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An efficient bond model for particle adhesion simulation in advanced manufacturing

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Abstract. The aim of the present work is to investigate the underlying structure of most common bond models used in particle dynamics, with an aim to enable their use in additive manufacturing simulation. In this context, in advanced manufacturing processes proper adhesion between particles requires certain stability requirements to be satisfied. Conversely, erroneous agglomeration resulting from particle adhesion may affect the particle-size spatial distribution and thereby compromise the mechanical properties of the manufactured piece. These constitute some of the reasons why particle adhesion continues to be a particularly important phenomenon in a wide range of engineering applications. In this work, we propose a simple bond model taking into account such considerations, with which we are able to capture inter-particle bonding very straightforwardly once a given bonding criterion is met. The derived stability conditions establish recommendations that can help the selection of proper parameter values (such as, but not only, the strength of the bond) for most common bond models, thereby guiding (or even avoiding) burdensome problem-dependent calibration. Numerical examples are provided to validate our scheme and explore its outcomes.

Keywords: Particles; bond model; adhesion; additive manufacturing; discrete element methods (DEM).

1 Introduction

The adhesion properties of powder particles may profoundly influence the quality of parts made by Additive Manufacturing (AM) processes [1]. In this context, adhesive bonding has become a key technology among the various industrial sectors (e.g., automotive, aerospace) that resort to AM due to its constant demand for lighter, more resistant, and environmentally friendly materials. In the small particles regime, wherein surface forces and near-field or long range interactions (i.e. electromagnetic interactions) dominate over gravitational forces and inertia effects (e.g., for a 1 μm diameter particle, the force of adhesion can easily exceed the force due to gravity by a factor greater than 10^6 [2]), bonding can be satisfactorily modelled through forces derived from well-established adhesion theories, like, e.g., the classical JKR (Johnson, Kendall and Roberts [3]) theory. For heavier particles, however, typically of the order of at least a few micrometers and higher (100μm<), gravity and inertia dominate [4], and such adhesion-theory based models are no longer satisfactory. In this regime, bonding is better represented through phenomenological mass-spring models, which provide an attractive force to interacting particles whenever they come into contact, usually with stiffness given through some (oftentimes ad-hoc) constitutive equation or based on especial considerations on the problem at hand. In the present work, we propose a simple (mass-spring) bond model able to capture inter-particle sticking very straightforwardly once a given bonding criterion is met. Our idea is to implement it in the near future within the discrete element method (DEM) formulation of Campello [5], [6] and [7], and then couple it with lumped heat-transfer equations for incorporation of thermal effects (e.g. due to temperature gradients and external heat sources, very relevant to AM processes) within the framework proposed in a recent work by the authors [8]. These two tasks will be accomplished in a forthcoming work by the authors, already under development. Here, instead, we will concentrate on the bond model itself, aiming to make it available for future use in advanced manufacturing simulation. Throughout the text, plain italic letters ($a, b, \ldots, \alpha, \beta, \ldots, A, B, \ldots$) denote scalar quantities, whereas boldface italic letters

($\boldsymbol{a}, \boldsymbol{b}, \ldots, \boldsymbol{\alpha}, \boldsymbol{\beta}, \ldots, \boldsymbol{A}, \boldsymbol{B}, \ldots$) denote vectors in a three-dimensional Euclidean space. The (standard) inner product of two vectors is denoted by $\boldsymbol{u} \cdot \boldsymbol{v}$, the norm of a vector by $\|\boldsymbol{u}\| = \sqrt{\boldsymbol{u} \cdot \boldsymbol{u}}$ and the absolute value of a scalar by $|a|$. Notation with a superposed dot is adopted to designate time derivatives.

2 Force potentials for attraction and repulsion

In several modeling approaches, such as molecular dynamics, pairwise attractive and repulsive interactions between particles of a system can be described through force potentials. For a particle i interacting with another j, if we only consider the central (normal) direction, we can say that i experiences a one-dimensional motion described by a coordinate r along this direction, in which it is both attracted to and repulsed from j, which in turn has coordinate r_j. In these conditions, force potentials representing the motion of i have the following general form

$$\psi(r) = c_1 |r - r_j|^{-m} - c_2 |r - r_j|^{-n} = c_1 \left(\frac{1}{|r - r_j|} \right)^m - c_2 \left(\frac{1}{|r - r_j|} \right)^n , \tag{1}$$

where $|r - r_j|$ is the distance between i and j and c_1, c_2, m and n are nonnegative constants ($c_1, c_2 \geq 0$ and $m, n \geq 0$). One well-known example of such potentials are the Mie´s potentials, of which the classic Lennard-Jones potential [9] is a special case. These potentials may likewise be written as

$$\psi(r) = \frac{k_1}{-\alpha_1 + 1} |r - r_j|^{-\alpha_1 + 1} - \frac{k_2}{-\alpha_2 + 1} |r - r_j|^{-\alpha_2 + 1} , \tag{2}$$

wherein the k´s and α´s are nonnegative. Accordingly, the force acting on i due to its interaction with j reads

$$f(r) = -\frac{d\psi}{dr} = k_1 |r - r_j|^{-\alpha_1} n - k_2 |r - r_j|^{-\alpha_2} n , \quad \text{with} \quad n = -\frac{d}{dr} |r - r_j| = \frac{r_j - r}{|r - r_j|} . \tag{3}$$

The positive term on the right hand side of $f(r)$ stands for the attractive part of the interaction, whereas the negative term for the repulsive one. A necessary and sufficient condition for the interaction to have an equilibrium configuration is that the potential have a stationary point $r = r_{eq}$, such that

$$\left. \frac{d\psi}{dr} \right|_{r_{eq}} = -f(r_{eq}) = k_1 |r_{eq} - r_j|^{-\alpha_1} - k_2 |r_{eq} - r_j|^{-\alpha_2} = 0 , \tag{4}$$

from which it follows

$$|r_{eq} - r_j| = \left(\frac{k_2}{k_1} \right)^{\frac{1}{\alpha_2 - \alpha_1}} . \tag{5}$$

In the eq. (5), r_{eq} represents the equilibrium position of i w.r.t. j in their central direction and $d_{eq} = |r_{eq} - r_j|$ is the equilibrium distance between them. A necessary and sufficient condition for r_{eq} to be stable is that the potential be a minimum at r_{eq}, i.e., $\psi(r)$ should be locally convex around r_{eq}. By imposing that the second derivative of ψ shall be positive at r_{eq}, and taking (5) into consideration, it follows that $\alpha_2 > \alpha_1$, which is the requirement for stability of the interaction. Still, by differentiation of eq. (4) we obtain the inflection point of the potential, r_{crit}, from which it follows that

$$|r_{crit} - r_j| = \left(\frac{\alpha_2 k_2}{\alpha_1 k_1} \right)^{\frac{1}{\alpha_2 - \alpha_1}} , \quad \text{where} \quad d_{crit} = |r_{crit} - r_j| \quad \text{is the critical distance of the interaction} . \tag{6}$$

3 Attraction and repulsion upon contact

In the interaction of two objects that are in contact, attractive forces might appear[1] besides the repulsive (contact) force they experience. Contact interactions between particles are often described through the amount of overlap (or local penetration) experienced by the particles, i.e., based on the distance between the centers of a potential contact pair. Models that follow such an approach are commonly referred to as *soft-sphere* models [5]. If we call such overlap by δ, and substitute $|r-r_j|^{-1}$ by δ in equation (3), we arrive at:

$$f(\delta) = k_1\delta^{\alpha_1}n - k_2\delta^{\alpha_2}n\,, \quad \text{where} \quad \begin{cases} k_1 & \text{is the stiffness of the atractive part} \\ k_2 & \text{is the stiffness of the repulsive part} \end{cases} \tag{7}$$

The equilibrium configuration of the interaction, if it exists, happens at an equilibrium overlap given by

$$\delta_{eq} = \left(\frac{k_1}{k_2}\right)^{\frac{1}{\alpha_2-\alpha_1}}. \tag{8}$$

Opposed to eq. (5), here the base of the exponentiation now has the stiffness of the attractive term on the numerator and that of the repulsive term on the denominator, as a consequence of the reciprocal analogy established between δ and $|r-r_j|$. By imposing δ_{eq} to be a stable configuration (similarly as done for r_{eq} in the previous section), we arrive at

$$\alpha_2 > \alpha_1\,, \tag{9}$$

i.e., the exponent of the contact term must always exceed that of the adhesion term. In addition, the critical overlap of the interaction (i.e., the overlap at which it loses stability) reads

$$\delta_{crit} = \left(\frac{\alpha_1 k_1}{\alpha_2 k_2}\right)^{\frac{1}{\alpha_2-\alpha_1}}, \text{ where } \delta \geq \delta_{crit} \text{ is mandatory for an ever-stable contact-adhesion interaction.} \tag{10}$$

If eq. (10) is satisfied and the bonding criterion is met[2], then the attractive-repulsive interaction arises and the bond is established, in which case it will evolve into a harmonic oscillation around the equilibrium configuration δ_{eq}. Such oscillation can be viewed as the motion of a one degree of freedom mass-spring oscillator governed by the following second-order differential equation

$$m^*\ddot{(\delta-\delta_{eq})} = -f(\delta-\delta_{eq}), \text{ or } m^*\ddot{x} = -f(x), \quad \text{with} \quad x = \delta-\delta_{eq} \quad \text{and} \quad m^* = \frac{m_i m_j}{m_i+m_j}, \tag{11}$$

where m^* is the effective mass of the oscillation and $-f$ is the (nonlinear) restoring force provided by the spring on m^*, which is given through eq. (7). A special case of the repulsive part of equation (7) is that of Hertzian contact (see Johnson [10]), which can be obtained by setting

$$k_2 = \frac{4}{3}E^*\sqrt{r^*} \quad \text{and} \quad \alpha_2 = \frac{3}{2}, \quad \text{where} \quad r^* = \frac{r_i r_j}{r_i+r_j} \quad \text{and} \quad E^* = \frac{E_i E_j}{E_j(1-\nu_i^2)+E_i(1-\nu_j^2)}, \tag{12}$$

where r^* and E^* are the so-called effective radius and effective elasticity modulus of the contacting pair (in which r_i and r_j are the radii of particles i and j, and E_i, E_j, ν_i and ν_j their elasticity moduli and Poisson coefficients, respectively). It follows that the equilibrium overlap is

[1] E.g., due to melting of their surface materials, or to chemical reactions that may ultimately glue or weld the bodies
[2] E.g., the temperatures of the particles reaching a certain critical temperature, like their melting temperature, or the concentration of chemical substances reaching a certain critical concentration.

$$\delta_{eq} = \left(\frac{k_1}{\frac{4}{3} E^* \sqrt{r^*}} \right)^{\frac{1}{3/2-\alpha_1}} , \tag{13}$$

whereas the critical overlap is

$$\delta_{crit} = \left(\frac{\alpha_1 k_1}{2E^* \sqrt{r^*}} \right)^{\frac{1}{3/2-\alpha_1}} \qquad \text{with} \qquad \alpha_1 < 3/2. \tag{14}$$

4 Our bond model for DEM advanced manufacturing applications

Based on equations (7) and (12), the bond model herein proposed has the following expression for the elastic part of the interaction (i.e.., the spring force):

$$\boldsymbol{f}_{ij}^{el} = -\frac{4}{3} E^* \sqrt{r^*} \delta_{ij}^{3/2} \boldsymbol{n}_{ij} + k_{adh} \delta_{ij}^{\alpha_{adh}} \boldsymbol{n}_{ij} , \tag{15}$$

where $\boldsymbol{f}_{ij}^{el}$ is the elastic force that acts on i due to its attraction-repulsion with j, $\boldsymbol{n}_{ij}$ is the central direction of the interaction (the unit vector that points from the center of i to the center of j) and k_{adh} and α_{adh} are the stiffness and the exponent of the adhesion part of the force, respectively. Let us now define a normalized overlap or deformation,

$$\varepsilon_{ij} = \frac{\delta_{ij}}{r^*}, \tag{16}$$

in which r^* is the effective radius of the pair, as given in eq. (12). Accordingly, the elastic force on i can be rewritten as

$$\boldsymbol{f}_{ij}^{el} = -\frac{4}{3} E^* r^{*2} \varepsilon_{ij}^{3/2} \boldsymbol{n}_{ij} + k_{adh} r^{*\alpha_{adh}} \varepsilon_{ij}^{\alpha_{adh}} \boldsymbol{n}_{ij} = -\bar{k}_{con} \varepsilon_{ij}^{3/2} \boldsymbol{n}_{ij} + \bar{k}_{adh} \varepsilon_{ij}^{\alpha_{adh}} \boldsymbol{n}_{ij} , \tag{17}$$

where

$$\bar{k}_{con} = \frac{4}{3} E^* r^{*2} \quad \text{and} \quad \bar{k}_{adh} = k_{adh} r^{*\alpha_{adh}} . \tag{18}$$

From (17), the equilibrium and critical deformations read

$$\varepsilon_{ij,\mathrm{eq}} = \left(\frac{\bar{k}_{adh}}{\bar{k}_{con}} \right)^{\frac{1}{3/2-\alpha_{adh}}} \quad \text{and} \quad \varepsilon_{ij,\mathrm{crit}} = \left(\frac{2}{3} \alpha_{adh} \frac{\bar{k}_{adh}}{\bar{k}_{con}} \right)^{\frac{1}{3/2-\alpha_{adh}}} , \tag{19}$$

and their corresponding overlaps are $\delta_{ij,\mathrm{eq}} = \varepsilon_{ij,\mathrm{eq}} r^*$ and $\delta_{ij,\mathrm{crit}} = \varepsilon_{ij,\mathrm{crit}} r^*$.

Remark: The value of the adhesion stiffness dictates how more or less overlapped the particles will be once the bond is established, i.e., it dictates the magnitude of $\varepsilon_{ij,\mathrm{eq}}$ or $\delta_{ij,\mathrm{eq}}$. It is not at all connected to whether the particles will or will not stick. In this latter aspect, what makes the particles stick (i.e., establish the bond) is having $\varepsilon_{ij} \geq \varepsilon_{ij,\mathrm{crit}}$ while at the same time fulfilling the bonding criterion (like having the particles´ temperatures attaining a certain critical temperature, as said before), irrespective of the value of k_{adh} (and, consequently, of $\bar{k}_{adh}$).

According to Hertz's contact theory, the maximum penetration of two contacting spheres of approaching velocity $v_{ij,\mathrm{rel}}$ (i.e., pre-collision relative velocity) in the absence of external forces is

$$\delta_{ij,\max} = \left(\frac{15 m^* v_{ij,\mathrm{rel}}^2}{16 E^* \sqrt{r^*}} \right)^{\frac{2}{5}} , \tag{20}$$

which follows from integration of the differential equation that describes their relative motion. By enforcing $\delta_{ij,\max} \geq \delta_{ij,\text{crit}}$, as to trigger the bond, it follows that

$$v_{ij,\text{rel}} > \left[\left(\frac{16E^* \sqrt{r^*}}{15m^*} \right)^{\frac{2}{5}} \left(\frac{\alpha_{adh} k_{adh}}{2E^* \sqrt{r^*}} \right)^{\frac{1}{3/2-\alpha_{adh}}} \right]^{\frac{5}{4}} . \tag{21}$$

Equation (21) is a necessary (although not sufficient) condition for the bond to be established. Additionally to the elastic force given by eq. (15) a viscous term is introduced in our model, which essentially represents a damper in the mass-spring oscillator, allowing the particles to dissipate their energy in the central direction. Considering a damper of damping constant d^*, we write this dissipative term as

$$\boldsymbol{f}_{ij}^{d} = -d^* \dot{\delta}_{ij} \boldsymbol{n}_{ij} , \tag{22}$$

where $\dot{\delta}_{ij}$ is the relative velocity of the particles in their central direction. In analogy with the equation of motion of a linear mass-spring-damper oscillator of mass m^*, stiffness k^* and damping constant d^*, we take

$$d^* = 2\xi^{bond} \sqrt{m^* k^*} , \tag{23}$$

in which ξ^{bond} is the damping rate of the oscillation, which is a model parameter that must be given. For the spring stiffness that enters the above equation, we take

$$k^* = -\frac{df_{ij}^{el}}{d\delta_{ij}} = 2E^* \sqrt{r^*} \delta_{ij}^{1/2} - \alpha_{adh} k_{adh} \delta_{ij}^{\alpha_{adh}-1} \quad \text{where} \quad f_{ij}^{el} = \left\| \boldsymbol{f}_{ij}^{el} \right\| \text{ is the force on the spring} . \tag{24}$$

From the above considerations, the total interaction force in this model reads

$$\boldsymbol{f}_{ij}^{tot} = \begin{cases} \boldsymbol{f}_{ij}^{con} + \boldsymbol{f}_{ij}^{d,con} , & IF\ \delta \leq \delta_{crit} \\ \boldsymbol{f}_{ij}^{el} + \boldsymbol{f}_{ij}^{d} , & IF\ \delta > \delta_{crit} \quad \text{and the bond criterion is met} , \end{cases} \tag{25}$$

where $\boldsymbol{f}_{ij}^{con}$ is the contact force in case there is no bonding, herein given by the purely Hertzian expression, and $\boldsymbol{f}_{ij}^{d,con}$ is its dissipative (viscous damping) term, given by

$$\boldsymbol{f}_{ij}^{d,con} = -d^{con} \dot{\delta}_{ij} \boldsymbol{n}_{ij} \quad \text{with} \quad d^{con} = 2\xi^{con} \sqrt{2E^* m^* \sqrt{r^*}} \delta_{ij}^{1/4} . \tag{26}$$

Here, ξ^{con} is the corresponding contact damping rate (i.e., the rate for purely contact interactions), which must be given. At the implementation level, similarly as it happens for damped, purely contact interactions, one should always check the consistency of the sign of the total interaction force. Accordingly, for $\delta_{ij} < \delta_{ij,\text{crit}}$, if $\boldsymbol{f}_i^{tot} \cdot \boldsymbol{n}_{ij} > 0$ then one must set $\boldsymbol{f}_i^{tot} = \boldsymbol{o}$, as to avoid an attractive contact force, which obviously makes no sense. For the same reason, for $\delta_{ij} > \delta_{ij,\text{crit}}$, if $\delta_{ij} > \delta_{ij,\text{eq}}$ and $\boldsymbol{f}_i^{tot} \cdot \boldsymbol{n}_{ij} > 0$, then $\boldsymbol{f}_i^{tot} = \boldsymbol{o}$, whereas if $\delta_{ij} < \delta_{ij,\text{eq}}$ and $\boldsymbol{f}_i^{tot} \cdot \boldsymbol{n}_{ij} < 0$, then $\boldsymbol{f}_i^{tot} = \boldsymbol{o}$ (this ensures an ever-restoring total interaction force for the bond).

5 Numerical examples

Let us illustrate the above bond model by analyzing two simple numerical examples with our (in-house) DEM code. We remark that more elaborate, multi-particle examples are currently being analyzed by the authors and shall appear soon in a forthcoming journal paper.

5.1 Bonding of two particles in a central collision (1): assessing the equilibrium configuration

Here we show one simple validation problem involving the bonding of two particles in a central collision. In particular, we want to evaluate whether the bond is established and, in case yes, if the expected equilibrium overlap

is attained for varying values of the bond damping rate ξ^{bond}, according to the formulation proposed in Sec. 4. Let us consider two same-sized particles with radii $r_i = 0.001\,\mathrm{m}$ approaching each other at a relative (central) velocity of 2.6 m/s (this is slightly greater than the critical velocity of eq. (21) and, thereby, should trigger the bond). The mass-density of the particles is $\rho_i = 2000\,\mathrm{kg/m^3}$ and their elastic properties are $E_i = 1\,\mathrm{GPa}$ and $\upsilon_i = 0$, respectively. The equilibrium overlap is set to $\delta_{ij,\mathrm{eq}} = 0.00005\,\mathrm{m}$, from which the adhesion stiffness $k_{adh} = 1.05\times10^5$ follows (the adhesion exponent adopted is $\alpha_{adh} = 1$). The time-step size adopted in the time numerical integration (explicit) was $\Delta t = 5\times10^{-7}\,\mathrm{s}$, whereas the final simulation time was $t = 0.005\,\mathrm{s}$. In Fig. 1, we plot the evolution of the particles´ overlap in time for different values of ξ^{bond} (only the relevant time interval is represented). As expected, we observe that not only the bond is established for all values of ξ^{bond}, but also the overlap converges to the predefined equilibrium overlap irrespective of ξ^{bond}. We can see, too, that for lower values of ξ^{bond} a greater amplitude around the equilibrium overlap is observed in the earlier stages of the interaction, which then progressively diminishes towards a static "stick" configuration. One should be careful with such great amplitudes because, if exaggerated, they may overcome the stable range of the interaction and thereby trigger instabilities and, in the extreme case, even lead to a loss of contact. This may be easily overcome in the model by adopting a sufficiently high value for ξ^{bond}, which will damp the oscillation from the beginning.

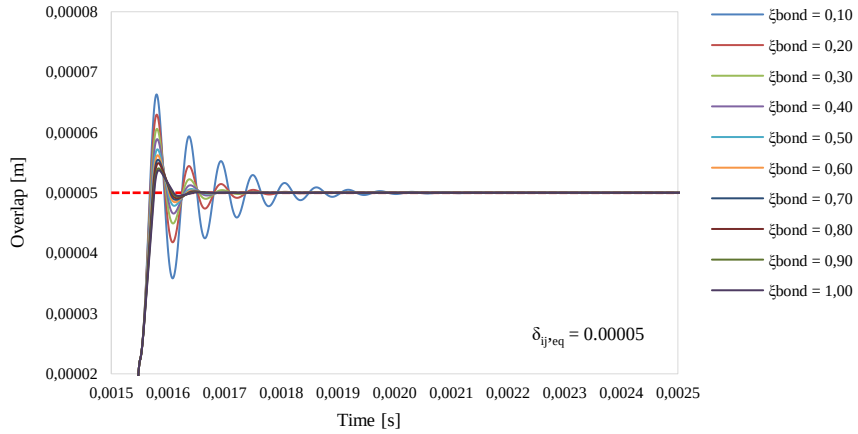

Figure 1. Example 5.1 Particles' overlap plotted against time.

5.2 Bonding of two particles in a central collision (2): parametric studies

Here we investigate the outcomes of a central collision in terms its coefficient of restitution for varying mass densities of the particles. The geometrical and material data are the same as from the previous example (except for the mass density), as well as the time-step size and the final simulation time. A critically damped bond ($\xi^{bond} = 1$) is assumed for all cases.

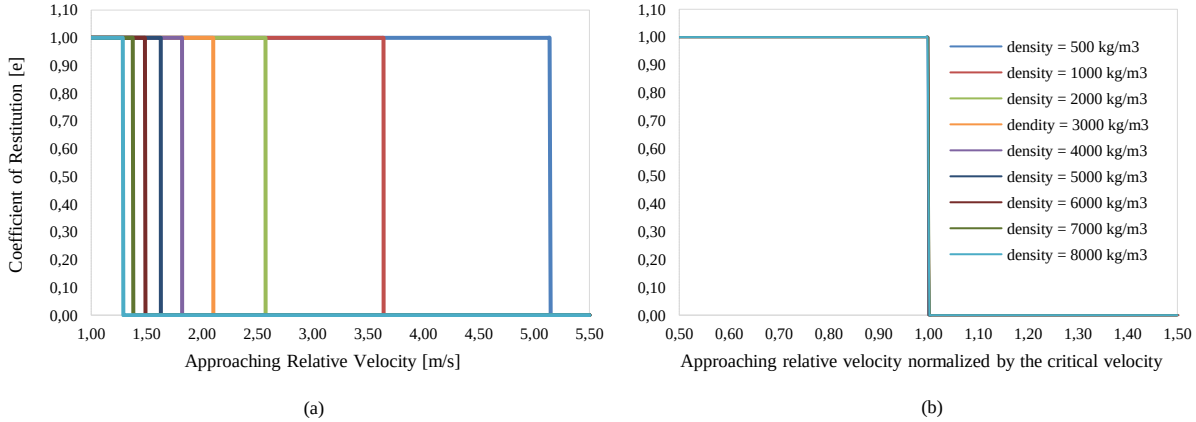

Figure 2. Example 5.2 Restitution coefficient *e* plotted as a function of the impact velocity. Analysis results.

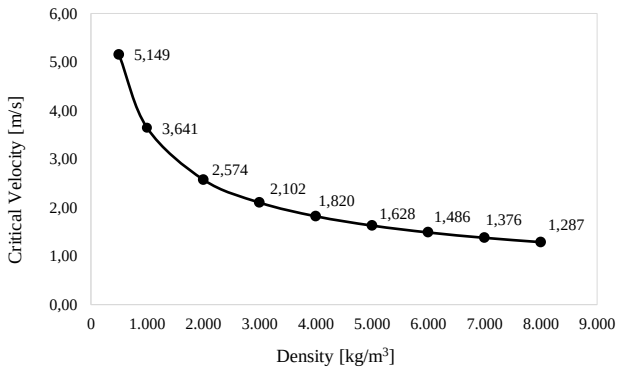

Figure 3. Values of critical velocities for each case

Table 1. Values of critical velocities

Density [kg/m^3]	Critical velocity [m/s]
500	5,149
1000	3,641
2000	2,574
3000	2,102
4000	1,820
5000	1,628
6000	1,486
7000	1,376
8000	1,287

As we can see from Fig. 2, the particles stick to each other irrespective of their mass density, as expected. Fig. 3 plots the critical velocities for each case, which is seen to be inversely proportional to the particles' densities (i.e., for lower density values a higher velocity is required to overcome the critical overlap δ_{crit} and thereby initiate the sticking regime).

6 Conclusions

The purpose of this work was to present the first results of an on-going research, intended to devise a mass-spring bond model to capture inter-particle bonding, aiming at advanced manufacturing applications. We find the model to be reasonably simple and straightforward to be implemented by engineers and analysts interested in the field. Also, as it could be seen from the first results, it proved to work very well for the purposes envisioned. The application of the model to the simulation of multi-particle systems (in particular, to AM processes) is under work and shall appear soon in a forthcoming paper by the authors.

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