdot \Delta y}{4} \cdot (Z_{i+1,j+1}^2 + Z_{i,j+1}^2 + Z_{i+1,j}^2 + Z_{i,j}^2) \tag{26}$$

Then, the integral $V_{Z^2} = \iint_A Z^2(x, y) dx dy$ is calculated by summation of every infinitesimal prism.

If a node is located at one of the 4 corners of the sample square, the only infinitesimal prism it is part of is the one located at the corner of the sample square. However, if a node is located on one of the four edges of the square sample, it is part of two different infinitesimal prisms; hence, it contributes twice to the total volume. Finally, if a node is interior to the sample square, i.e., it does not belong to either an edge or a corner of the sample square, then it belongs to four different infinitesimal prisms, contributing to the total volume four times. Hence, S_q is given by

$$S_q = \sqrt{\frac{1}{A} V_{Z^2}} \tag{27}$$

Similarly, the arithmetical mean height (S_a), skewness (S_{sk}) and kurtosis (S_{ku}) are calculated by:

$$S_a = \frac{1}{A} \iint_A |Z(x, y)| dx dy \tag{28}$$

$$S_{sk} = \frac{1}{S_q^3} \left[\frac{1}{A} \iint_A Z^3(x, y) dx dy \right] \tag{29}$$

$$S_{ku} = \frac{1}{S_q^4} \left[\frac{1}{A} \iint_A Z^4(x, y) dx dy \right] \tag{30}$$

Skewness (S_{sk} -unitless) represents the degree of symmetry of the surface heights about the mean plane. Skewness' sign indicates the peak or valley predominance of a surface. Negative skewness values indicate an upwards-deviated distribution, i.e., a surface with deep valleys and smoother, more even plateaus. Positive skewness indicates a downwards-deviated distribution, i.e., a surface with high peaks with smoother and less steep valleys.

Kurtosis (S_{ku} -unitless) is used to evaluate sharpness in the height distribution. More specifically, $S_{ku} > 3$ indicates the presence of inordinately high peaks/deep valleys or lack thereof ($S_{ku} < 3$) making up the texture. For normally distributed surface heights (i.e., bell

curve), S_{sk} is 0, and S_{ku} is 3. Surfaces described as gradually varying, free of extreme peaks or valley features, tend to have $S_{ku} < 3$ [43].

Skewness is useful for monitoring the effect of wear on a surface (e.g., evaluating the abrasion and oil sump of lubricants for slide planes), while kurtosis is used for spotting the presence of either peak or valley defects that may occur on a surface [44,45].

Other useful surficial parameters, like the peak-to-valley roughness (S_z), the maximum peak height (S_p) and the maximum peak depth (S_v), mostly identify the magnitude of the largest defects of the surface and fail to examine the consistency and evenness of the surface, which the aforementioned metrics examine more accurately.

2.3.4. True Packing Density

The packing density, or compaction ratio, is directly connected to the finished parts' density and microhardness [46].

In many works, "theoretical" packing density is calculated by dividing the mass of a layer by the theoretical volume of the layer, which is calculated by multiplying its border dimensions along the three axes, x , y and z [47,48]. However, the actual layer height differs from the theoretical layer height (see Section 2.3.1). Theoretical packing density is an indicator of how well the powder layer is "filled" but fails to show how well the particles themselves have been arranged in order to increase their coordination numbers and minimize the air gaps between them. In this work, the true packing density is calculated by using the actual instead of the theoretical layer thickness (see Equations (31) and (32)).

$$PD\left(\frac{\text{kg}}{\text{m}^3}\right) = \frac{m_{\text{LAYER}}}{V_{\text{LAYER}}} = \frac{1}{V_Z} \sum_{i=1}^{n_{\text{particles}}} m_{\text{particle},i} \quad (31)$$

$$PD(\%) = \left(\frac{PD\left(\frac{\text{kg}}{\text{m}^3}\right)}{\rho_{\text{powder, BULK}}} \right) \cdot 100\% \quad (32)$$

3. Results

3.1. Design of Experiments

The Taguchi DoE is a statistical tool used to reach conclusions when it comes to the effect of various factors on the result of an experiment with regard to some quality criterion that is set beforehand. The number of factors and the number of each factor's levels leads to the selection of an orthogonal array (OA) suitable to accommodate all the necessary combinations of the factors' levels in order to reach solid outcomes [49].

Four variables are examined:

- *Translational speed of the doctor blade* along the deposition (x) axis (u_{tr}), examined at three levels: 0.01 m/s, 0.05 m/s, 0.1 m/s. These levels were selected according to the current industrial SLS/SLM machines' powder deposition speed standards. These were validated in both the prototype SLS/SLM powder deposition system designed [1,42] as well as via the industrial SLM machine of the Laboratory of Manufacturing Engineering of the School of Mechanical Engineering of NTUA (Z-rapid iSLM280, ZRapid, Suzhou, China).
- *Vibrational frequency of the doctor blade* along the vertical (z) axis (f_{vib}), examined at three levels: 500 Hz, 1000 Hz, 2000 Hz. The frequencies selected were relatively low compared to, say, ultrasound frequencies to maintain a reasonably high simulation timestep. Furthermore, the simulations seek to examine whether a low-frequency-vibrating doctor blade benefits powder spreading compared to vibration-less deposition, which is the common powder deposition method encountered in the industry. Preliminary testing of vibration-less doctor blade powder deposition examined the deposited layer's quality for a flat doctor blade at two different translational speed levels, i.e., 0.08 m/s, typical of commercial machines (see Figure 10a) and 0.01 m/s (see Figure 10b). The cross-check between vibration-less and oscillating recoater deposition proved that vibration enhances the homogeneity and evenness of the deposited layer.

- *Vibrational amplitude of the doctor blade along the vertical (z) axis (A_{vib})*, examined at three levels: 1 μm , 2.5 μm , 5 μm . The amplitude values were selected in such a way that they are equal or less to the minimum particle diameter (5 μm), thus making it impossible for powder particles to escape behind the doctor blade via the gap between the doctor blade and the back border plate.
- *Angle of relief of the doctor blade (θ_{rel})*, examined at three levels: 0°, 5°, 10°. The geometry of the doctor blade is a quasi-cubic 3D shape with a 1 mm side (see Figure 11). The feature differentiating it from a cube is its angle of relief, beginning after a 100 μm horizontal flat area, implemented to enhance the vibration's powder compaction effect. Had this horizontal area not existed in the 5- and 10-degree doctor blades, negligible powder compaction would have been achieved via the blade's edge. Furthermore, this would render the simulation non-realistic since no sharpened blades are used for powder deposition. The size of this feature (100 μm) was selected to be 25 μm larger than the largest particle diameter (75 μm).

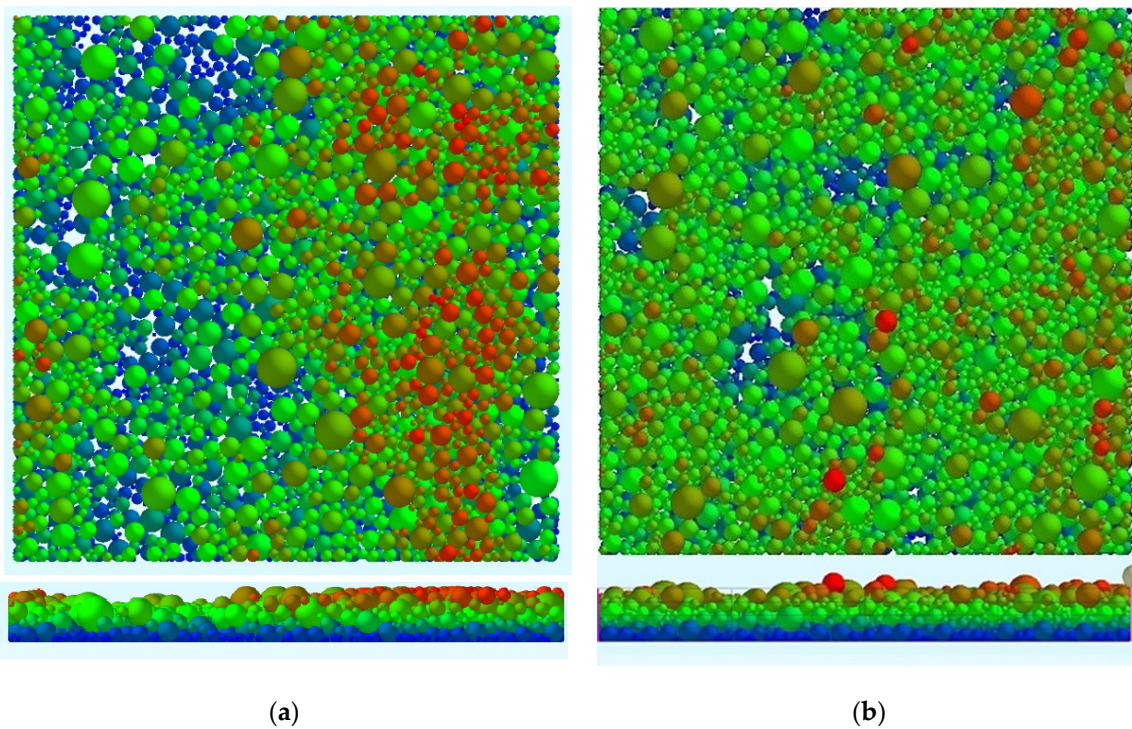


Figure 10. Powder deposition example (top and side views) with a non-vibrating doctor blade at deposition speed of: (a) 0.08 m/s; (b) 0.01 m/s.

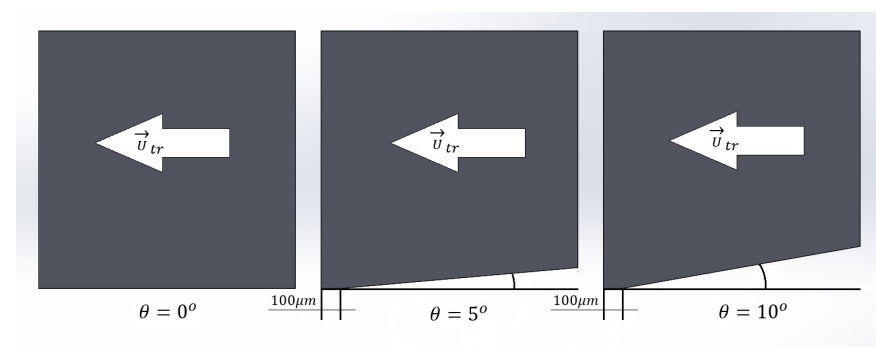


Figure 11. Side view of the doctor blade. Depiction of the angle of relief and the blade's profile.

The blade design resembles the relatively thick, commercially available doctor blades. Figure 11 shows that, as the angle increases, the secondary contact surface between the

blade and the particles decreases. The primary contact surface is the left vertical doctor blade’s surface, which forces the powder slope to move toward the direction of \vec{u}_{tr} . The secondary contact surface is the area that applies vertical pressure via vibration onto the powder layer, i.e., the 100 μm wide strip and the fraction of the inclined surface behind this strip that interacts with the particles via the vibrational and adhesive forces. When the relief angle equals 0° , the secondary contact area is equal to the entire 1 mm^2 of the doctor blade bottom area, while when the relief angle increases, the secondary contact area decreases to 0.1 mm^2 plus the decreasing inclined contact zone, as described above.

The goal is to optimize the response of all quality criteria simultaneously. This is not a trivial feat since each response is individually optimized at different levels. This work attempts to find global optimum levels of the spreading variables for all of the quality criteria to achieve the best possible outcome. Initially, each of the four responses is examined separately.

Table 6 presents the setup of the powder spreading simulations in an L27 Taguchi orthogonal array. The L27 provides the capability of examining three interactions, which is enough for this case study. Examining more interactions would overcomplicate the design and lead to a number of trials comparable to the full factorial design. The quality criteria are described in Sections 2.3.1–2.3.4, namely LTD, SCR, S_q -RMS and PD. The quality loss function is the lower, the better for LTD and S_q -RMS, and the higher, the better for SCR and PD. S_a , S_{sk} and S_{ku} are also presented since they provide useful observations. The regression equations are calculated using the Minitab™ (version 17) software. All regressions used four continuous predictors, i.e., the four variables of the Taguchi DoE; according to these, four linear terms and three interaction terms were used, as shown in Tables A1–A5 of Appendix A.

3.2. Shear Modulus Sensitivity

EDEM™ tutorials suggest an initial value of G around $1 \cdot 10^7$ Pa since the actual value drastically decreases the timestep (see Section 2.1.1). The suggested G value ranges between $1 \cdot 10^6$ Pa and $1 \cdot 10^9$ Pa.

In Table 7, both the critical timestep and the total simulation time of the three repetitions of Trial #9 of the Taguchi DoE are presented, along with the surface quality criteria of the deposited layer.

Table 7. Calculated timesteps and surface quality criteria for various G values. The settings used were those of trial #9 of the Taguchi L27 array for powder spreading, i.e., $U_{tr} = 0.01\text{ m/s}$, $f_{vib} = 2000\text{ Hz}$, $A_{vib} = 5\text{ }\mu\text{m}$ and $\theta_{rel} = 5^\circ$.

REP #	r_{min} (μm)	ρ ($\frac{\text{Kg}}{\text{m}^3}$)	ν	β	G (Pa)	Δt_c (nsec)	t_{sim} (h)	LTD (μm)	SCR (%)	S_q (μm)	PD (% of BD)
1	2.5	3820	0.3	0.9255	10^7	165.861	2.5	21.5 (+18.8%)	99.3 (−0.1%)	16.4 (+10%)	67.8 (+0.6%)
2	2.5	3820	0.3	0.9255	1.5×10^8	42.825	25	18.9 (+4.4%)	99.4 (\equiv)	15.8 (+6%)	67.4 (\equiv)
3	2.5	3820	0.3	0.9255	1.5×10^{11}	1.354	168	18.1	99.4	14.9	67.4

Three orders of magnitude G reduction caused the simulation duration to drop tenfold, from 168 h to 15 h, while only |LTD| and S_q were minimally affected (increased by 4.4% and 6%, respectively). By a further G decrease by another order of magnitude, again only |LTD| and S_q increased by a further 14.4% and 4%, respectively; the percentages are calculated as a fraction of their real-world G simulation (repetition #3) values.

To keep the duration of the 27 Taguchi trials within acceptable limits, the smallest G value was selected. The results deviate substantially only for |LTD| (18.8%), but not at such a level to justify running simulations that last 12 (25/2.5) or 67 (168/2.5) times more. The study remains “on the safe side”, because, by decreasing G , the quality of the layer

seems to deteriorate. If the surface quality is considered acceptable by the 10 MPa G value, then the layer produced by the real-world G value will be of higher quality, also rendering it acceptable.

3.3. ANOVA Results and Discussion

Figures 12 and 13 present the results corresponding to means and signal-to-noise-ratio, respectively. The former depicts the average response for each combination of control factor levels, while the latter is the ratio of the mean (signal) to the standard deviation (noise). Hence, the means plot shows the average performance, while the SNR plot shows the variance from the design. Additionally, Tables A1–A3 depict the ANOVA results for the LTD, SCR and RMS, respectively.

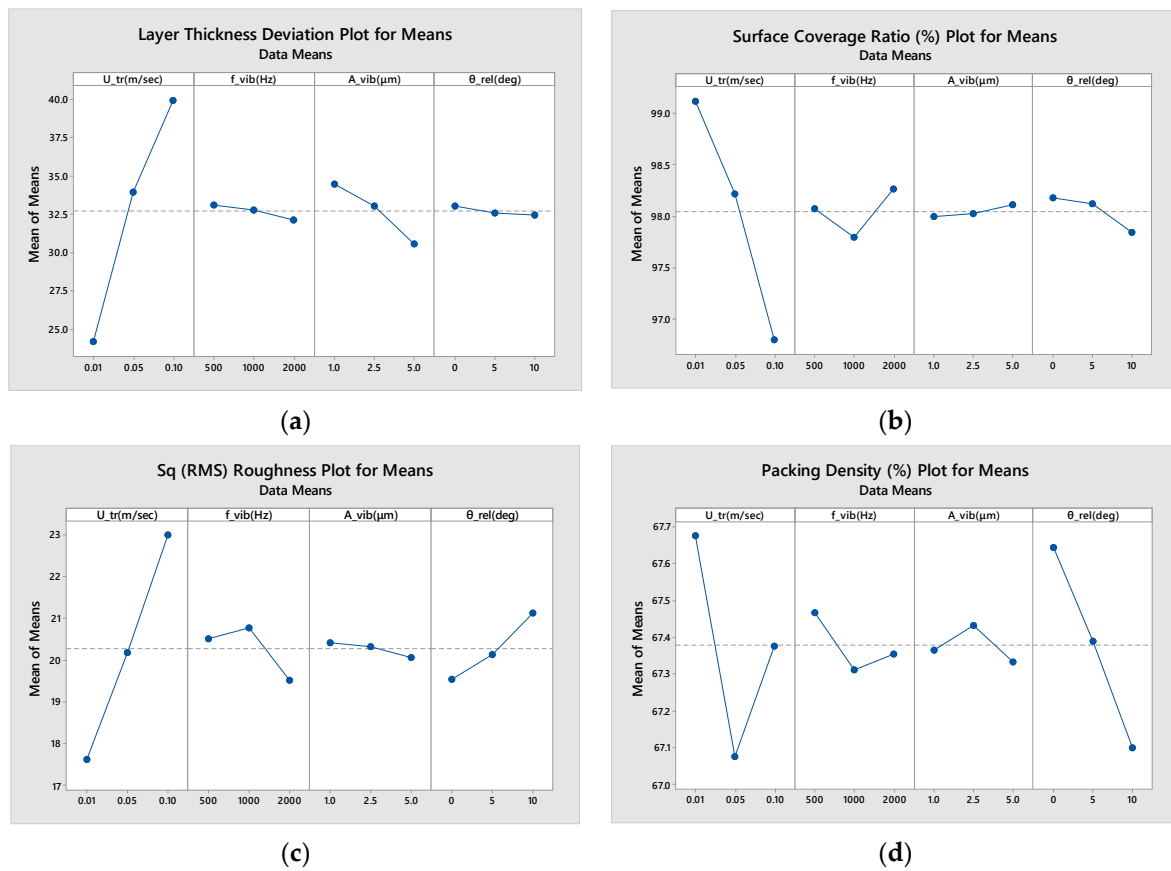


Figure 12. Means of the quality criteria: (a) LTD; (b) SCR; (c) RMS; (d) PD.

Figures 12 and 13 deduce that none of the four factors has a statistically important impact on the true packing density, which ranges from 66.8% to 68.4%, while the mean PD value varies between 67% and 67.7%. Indeed, the powder’s compressing mechanism relies mostly on gravity, since even the vibrating blade only momentarily pushes the layer downwards and then moves upwards again.

The blade vibrates between $z_{low} = h_{l,th}$ and $z_{high} = (h_{l,th} + A_{vib})$; hence, it does not compress the layer below the actual layer thickness level. Even though the theoretical packing density varies in an inversely proportional manner compared to the layer thickness deviation, the true packing density will not be examined as a quality criterion since it was proven that the four factors do not substantially affect it. The fact that the true PD remains unchanged might be caused by the small particle size, since the cohesive forces are large enough to prevent the gravitational forces from increasing the coordination number of each individual particle during the recoater’s compressive motion.

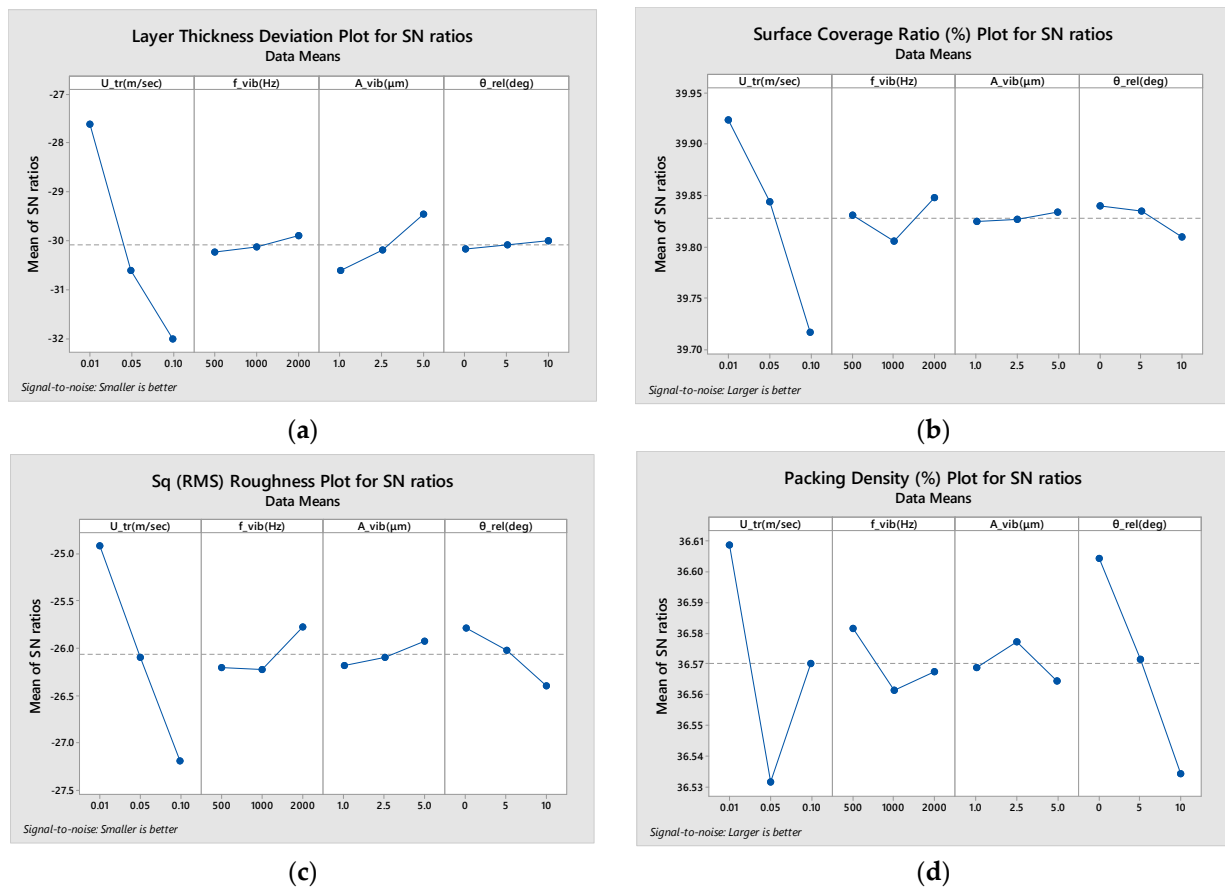


Figure 13. Signal-to-noise ratios: (a) LTD; (b) SCR; (c) RMS; (d) PD.

3.3.1. Layer Thickness Deviation

The “Contribution” column of the ANOVA for the |LTD| (Table A1) shows that |LTD| is primarily affected by u_{tr} (87.49%) and much less by A_{vib} (5.70%). f_{vib} and θ_{rel} contribute negligibly, at 0.36% and 0.12%, respectively, similar to the interactions between the factors. The only interactions examined are the interactions between u_{tr} and the other factors, since it is obviously the most impactful factor. Clearly, the smaller u_{tr} and the larger A_{vib} are, the more the actual layer thickness approaches the theoretical layer thickness.

Figure 14 shows that u_{tr} - A_{vib} and u_{tr} - f_{vib} interaction plots have approximately parallel lines; hence, they demonstrate a low degree of interaction, only traceable at higher speeds. Both couples show no interaction at low- and middle-speed levels; however, at higher speeds, it becomes more beneficial to maintain a low frequency and high amplitude. The interaction between u_{tr} and θ_{rel} reveals that, at low and high speeds, sharper blades with large angles of relief perform better, while, at middle speeds, the optimum performance belongs to the flat-bottomed blade.

3.3.2. Surface Coverage Ratio

Figures 12 and 13 show that SCR, like |LTD|, is primarily influenced by the u_{tr} (78.44% contribution, Table A2). Again, an increase in u_{tr} causes a decrease in SCR, deteriorating the layer quality.

Table A2 proves that θ_{rel} , f_{vib} and A_{vib} play a small role (1.60%, 1.02% and 0.19%, respectively) in terms of SCR. Figure 15 proves that the pair u_{tr} - θ_{rel} has negligible interaction; the flat-bottomed blades show better results at all speeds. However, for both the pairs u_{tr} - f_{vib} and u_{tr} - A_{vib} , there only is no interaction at low and middle speeds, and SCR is positively affected by higher frequency amplitude. Contrariwise, at greater u_{tr} values, this trend gets reversed in terms of A_{vib} ; smaller amplitudes give better SCR at maximum speed.

In terms of f_{vib} , middle-frequency levels drastically deteriorate SCR at maximum u_{tr} , leading to the conclusion that the natural frequency of the system is located at approximately 1000 Hz.

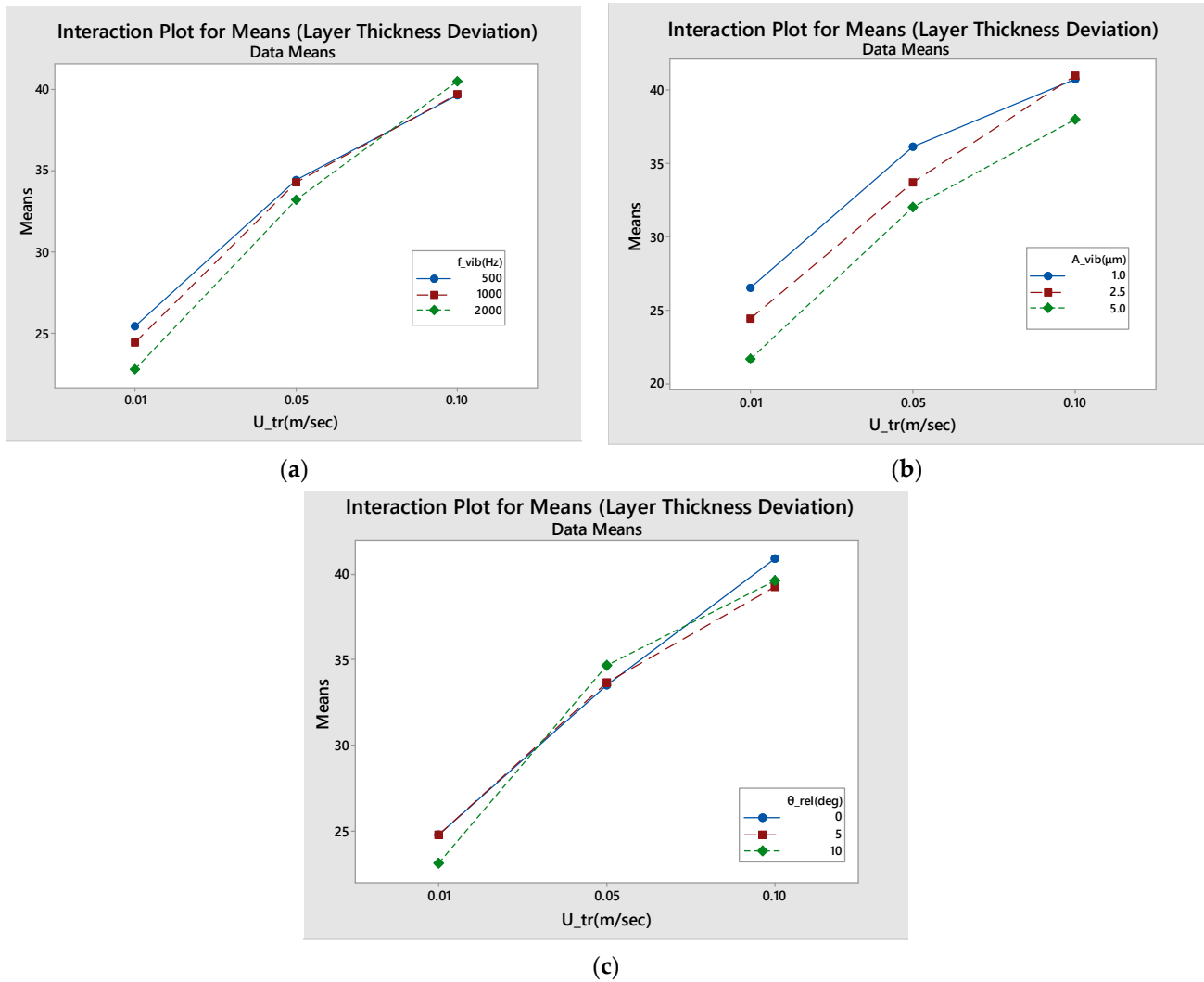


Figure 14. Interaction plots for means of $|LTD|$: (a) u_{tr} - f_{vib} ; (b) u_{tr} - A_{vib} ; (c) u_{tr} - θ_{rel} .

The regression’s error is higher than 10%, probably because of the high inherent complexity of the process. However, this does not harm the credibility of the results, as shown in the calculated deviation between the simulation and the expected regression value (see Table 8).

Table 8. Regression vs. simulation performance of optimum parameter sets for the three different quality criteria.

Optimum	u_{tr} (m/s)	f_{vib} (Hz)	A_{vib} (μm)	θ_{rel} ($^{\circ}$)	Regression Optimum	Simulation Optimum	Deviation (sim-reg)/reg	ANOVA Regression Error
$ LTD $	0.01	2000	5	10	20.8 μm	20.4 μm	-1.9%	5.32%
SCR	0.01	2000	5	0	99.54%	99.33%	-0.2%	15.52%
S_q -RMS	0.01	2000	5	0	15.8 μm	15.7 μm	-0.6%	15.67%

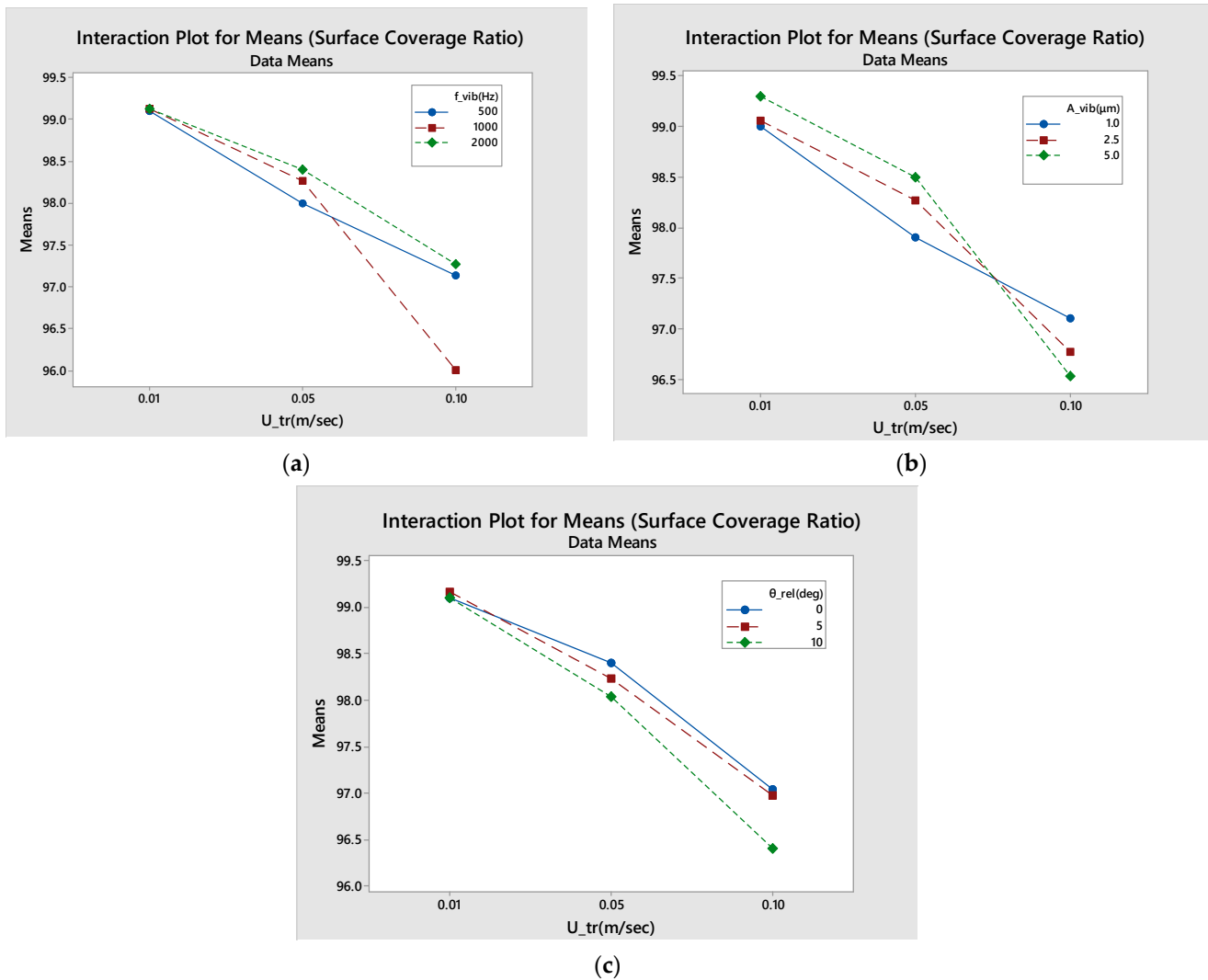


Figure 15. Interaction plots for means of SCR: (a) u_{tr} - f_{vib} ; (b) u_{tr} - A_{vib} ; (c) u_{tr} - θ_{rel} .

3.3.3. RMS Surface Roughness

Figures 12 and 13 for S_q -RMS show that the smaller u_{tr} is, the smaller S_q is; hence, the better the surface quality. S_q is affected more by θ_{rel} compared to previous criteria. Indeed, flatter blades tend to create smoother surfaces due to the increased contact zone between them and the surface. Again, high frequency and amplitude levels show better results in terms of S_q .

Table A3 shows that u_{tr} is again the prevalent, affecting factor (65.79%); however, θ_{rel} and the f_{vib} are also important (5.61% and 2.89% contribution, respectively). Despite the weak influence of A_{vib} (0.32%), its interaction with u_{tr} is quite significant (6.37%).

Interestingly, as seen in Figure 16c, even though at low u_{tr} , the effect of different θ_{rel} is negligible on S_q ; as the speed increases, the worse the results that are achieved via sharper blades. Furthermore, while between low and medium speeds, there seems to be no u_{tr} - f_{vib} or u_{tr} - A_{vib} interaction, this changes between medium and high-speed levels. While at low and medium speeds, it is beneficial to apply high A_{vib} , at high u_{tr} , it is beneficial to opt for a lower A_{vib} . This is possibly due to the high amount of kinetic energy fed towards the particles, which surpasses a threshold, leading to an unstable powder bed behavior increasing the surficial defects.

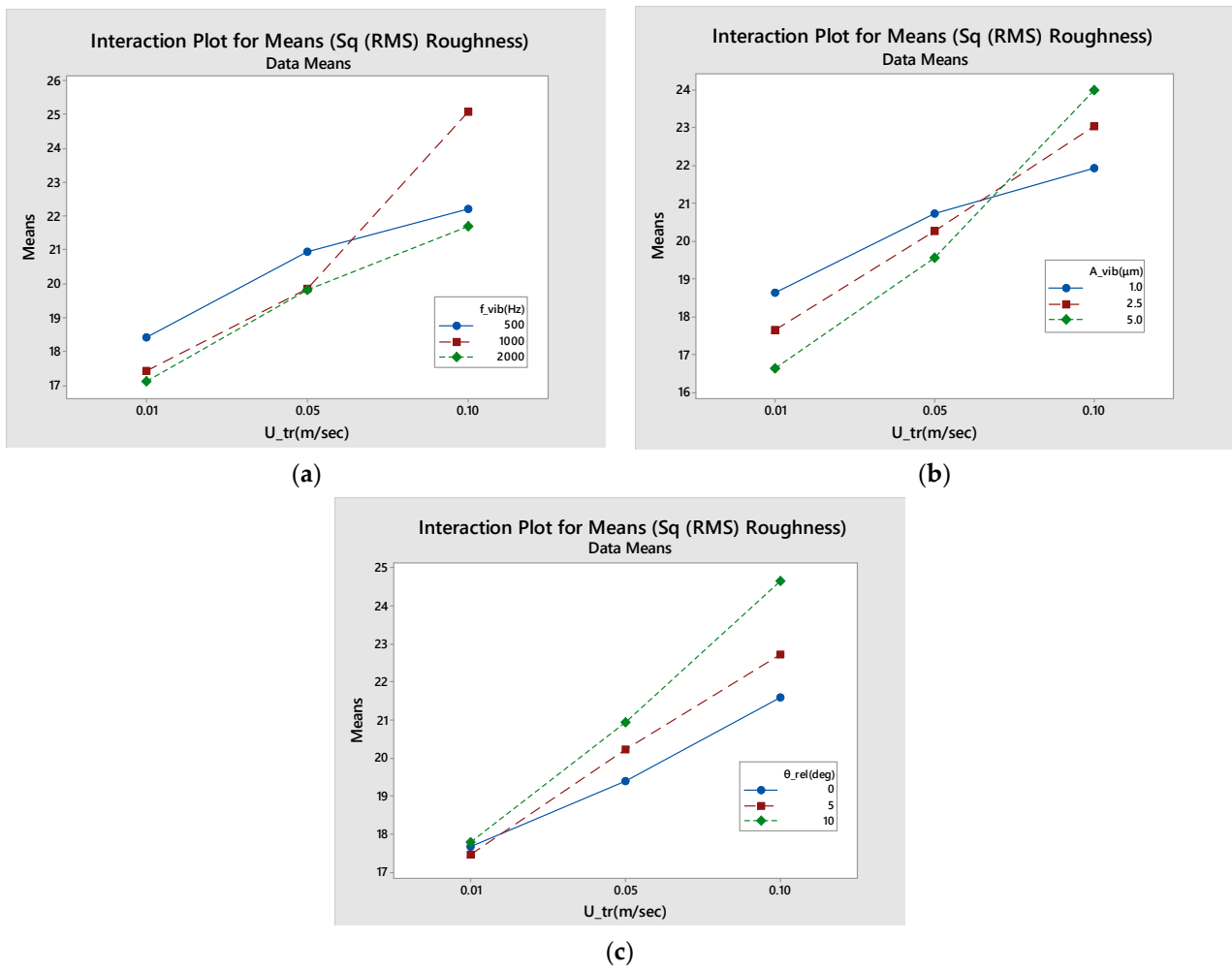


Figure 16. Interaction plots for means of S_q -RMS: (a) u_{tr} - f_{vib} ; (b) u_{tr} - A_{vib} ; (c) u_{tr} - θ_{rel} .

The error surpasses 10% due to the process complexity; however, this does not harm the credibility of the experiment and the validity of the results and conclusions (see Table 8).

In conclusion, if it is absolutely necessary to vastly increase the spreading speed (e.g., for production reasons), the negative outcome in terms of S_q -RMS and SCR can be partially compensated by opting for flat-bottomed blades and reducing A_{vib} while maintaining high f_{vib} . This leads to a slight $|LTD|$ increase, which is easily countered via adjusting the downwards motion of the fabrication piston, i.e., increasing $h_{l,th}$, while poor SCR and S_q -RMS signify important surficial defects, possibly inheritable to the next layers.

4. Discussion

Process Parameter Optimization

The optimum parameter sets for all three quality criteria is by $\frac{3}{4}$ identical (referring to u_{tr} , f_{vib} and A_{vib}) at $u_{tr} = 0.01$ m/s, $f_{vib} = 2000$ Hz, $A_{vib} = 5$ μm with the observation that flat-bottomed blades promote optimum SCR and S_q -RMS, while sharp blades promote higher $|LTD|$, compromising the other two (see Table 9).

Table 6 reveals that all trials have negative S_{sk} , as expected, since the top hemispheres of the particles create surfaces with smoother, rounder plateaus and deeper, sharper valleys, with an upper-side deviated distribution. Furthermore, almost every trial features $S_{ku} > 3$ (apart from #23 and #24), which is also expected, indicating the presence of inordinately deep valleys since the valleys reach the substrate at uncovered nodes.

Table 9. Performance comparison of optimum $|LTD|$, SCR and S_q values (reg: “regression”; sim: “simulation”).

OPTIMUM	u_{tr} (m/s)	f_{vib} (Hz)	A_{vib} (μm)	θ_{rel} (deg)	$ LTD _{reg}$ ($ LTD _{sim}$)	SCR_{reg} (SCR_{sim})	S_{q-reg} (S_{q-sim})	$S_{sk_{sim}}$	$S_{ku_{sim}}$
$ LTD $	0.01	2000	5	10	20.8 (20.4)	99.51 (99.29)	15.9 (16.5)	-1.412	6.304
SCR	0.01	2000	5	0	21.4 (22.1)	99.54 (99.33)	15.8 (15.7)	-1.543	6.530
S_q -RMS	0.01	2000	5	0	21.4 (22.1)	99.54 (99.33)	15.8 (15.7)	-1.543	6.530

After arranging the lines of Table 6 by ascending (i) S_{sk} and (ii) S_{ku} order, respectively, the three quality criteria are plotted versus S_{sk} and S_{ku} , respectively, in Figures 17 and 18. Each set of points is approximated linearly via the least-squares method, and the coefficients of determination (R^2) can be seen on the plot.

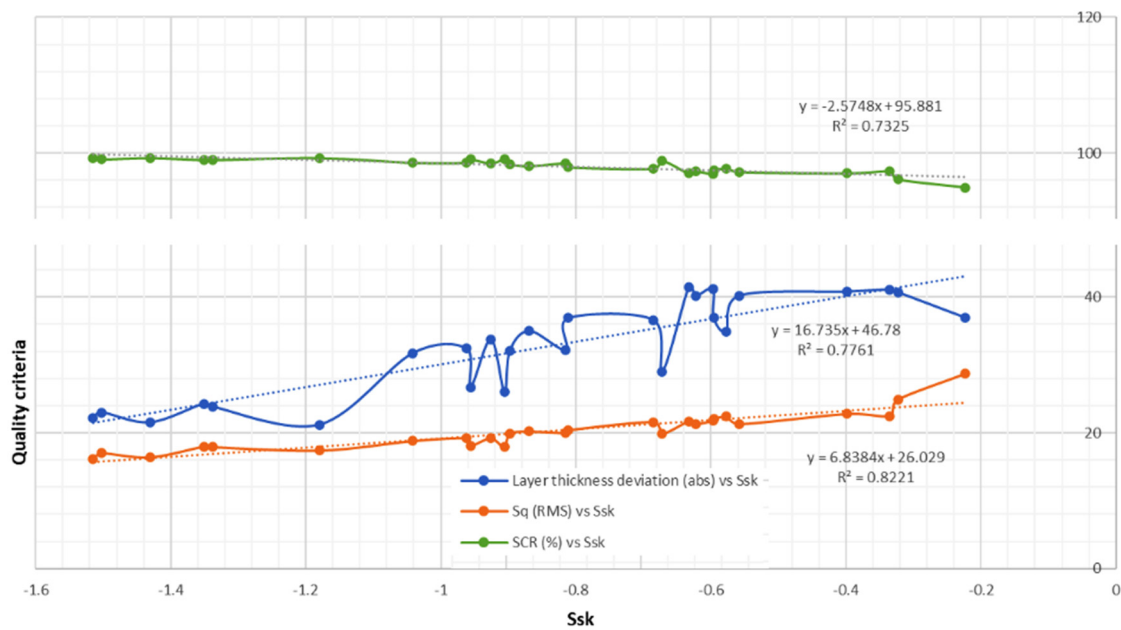


Figure 17. Quality criteria vs. S_{sk} .

The skewness plot reveals that, as the layer’s quality deteriorates (an increase in $|LTD|$ and S_q -RMS; decrease in SCR), S_{sk} increases, approaching zero from the negative side. Similarly, the kurtosis plot reveals that the lower the layer quality, the smaller S_{ku} becomes, approaching zero from the positive side. Figures 17 and 18 provide the least-squares linear approximation of the three quality criteria versus S_{sk} and S_{ku} . Therefore, S_{sk} and S_{ku} serve as equivalent indicators of surface quality.

A weighted means (WM) of $|LTD|$, $(100-SCR)$ and S_q -RMS is used for optimization after they are normalized in the range 0–1 (see Equations (33) and (34)).

$$WM_{S_{sk}} = w_{|LTD|_n - S_{sk}} \cdot |LTD|_n + w_{(100-SCR)_n - S_{sk}} \cdot (100 - SCR)_n + w_{S_{q_n} - S_{sk}} \cdot S_{q_n} \quad (33)$$

$$WM_{S_{ku}} = w_{|LTD|_n - S_{ku}} \cdot |LTD|_n + w_{(100-SCR)_n - S_{ku}} \cdot (100 - SCR)_n + w_{S_{q_n} - S_{ku}} \cdot S_{q_n} \quad (34)$$

These WMs and the experiment are connected via plotting the WMs vs. the respective S_{sk} and S_{ku} values because of the observation that the smaller (negative) S_{sk} and the larger (positive) S_{ku} values become, the higher the layer quality.

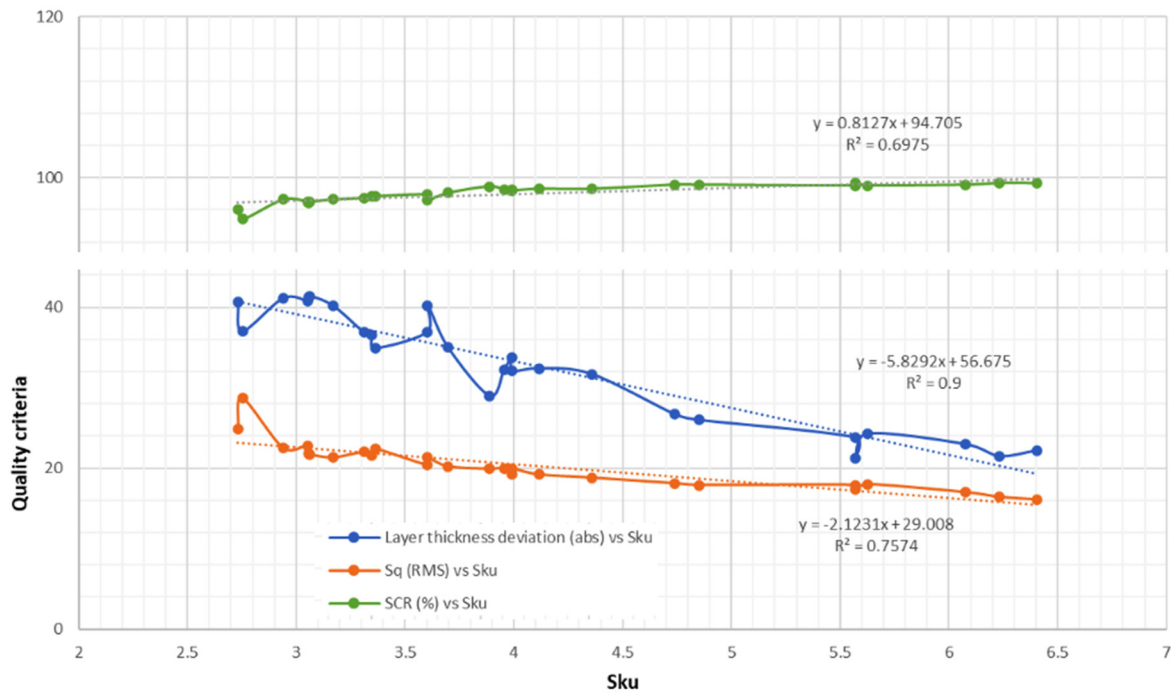


Figure 18. Quality criteria vs. Sku.

A simple algorithm combines the three weights, given that their sum must always be equal to 1, aiming to develop a line via the least-squares method, which gives the best fit (highest coefficient of determination (R^2) value) among all the possible lines created by various weight combinations. The algorithm has a 0.05 weight-increment step. The weight combinations that lead to the best-fit lines are the following:

$$\left\{ \begin{array}{l} w_{|LTD|_n-Ssk} = 0.35 \\ w_{(100-SCR)_n-Ssk} = 0.05 \\ w_{Sq_n-Ssk} = 0.60 \end{array} \right\} WM_{Ssk} = 0.6449 \cdot Ssk + 0.9549 \quad R^2 = 0.8869$$

$$\left\{ \begin{array}{l} w_{|LTD|_n-Sku} = 0.40 \\ w_{(100-SCR)_n-Sku} = 0.20 \\ w_{Sq_n-Sku} = 0.40 \end{array} \right\} WM_{Sku} = -0.1497 \cdot Sku + 1.1224 \quad R^2 = 0.9499$$

The line depicting WM_{Ssk} versus Ssk is an increasing function of Ssk (see Figure 19). Since the higher the (negative) Ssk value, the higher the layer quality, it is concluded that the smaller the quantity $(0.35 \cdot |LTD|_n + 0.05 \cdot (100 - SCR)_n + 0.60 \cdot Sq_n)$, the better the layer quality, according to Ssk .

Similarly, the line depicting WM_{Sku} versus Sku is a decreasing function of Sku (see Figure 20). Since the higher the (positive) Sku value, the higher the layer quality, it is concluded that the smaller the quantity $(0.40 \cdot |LTD|_n + 0.20 \cdot (100 - SCR)_n + 0.40 \cdot Sq_n)$, the better the layer quality, according to Sku .

Both Ssk and Sku lead to similar observations with regard to WM_{Ssk} and WM_{Sku} that need to be minimized in order to optimize the layer's quality. The weights calculated are similar to the qualitative importance that an expert in AM would assign to them. SCR is the least important since it detects the extent to which large surface defects exist within the layer. Such defects can be caused by dragging an agglomerate along the surface, creating a groove that leaves the substrate visible, drastically decreasing the SCR . However, such defects are easily avoidable by implementing proper sieving of the powder prior to recoating. Despite the possibility of such defects being catastrophic for the surface quality, since they are usually inherited from layer to layer and cause serious defects in the geometrical accuracy

or even the feature geometry of the finished part, the easiness in their avoidance renders them quite uncommon. That is why it is assigned the lowest weight, at 0.05 and 0.2, for Ssk and Sku evaluation, respectively.

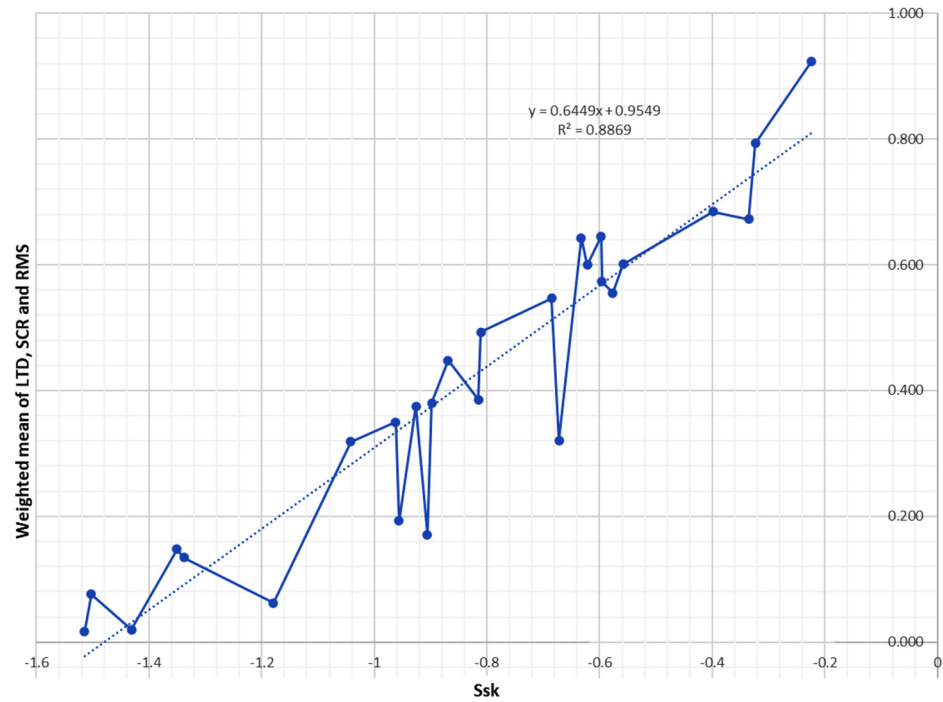


Figure 19. Best-fit line WM_{Ssk} versus Ssk.

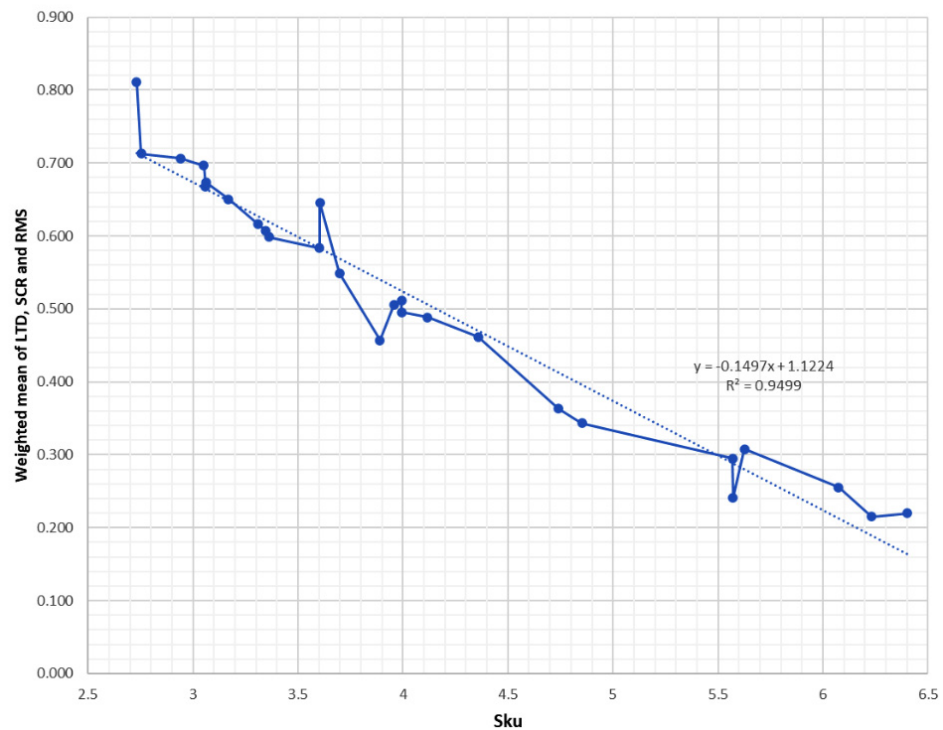


Figure 20. Best-fit line WM_{Sku} versus Sku.

Secondly, $|LTD|$ shows how lower the mean line of the layer’s surface is compared to the plane of the theoretical layer thickness. It is important since it is directly connected to the layer’s PD_{th} . Despite being important, it can be countered by appropriately adjusting (increasing) the $h_{l,th}$ by increasing the vertical downwards displacement of the fabrication

piston so as to achieve the desired h_1 . Hence, it is assigned a medium weight, at 0.35–0.4 for Ssk and Sku evaluation, respectively.

S_q -RMS quantifies layer evenness and homogeneity, showing whether the finished surface will have a high or low roughness value. High S_q -RMS values cannot lead to serious inherited defects throughout the layers; however, they can affect the surface quality of the finished part, making it necessary to be post-processed in order for it to become ready for use. Furthermore, S_q -RMS is the most consistent quality criterion, as it will identify, without fail, large areas where the layer’s surface is below or above the mean line, identifying intense spreading fluctuations during the powder–recoater interaction. Hence, it is assigned the highest weight, at 0.6 and 0.4, for Ssk and Sku evaluation, respectively.

In conclusion, the empirical approach of the method agrees with the calculated analytical results after the statistical analysis. Ssk and Sku can be used solely in conjunction with the weighted means of the three quality criteria in order to examine the general quality of the layer. Examining Ssk or Sku is equivalent to examining a weighted mean of the three normalized quality criteria, $|LTD|_n$, $(100-SCR)_n$ and $(S_q-RMS)_n$. The weights are in agreement with the ones that would have been chosen by experts in the field. Table 9 is completed via the regression–validation simulations. Both Ssk and Sku indicate that the optimum parameter level combination for the SCR and RMS values leads to a layer quality higher than that corresponding to the parameter values optimizing $|LTD|$. Hence, the optimum parameter level combination is: $u_{tr} = 0.01$ m/s, $f_{vib} = 2000$ Hz, $A_{vib} = 5$ μ m, $\theta_{rel} = 0^\circ$.

The vibration’s positive effect on the spreading outcome is proven by comparing the optimum level combination with a vibration-less trial where optimum values for u_{tr} and θ_{rel} are chosen. Metrics/visual evaluation are shown in Table 10 and Figure 21, respectively.

Table 10. Vibration-less vs. vibration-assisted performance (reg: “regression”; sim: “simulation”).

	u_{tr} (m/s)	f_{vib} (Hz)	A_{vib} (μ m)	θ_{rel} (deg)	$ LTD _{reg}$ ($ LTD _{sim}$)	SCR_{reg} (SCR_{sim})	S_{q-reg} (S_{q-sim})	Ssk _{sim}	Sku _{sim}
NO VIB.	0.01	0	0	0	- (28.9)	- (98.56)	- (20.9)	−0.716	3.962
OPTIMUM	0.01	2000	5	0	21.4 (22.1)	99.54 (99.33)	15.8 (15.7)	−1.543	6.530

The optimum level combination determined by Taguchi analysis is superior to its equivalent vibration-less trial by every quality criterion, including Ssk and Sku. A top-view examination of the layers shows multiple surface defects in the vibration-less layer, as the SCR indicates. These are located behind larger particles, revealing the detrimental effect of large particle dragging. Vibration alleviates large particle and agglomerate dragging and partially breaks down agglomerates, decreasing the defective areas.

In the vibration-less trial, the height of the particles displays higher randomness, with many particle centers being over $h_{l,th}$, as shown in the legend. Contrariwise, the particles in the optimum vibration-assisted trial have a uniform height, with the color showing much less variation, while the top of most particles is just contacting $z = h_{l,th}$ plane (see Figure 21b). The positive effect of vibration, combined with the fact that the layer’s PD_{th} increases with applied vibration, solely via the decrease in the $|LTD|$ and not via increased particle packing, which is proven to be negligible, come in agreement with the findings in [50], who proved these via DEM simulations for both a vibrating roller and a vibrating doctor blade recoater.

Since Ssk and Sku serve as general layer quality indicators, ANOVA for these is provided in Tables A4 and A5, respectively, while Equations (35) and (36) provide the regression Equations.

$$|Ssk| = 0.587 - 0.90u_{tr} + 0.000295f_{vib} + 0.1455A_{vib} + 0.0112\theta_{rel} - 0.00318u_{tr}f_{vib} - 1.222u_{tr}A_{vib} - 0.00901A_{vib}\theta_{rel} \quad (35)$$

$$Sk_u = 3.498 - 9.95u_{tr} + 0.000656f_{vib} + 0.4665A_{vib} + 0.0582\theta_{rel} - 0.00613u_{tr}f_{vib} - 3.07u_{tr}A_{vib} - 0.0273A_{vib}\theta_{rel} \quad (36)$$

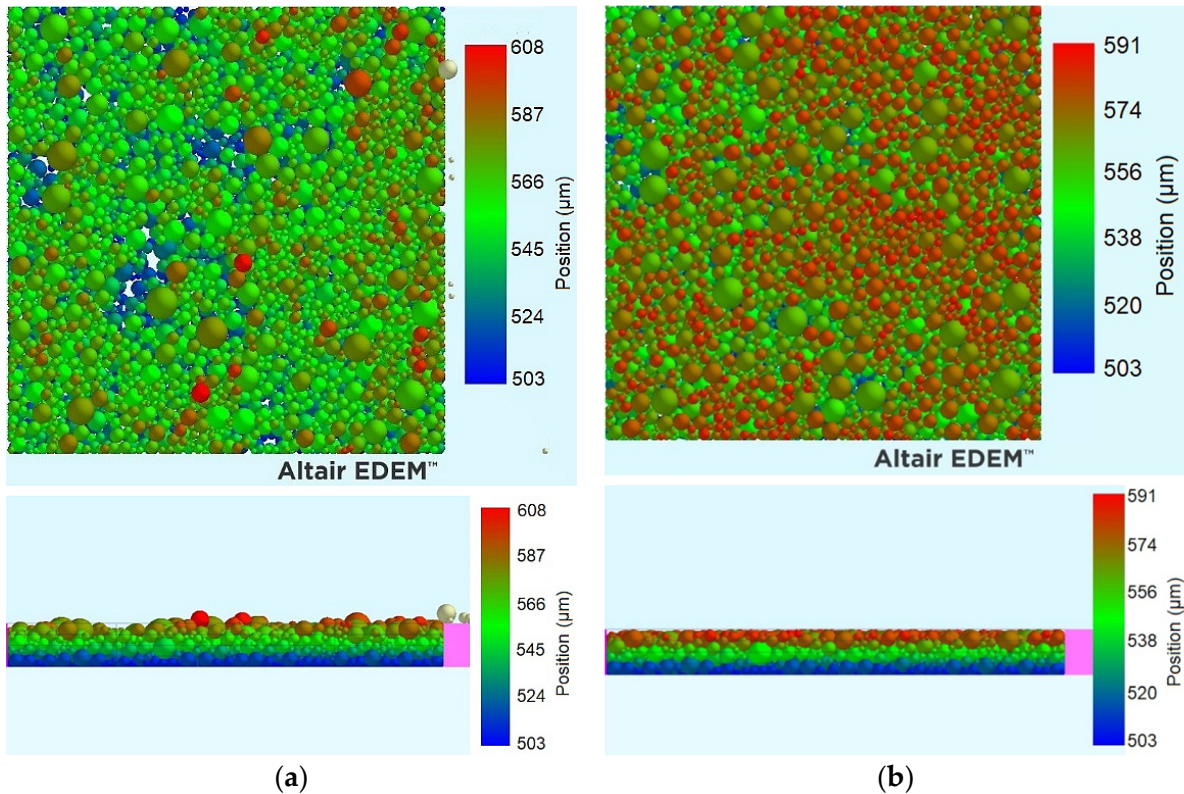


Figure 21. Layer quality comparison: (a) vibration-less (top and side); (b) vibration-assisted optimum (top and side). (Note: Magenta: back border plate; pink: front border plate).

The regression equations above were calculated in order to minimize the error of the ANOVA. More specifically, the interactions were selected to maximize the sum of the contribution column of the ANOVA table, hence minimizing the error of the regression equation.

By using Equations (35) and (36), it is confirmed that the optimum parameter combination is the one shown in Table 10. The regression optimum values are as follows: $Ssk_{opt,reg} = -1.771$, $Sk_{u_{opt,reg}} = 6.766$.

The simulation-calculated optimum values are as follows: $Ssk_{opt,sim} = -1.543$, $Sk_{u_{opt,sim}} = 6.530$.

The deviation between the simulation and the regression-calculated optimum values is -12.9% and -3.5% for skewness and kurtosis, respectively. Kurtosis' value is within the 8.77% , while skewness slightly exceeds the 9.26% error predicted by ANOVA. However, this is not considered to be a very important error, even though it is indicative of the fact that kurtosis might be a more reliable indicator of layer quality, which was also revealed by the R^2 values of the best-fit lines.

5. Conclusions

This work utilizes DEM simulations in conjunction with robust statistical analysis in the form of Taguchi DoE with subsequent ANOVA to evaluate the effect of spreading parameters on the deposited layer quality for PBF processes. Pertinent individual contributions are itemized as follows.

- A method is presented for connecting D_{10} , D_{50} and D_{90} of a powder to specific lognormal distribution parameters to accurately define the particle size distribution.
- Different ways of maximizing the timestep were exploited to minimize the computational time without affecting the validity of the results.
- The powder cohesion is parametrized to achieve realistic behavior of the powder.

- An appropriate contact model is selected based on powder characteristics.

The quality of the spread layer is proven to deteriorate with the spreading speed increase. Furthermore, oscillation of the doctor blade recoater promotes even flattening of the deposited layer and lower RMS roughness values, along with higher surface coverage ratios.

Different weighted means of the three quality criteria, namely LTD, SCR and RMS, have been proven to be connected to the layer’s surface areal skewness and kurtosis. Furthermore, skewness and kurtosis were proven to serve as general quality criteria for a deposited surface. The lower the (negative) skewness and the higher the (positive) kurtosis values, the higher the quality of the layer.

As a future step, Taguchi experiments using a prototype and a commercial powder deposition system are aimed at evaluating the layers via 3D white light scanning in order to cross-check the simulation results with actual experimental results on a larger scale.

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Appendix A

Table A1. ANOVA for |LTD|.

Source	DoF	SeqSS	Contribution	Adj SS	Adj MS	F-Value	p-Value
Regression	7	1182.59	94.68%	1182.59	168.941	48.33	0.000
U_{tr} (m/s)	1	1092.82	87.49%	65.78	65.783	18.82	0.000
f_{vib} (Hz)	1	4.51	0.36%	14.28	14.284	4.09	0.058
A_{vib} (µm)	1	71.25	5.70%	37.67	37.668	10.78	0.004
θ_{rel} (deg)	1	1.56	0.12%	0.65	0.653	0.19	0.670
U_{tr} (m/s)*f_{vib} (Hz)	1	9.77	0.78%	9.77	9.772	2.80	0.111
U_{tr} (m/s)*A_{vib} (µm)	1	2.66	0.21%	2.66	2.659	0.76	0.394
U_{tr} (m/s)*θ_{rel} (deg)	1	0.01	0.00%	0.01	0.014	0.00	0.950
Error	19	66.42	5.32%	66.42	3.496		
Total	26	1249.01	100.00%				

Table A2. ANOVA for SCR.

Source	DoF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	p-Value
Regression	7	264.644	84.48%	264.644	378.063	14.77	0.000
U_{tr} (m/s)	1	245.720	78.44%	13.689	136.885	5.35	0.032
f_{vib} (Hz)	1	0.3201	1.02%	0.0051	0.00512	0.02	0.889
A_{vib} (µm)	1	0.0581	0.19%	0.6210	0.62098	2.43	0.136

Table A2. Cont.

Source	DoF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	p-Value
θ_{rel} (deg)	1	0.5000	1.60%	0.0021	0.00213	0.01	0.928
U_{tr} (m/s)* f_{vib} (Hz)	1	0.0922	0.29%	0.0922	0.09218	0.36	0.556
U_{tr} (m/s)* A_{vib} (μm)	1	0.6259	2.00%	0.6259	0.62591	2.45	0.134
U_{tr} (m/s)* θ_{rel} (deg)	1	0.2961	0.95%	0.2961	0.29611	1.16	0.296
Error	19	48.630	15.52%	48.630	0.25595		
Total	26	313.274	100.00%				

Table A3. ANOVA for S_q -RMS.

Source	DoF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	p-Value
Regression	7	166.032	84.33%	166.032	237.188	14.60	0.000
U_{tr} (m/s)	1	129.530	65.79%	0.514	0.5136	0.32	0.580
f_{vib} (Hz)	1	5.696	2.89%	1.853	18.529	1.14	0.299
A_{vib} (μm)	1	0.632	0.32%	11.329	113.287	6.97	0.016
θ_{rel} (deg)	1	11.045	5.61%	0.050	0.0504	0.03	0.862
U_{tr} (m/s)* f_{vib} (Hz)	1	0.000	0.00%	0.000	0.0000	0.00	0.996
U_{tr} (m/s)* A_{vib} (μm)	1	12.539	6.37%	12.539	125.390	7.72	0.012
U_{tr} (m/s)* θ_{rel} (deg)	1	6.590	3.35%	6.590	65.902	4.06	0.058
Error	19	30.860	15.67%	30.860	16.242		
Total	26	196.892	100.00%				

Table A4. ANOVA for |Ssk| in powder spreading.

Source	DoF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	p-Value
Regression	7	314.077	90.74%	314.077	0.448681	26.61	0.000
U_{tr} (m/s)	1	238.472	68.90%	0.00401	0.004008	0.24	0.631
f_{vib} (Hz)	1	0.16578	4.79%	0.29422	0.294217	17.45	0.001
A_{vib} (μm)	1	0.09149	2.64%	0.33803	0.338033	20.05	0.000
θ_{rel} (deg)	1	0.09188	2.65%	0.01437	0.014371	0.85	0.367
U_{tr} (m/s)* f_{vib} (Hz)	1	0.15900	4.59%	0.14302	0.143016	8.48	0.009
U_{tr} (m/s)* A_{vib} (μm)	1	0.14879	4.30%	0.14879	0.148786	8.82	0.008
U_{tr} (m/s)* θ_{rel} (deg)	1	0.09911	2.86%	0.09911	0.099110	5.88	0.025
Error	19	0.32040	9.26%	0.32040	0.016863		
Total	26	346.117	100.00%				

Table A5. ANOVA for S_{ku} in powder spreading.

Source	DoF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	p-Value
Regression	7	301.817	91.23%	301.817	43.117	28.25	0.000
U_{tr} (m/s)	1	243.774	73.69%	0.4860	0.4860	3.18	0.090
f_{vib} (Hz)	1	11.329	3.42%	14.524	14.524	9.52	0.006
A_{vib} (μm)	1	20.368	6.16%	34.737	34.737	22.76	0.000

Table A5. Cont.

Source	DoF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	p-Value
θ_{rel} (deg)	1	0.1624	0.49%	0.3852	0.3852	2.52	0.129
U_{tr} (m/s)* f_{vib} (Hz)	1	0.6266	1.89%	0.5332	0.5332	3.49	0.077
U_{tr} (m/s)* A_{vib} (μm)	1	0.9391	2.84%	0.9391	0.9391	6.15	0.023
A_{vib} (μm)* θ_{rel} (deg)	1	0.9064	2.74%	0.9064	0.9064	5.94	0.025
Error	19	28.999	8.77%	28.999	0.1526		
Total	26	330.816	100.00%				

Appendix B

Table A6. Table of variables and abbreviations.

Context	Description/Definition	Symbol/Abbreviation	Unit	Equations	Tables
General	Additive manufacturing	AM	-	-	-
	Selective Laser Sintering/Selective Laser Melting	SLS/SLM	-	-	-
	Powder Bed Fusion	PBF	-	-	-
	Powder deposition system	PDS	-	-	-
	Analytic Hierarchy Process	AHP	-	-	-
	Discrete Element Method/Modelling	DEM	-	-	-
	Design of Experiments	DoE	-	-	-
	Analysis of Variance	ANOVA	-	-	(Tables A1–A5)
	Particle size distribution	PSD	-	-	(Table 2)
	Hertz–Mindlin with JKR contact model	JKR	-	-	(Table 1), (Table 4)
	Derjaguin–Muller–Toporov contact model	DMT	-	-	(Table 1)
	Bradley–Derjaguin contact model	BD	-	(10)	(Table 1), (Table 4)
	Maugis–Dugdale analytical contact model	MD	-	-	(Table 1)
	Layer thickness deviation	LTD	μm	(22)	(Tables 6–10)
	Surface coverage ratio	SCR	(%)	(24)	(Tables 6–10)
	Root-mean-square surficial areal roughness	S_q -RMS	μm	(25), (27), (29), (30)	(Tables 6–10)
	Arithmetical Areal Surficial Mean Height	S_a	μm	(28)	(Table 6)
	Areal Surficial Skewness	S_{sk}	-	(29), (35)	(Tables 6, 9 and 10)
	Areal Surficial Kurtosis	S_{ku}	-	(30), (36)	(Tables 6, 9 and 10)
	Layer	True packing density	PD_{tr} (PD)	(%)	(31), (32)
Theoretical packing density		PD_{th}	(%)	-	-
Real layer height/thickness		h_l	μm	(22), (23)	-
	Theoretical layer height/thickness	$h_{l,th}$	μm	(22)	-

Table A6. Cont.

Context	Description/Definition	Symbol/ Abbreviation	Unit	Equations	Tables
Material properties	Shear modulus	G	Pa	(1)	(Tables 3 and 7)
	Young's modulus	E	Pa	(18), (21)	(Tables 3 and 4)
	Poisson ratio	ν	-	(2), (18), (21)	(Tables 3 and 7)
	Powder bulk density	ρ	kg/m ³	(1), (32)	(Tables 2 and 7)
	Coefficient of restitution of materials A–B	$c_{r,A-B}$	-	-	-
	Coefficient of rolling friction of materials A–B	$c_{rf,A-B}$	-	-	-
	Coefficient of static friction of materials A–B	$c_{sf,A-B}$	-	-	-
	Equilibrium separation in Lennard–Jones potential	z_0		(8), (10)	(Table 3)
Particle size and distribution	Particle diameter distribution percentile (X%)	D_X	μm	(14)–(16)	(Table 2)
	Lognormal distribution's mean	μ_X	μm	(11), (12)	-
	Lognormal distribution's standard deviation	σ_X	μm	(12)	-
	Cumulative lognormal distribution function	F_X	-	(13)–(16)	-
Particle contact model	Effective Young's modulus of contacting particles	E^*	Pa	(5)–(8), (18)	(Table 3)
	Effective radius at the point of interparticle contact	R^*	m	(4)–(8), (10), (17), (20)	(Tables 3 and 4)
	Work of adhesion	Γ	J/m ²	(4), (6)–(10), (20), (21)	(Tables 3 and 4)
	Contact patch radius	α	μm	(6), (7)	-
	Relative particle approach	δ_n	μm	(3), (7), (10)	-
	Relative particle approach at tear-off point	δ_{to}	μm	(3), (5), (19), (21)	(Tables 3 and 4)
	Normal force of particles in contact (JKR model)	F_n^{JKR}	N	(3), (6)	-
	Pull-off force of particles in contact (JKR model)	F_{po}^{JKR}	N	(3), (4)	-
	Pull-off force	F_{po}	N	(5), (20)	(Table 4)
	Tabor's parameter	μ	-	(8)	(Tables 1, 3 and 4)
	Tensile load	T	N	(10)	-
Simulation	Minimum particle radius in simulation	r_{min}	μm	(1)	(Table 7)
	Rayleigh critical timestep	Δt_c	nsec	(1)	(Table 7)
	Physical radius	$R_{particle}$	μm	(19)	-
	Contact radius	$R_{c,EDEM}$	μm	(19)	-
	Average particle radius (lognormal normalization)	R_{ave}	μm	-	(Table 3)

Table A6. Cont.

Context	Description/Definition	Symbol/ Abbreviation	Unit	Equations	Tables
Taguchi-DoE	Translational deposition speed of the doctor blade	u_{tr}	m/sec	(35), (36)	(Tables 6 and 8–10)
	Vertical vibrational frequency of the doctor blade	f_{vib}	Hz	(35), (36)	(Tables 6 and 8–10)
	Vertical vibrational amplitude of the doctor blade	A_{vib}	μm	(35), (36)	(Tables 6 and 8–10)
	Angle of relief of the doctor blade	θ_{rel}	deg.	(35), (36)	(Tables 6 and 8–10)

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