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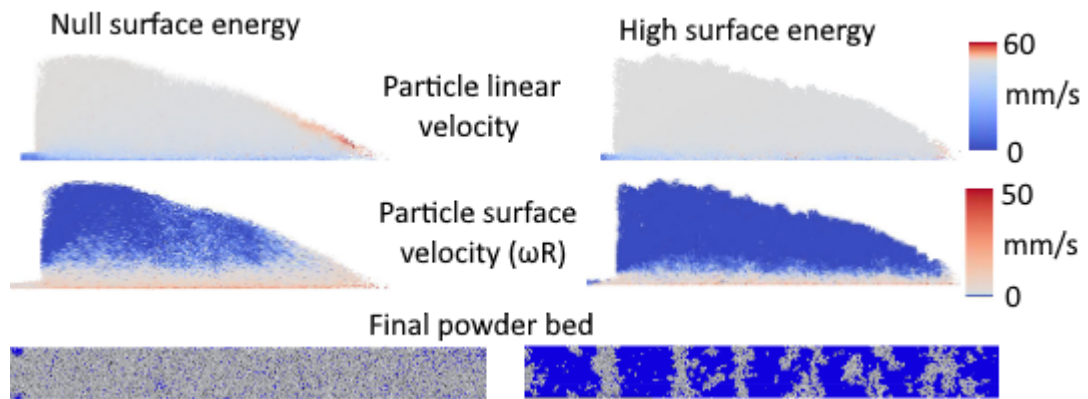
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## Graphical Abstract

### Identification of the influential DEM contact law parameters on powder bed quality and flow in additive manufacturing configurations

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## Highlights

### **Identification of the influential DEM contact law parameters on powder bed quality and flow in additive manufacturing configurations**

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- Effective surface energy between powder particles is a key parameter to assess bed-forming ability.
- Rolling friction between particles also contributes significantly to powder bed quality.
- A sliding friction above 0.4 is required to counter powder resistance and ensure deposition.
- The heap profile ahead of the blade can be a good predictor of powder spreadability.
- The observed size segregation on the fabrication plate can be traced to powder motion during the feeding stage.

# Identification of the influential DEM contact law parameters on powder bed quality and flow in additive manufacturing configurations

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## Abstract

The main objective of the present manuscript is to implement DEM simulations of powder spreading in an Additive Manufacturing process. A numerical sensitivity analysis is carried out in order to identify the contact law parameters that impact most on powder bed quality. Tested parameters are surface energy, as well as sliding, rolling and restitution coefficients. It is seen that effective surface energy between powder particles is a key parameter to assess bed-forming ability, but that it is also necessary to consider rolling and sliding frictions for an accurate modeling of the spreading phenomena. In addition, our simulations allow a better understanding of the size segregation issues during the feeding and deposition stages. Finally, we describe the effect of the contact law parameters on the heap profile. We identify various powder flow zones within the heap, and show that heap profile can be a predictor of powder bed quality.

*Keywords:* Powder Spreading, Discrete Element Method, Contact Law, Adhesion, Sliding Friction, Rolling Friction

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## 1. Introduction

A number of Additive Manufacturing (AM) processes (e.g. Powder bed fusion (PBF) and Metal Binder Jetting (MBJ)) are manufacturing processes that allow the production of metallic parts from powder by successive spreading and densification of powder layers. Other materials can be also used in powder bed based AM techniques, such as polymers with Selective Laser Sintering (SLS) or Multi Jet Fusion (MJF). All those processes enable the production of complex shapes, making them useful for a variety of applications. The first critical step in powder bed based AM processes is powder spreading, which is commonly assumed to lead to denser and smoother surfaces of the final parts if it is even and homogeneous [1]. Powder paving marks the initial state before heat densification in the case of PBF or binder absorption in the case of MBJ [2, 3]. For L-PBF (Laser-PBF), powder layer quality is critical for final part density only in case of packing density under a certain threshold [4]. Even if the gas flow around laser beam and melt pool leads to denudation of the powder layer along the laser path, passage through the liquid state allows to some extent a smoothing of the density variations. However, large empty patches and inhomogeneities can not be corrected by fusion [5, 6]. Moreover, powder bed roughness is correlated with final L-PBF part roughness [4]. In MBJ, the shrinkage during sintering largely depends on the distribution of the green part porosity. Therefore, the achievement of a homogeneous bed is of paramount importance as variations in porosity between layers may cause distortions of the final printed part. Even more important, as opposed to the case of fusion, low densities and inhomogeneities can not be corrected by sintering. On the other hand, excessive densities makes binder absorption more difficult, which makes green parts brittle and harder to handle [3]. Therefore, an optimal bed density is a compromise between the possibility of reaching a large density after sintering and the capacity for binder absorption

28 within the bed.

29 The spreading mechanisms depend on powder characteristics, such as powder  
30 morphology and size distribution. An a priori counterintuitive fact is that powder  
31 flowability measured with dedicated qualification equipment is not necessarily  
32 correlated with powder spreadability during process [1, 7, 8]. From a general  
33 standpoint, a water atomized powder-spreading results in low packing density  
34 and high layer roughness, because of the low particle sphericity [9]. In addition,  
35 a powder with a wide Particle Size Distribution (PSD) can be beneficial for  
36 adequate layer formation. For bimodal distribution, a small amount of fine  
37 particles has a positive effect on bed density and smoothness as it allows filling  
38 of the voids within the bed. However, over a certain fraction of small particles  
39 Van der Waals forces become too important, leading to particle agglomeration  
40 and a poor powder bed quality [7]. In principle, an optimal fine fraction can be  
41 identified, depending on the original powder PSD [3].

42 The geometry of the spreading device can have a significant impact on pow-  
43 der bed quality. Rollers based on counter-rotating movement allow particles to  
44 rearrange; however, they increase particle segregation and require a minimum  
45 spreading height, typically over  $1.8 \times D_{90}$ ,  $D_{90}$  representing the 90th volume-  
46 percentile of the considered powder [10]. An increased roller diameter results in  
47 a larger compression force on the powder bed [11]. Concerning metallic scrapers,  
48 an angle of attack between  $5^\circ$  and  $15^\circ$  allows an appropriate compaction [12].  
49 Haeri [13] simulated an elliptic blade profile, and obtained better results than  
50 with a roller. According to Wang et al. [14], a round blade gives a better per-  
51 formance than rollers and angled blades. From a process standpoint, the main  
52 parameters that can be optimized are the nominal spreading height and spread-  
53 ing device velocity. Indeed, the largest particles of a distribution (typically over  
54 the  $D_{90}$ ) fix the minimum layer thickness [9]. Moreover, an increase of the nom-

55 inal height and a reduction of the spreading speed lead to denser and smoother  
56 powder bed [15]. However, in L-PBF the actual spreading height is often far  
57 away from the nominal spreading height set by the machine user. A first factor  
58 accounting for such a difference is powder densification upon melting. Actual  
59 spreading height values increase during the first layers. Then, a steady state is  
60 reached after about ten layers [16, 17]. Nominal height and spreader velocity  
61 can also contribute to this difference.

62 An optimization of the powder bed quality can be achieved through a numer-  
63 ical simulation of the spreading process. The Discrete Element Method (DEM)  
64 (see e.g. [18]) allows a mathematical representation of the dynamic behavior of  
65 a set of particles where each powder particle is considered independently, their  
66 motions being derived from the integration of Newton’s law. It thus allows the  
67 modeling of powder spreading and the investigation of physical phenomena such  
68 as powder flow dynamics and force arches [10, 17, 19]. A common characteristic  
69 feature of DEM modeling is that the shape of the particles is assumed spherical,  
70 the constitutive contact laws being expressed on the basis of a theoretical inter-  
71 penetration [18]. All the interactions between particles are expressed through  
72 those contact laws. The technique has been widely used to model powder bed  
73 formation in additive manufacturing configurations [14, 15, 19–21].

74 During spreading, a powder heap can be observed in front of the blade.  
75 Previous works have highlighted different heap zones in terms of flow behavior.  
76 Avalanche or free-flowing zone is observed close to the upper part, specially near  
77 the front of the powder heap [10, 20], whose shape farthest away from the blade  
78 can be characterized by a Recoating Angle (RA) [20, 22] also called Dynamic  
79 Repose Angle [23, 24]. Just over the plate, a deceleration zone contains the  
80 particles that are slowed down due to the effect of plate friction. Over this  
81 deceleration zone, a quasi-static or slow flow zone [10] covers the majority of the

82 heap and is characterized by an almost zero particle velocity in the blade frame.  
83 Finally, in the vicinity of the blade gap with the plate, a shear stress region  
84 contains force arches that partially govern effective powder deposition [17, 20].

85 A complexity of the DEM technique is that, depending on the contact law im-  
86 plemented, a large number of parameters are often necessary as inputs in the sim-  
87 ulation. For example, the Hertz-Mindlin contact with Johnson Kendall Roberts  
88 (JKR) adhesion model requires no less than 6 parameters, namely Young’s mod-  
89 ulus, Poisson’s ratio, effective surface energy, restitution coefficient, and then  
90 sliding and rolling friction coefficients [25–27]. Moreover, in powder spreading  
91 simulations, contact parameters between powder particles, powder and the plate  
92 as well as powder and the blade are expected to be different.

93 Whenever possible, it is of course preferable to independently measure the  
94 constitutive parameters through the design of specific experiments that can be  
95 interpreted on a physical basis. An example is the drop test method for effective  
96 surface energy [28]. Another approach is based on calibration by flow experi-  
97 ments and macroscopic metrics. However, the number of necessary parameters  
98 is such that a priori assumptions on the physical phenomena to account for are  
99 necessary. Many routines of calibration are proposed in the literature, essen-  
100 tially based on packing density, and static and dynamic Angle of Repose (AOR)  
101 [20, 29, 30]. The use of a powder rheometer with shear cell or impeller blade is  
102 also possible [31, 32]. Choice of calibration experiments must feature dynamic  
103 and static behavior in order to cover various powder flow aspects, as static and  
104 dynamic Angle of Repose [1, 20].

105 The main objective of the present manuscript is to carry out a numerical  
106 sensitivity analysis in order to determine contact law parameters that have the  
107 greatest impact on powder bed quality. Tested parameters are effective sur-  
108 face energy, restitution coefficient, and sliding and rolling friction coefficients.



109 Here a particular attention is paid to the discrimination between the various  
110 types of contact frictions, namely *powder/powder*, *powder/building plate* and  
111 *powder/spreading blade*. Indeed, because of different surface characteristics be-  
112 tween particles and bulk material it appears necessary to address this point in  
113 detail. Regarding the *powder/spreading blade* contact, it is expected to be very  
114 much geometry dependent [13, 29], and would require a dedicated analysis, which  
115 is outside the scope of the present manuscript. On the other hand, there is a  
116 lack of knowledge about *powder/plate* interaction; therefore, focus will be on this  
117 issue. The second objective of our work is to describe the effect of the contact  
118 law parameters on the heap profile, through an in-depth analysis of slope angle  
119 measurements. Thanks to particle velocity and rotation, flow zones within the  
120 heap can be identified. Then, powder flowability and plate friction can be linked  
121 to powder flow, heap profile and finally powder bed quality.

122 The modeled powder is a thin 316L stainless steel metallic powder commonly  
123 used in L-PBF. To carry out the proposed objectives, we decided to focus on a  
124 simple fixed geometry set-up, thus allowing the implementation of a large number  
125 of numerical simulations with many contact law parameter sets. A powder bed  
126 analysis routine is used to post-process raw DEM data. The powder bed quality  
127 will be characterized in terms of height, density and their variations along the  
128 spreading direction. Particle size segregation is also investigated. Then, contact  
129 law parameters are discussed in term of variation ranges and associated powder  
130 physical properties. Finally, the effect of contact law parameters are presented  
131 within a global analysis of particle movement allowed by DEM data to gain some  
132 insights on the effect of these contact parameters on powder flow dynamics.

**Nomenclature (SI units are used here, relevant prefixes (milli, micro...) have been used in the text)**

**DEM calculation and contact laws :**

$m_i$	kg	Mass of a particle $i$
$\vec{x}_i$	m	Position of a particle $i$
$\vec{F}_i$	N	Sum of forces acting on a particle $i$
$t$	s	Time
$I_i$	kg m <sup>2</sup>	Moment of inertia of a particle $i$
$\vec{\omega}_i$	rad/s	Angular velocity of a particle $i$
$\vec{M}_i$	kg m <sup>2</sup> /s <sup>2</sup>	Sum of moments acting on a particle $i$
$\vec{F}_n$	N	Contact normal force between two particles $i$ and $j$
$E$	Pa	Young's modulus
$\nu$	dimensionless	Poisson's ratio
$R_i$	m	Radius of a particle $i$
$\delta_n$	m	Overlap for a contact between two particles $i$ and $j$
$\gamma$	J/m <sup>2</sup>	Effective surface energy
$\eta$	kg/s	Damping factor
$e$	dimensionless	Restitution coefficient
$\vec{F}_t$	N	Tangential force at a contact between two particles $i$ and $j$
$\vec{\delta}_t$	m	Tangential relative displacement for a contact between two particles $i$ and $j$
$G$	Pa	Shear modulus
$\mu_{sl}$	dimensionless	Sliding friction coefficient of a contact between two particles $i$ and $j$
$\vec{M}_{ro}$	N m	Moment due to rolling resistance for a contact between two particles $i$ and $j$

$\mu_{ro}$	dimensionless	Rolling friction coefficient of a contact between two particles $i$ and $j$
$g$	m/s <sup>2</sup>	External acceleration (gravity)
$\rho$	kg/m <sup>3</sup>	Density

**Contact types for  $\mu_{sl}$  and  $\mu_{ro}$  :**

$po/po$		Contacts between powder particles
$po/pl$		Contacts between powder particles and plates (feeding and building)
$all$		All contacts : $po/po$ , $po/pl$ then contacts between powder and blade

**Simulation condition :**

$L$	m	Length along x axis, blade moving direction
$W$	m	Width along y axis, direction normal to periodic boundaries
$H$	m	Height along z axis, direction of the gravity
$\Delta t$	s	Time step
$v$	m/s	Velocity (blade)

**Contact law parameters illustration :**

$\overrightarrow{F_{n,pull-off}}$	N	Pull off force due to JKR adhesion term [27]
$n_s$	dimensionless	Sides of a polygon (Estrada theory [33])

**Results characterization**

$a$	m	Grid parameter
$\bar{H}$	m	Mean height of powder bed
$\bar{\varphi}$	dimensionless	Mean relative powder bed density
$D_{43}$	m	Volume moment mean diameter
$RA_{attack}$	rad	Recoating Angle (front of heap)

	$RA_{HL}$	rad	Recoating Angle (Global on heap)
136	$\vec{v}$	m/s	Linear velocity (particle)
	$\vec{v}_s$	m/s	Surface velocity (particle)

## 137 2. Methodology

### 138 2.1. Discrete Element Method, contact laws

MUSEN is a DEM open-source software used for numerical simulation. It allows GPU computation saving time compared to CPU computation [34]. Each particle  $i$  is spherical and defined by its position  $\vec{x}_i$  and angular velocity  $\vec{\omega}_i$ . At each time step  $\Delta t$ , those values are updated from the sum of forces  $\vec{F}_i$  and moments  $\vec{M}_i$  acting on each particle  $i$  [35]:

$$m_i \frac{d^2 \vec{x}_i}{dt^2} = \vec{F}_i, \quad I_i \frac{d\vec{\omega}_i}{dt} = \vec{M}_i \quad (1)$$

139  $m_i, I_i$  are the mass and moment of inertia of the particle  $i$ . Forces  $\vec{F}_i$  and  
 140 moments  $\vec{M}_i$  result from contacts with walls or particles and gravity. Contact  
 141 laws are used to compute all of the interactions between particles and between  
 142 particles and surfaces.

The resulting normal contact force on particle  $i$  takes into account an elastic repulsion with damping; it is calculated using Hertz-Mindlin contact law [25, 26]. Following Johnson, Kendall, and Roberts, [27], thereafter referred to as JKR, an additional adhesion term is considered:

$$\vec{F}_n = \left( -\frac{4\sqrt{R^* \delta_n^3 E^*}}{3} + \sqrt{8\pi E^* \gamma \sqrt{\delta_n^3 R^{*3}} - \eta_n \delta_n} \right) \vec{n} \quad (2)$$

$E^*$  and  $R^*$  are the equivalent Young's modulus and equivalent radius of the considered contact. Table 1 gives the formulae for equivalent quantities.  $\delta_n$  is the normal overlap,  $\gamma$  is the effective surface energy of decohesion between two

particles [18] and  $\eta_n$  is the normal damping factor, defined from the restitution coefficient  $e$  :

$$\eta_n = \frac{1.8257 \ln(e)}{\sqrt{\pi^2 + \ln^2(e)}} \sqrt{2m^* E^* \sqrt{R^* \delta_n}} \quad (3)$$

$e$  is the ratio between particle velocity after and before a collision ( $= v/v_0$ ).  $m^*$  is the equivalent mass. The Hertz-Mindlin model is also used to calculate tangential force at the contact. Tangential contact is elastic with damping until a sliding limit given by Coulomb law:

$$\begin{cases} \vec{F}_t = -8G^* \sqrt{R^* \delta_n} \vec{\delta}_t - \eta_t \vec{\delta}_t \\ \text{if } |\vec{F}_t| > \mu_{sl} |\vec{F}_n| \text{ then } \vec{F}_t = \mu_{sl} |\vec{F}_n| \frac{\vec{F}_t}{|\vec{F}_t|} \end{cases} \quad (4)$$

$\vec{\delta}_t$  is the tangential relative displacement,  $G^*$  is the equivalent shear modulus,  $\mu_{sl}$  is the sliding friction coefficient. Then,  $\eta_t$  is the tangential damping factor calculated from  $e$  :

$$\eta_t = \frac{3.6514 \ln(e)}{\sqrt{\pi^2 + \ln^2(e)}} \sqrt{2G^* m^* \sqrt{R^* \delta_n}} \quad (5)$$

Rolling friction generates a moment against angular velocity. It is dependent on the contact normal force and the rolling friction coefficient  $\mu_{ro}$  :

$$\vec{M}_{ro} = -\mu_{ro} |\vec{F}_n| R_i \frac{\vec{\omega}_i}{|\vec{\omega}_i|} \quad (6)$$

Then,  $F_i$  and  $M_i$  introduced in Eq. (1) can be deduced from Eqs. (2),(4) and (6) summing over all contacts with neighbor particles  $j$ .

$$\begin{cases} \vec{F}_i = \sum_j (\vec{F}_n + \vec{F}_t) + m_i \vec{g} \\ \vec{M}_i = \sum_j (\vec{M}_{ro} - R_i \vec{F}_t \wedge \vec{n}) \end{cases} \quad (7)$$

**Table 1.** Expressions used to calculate equivalent quantities for a contact between two particles  $i$  and  $j$ .

Quantity	Expression
Equivalent Young's modulus	$E^* = \left( \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j} \right)^{-1}$
Equivalent contact radius	$R^* = R_i R_j / (R_i + R_j)$
Equivalent mass	$m^* = m_i m_j / (m_i + m_j)$
Shear modulus	$G_i = E_i / (2(1 + \nu_i))$
Equivalent shear modulus	$G^* = \left( \frac{2-\nu_i}{G_i} + \frac{2-\nu_j}{G_j} \right)^{-1}$

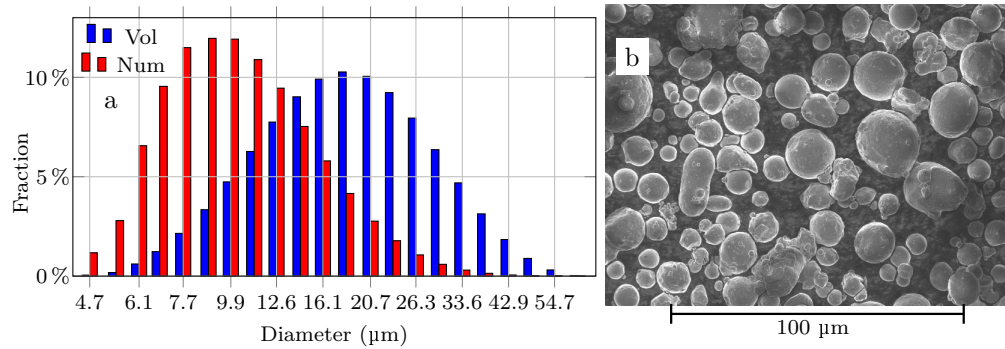
143 *2.2. Simulation conditions*

144 *2.2.1. Powder supply*

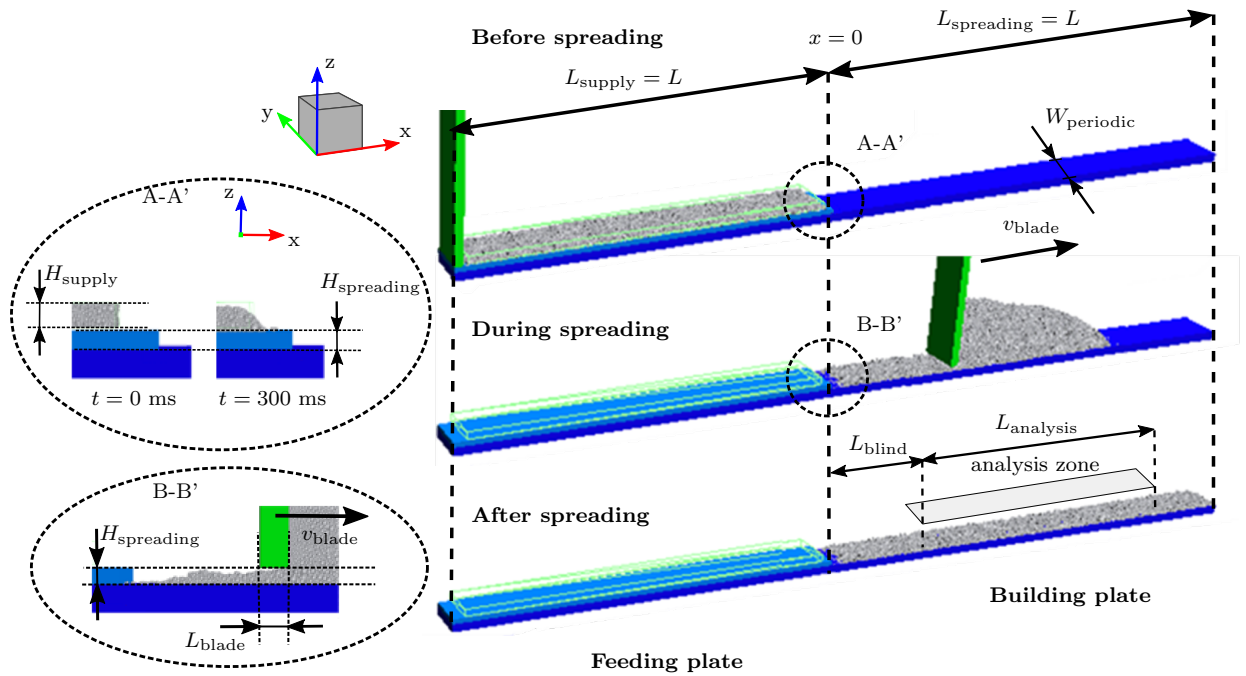
145 Even though no experimental work is reported within the present work, it  
146 appeared a priori interesting to model an actual commercial powder commonly  
147 used in L-PBF practice and to use measured characteristics as input for the  
148 simulations. In this study, a gas atomized (GA) 316L stainless steel powder  
149 provided by Sandvik is therefore modeled. The volume-based powder size dis-  
150 tribution (PSD) is measured by laser diffraction in ethanol following the ISO  
151 13320 standard (Mastersizer 2000 Malvern<sup>®</sup>). Volumetric D10, D50 and D90  
152 are equal to **10/18/32**  $\mu\text{m}$  respectively. SPAN = (D90-D10)/D50 is equal to  
153 **1.2** [36]. The volume-based distribution in the form of size classes is converted  
154 to number-based distribution, as shown in Fig. 1.

155 *2.2.2. Geometry*

156 Simulation set-up at different stages is illustrated in Fig. 2. Table 2 provides  
157 the different geometrical dimensions and values related to simulation setup. An  
158 external acceleration  $g$  corresponding to gravity is set to  $9.81 \text{ m s}^{-2}$  along z-axis.  
159  $W_{\text{periodic}}$  is the distance between periodic boundaries. It is set as 10 times the  
160 size of the D99.5, which is the diameter of the 0.5% largest particles in volume



**Fig. 1.** Powder supply : (a) Volume and number based Powder Size Distribution (PSD) and (b) powder observed by SEM (secondary electrons)



**Fig. 2.** Spreading simulation geometry at different stages, at  $t = 0$  ms,  $t = 750$  ms and  $t = 1$  s. x-axis length is cut to help representation. A-A' and B-B' zooms show the transition between both plates

**Table 2.** Spreading simulation dimensions and fixed parameters.

Dimensions	Value
$L_{\text{supply}} = L_{\text{spreading}} = L$ (mm)	15
$W_{\text{periodic}}$ ( $\mu\text{m}$ )	500
$V_{\text{blade}}$ ( $\mu\text{m/s}$ )	50
$L_{\text{blind}}$ (mm)	4
$L_{\text{analysis}}$ (mm)	9
$H_{\text{supply}}$ ( $\mu\text{m}$ )	90
$H_{\text{spreading}}$ ( $\mu\text{m}$ )	60
$L_{\text{blade}}$ ( $\mu\text{m}$ )	100
$g$ ( $\text{m s}^{-2}$ )	9.81
$\Delta t$ (ns)	8

161 [7, 12, 19]. The spreading length  $L$  is set to 15 mm. Such a spreading length  
162 is small compared to a real building plate. However, the simulation of a 10  
163 cm-long spreading would require too much computing resources. In order to  
164 investigate spreading length effect, one spreading is done with reference powder  
165 parameters (introduced in section 2.3.5) and twice the reference length, i.e. 30  
166 mm. As visible in Fig. 2(B-B'), the step between feeding and building plate  
167 influences results at the beginning of the bed, therefore the analysis zone starts  
168 at a distance  $L_{\text{blind}}$  from the feeding plate. It allows skipping the first millimeters,  
169 where transients in the spreading flow could be observed. The rectangular blade  
170 has a thickness  $L_{\text{blade}}$  of 100  $\mu\text{m}$ . As mentioned earlier, the focus of the present  
171 work is not on *powder/blade* interactions; therefore, it was decided to use a  
172 generic blade geometry in all simulations.

173 Initial powder generation takes place in a 90  $\mu\text{m}$  high box slightly raised over  
174 the feeding plate in order to avoid interactions with walls at the first time step.  
175 First, particles are randomly packed setting a 50% porosity inside the box with  
176 the specified PSD. At  $t=0$  particles are released and left to settle on the feeding



177 plate. The small initial drop and a 300 ms rest time before blade movement  
 178 allows an equilibrium state to be reached with respect to gravity [15]. After  
 179 complete spreading, the simulation continues for 100 ms to allow the powder  
 180 bed to settle. Unless specified otherwise, the material parameters of the blade  
 181 and the plate are the same as powder particles.

182 Spreading height  $H_{\text{spreading}}$  is set to 60  $\mu\text{m}$ , a value typical of L-PBF processes  
 183 that is approximately two times the D90 of powder; however, some rare particles  
 184 (0.03% in volume) are larger than the gap. Depending on the initial bed porosity,  
 185 laser densification on such a 60  $\mu\text{m}$  layer should result in a final solidified layer of  
 186 20-30  $\mu\text{m}$ . In an actual L-PBF process, after few layers (5 to 10), the solidified  
 187 thickness would approach the spreading height [16]. Therefore, our choice of  
 188  $H_{\text{spreading}}$  set to 60  $\mu\text{m}$  allows typical values relevant for the L-PBF processes to  
 189 be covered, both in transient and steady state modes. Blade velocity is fixed to  
 190 50 mm/s, again a typical value for L-PBF processes.

### 191 2.2.3. Time step and fixed powder parameters

192 Time step is set to the value recommended by MUSEN [34], which is 10%  
 193 of the smallest Rayleigh time for the considered particle distribution. Rayleigh  
 194 time is defined as the time needed for a shear wave to propagate through a solid  
 195 particle [37, 38]. It can be calculated as a function of the Young's modulus,  
 196 density, Poisson ratio and particle radius:

$$\Delta t = 0.1 * \min \left\{ \frac{\pi * R_i * \sqrt{2\rho(1 + \nu_i)}}{\sqrt{E_i}(0.163\nu_i + 0.8766)} \right\} \quad (8)$$

197 Let us recall that simulated powder consists of perfect spherical particles,  
 198 with a PSD in number given in Fig. 1. Since Young's Modulus, density and  
 199 Poisson ratio are well known materials properties, 316L alloy standard values  
 200 are used for our simulation and fixed [19]. However, for simulation purposes,

201 Young’s Modulus can be decreased by some orders of magnitude in order to  
202 increase the time step and so decrease computational time. Based on Chen et al.  
203 work [39], Young’s modulus is decreased by 3 orders of magnitude. Even at this  
204 reduced value, it still complies with the standard criterion on maximal relative  
205 overlap over all particles at each time step [38]:

$$\frac{\max(\delta_{n,i})}{2R_i} < 0.01 \quad (9)$$

206 The other option for time step increase, namely material density increase, is  
207 not possible in our present spreading configuration, as the particle flow can not  
208 be considered quasi-static [18].

### 209 *2.3. Studied powder contact law parameters*

210 As opposed to the macroscopic parameters discussed just above, the values  
211 of effective surface energy, restitution coefficient, as well as sliding and rolling  
212 coefficients are intrinsically dependent on the fact that the material is in powder  
213 form. An independent determination of the parameter set for a given powder  
214 would be a formidable task, as it is generally not possible to focus on a single  
215 physical property without the need to consider the effect of other parameters.  
216 Quite generally, what is done in the literature relies on a single macroscopic  
217 experiment to calibrate a simulation parameter, assuming rather arbitrarily the  
218 effect of the others to be limited. Such an approach was followed for instance  
219 by Meier et al.[30], who used Angle of Repose (AOR) data to determine the  
220 effective surface energy ( $\gamma$ ). However, a limitation of this approach is that it is  
221 necessary first to know rolling friction coefficient ( $\mu_{ro}$ ) to accurately determine  
222  $\gamma$  [40]. Therefore, the approach of the present paper is to conduct a sensitivity  
223 analysis on a wide parameter range to identify general trends on the relative  
224 influence of contact law parameters.

225 *2.3.1. Effective surface energy*

226 The drop test method developed by Zafar et al. allows measurement of the  
227 effective surface energy of a particle [28]. Drop test is based on equilibrium  
228 between JKR pull-off force shown in Eq. (10) [27] and particle deceleration force  
229 due to an impact. Nan et al.[19] determined this value at 9 mJ/m<sup>2</sup> for 316L  
230 powder. However, this value cannot be directly used, due to the Young's Modulus  
231 reduction, mentioned above. Indeed, despite an unchanged pull-off force from  
232 a physical standpoint, adhesion work would numerically increase because of the  
233 larger overlapping allowed by softer particles. Eq. (11) shows the scaling law  
234 between surface energy and Young's modulus [41, 42]. The initial value of 9  
235 mJ/m<sup>2</sup> is scaled to 0.5 mJ/m<sup>2</sup> by using a simulation Young's modulus equal to  
236 0.2 GPa.

$$\overrightarrow{F_{n,\text{pull-off}}} = -3/2 \pi \gamma R^* \quad (10)$$

$$\gamma_{\text{simu}} = \gamma_{\text{exp}} \left( \frac{E_{\text{simu}}}{E_{\text{exp}}} \right)^{2/5} \quad (11)$$

237 In the present work, surface energy varies between 0 and 1 mJ/m<sup>2</sup>. This  
238 large interval allows coverage of studies ignoring adhesion [43, 44] up to the  
239 higher value found in the literature for 316L powder [45]. Interestingly, most of  
240 studies describing the same issue use a surface energy with an order of magnitude  
241 of 0.1 mJ/m<sup>2</sup> by taking into account the Eq. (11) [19, 46, 47].

242 *2.3.2. Sliding friction coefficient*

243 Sliding friction coefficient can be influenced by particles' surface roughness.  
244 As explained by Shaheen et al.[47], the increase of surface roughness will cause  
245 a reduction of the contact area. Thus, normal pressure will increase for a given

246 contact force. Plastic deformation is then possible, increasing tangential force be-  
247 fore sliding. Yim et al.[20] confirmed this assumption by calibrating two powders  
248 with different roughness. Roughness was measured by Atomic Force Microscopy.  
249 Then, DEM parameters were calibrated by static and dynamic Angle of Repose.  
250 Another approach consists in the gluing of powder on a substrate, which allows  
251 direct measurement of sliding friction, because particles cannot roll. Friction  
252 can be implemented against a substrate, e.g. a plate manufactured by powder  
253 bed fusion [19, 48] or against a similarly glued powder [31]. Slope between nor-  
254 mal  $F_T$  and tangential forces  $F_N$  is obtained by measuring an angle of sliding  
255 with different applied weights [19, 48] or tangential force [31]. In principle, the  
256 particle sliding coefficient is equal to the global sliding coefficient of the exper-  
257 iment ( $F_N/F_T$ ) and can be used directly as  $\mu_{sl}$  [31, 48]. In the present work,  
258 tested sliding friction coefficients range in the interval [0.2, 1.2] as proposed in  
259 the literature [21, 29, 48, 49].

### 260 2.3.3. *Rolling friction coefficient*

261 Rolling friction is known to be highly dependent on particle morphology  
262 [47]. It can be measured from the travel distance of a particle rolling on a  
263 plane [40]. However, such a travel distance measurement does not work for  
264 highly non-spherical particles from Water Atomization (WA) processes because  
265 of the incapacity of those particles to roll [50]. For non-cohesive powder, rolling  
266 friction can be calibrated from the Angle of Repose [50]. From automated image  
267 analyzer, rolling friction coefficient can be computed using powder eccentricity  
268 [50–52].

269 To account for the dependence of rolling friction on particle morphology,  
270 polygonal particles can be represented in 2D simulation by round particles with  
271 a rolling friction coefficient linked to the number of sides  $n_s$  of polygons [33]:

$$\mu_{\text{ro}}^{\text{estrada}} = (1/4) \tan(\pi/2n_s) \quad (12)$$

272 Here, the tested rolling friction coefficients are [0,0.01,0.05,0.2]. By consid-  
 273 ering the above formula, they would correspond to a perfect circle and polygons  
 274 with respectively 40, 8 and 2.3 sides. The last value has of course no physical  
 275 meaning but it is proposed to model a highly non-spherical powder like water-  
 276 atomized powder.

277 In the literature, rolling friction coefficients are often set between 0.005 and  
 278 0.1 [14, 20, 21, 48]. Sometimes rolling resistance is ignored, which corresponds  
 279 to a zero rolling friction coefficient [15].

#### 280 *2.3.4. Restitution coefficient*

281 Restitution coefficient is defined as the ratio of the particle velocity after and  
 282 before a collision [26]. In practice, it can be measured following the impact of  
 283 particles on a plane with a high-speed camera. Nan et al. measured a restitution  
 284 coefficient for 316L powder of  $0.64 \pm 0.084$  [19]. In order to investigate restitu-  
 285 tion coefficient ( $e$ ) effects, four values were tested in the [0.1,0.9] range, such a  
 286 large interval comprising most of the values used in the literature for metallic or  
 287 polymeric materials [13, 21, 29, 46, 47, 49]. In most DEM parameters sensitivity  
 288 analysis,  $e$  is assumed not to have a real impact and kept fixed between 0.3 and  
 289 0.9 [30, 47, 53]; moreover, it could be reduced to 0.1 to stabilize the simulation  
 290 [49].

#### 291 *2.3.5. Variation range*

292 To sum things up, all reference parameters for contact laws are chosen ac-  
 293 cording to values given in the literature. Variation ranges are wide in order to  
 294 cover many different values used in literature. All reference parameters (fixed  
 295 and modified) as well as variation range are presented in Table 3. Parameters are

296 first changed for all contact types simultaneously (results referred to *all* contact  
297 types in the following). However, since as mentioned before contact parame-  
298 ters between two powder particles or between a powder particle and the plate  
299 or blade are expected to be different, they will also be modified independently  
300 for each contact type. In that case, when a parameter is modified, all others  
301 are kept identical to their reference value, and the results will be presented as  
302 *powder/powder* (*po/po*) and *powder/plate* (*po/pl*) contact.

303 For surface energy simulations, we only considered *po/po* contact. It may  
304 appear a priori surprising to neglect powder adhesion on blade and plate, but  
305 when the present work was initiated, the MUSEN software did not allow non-  
306 zero surface energy for these contacts. We thus decided to proceed modeling only  
307 *powder/powder* adhesion. Fortunately, when updates of MUSEN were afterwards  
308 implemented, it was checked on a number of test cases that the results were  
309 not significantly modified when accounting for powder blade and powder plate  
310 adhesion. In any case, the conclusions drawn in the manuscript can be expected  
311 to hold. Sliding and rolling friction parameters will be first modified for all  
312 contact types at the same time (*all*). Then, the ones that are more influential will  
313 be modified independently for *powder/powder* (*po/po*) and *powder/plate* (*po/pl*)  
314 contact. Finally, the contact parameters between powder and blade are not  
315 investigated because the study of the effect of blade geometry is, as mentioned  
316 earlier, beyond the scope of this work [10, 12, 14].

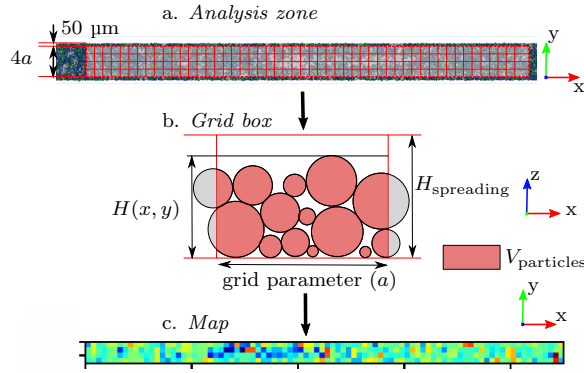
## 317 2.4. Powder bed characterization

### 318 2.4.1. Height and density

319 In powder bed fusion process, powder bed density, height and roughness are  
320 key descriptors of powder bed quality and used by most authors [10, 15, 17, 21,  
321 47]. In addition, in an L-PBF configuration, segregation could lead to differential  
322 laser interaction as a function of the horizontal position over the powder bed. It

**Table 3.** Reference powder parameters and variation range.

Parameter	Symbol	Reference value	Variation range
Young's Modulus (Pa)	$E$	$2 * 10^8$	–
Particle density (kg/m <sup>3</sup> )	$\rho$	7900	–
Poisson's ratio	$\nu$	0.3	–
Effective surface energy (mJ/m <sup>2</sup> )	$\gamma$	0.5 [19]	[0; 1] [21, 43]
Sliding friction coefficient	$\mu_{sl}$	0.7 [46]	[0.2; 1.2] [29, 48]
Rolling friction coefficient	$\mu_{ro}$	0.05 [47]	[0; 0.2] [15, 20]
Restitution coefficient	$e$	0.6 [19, 21]	[0.1; 0.9] [23, 49]



**Fig. 3.** Powder bed analysis with grid for height and density.

323 could create molten pool heterogeneity and then pores [10]. For this study, our  
 324 choice is to measure powder bed density, height and segregation.

325 Height and density analysis routine used here is inspired by the work of Meier  
 326 et al.[15]. First, the bed is voxelized at a resolution of 1 micrometer. Then, a  
 327 grid presented in Fig. 3 with a 100 µm parameter ( $a$ ) is selected to consider only  
 328 significant variations. Indeed, a typical laser spot diameter used in L-PBF is 100  
 329 µm, and besides such a 100 µm grid parameter is sufficiently large to encompass  
 330 a statistically relevant number of particles. The 50 µm margin on each side

331 avoids numerical artifacts from periodic boundaries.

332 Density and height are determined on each grid box. Local height  $H(x, y)$   
333 is the maximum value for a box as seen in Fig. 3(b). Local box density  $\varphi(x, y)$   
334 is defined as the volume occupied by particles over the complete box volume  
335 calculated with  $H(x, y)$  as height as seen in Eq.(13). Using local height  $H(x, y)$   
336 allows the removal of the height effect on density values. For boxes where height  
337 is zero, a situation met when no particles are in the box, the density is fixed to 0.  
338 Then, height and density averages ( $\bar{H}$  and  $\bar{\varphi}$ ) are computed as well as standard  
339 deviations over all boxes.

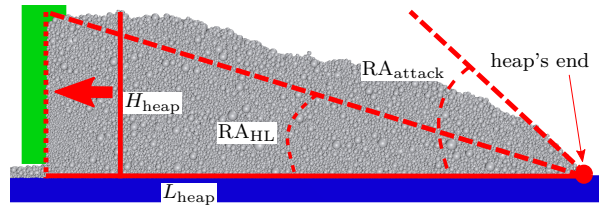
$$\varphi(x, y) = \frac{V_{\text{particles}}(x, y)}{a^2 H(x, y)} \quad (13)$$

#### 340 2.4.2. Segregation

341 Segregation is a known phenomenon in granular systems and experimentally  
342 observed in the powder bed spreading process [9]. Segregation occurs when parti-  
343 cles composing a granular media have different properties like size, shape or den-  
344 sity [54]. In our case, only size differentiates particles. Percolation-mechanisms  
345 can be invoked to explain size segregation. Thanks to gravity, small particles  
346 move through voids kept between large particles [55]. A consequence on pow-  
347 der bed spreading is the preferential deposition of small particles in the first  
348 section of the bed [10]. As a matter of fact, DEM allowed the confirmation of  
349 percolation-induced segregation during powder spreading [21]. To quantify seg-  
350regation, the volume moment mean diameter  $D_{43}$  is calculated all along the bed  
351 inside fixed length divisions. It is computed from particle radius as follows in  
352 Eq. (14); it is the average diameter weighted by volume.

$$D_{43} = 2 \left( \frac{\sum_i R_i^4}{\sum_i R_i^3} \right) \quad (14)$$





**Fig. 4.** Recoating Angles description:  $RA_{HL}$  and  $RA_{attack}$ .

353 *2.5. Powder heap characterization*

354 In this study, the powder heap is characterized by two Recoating Angles  
 355 (RA). Indeed, a simple fitting of the heap top surface, as done by Chen et  
 356 al.[23], is not possible because of the complex observed heap shapes. We thus  
 357 decided to define both a global and a local RA, both angles being represented in  
 358 Fig. 4. A global heap angle called  $RA_{HL}$  is derived using the height  $H_{heap}$  and  
 359 the length ( $L_{heap}$ ) of the powder heap:

$$RA_{HL} = \arctan(H_{heap}/L_{heap}) \quad (15)$$

360 The local Angle of attack  $RA_{attack}$  corresponds to the angle at the end of the  
 361 powder heap, where the end of the heap is identified as the first point without  
 362 powder from the blade. To define this angle, a moving average of the heap  
 363 height along x-axis first smooths the heap surface. The nominal half-width of  
 364 the moving average is arbitrarily fixed to 200  $\mu\text{m}$ , except near the end of the  
 365 heap where it is adaptative. Then, the  $RA_{attack}$  is the maximum slope angle  
 366 calculated between two points separated by the previous half-width.

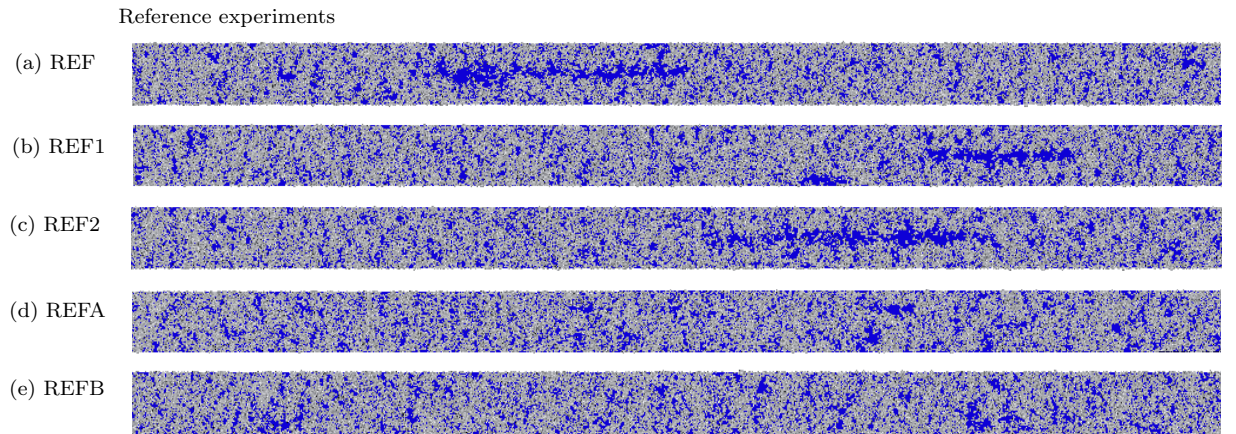
### 367 **3. Results**

#### 368 *3.1. Numerical standard deviation*

369 In order to estimate relevant error bars on the results that will be discussed,  
370 it appeared interesting to run identical simulations to check the reproducibility  
371 of the observed results. Indeed, starting from an exactly identical generation,  
372 tiny iterative numerical discrepancies over the  $10^8$  time steps occurring during  
373 a simulation are likely to come to slight different results. In addition, slightly  
374 different initial conditions (see particle generation procedure) can also lead to  
375 deviations. In order to quantify these mechanisms, 3 runs of simulation with  
376 reference powder parameters introduced in [Table 3](#) were first done using the same  
377 initial state of the particles (REF,REF1,REF2). In addition, to evaluate the  
378 deviation due to the slight variation within the initial state, 2 more simulations  
379 are run from different initial particle generations keeping the same generation  
380 box, porosity and PSD (REFA,REFB). Then, particles are randomly packed  
381 running from scratch the same filling algorithm, but with same specifications.

382 At first, slight but significant differences are observed: for instance, an iso-  
383 lated elongated empty patch, due to a particle larger than the gap in front of the  
384 blade, is well visible on [Fig. 5\(a\)](#). This large particle was blocked for some time,  
385 preventing flow and deposition of particles. After some millimeters, this particle  
386 is finally set free, releasing particle flow. This particle crossing the blade gap  
387 briefly increases forces measured on the blade by 2 orders of magnitude. Inter-  
388 estingly, for exactly the same initial conditions, the REF1 and REF2 runs also  
389 exhibit elongated empty patches but at different locations, meaning that small  
390 iterative discrepancies have to be involved. However, elongated empty patches  
391 are not observed on runs REFA and REFB, meaning that slight differences in  
392 terms of particle generation may have a significant effect.

393 [Table A.1](#) in the appendix details the density, height and RA results as well as



**Fig. 5.** Raw powder beds from different reference simulations. The plate is blue and particles are gray.

394 average and standard deviation over those 5 simulations. Fortunately, the above  
 395 mentioned differences do not translate to very large variations when analyzed on  
 396 a statistical basis. Anticipating the results to be presented below, the error bars  
 397 corresponding to the standard deviations observed on those 5 spreadings will be  
 398 seen to be quite low compared to variations due to contact law sensitivity. In the  
 399 following, when comparison is made to a reference, the REF simulation serves  
 400 as the basis.

### 401 *3.2. Overview of the powder bed*

402 Turning to the effect of contact law parameters, a first overview on simula-  
 403 tions carried out changing all contacts simultaneously is shown in Fig. 6. It allows  
 404 the visualization of some important phenomena that will be discussed later on.  
 405 More generally, it is worth stating that isolated empty patches previously dis-  
 406 cussed for the reference bed are observed on many high quality continuous beds  
 407 because of particles larger than the gap, as visible in Fig. 6(a,b,i). Despite an  
 408 overall satisfactory quality of the powder bed, larger particles may occasionally  
 409 stay jammed because of their size.

410 A high surface energy leads to empty patches larger than 100  $\mu\text{m}$ , see Fig. 6(d).  
411 Therefore, some boxes of the grid will be empty, meaning a larger variation of  
412 height and density along the bed. A low sliding friction coefficient does not allow  
413 particles to stick on the plate; it results in no powder deposition, see Fig. 6(e).  
414 High rolling resistance creates many small empty patches uniformly distributed  
415 on bed, see Fig. 6(j). Qualitatively, the higher the sliding friction and the lower  
416 the rolling friction, the better the homogeneity of the powder bed.

### 417 3.3. Height and density

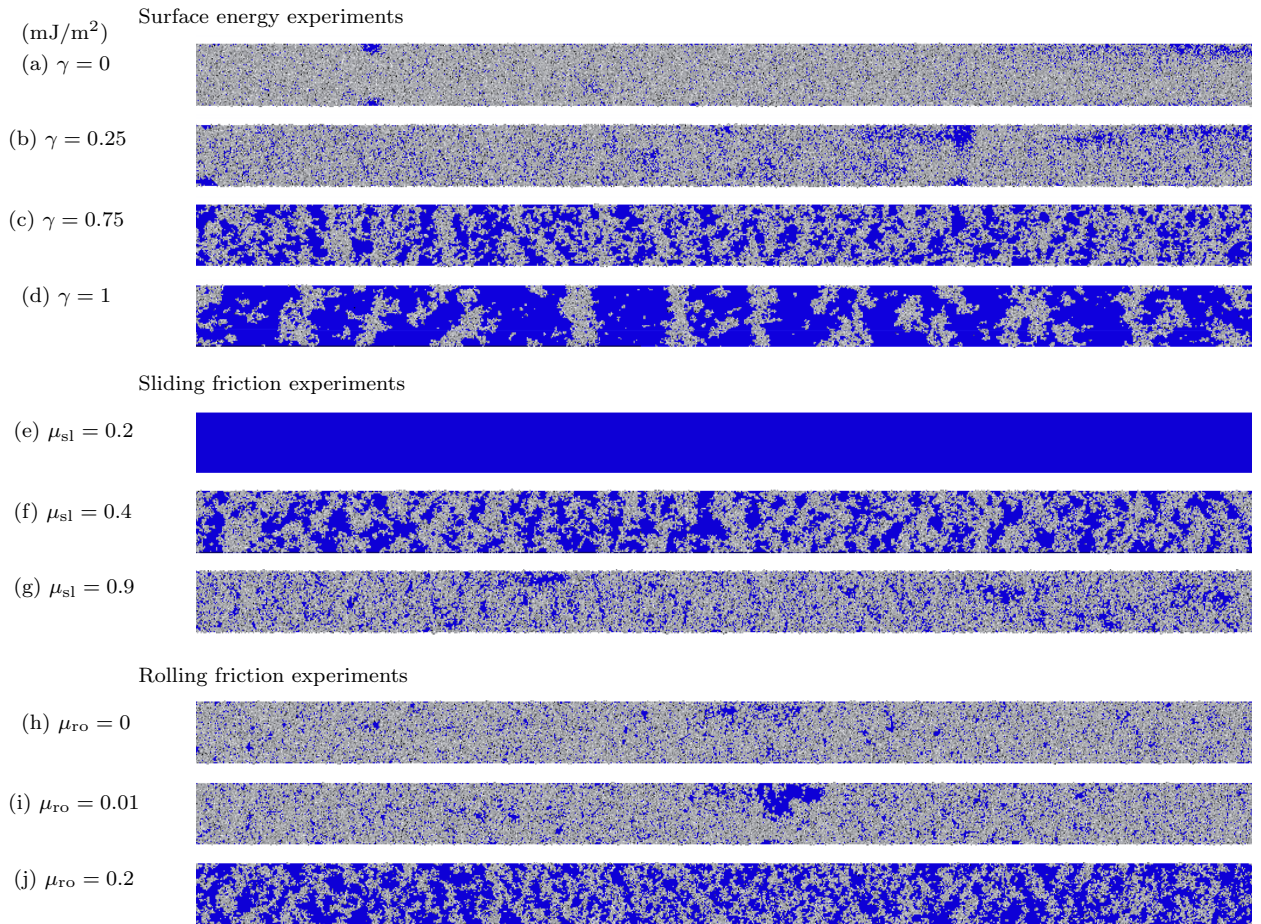
418 Bed height and density results are presented in Fig. 7. Mean height and  
419 density ( $\bar{H}$  and  $\bar{\varphi}$ ) are plotted against the various parameters. In addition, as  
420 mentioned above, sliding and rolling friction coefficients are modified indepen-  
421 dently for each contact type. Effects of *powder/powder* ( $po/po$ ), *powder/plate*  
422 ( $po/pl$ ) and *all* contacts parameters are respectively plotted in red, blue and  
423 green. Let us also recall that for surface energy simulations, we only considered  
424  $po/po$  contacts.

#### 425 3.3.1. Spreading length effect

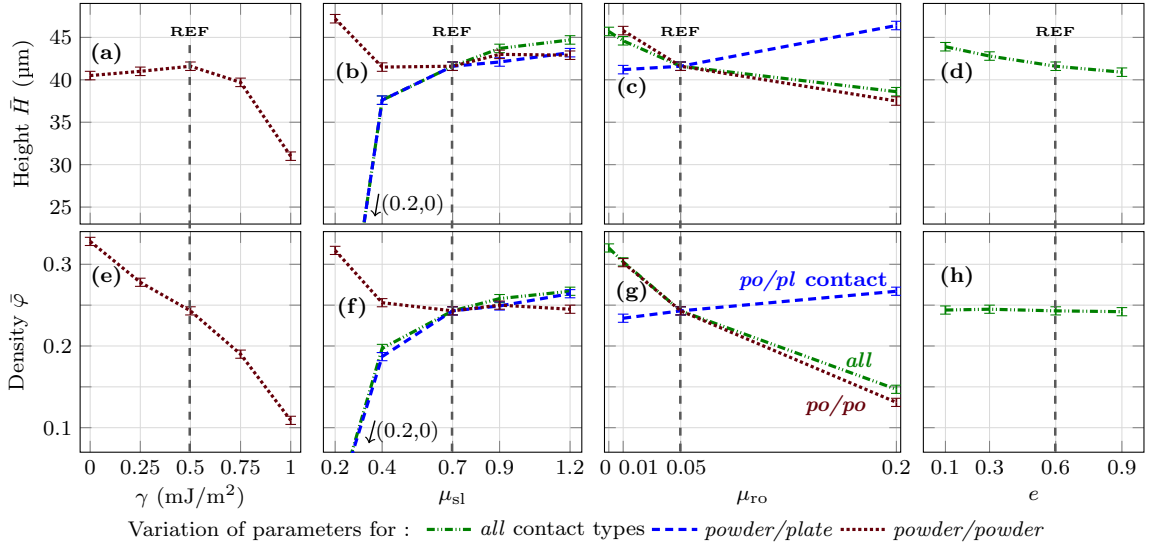
426 For the 30 mm bed, the blind length  $L_{\text{blind}}$  is unchanged. However, the analy-  
427 sis zone is 15 mm longer. The measured height and density of the 30 mm bed are  
428 not very different when compared to the 15 mm length simulations. This there-  
429 fore supports our assumption that 15 mm is long enough to be representative of  
430 the powder deposition in terms of height and density.

#### 431 3.3.2. Effective surface energy effect

432 In order to quantify the effect of effective surface energy, powder parameters  
433 are kept to their reference values except  $\gamma$ , which is equal to  $[0, 0.25, 0.5, 0.75, 1]$ .  
434 Effect on mean height and density are shown in Fig. 7(a and e). For surface  
435 energy under 0.5  $\text{mJ}/\text{m}^2$ , the mean height ( $\bar{H}$ ) is not significantly affected staying



**Fig. 6.** Raw powder beds from different simulations with different coefficient values. Only *powder/powder* contacts are modified for surface energy simulations. For sliding and rolling friction coefficients, all contact types are modified.



**Fig. 7.** Effects of surface energy, sliding, rolling and restitution coefficients on mean spread height ( $\bar{H}$ ) and density ( $\bar{\varphi}$ ).

436 around  $2/3$  of  $H_{\text{spreading}}$ . On the other hand, the mean density ( $\bar{\varphi}$ ) is linearly  
 437 affected in the all range going from 0.33 for  $\gamma = 0$  mJ/m<sup>2</sup> to 0.11 for  $\gamma = 1$   
 438 mJ/m<sup>2</sup>. The height and density variations along the powder bed barely exceed  
 439 the scatter observed on reference experiments.

440 Bed is denser and smoother for  $\gamma$  values less than 0.5 mJ/m<sup>2</sup>. Between  
 441 0.5 and 1 mJ/m<sup>2</sup> mean density and height jointly decrease, whereas deviations  
 442 increase. The density standard deviation over grid boxes takes values closes  
 443 to the mean density ( $\bar{\varphi}$ ) whereas the height standard deviation reaches half-  
 444 mean height ( $\bar{H}/2$ ), a situation characteristic of a poor bed quality with large  
 445 voids zones. When the effective surface energy takes values between 0.75 and 1  
 446 mJ/m<sup>2</sup>, the powder bed will become irregular with empty grid boxes as visible  
 447 in Fig. 6(d). Those empty patches are the worst situation for powder melting.  
 448 This result confirms the predominance of the surface energy effect according to  
 449 previously published studies [15, 47].

450 *3.3.3. Sliding friction effect*

451 Results are shown in Fig. 7(b and f). First, we consider the friction coefficient  
452 to be the same for all contacts (i.e. *po/po*, *po/pl* as well as *powder/blade*  
453 contacts): it is denoted  $\mu_{sl,all}$ . Over  $\mu_{sl,all} = 0.7$  a quasi plateau is observed for  
454 density ( $\bar{\varphi} = 25\%$ ) and height ( $\bar{H} = 2/3 H_{spreading}$ ). For  $\mu_{sl,all}$  lower than 0.7 a  
455 powder bed degradation is observed until that powder is totally pushed out the  
456 plate when  $\mu_{sl,all} = 0.2$ . For  $\mu_{sl,all} = 0.4$ , the decreases are about 10% from the  
457 plateau value for the height and about 25% for the density.

458 Interestingly, modifying the sliding friction coefficient only for contacts be-  
459 tween powder and plate leads to the same results. Sliding friction coefficient  
460 between powder and plate appears to be a key material parameter. A sliding  
461 friction around 0.4 with plate is required for the plate to hold the powder parti-  
462 cles and achieve a satisfactorily spreading powder.

463 Moreover, a *powder/powder* sliding friction ( $\mu_{sl,po/po}$ ) ranging from 0.4 to  
464 1.2 shows no effect, suggesting a powder displacement by rolling. When the  
465 sliding friction coefficient with plate is large enough, a low sliding friction between  
466 powder particles (see  $\mu_{sl,po/po} = 0.2$  case) improves mean height by 15% and  
467 density by 25%. Powder displacement by sliding is probably allowed in that  
468 case.

469 *3.3.4. Rolling friction effect*

470 As for the sliding friction coefficient, the effect of the rolling friction ( $\mu_{ro}$ )  
471 was studied on *all*, *po/po* and *po/pl* contact types. Firstly, as seen in Fig. 7(c  
472 and g), height and density are continuously affected in the whole range of  $\mu_{ro,all}$ ,  
473 going from 0.33 to 0.15 for density and from 45  $\mu\text{m}$  to 38  $\mu\text{m}$  for height. However  
474 height and density variation along bed remain limited compared to the case of  
475 high surface energy (1  $\text{mJ}/\text{m}^2$ ) simulation.

476 A modification of only the *powder/powder* rolling friction coefficient ( $\mu_{ro,po/po}$ )

477 amplifies the variation already observed for  $\mu_{ro,all}$ . Collective behavior is then  
478 essentially governed by *powder/powder* contacts. This suggests that spreading  
479 a powder that rolls with difficulty, such as water atomized powder for exam-  
480 ple, would lead to looser but continuous beds that could potentially fulfill the  
481 requirements for an L-PBF process.

482 On the other hand, an increase of the *powder/plate* rolling friction coefficient  
483 ( $\mu_{ro,po/pl}$ ) is beneficial for bed quality. For instance a value of  $\mu_{ro,po/pl} = 0.2$   
484 improves both density and height by 10% compared to the reference value.

### 485 3.3.5. Restitution coefficient

486 As seen in Fig. 7(d and h), the variation of the restitution coefficient between  
487 0.1 and 0.9 has a negligible impact. Our conclusion is that, at least for our process  
488 conditions, its determination is not an issue in this interval for powder spreading  
489 experiment.

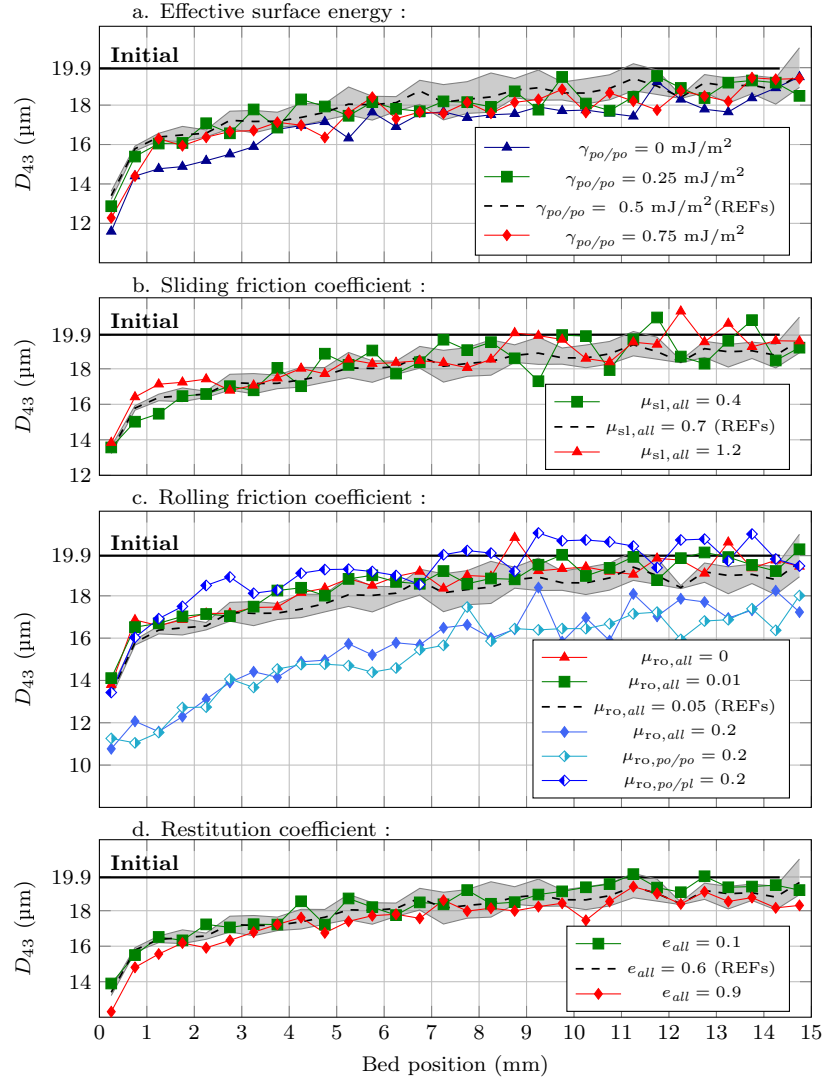
## 490 3.4. Segregation

### 491 3.4.1. Powder parameters effects

492 From now on, since it will be seen that most relevant segregation phenomena  
493 take place within the first few millimeters, the analysis zone will start at the very  
494 beginning of the building plate. In other words, as opposed to what was done  
495 previously, we will not consider a blind zone from the feeding plate. The volume  
496 moment mean diameter of particles  $D_{43}$  along the powder bed is plotted in  
497 Fig. 8. All parameter sets lead to the preferential deposition of smaller particles  
498 at the beginning of spreading. In the first 3 millimeters of the powder bed,  
499  $D_{43}$  approximately increases from 70% to 85% of its initial value (19.8  $\mu\text{m}$ ) as  
500 calculated from the starting powder characteristics. Then, the mean volume  
501 diameter reaches a plateau at 90% to 95% of this initial value.

502 Starting with surface energy, it is seen that segregation is not very sensitive  
503 to the value of  $\gamma$ . Only at a zero surface energy a somewhat smaller  $D_{43}$  on





**Fig. 8.** Volume moment mean diameter  $D_{43}$  along powder bed for different simulations. Bed is divided in 30 boxes of  $500 \mu\text{m}$  long. The dashed line and the gray shaded zone respectively represent the average and the minimum-maximum spread for the 5 simulations with reference parameters (REFs).

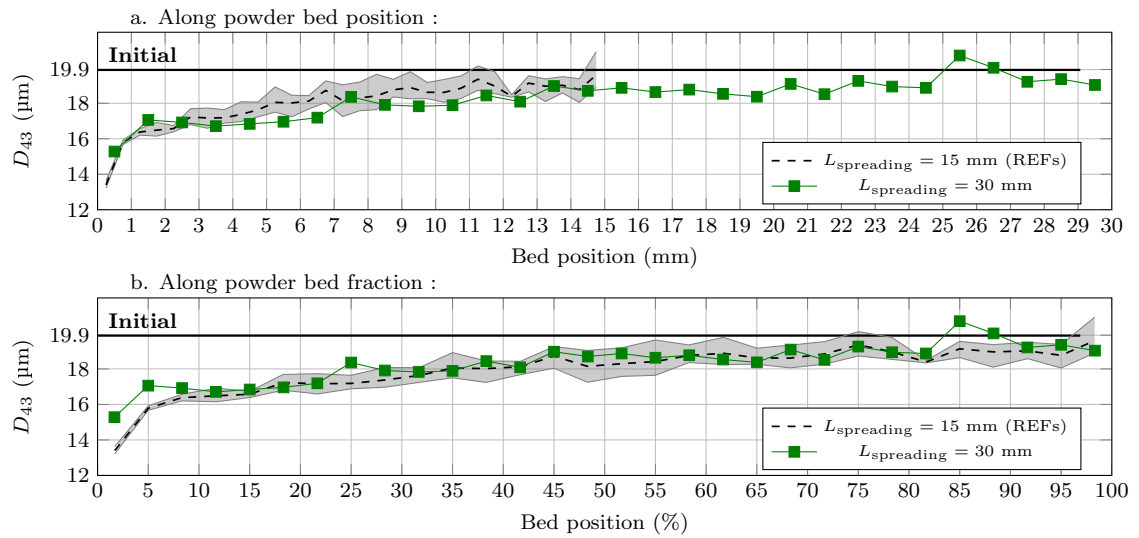
504 the first 4 mm of the bed can be observed. This can be interpreted stating that  
505 without adhesion, smallest particles are free to move between larger ones. The  
506 simulation with the effective surface energy equal to 1 mJ/m<sup>2</sup> is not plotted.  
507 As mentioned earlier, the powder bed presents large empty patches visible in  
508 Fig. 6(d) which make the curve chaotic. Moreover, in this case segregation can  
509 be considered a minor issue compared the voids that plague bed quality.

510 As observed for surface energy, the effect of sliding and restitution coefficients  
511 on segregation is quite limited. Regarding rolling friction, a high coefficient  
512 ( $\mu_{ro,all} = 0.2$ ) leads to the largest segregation.  $D_{43}$  is initially smaller than for  
513 other simulations at the beginning of deposition. In addition, the increase is  
514 slower leading to a significant and continuous evolution until half of the bed  
515 length. Then, it stabilizes around 85% of the initial value. The effect of the  
516 rolling coefficient is again due to *powder/powder* contacts. Indeed, curves for *all*  
517 and *po/po* contacts are nearly overlapped.

518 To sum things up on segregation issues, since the observed variations take  
519 place within the first few millimeters of the building plates where parts are  
520 rarely positioned in practice, it can be stated that segregation should not be  
521 a critical issue, at least for spherical powders from a gas atomization process.  
522 On the other hand, less spherical particles from a water atomization process  
523 with a higher rolling friction coefficient could segregate on longer distances and  
524 potentially induce variations of the received laser power which could be an issue  
525 for part manufacturing.

#### 526 3.4.2. Spreading length effect

527 As done in Fig. 8, Fig. 9 shows the effect of the spreading length on seg-  
528regation. Two spreads of 15 mm and 30 mm length in REF conditions are  
529 represented, where the volume moment mean diameter of particles  $D_{43}$  is plot-  
530 ted as a function of either bed length in mm or bed length fraction (normalized



**Fig. 9.** Volume moment mean diameter  $D_{43}$  along powder beds for reference parameter set with two spreading lengths. a/ Diameter is plotted along powder bed position, each box is 500  $\mu\text{m}$  long. b/ Diameter is plotted along powder bed fraction, bed is divided into 30 boxes. The dashed line and the gray shaded zone respectively represent the average and the minimum-maximum spread for the 5 simulations with reference parameters (REFs).

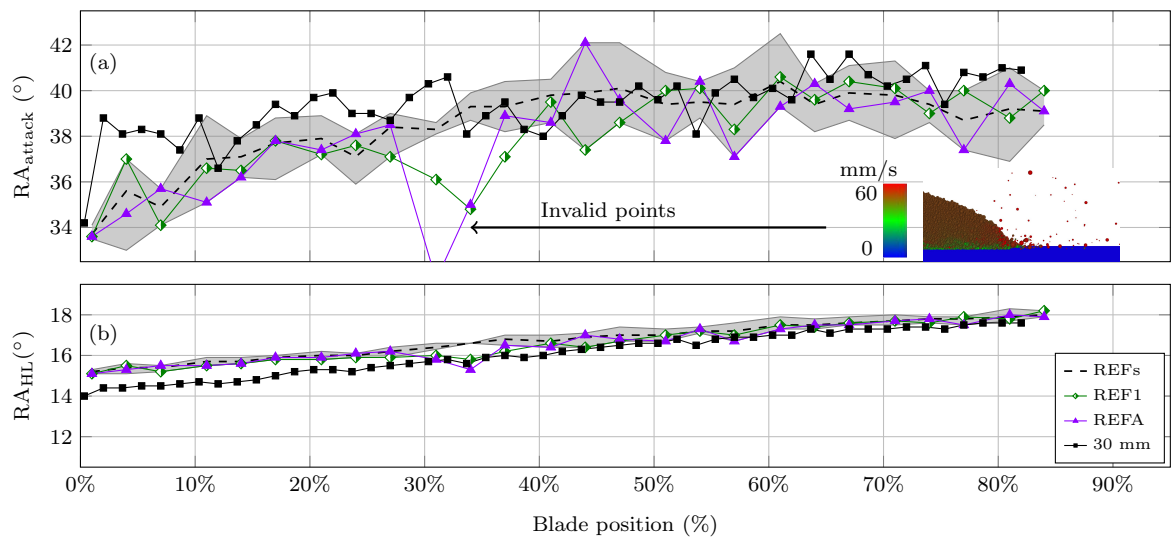
531 by spreading length). During the first 3 mm,  $D_{43}$  curves overlap when using  
532 the bed length in mm as x-axis. On the other hand, after these first 3 mm,  
533 curves overlap when using the bed length fraction as the x-axis. Interestingly,  
534 the Root Mean Square Deviation RMSD between 15 mm and 30 mm geometries  
535 is reduced by considering fractions instead of lengths. The rate of reduction is  
536 between 13% and 55% for different reference simulations. Apart from the first  
537 few millimeters of spreading, this points to a better physical description of the  
538 segregation phenomena using normalized spreading lengths.

### 539 *3.5. Recoating Angles (RA)*

#### 540 *3.5.1. RA stability along spreading*

541 Heap profile evolves during spreading.  $RA_{\text{attack}}$  and  $RA_{\text{HL}}$  are respectively  
542 plotted in the Fig. 10(a and b) all along spreading process for reference parameter  
543 simulations as well as for the 30 mm geometry simulation. The insert of Fig. 10  
544 enlightens the effect of particle ejections that take place in the vicinity of the  
545 heap's front end. Our moving average procedure (see Fig. 4) then fails, leading  
546 to outlier points that were removed from the RAs calculation.  $RA_{\text{HL}}$  is seen  
547 to increase in a linear manner. Therefore, a linear regression is implemented to  
548 characterize the evolution of this angle. The data from the 15 mm and 30 mm  
549 do not overlap, meaning that the measured slope is depending on the quantity  
550 of powder involved. However, the 15 mm and 30 mm data reach a similar value  
551 at the final spreading length. Then, for further comparisons of parameter sets  
552 results,  $RA_{\text{HL}}$  is characterized by the intercept value of the linear regression  
553 taken at 100% of the spreading length. It has to be noted that this observation  
554 is likely due to our choice of simulation conditions with feeding length equal  
555 to spreading length, but we nevertheless consider this value fit for comparison  
556 purposes.

557  $RA_{\text{attack}}$  presents a fast increase at the beginning of the building plate. After



**Fig. 10.**  $RA_{\text{attack}}$  and  $RA_{\text{HL}}$  along bed for reference simulations. The dashed line and the gray shaded zone respectively represent the average and the minimum-maximum spread for the 5 simulations with reference parameters (REFs). Invalid points between 31% and 38% for REF1 and REFA are removed from average, min and max calculations.

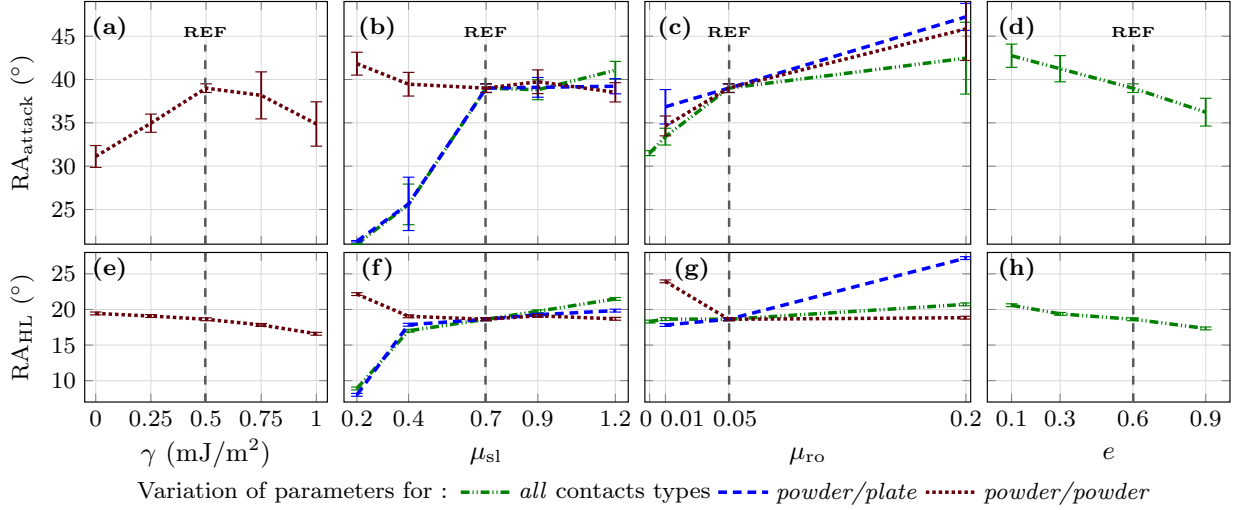
558 the first millimeters,  $RA_{\text{attack}}$  no longer increases, but it is still subjected to  
559 significant variations. Beyond 20% of the powder bed, average and standard  
560 deviation of the  $RA_{\text{attack}}$  are  $39.2^\circ$  and  $1.2^\circ$  for reference simulations.  $RA_{\text{attack}}$   
561 is roughly the same between both 15 mm and 30 mm geometries over 20% of the  
562 spreading length.

563 The  $RA_{\text{attack}}$  relative standard deviation around its mean value is 3% after  
564 the first 20% of spreading length, whereas for  $RA_{\text{HL}}$  it is about 1% around the  
565 fitting line. The higher value in the case of  $RA_{\text{attack}}$  is likely due to the fact that  
566 this indicator is sensitive to a powder behavior at the end of the heap involving  
567 only some hundreds of flowing particles in the avalanche zone. Avalanche is  
568 not continuous and subject to accelerations and decelerations, leading to strong  
569  $RA_{\text{attack}}$  variations during spreading. On the other hand, the  $RA_{\text{HL}}$  involves  
570 powder rearrangement at the scale of the whole heap; it is less sensitive to  
571 individual events compared to  $RA_{\text{attack}}$ . Therefore,  $RA_{\text{attack}}$  and  $RA_{\text{HL}}$  can be  
572 considered as complementary indicators to characterize the heap profile.

### 573 3.5.2. Powder parameters effects

574 RA sensitivity analysis results are presented in Fig. 11 following the same  
575 rules used for height and density in Fig. 7. Both Recoating Angles ( $RA_{\text{attack}}$ ,  
576  $RA_{\text{HL}}$ ) are plotted for all simulations. Variations of each powder parameter  
577 around reference value are plotted. Sliding and rolling friction coefficients are  
578 differentiated between *powder/powder* and *powder/plate* contacts.

579 To compare different parameter sets together, the heap profile is measured  
580 at 6 times locations between  $t = 600$  ms and  $t = 850$  ms. Those time steps  
581 are uniformly distributed between 0% and 84% of the blade displacement on the  
582 building plate as presented by Fig. 10. Our choice is made to avoid end effects  
583 on the comparison between parameter sets as the heap can be considered to be  
584 in a transient state before 17%. The spread associated to the above sampling is



**Fig. 11.** Effects of surface energy, sliding, rolling and restitution coefficient on both definitions of RAs.

585 less than  $1^\circ$  for  $RA_{\text{attack}}$ , and less than  $0.2^\circ$  for  $RA_{\text{HL}}$ .

586 The error bars on the figure correspond to the standard deviation calculated  
 587 on those 6 points for each simulation. It should be noted that when considering  
 588 the whole set of reference simulations, the observed spread is equivalent.

589 As seen in Fig. 11, almost all simulations lead to similar effects on  $RA_{\text{attack}}$   
 590 and  $RA_{\text{HL}}$ . Starting from the restitution coefficient, a larger value of  $e$  amounts  
 591 to increased particle velocities after collisions, and thus to a facilitated rear-  
 592 rangement of the heap by particle flow. Therefore, both angles are smallest for  
 593  $e = 0.9$ .

594 Sliding friction coefficient  $\mu_{\text{sl}}$  has an impact for *powder/plate* contact type  
 595 as for height and density analysis. *All* and *powder/plate* contact types points  
 596 again overlap. An insufficient sliding friction coefficient between powder and  
 597 plate leads to low  $RA_{\text{attack}}$  and  $RA_{\text{HL}}$ . Forces between plate and heap are not  
 598 large enough to raise the powder heap upwards on the blade.

599 According to Fig. 11(g), the rolling friction coefficient has no impact on  $RA_{\text{HL}}$

600 for the *all* contact types configuration. However, each contact type has his own  
 601 effect. Reducing  $\mu_{ro,po/po}$  will reduce internal forces inside powder, facilitating  
 602 the raise of the heap on the blade and thus higher  $RA_{HL}$ . On the other hand, re-  
 603 ducing  $\mu_{ro,po/pl}$  facilitates powder rolling on plate. Therefore, the heap stretches,  
 604 and the  $RA_{HL}$  is smaller.  $RA_{attack}$  is reduced when rolling friction is reduced for  
 605 *powder/powder* contacts as well as for *powder/plate*.

606 The effective surface energy has a slight effect on  $RA_{HL}$ , an increase of  $\gamma$   
 607 leads to a moderate decrease of  $RA_{HL}$ . Regarding  $RA_{attack}$ , a maximum value  
 608 is observed for  $0.5 \text{ mJ/m}^2$ . The bell-shaped curve results from a change in flow  
 609 regime around  $0.5 \text{ mJ/m}^2$ . All these results will now be discussed with a focus on  
 610 particle velocities that will allow a better understanding of the involved physical  
 611 phenomena.

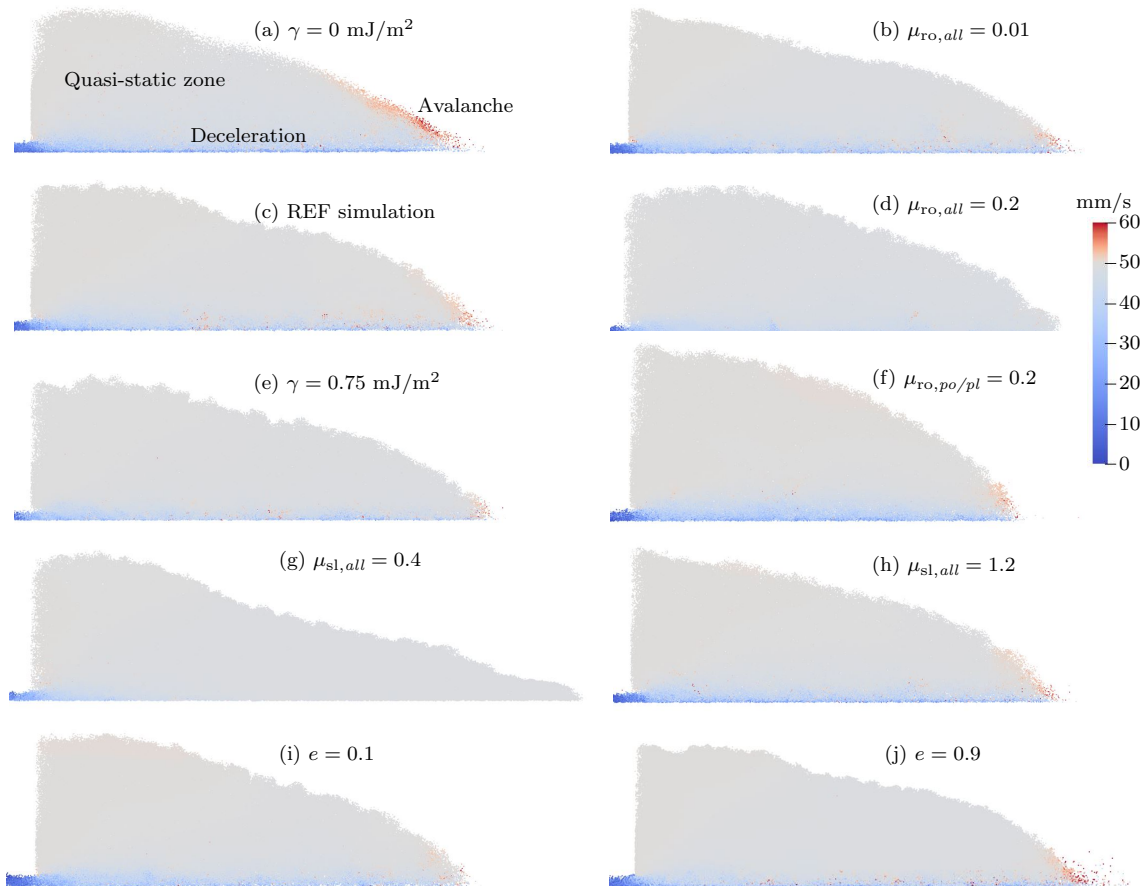
### 612 3.6. Powder flow zones

613 Regarding the norm of linear velocity, different flow zones can be identified  
 614 in powder heaps presented in Fig. 12, as were first observed by Zhang et al. and  
 615 Yim et al.[10, 20]. First, it can be seen that most of the particles are in the  
 616 quasi-static zone, where their velocities are close to that of the blade velocity,  
 617 namely  $50 \text{ mm/s}$ , color code in gray in the figure. In addition, particle motion  
 618 can also be characterized by their rolling velocities measured on their surfaces as  
 619 characterized by Eq. (16). In the quasi-static zone, the rolling velocity of those  
 620 particles, in blue in Fig. 13, is almost zero, further supporting the assumption  
 621 of quasi-static behavior according in the blade frame of reference.

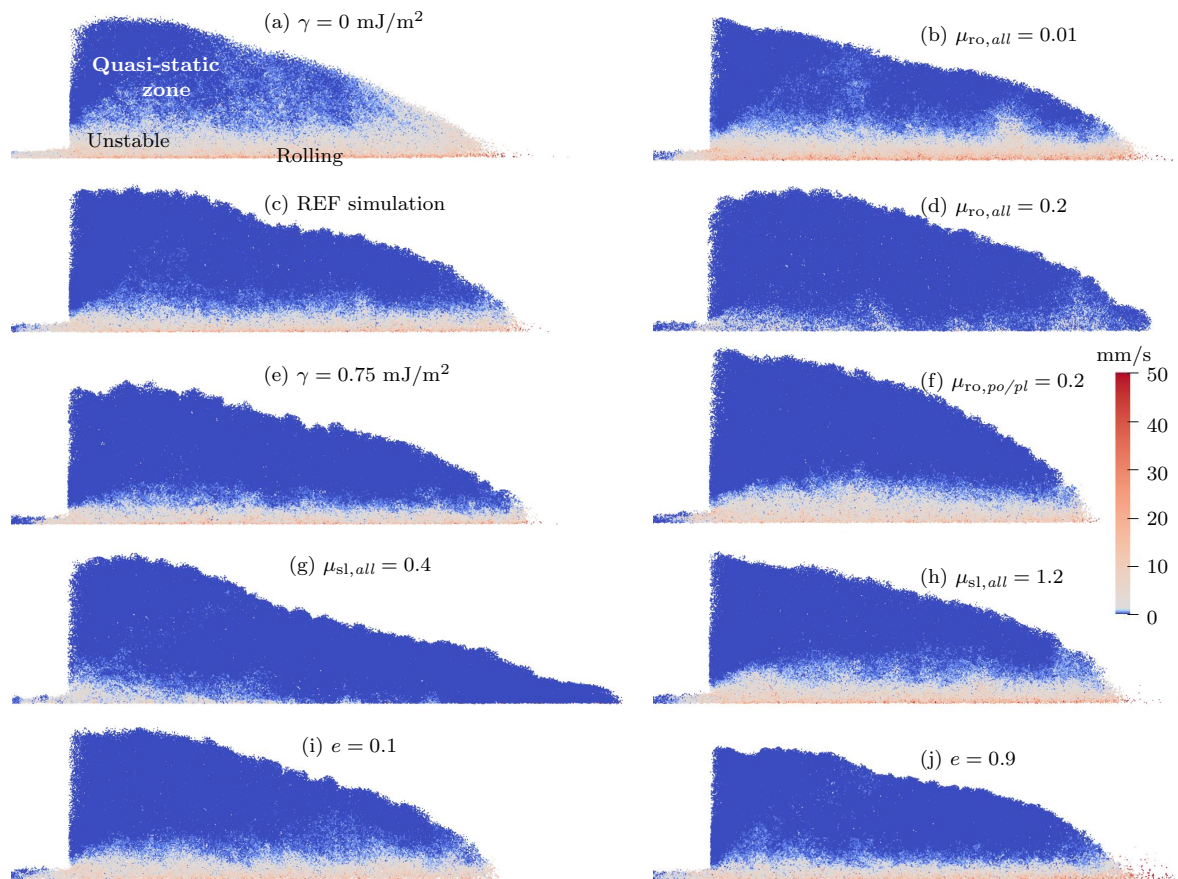
$$\vec{v}_{s,i} = \vec{\omega}_i R_i \tag{16}$$

622 The second zone is the free-flowing zone, also called avalanche zone [10, 20].  
 623 It is composed by particles with color code in red in front of the bed, with linear





**Fig. 12.** Linear velocity of particles in the building plate frame,  $t = 750$  ms. Each simulation is specified. Different flowing zones can be identified, particles moving at blade velocity (50 mm/s) are in the quasi-static zone. Particles faster than blade are in the avalanche zone. Then, particles slower are in the deceleration zone.



**Fig. 13.** Surface velocity  $\|\vec{v}_s\|$  of particles,  $t = 750$  ms. Each simulation is specified. Different flowing zones can be identified, particles with no surface velocity are in the quasi-static zone. Particles presenting a non null surface velocity, approximately between 1 and 10 mm/s, are in the unstable zone. Then, a thin rolling band is composed of particles with an high surface velocity over 20 mm/s.

624 velocities higher than the blade-spreading rate (see Fig. 12). Interestingly, this  
625 zone is not observed for all parameter sets, as its existence requires a sufficient  
626 powder flowability combined with a sufficiently raised upward heap. This last  
627 assumption is illustrated by the case  $\mu_{sl,all} = 0.4$ , where the plate friction is  
628 too small, resulting in a heap that is not raised upwards enough at the front of  
629 the bed. Therefore, the slope necessary for powder avalanche is too small, and  
630 particles do not fall.

631 The last zone is characterized by the deceleration of particles in the vicinity  
632 of the plate, with linear velocities smaller than the one of the blade (see color  
633 code blue in Fig. 12). An interesting finding of our simulations is that this zone  
634 extends all along the powder heap for favorable spreading conditions. In such  
635 cases, a specific behavior can be identified in the immediate vicinity of the plate,  
636 where the linear and surface velocities of the particles are similar, taking values  
637 between 20 and 40 mm/s and indicating a perfect rolling of the particles appears  
638 on the plate surface. Furthermore, above the building plate, powder instabil-  
639 ity extends for hundreds of micrometers along the vertical axis, translating to  
640 surface velocities between 1 and 10 mm/s (see Fig. 13). The extension of this  
641 instability zone depends on the interactions within the powder heap. For un-  
642 favorable powder spreading (e.g. in cases  $\mu_{sl,all} = 0.4$  or  $\mu_{ro,all} = 0.2$ , particle  
643 deceleration takes place only in the vicinity (say first hundreds of micrometers)  
644 of the blade and without easy rolling on plate. This final deceleration just be-  
645 fore passing through blade gap is probably due to shear stress created by the  
646 blade as described by Yim et al.[20]. In any case, it appears that the extent  
647 of this deceleration zone can be a good predictor of bed quality. Finally, even  
648 though outside the scope of the present work, it can be stated that improving  
649 the shear stress distribution in this ultimate deceleration zone could be achieved  
650 by optimizing the blade geometry [12, 13].

651 All contact law parameters are seen to modify powder flow in a specific way.  
652 On the one hand, a high effective surface energy limits the extension of powder  
653 instability over the deceleration zone, increasing the size of the quasi-static zone.  
654 On the other hand, a zero effective surface energy leads to a large deceleration  
655 zone.

656 The restitution coefficient does not significantly modify the deceleration zone,  
657 even if tiny red dots are visible within the deceleration zone in Fig. 12(j) for  
658  $e = 0.9$ , representative of some bouncing contacts and interactions between  
659 particles. Moreover, those bouncing contacts favor particle flow, as seen at the  
660 front of the heap in the avalanche zone.

661 Sliding and rolling friction coefficients play a key role on the velocity profile  
662 in the deceleration zone. A low sliding friction coefficient prevents particles from  
663 rolling, the same observation being made for  $\mu_{ro,all} = 0.2$  albeit with a different  
664 heap profile. A low rolling friction coefficient or a high sliding friction coefficient  
665 do the opposite, a more visible rolling layer can be observed as a red line, e.g. in  
666 Fig. 13(b). Nevertheless, this effect is more visible with low rolling coefficient.  
667 The case  $\mu_{ro,po/pl} = 0.2$  is peculiar, as particles stop rolling on the plate, see  
668 Fig. 13(f), but deceleration remains nevertheless possible as seen in Fig. 12(f).  
669 There is a significant extension of the unstable zone over the deceleration area  
670 showing a good particle flow over a high friction plate.

## 671 4. Discussion

### 672 4.1. Towards an optimum heap profile for good powder bed quality

673 Powder bed quality thus seems to be governed by the particle behavior within  
674 the deceleration zone above the build plate. More precisely, a large deceleration  
675 zone with rolling particles is seen to be correlated with a good powder bed  
676 quality in terms of height and density. Moreover, it appears that the heap profile

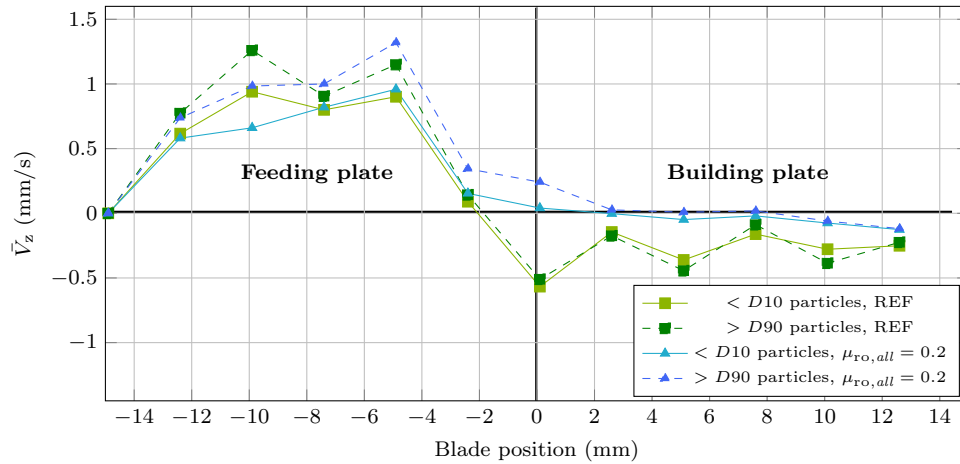
677 is controlled by powder behavior within the deceleration and avalanche zones.  
678 First, friction with the plate leads to an upward motion of the powder heap and  
679 an increase of the  $RA_{HL}$ . Then, powder can freely flow if heap is sufficiently  
680 raised upward, creating the avalanche.

681 The avalanche itself is characterized by the  $RA_{attack}$ , which depends on pow-  
682 der properties, especially surface energy and rolling friction. Those parameters  
683 are also paramount for standard angle of repose experiments [30, 40], suggest-  
684 ing similar mechanisms. However, it should be noted that the  $RA_{attack}$  has no  
685 meaning if there is no avalanche zone, i.e. when particles do not flow. From the  
686 different characteristics of the powder heap, a global and a local angle of attack,  
687 it seems possible to foresee final bed quality.

688 In this respect, the perfect heap has a maximum  $RA_{HL}$  - characteristic of a  
689 high interaction with the plate - and a minimum  $RA_{attack}$  - characteristic of easy  
690 flowing powder. A maximal  $RA_{HL}$  with minimal  $RA_{attack}$  corresponds to a right-  
691 angled triangle, with the hypotenuse being the heap top surface. Simulations  
692 with  $\gamma = 0 \text{ mJ/m}^2$  or  $\mu_{ro,all} = 0.01$  shown in Fig. 12(a and b) approach this  
693 perfect shape. They have a small  $RA_{attack}$  and a high  $RA_{HL}$  as seen in Fig. 11.  
694 In addition, they present ones of the best bed height and density of the analysis  
695 (see Fig. 7).

#### 696 4.2. Where does segregation take place?

697 The detailed study of flow phenomena within the heap also allows the issue  
698 of the origin of segregation to be addressed. Indeed, segregation observed in  
699 Fig. 8 can be accounted for invoking a differential velocity between small and  
700 large particles, which results in a mean height, characterized as the average posi-  
701 tion along z-axis, lower for small particles than for large particles. Accordingly,  
702 Fig. 14 and Fig. 15 show respectively the mean velocity along z-axis and the  
703 mean height for the smallest (below D10) and the largest (above D90) particles



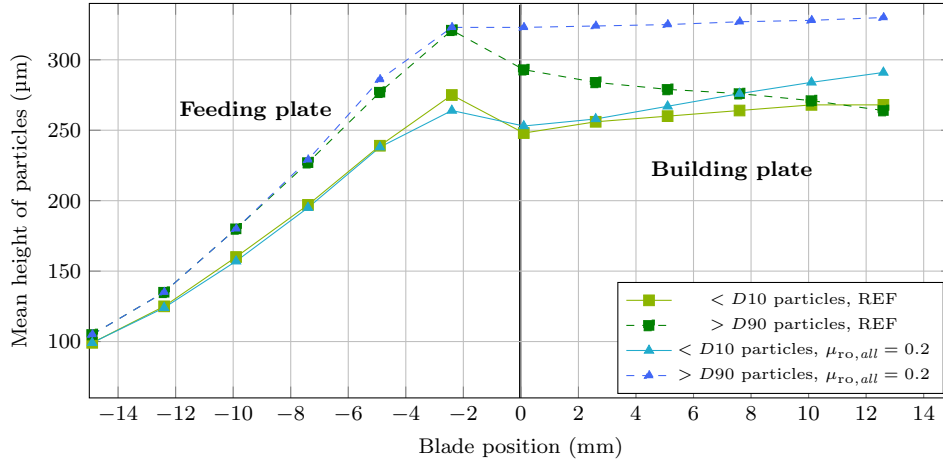
**Fig. 14.** Mean particle velocity along z-axis during blade movement, including powder feeding and spreading. Velocities are plotted for particles smaller than D10 and larger than D90.

704 within the heap during the spreading process for the reference powder parameter  
 705 set and a high rolling friction case.

706 During powder feeding between -15 and 0 mm, the blade gathers particles on  
 707 the feeding plate and pushes them forward to form a powder heap. The vertical  
 708 mean velocity  $\bar{V}_z$  is positive for both large and small particles corresponding  
 709 to the heap formation, but with a large speed difference between smallest and  
 710 largest particles. Thus, as seen in Fig. 15, the mean height of all particles  
 711 increases but more for the largest particles, inducing segregation.

712 Both plotted simulations show a similar behavior during feeding. The first  
 713 difference that can be observed between the reference (REF) and the high rolling  
 714 resistance ( $\mu_{ro,all} = 0.2$ ) simulations is from -2 and 0 mm, a region corresponding  
 715 to the transition between the feeding and the building plate, where there is a  
 716 step of spreading height. In this region, the drop in vertical velocity is much  
 717 higher for both size classes in the REF simulation, down to negative values.

718 In the powder spreading zone from 0 to 15 mm, starting from the REF



**Fig. 15.** Mean particle position along z-axis during blade movement, including powder feeding and spreading. Positions are plotted for particles smaller than D10 and larger than D90.

719 simulation, all particle velocities are nearly the same and negative as visible in  
 720 Fig. 14. However, the particles mean heights move in different ways (see Fig. 15):  
 721 upwards for the smallest particles and downwards for the largest. To account for  
 722 such a finding, let us notice that small particles, which are initially segregated  
 723 at the bottom of the heap, are deposited first. Thus, their mean height increases  
 724 because particles in the bed are ousted from the average calculation. At the end  
 725 of the building plate, the heap is well mixed for REF simulation. Indeed, mean  
 726 heights for largest and smallest particles are nearly the same.

727 As for the spreading behavior in the high rolling resistance simulation  $\mu_{ro,all} =$   
 728 0.2, particle velocity remains just below zero from 0 to 15 mm, contrary to  
 729 reference simulation that exhibited significantly lower values. This is a result of  
 730 a reduced powder flow for the high rolling resistance simulation. In that case,  
 731 there is an increase in mean position even for the large particles during spreading.  
 732 It results in a higher mean position along z-axis for all particles, and a segregated  
 733 powder heap at the end of spreading as opposed to the reference case.

## 734 5. Conclusion

735 In this work, the effect of contact law parameters on powder spreading is nu-  
736 merically investigated using DEM simulations. Regarding powder bed quality,  
737 the effective surface energy is the most important contact law parameter. Its  
738 variation between 0 and 1 mJ/m<sup>2</sup> leads to a linear reduction of the density by  
739 a factor of more than 2; in addition, discontinuous powder bed are observed for  
740 values over 0.75 mJ/m<sup>2</sup>. For a meaningful simulation of actual powder spread-  
741 ing, an accurate determination of its value is paramount. The impact of the  
742 rolling friction coefficient is also paramount for contacts between powder parti-  
743 cles. In the tested range,  $\mu_{To}$  impact is of the same order than for surface energy.  
744 Its determination should thus be carried out using characterization techniques  
745 involving only powder particles. On the other hand, the impact of the sliding  
746 friction coefficient is more important for contacts between powder and building  
747 plate than between powder particles. Its characterization should be done for  
748 this contact type, confirming the validity of the approach of Nan et al.[19]. A  
749 minimal value of sliding friction around 0.4 with the plate is necessary in order  
750 to deposit the powder on plate. Finally, the restitution coefficient does not have  
751 a significant impact on powder bed quality; its determination is not a first order  
752 issue.

753 As for heap characterization, the three flowing zones identified in previous  
754 works [10, 20] were indeed observed in our simulations. But we showed that,  
755 depending on the contact law parameters, the avalanche and deceleration zones  
756 do not always exist. The deceleration zone is where the plate slows powder  
757 particles by friction, its presence is essential for adequate powder deposition.  
758 Therefore, in the case of simple geometries where the blade has no significant  
759 compaction effect, a characterization of this zone of friction between powder  
760 and plate looks essential. Interestingly, our work allows to make a connection



761 between bed quality and heap shape.

762 The effect of geometry was also verified by doubling the simulation length,  
763 which was seen to lead to insignificant variation in terms of height and density.  
764 As for particle flow within the heap, the doubling of the simulation length leads  
765 to small differences on particle size segregation and RA. Our simulations showed  
766 that the mechanisms leading to size segregation on the building plate have their  
767 origin in flow phenomena occurring during the formation of the heap on the  
768 feeding plate. This issue is therefore highly dependent on the simulation choices  
769 and the modeled geometry.

770 These findings can further enhance characterization protocols of AM pow-  
771 ders in order to determine the ability of a given powder to be properly spread  
772 on a given surface, namely in terms of powder flowability and plate friction. As  
773 for perspectives, the present work points to the necessity of adequately charac-  
774 terizing the spreading conditions. As such, studies of deposition on an actual  
775 solidified part, as opposed to a bare plate, would be of interest. More precisely,  
776 a characterization of the rolling friction coefficient between powder and a solid-  
777 ified part is still unexplored and looks as essential for the simulations' accuracy.  
778 Further works on the ability of the heap shape to predict spreading quality  
779 through the identification of new descriptors should also be carried out. Finally,  
780 our methodology could be extended to include the effect of different spreading  
781 devices, e.g. blades of various shapes and orientations, as well as rollers.

## 782 **6. Acknowledgments**

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**Table A.1.** Deviation tests results for height, density and Recoating Angles.

Simulation	$\bar{H}$ $\mu m$	$\bar{\varphi}$	RA <sub>attack</sub>	RA <sub>HL</sub>
REF	41.6	0.243	39.0°	18.6°
REF1	42.5	0.243	39.5°	18.8°
REF2	41.8	0.242	38.6°	18.9°
REFA	42.3	0.249	38.5°	18.4°
REFB	42.0	0.252	39.7°	18.7°
Estimation of the results deviations between REF, REF1, REF2, REFA and REFB :				
Mean Value	42,0	0,246	39.1°	18.7°
Standard deviation	0,4	$4 * 10^{-3}$	0.5°	0.2°
Relative standard deviation	0.9 %	1.8 %	1.5 %	1.1 %

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