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On the Adhesive JKR Contact and Rolling Models for Reduced Particle Stiffness
Discrete Element Simulations

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Abstract
Discrete Element Method (DEM) simulations are a promising approach to accurately predict agglomeration and deposition of micron-sized adhesive particles. However, the mechanistic models in DEM combined with high particle stiffness for most common materials require time step sizes in the order of nano seconds, which makes DEM simulations impractical for more complex applications.

In this study, analytically derived guidelines on how to reduce computational time by using a reduced particle stiffness are given. The guidelines are validated by comparing simulations of particles with and without reduced particle stiffness to experimental data. Then two well-defined test cases are investigated to show the applicability of the guidelines.

When introducing a reduced particle stiffness in DEM simulations by reducing the effective Young’s modulus from $E$ to $E_{\text{mod}}$, the surface energy density $\gamma$ in the adhesive Johnson-Kendall-Roberts (JKR) model by Johnson et al. [1] should be modified as $\gamma_{\text{mod}} = \gamma (E_{\text{mod}}/E)^{2/5}$. Using this relation, the stick/rebound threshold remains the same but the collision process takes place over a longer time period, which allows for a higher time step size. When rolling motion is important, the commonly used adhesive rolling resistance torque model proposed by Dominik and Tielens [2, 3], Krijt et al. [4] can be used by modifying the contact radius ratio $(a/a_0)^{3/2}$ to $(a_{\text{mod}}/a_{0,\text{mod}})^{3/2}$, whilst keeping the other terms unaltered in the description of the rolling resistance torque $M_{r,\text{mod}} = -4F_C (a/a_0)^{3/2}$. Furthermore, as the particle stiffness is reduced from $E$ to $E_{\text{mod}}$, the time period for collisions (or oscillations when particles stick upon impact) $\Delta t_{\text{col}}$ is found to vary as $\Delta t_{\text{col,mod}} = \Delta t_{\text{col}} (E/E_{\text{mod}})^{2/5}$. As the collision duration and the collision time step size are directly related, this criterion can be used to estimate how much the time step size can be changed as a reduced particle stiffness is introduced.

Introducing particles with a reduced particle stiffness has some limitations when strong external forces are acting to break-up formed agglomerates or re-entrain particles deposited on a surface out into the free stream. Therefore, care should be taken in flows with high local shear to make sure that an external force, such as a fluid drag force, acting to separate agglomerated particles, is several orders of magnitude lower than the critical force required to separate particles.

Keywords: Discrete Element Method, Reduced particle stiffness, Adhesive particles, JKR adhesive model, Rolling resistance torque, Computational efficiency

1. Introduction
Discrete Element Method (DEM) simulations are typically used to accurately predict the motion of particles in systems with high local particle volume fraction where particle-particle collisions are important. Recently, the motion of adhesive particles has received increased attention [5] due to the wide range of applications which include, but are not limited to, particulate fouling layers in heat exchangers, food processing, sediment transport, aerosol modelling, fluidized beds and dust coagulating to form early stages of planets in space. As opposed to other methods, DEM simulations resolve particle-particle collisions directly using a mechanistic approach. As each particle-particle collision is resolved over numerous time steps, the required computational time is high compared to other methods [6]. A widely used approach to decrease computational costs is to decrease the particle stiffness, namely Young’s modulus, and thereby make collisions take place over longer time periods allowing for an increased time step size. For collisions involving non-adhesive particles, numerous studies suggest that the particle stiffness can be reduced by several orders of magnitude without altering the collisions in terms of separating velocity after collision [7, 8]. However, when introducing adhesive particles, recent studies have pointed out that a reduced particle stiffness has to be balanced by a reduced adhesive force. Therefore, Kobayashi et al. [9]...
introduced a dynamic van der Waals adhesion model upon collision that scales the adhesive force $F_{ad}$ according to the square root of the ratio of particle spring constants $k$ as:

$$F_{ad,mod}/F_{ad} = \sqrt{k_{mod}/k},$$

where subscript $mod$ denotes modified values. Gu et al. [8] extended the work and included the fact that the van der Waals force is effective over a finite distance before the particles come into physical contact. Common for these studies is the fact that they assume particle deformation to play a negligible role on the adhesive force upon collision. This assumption is valid for sufficiently small particles, where particle deformation is negligible [10].

When the particle diameter is large (typically $d_p > 10 \text{ µm}$), particle deformation cannot be neglected when describing the adhesive force. The importance of particle deformation on the adhesive behaviour is described by Tabor [11] through the dimensionless Tabor parameter $\lambda_T$, where $R, \gamma, E$ and $D_{min}$ define effective particle radius, surface energy density, effective Young’s modulus and minimum atomic separation distance between particles (typically taken to be 1.65 Å [12, 13]):

$$\lambda_T = \left(\frac{4R\gamma^2}{E^2D_{min}}\right)^{1/3}$$

$$\frac{1}{R} = \frac{1}{r_i} + \frac{1}{r_j}, \quad \frac{1}{E} = \frac{1 - \nu_i^2}{E_i} + \frac{1 - \nu_j^2}{E_j}$$

where $r$ and $\nu$ refer to particle radius and Poisson’s ratio respectively and subscripts $i$ and $j$ refer to particle $i$, $j$. The study by Johnson and Greenwood [10] shows that the adhesive Johnson-Kendall-Roberts (JKR) model by Johnson et al. [1] is valid for $\lambda_T > 3$, the Derjaguin-Muller-Toporov (DMT) model by Derjaguin et al. [14] is valid for $\lambda_T < 0.1$ and the model by Maugis [15] is valid in between the two when $0.1 \leq \lambda_T \leq 3$.

With an increasing number of studies on collisions of adhesive particles being carried out, the aim of this paper is to emphasise the importance of reducing the particle adhesiveness when a reduced particle stiffness is introduced. For this purpose an analytically derived criterion on how to adjust the surface energy density to account for a reduced particle stiffness for collisions in the JKR limit ($\lambda_T > 3$) is presented. This paper is structured as follows: Firstly, the adhesive DEM modelling framework is briefly outlined. Secondly, the criterion on how to reduce particle stiffness is presented for both collisions and rolling behaviour. Thirdly, numerical simulations of adhesive particles are compared to experimental data found in literature. Lastly, two simple test cases are investigated in more details to show the applicability of the proposed criterion. These test cases represent types of collisions commonly encountered in the particle agglomeration and deposition processes:

1. Binary head-on adhesive particle/particle or particle/wall collisions forming agglomerates or deposition.

2. Collisions of single adhesive particles with a wall. Here the particles are affected by a constant external force parallel to the wall (e.g. a gravity force, time-independent fluid force or a constant magnetic force). Here focus is on the rolling resistance torque, which causes particles to stick to a surface, despite being affected by a constant force.

2. Modelling Framework

The translational and rotational motion of particles is obtained using the DEM, where Newton’s equation of motion is solved to obtain the instantaneous translational and rotational position for each particle:

$$m\frac{d^2x}{dt^2} = F_{con} + F_{ext}$$

$$I\frac{d\omega}{dt} = M_{con} + M_t$$

where the forces contributing are the contact force upon impact $F_{con}$ and an external force $F_{ext}$ which could represent a gravity force, a time-independent fluid force or a constant magnetic force. Likewise, the total torque is the sum of a contact torque $M_{con}$ and a rolling resistance torque $M_t$. The contact force is split into normal and tangential contributions ($F_{con,n}$ and $F_{con,t}$), where the normal contact force is the sum of a spring force, an adhesive force and a damping force contribution:

$$F_{con,n} = F_{spring,n} + F_{jkr,n} + F_{damp,n}$$

In the tangential direction, spring and damping force contributions are taken into account through:

$$F_{con,t} = F_{spring,t} + F_{damp,t}$$

Figure 1 gives an overview of the force contributions acting on a particle upon collision with another particle (partly shown on the left).

2.1. Adhesive contact between particles and a surface

Numerous approaches have been suggested to account for an adhesive force. Common for the approaches is that they rely on a surface energy density $\gamma$ to describe the adhesive force. For small $\lambda_T$, the contact independent van der Waals formulation by Hamaker [16] is used in studies such as [8, 9, 17, 18] to account for the adhesive force. For higher $\lambda_T$ (softer particles), the contact dependent adhesive JKR force proposed by Johnson et al. [1] is used in studies such as [19, 20]. In the present study, focus is on the simplified JKR model suited for DEM simulations and used in studies such as [13, 21, 22]. The simplified JKR model has the same force-displacement relation as the original model, requires the same $8/9$ of the critical force $F = (8/9)F_C = (8/9)3\pi R_T^2$ to break contact but assumes contact is broken as soon as the normal overlap becomes negative in the particle separation process. At
where the contact normal force by dissipating kinetic energy in the thermore, a normal damping force contributes to the which can be solved using an iterative approach or the overlap $\delta_n$ where the relation between contact radius $a$ and normal force, the contact radius is given by [23]:

$$a_0 = \left(\frac{9\pi\gamma R^2}{E}\right)^{1/3}$$

(7)
as in the original JKR model. The normal spring force described by the Hertzian contact model is modified as follows due to an adhesive force:

$$F_{\text{spring},n} = -\frac{4E}{3R}a^3 n$$

(8)

$$F_{\text{damp},n} = -2\frac{5}{6}\beta \sqrt{S_n} m v_n$$

(11)

where $\beta$ accounts for the energy lost upon collision through the coefficient of restitution $e$ while $S_n$ takes the particle properties into account:

$$\beta = \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}}$$

(12)

$$S_n = 2E\sqrt{R\delta_n}$$

(13)

where $m$ is particle mass, $v_n$ is the relative normal velocity, and $n$ is the normal unit vector. In the tangential direction, the spring force contribution is:

$$F_{\text{spring},t} = -S_t \Delta s_t$$

(14)
deck $\Delta s_t$ is tangential displacement between the particles and $S_t = 8G\sqrt{R\delta_n}$ with the effective shear modulus $G$:

$$\frac{1}{G} = \frac{2 - \nu_t}{G_i} + \frac{2 - \nu_t}{G_j}$$

(15)

Where the shear moduli for particle $i,j$ are related to the Young’s modulus through $G_i = E_i/(2(1 + \nu_i))$ and $G_j = E_j/(2(1 + \nu_j))$. Likewise, energy is dissipated in the tangential direction by a damping force:

$$F_{\text{damp},t} = -2\sqrt{\frac{5}{6}} \beta \sqrt{S_t} m v_t$$

(16)

where $v_t$ is the relative tangential velocity of the particles. In the case of adhesive contact, the tangential force is truncated to fulfil [24, 25]:

$$|F_{\text{con},t}| \leq \mu_s |F_N + 2F_C|$$

(17)

where $\mu_s$ is the sliding friction coefficient.

2.2. Adhesive rolling, sliding and twisting resistance

To predict the formation of agglomerates or particles sticking to a wall, a description of adhesive rolling plays a major role [2–4]. Due to the small particle inertia of micron-sized particles, twisting (rotation along the axis connecting two particles) and sliding (relative tangential motion without rotation) are less important than rolling, to accurately predict formation/break-up of agglomerates [19, 26]. Therefore, focus is on the adhesive rolling behaviour and how to modify the adhesive rolling resistance model to account for the reduced particle stiffness.

When a particle is in normal equilibrium with a wall, the centre of contact and projected centre of gravity are coincident, see figure 2(a). However, when an external force $F_{\text{ext}}$ is applied, a small shift between the centre of contact and projected centre of gravity will build up, as illustrated in figure 2(b). The result of this asymmetric contact region is a torque $M_c$ opposing rotation and trying to obtain the symmetric contact region as in figure 2(a). If the particle is rolled less than a critical rolling displacement ($\xi < \xi_{\text{crit}}$), the particle rolls back to obtain the same contact point when the external force is removed. However, when the particle is rolled a distance longer than the critical rolling displacement ($\xi > \xi_{\text{crit}}$), the particle is moved irreversibly. While Dominik and Tielens [2, 3] suggest a critical rolling displacement in the order of an atom diameter, the more recent study by Krijt et al. [4] relates the critical rolling displacement to the equilibrium contact radius $a_0$ and a material dependent adhesion hysteresis parameter $\Delta \gamma/\gamma$ to obtain improved experimental agreement through:

$$\xi_{\text{crit}} = \frac{a_0 \Delta \gamma}{12}$$

(18)
In general as a particle rolls, the rolling displacement \( \xi \) is obtained by integrating the rolling velocity:

\[
\xi = \left( \int_{t_0}^{t_1} \mathbf{v}_L(t) \, dt \right) \cdot \mathbf{r}_i
\]  

(19)

where the rolling velocity \( \mathbf{v}_L \) is defined as:

\[
\mathbf{v}_L = R (\omega_i - \omega_j) \times \mathbf{n} + \frac{1}{2} \frac{r_j - r_i}{r_i + r_j} \mathbf{v}_S
\]  

(20)

which can conveniently be implemented into the DEM method by incremental changes between two successive time steps. The rolling resistance torque is then given by [2, 3]:

\[
M_t = \begin{cases} 
  k_r \xi & \text{if } \xi < \xi_{\text{crit}} \\
  k_r \xi_{\text{crit}} & \text{if } \xi \geq \xi_{\text{crit}}
\end{cases}
\]  

(21)

with rolling stiffness \( k_r = 4F_C (a_i/a_0)^{3/2} \). As the rolling displacement \( \xi \) cannot exceed the critical rolling displacement \( \xi_{\text{crit}} \), the rolling displacement is numerically truncated to fulfil:

\[
|\xi| \leq |\xi_{\text{crit}}|
\]  

(22)

3. Reduced Particle Stiffness

3.1. Modified adhesive JKR model for reduced particle stiffness

When a reduced particle stiffness is introduced in DEM simulations, the particles will inevitably overlap more during collision. If the surface energy density \( \gamma \) is left unchanged, the result is a more adhesive collision as the kinetic energy lost upon collision is increased significantly. Therefore, a reduced particle stiffness has to be balanced by a reduced surface energy density for the outcome of the collision to remain the same. For the separation energy required to separate two particles in contact to remain constant, the following criterion has to be fulfilled:

\[
\int_0^{\delta_{n,0}} (F_{\text{mod}} + F_{\text{spring}}) \, d\delta_n = \int_0^{\delta_{n,0,\text{mod}}} (F_{\text{mod}} + F_{\text{spring,mod}}) \, d\delta_n
\]  

(23)

where \( \delta_{n,0} = (1/3)a_0^2/R \) is the normal overlap at equilibrium. Inserting expressions for \( F_{\text{mod}} \) and \( F_{\text{spring}} \) from equation (8) and (9) with the contact radius given by equation (10) into equation (23) gives an expression for the modified surface energy density as a result of modified effective Young’s modulus:

\[
\gamma_{\text{mod}} = \gamma \left( \frac{E_{\text{mod}}}{E} \right)^{2/5}
\]  

(24)

Details on how this derived from (23) are given in appendix A. The result in (24) is actually the same criterion Gu et al. [8] found for the contact independent van der Waals formulation [16] \( F_{\text{vdW}} = A_H R/(6D_{\text{min}}^2) \) with the effective Hamaker constant \( A_H = 24\pi D_{\text{min}}^2 m^5 \). Figure 3 shows a comparison of the original JKR model, the JKR model with reduced particle stiffness and the JKR model with reduced particle stiffness and reduced surface energy density using equation (24). As the figure shows, by only reducing the particle stiffness (by the Young’s modulus \( E \)) the same force \( F_N = -(8/9)F_C \) is required to break contact. However, the equilibrium overlap is increased significantly as \( \delta_{n,0,\text{mod}} = (1/3)a_0^2/\sqrt{3}R = (3\pi^2\gamma^2/R/E_{\text{mod}}^{1/2})^{1/3} \). By reducing both the stiffness and adhesiveness (by the surface energy density \( \gamma \)) using equation (24), the force-displacement relation is changed so that the separation energy remains the same as in the original model. The result is a higher overlap distances during collision and consequently larger time step sizes. However, the normal force required to break contact is reduced to
It should be noted that as a natural consequence of introducing a reduced particle stiffness, the particles will travel longer distances upon collision due to the changed force-displacement relation, see figure 3. When collisions with a plane wall at an oblique angle are considered, the result is particles travelling a slightly longer distance before coming to rest. However, this is typically not of importance in DEM simulations involving many particles.

4. Validation by Experimental Data

Collisions of small spheres have been studied thoroughly. At sufficiently low impact velocities, the collisions are dominated by adhesive forces in the contact region resulting in sticking behaviour, where the effective coefficient of restitution $e_{\text{eff}}$ is zero. At higher impact velocities when the particles are unable to stick, the effective coefficient of restitution increases rapidly with increasing impact velocity. At sufficiently high velocities where the collisions become increasingly unaffected by adhesive forces, the effective coefficient of restitution approaches the coefficient of restitution $e$.

In the following, simulation results obtained by integrating (3) for both non-modified and modified stiffness using (24) are compared to experimental data presented by Dahneke [27]. As noted by Krijt et al. [28], expected collision outcomes typically differ slightly from experiments as even small imperfections in particle or wall material result in a non-perfect collision. Therefore, the fitted values suggested by Krijt et al. [28] are used when comparing to experiments. Figure 5 shows how the simulation results with both non-modified and modified stiffnesses compare to experimental data.

Figure 5 shows that the DEM methodology described above is capable of predicting the effective coefficient of restitution. Furthermore, by reducing the particle stiffness from $E$ to $E_{\text{mod}}$ and modifying the surface energy density by analytical solution in (24), the exact same results are indeed obtained. More details on how introducing softer particles allows for a higher time step size are given in section 6.

5. Test Cases

5.1. Dimensionless quantities

To generalise the analysis, particle properties are reported based on a set of dimensionless quantities that control different aspects of the adhesion and rolling processes, which ultimately govern the agglomeration and deposition processes. Based on the effective Young's modulus $E$, effective radius $R$, relative particle velocity before impact $v$, particle density $\rho_p$, collision angle $\psi$, and coefficient of restitution $e$, the adhesion process is fully described. The above mentioned parameters form three governing parameters: an elasticity parameter describing the ratio between particle stiffness and particle

Figure 4: Comparison of torque-rolling distance relations using the original JKR model and different modified versions: — — Original adhesive rolling resistance torque model by [2–4]; ····· Reduced Young’s modulus and modified surface energy density given by the criterion in equation (24).
The effective coefficient of restitution $e_{\text{eff}}$ is defined as the ratio between particle adhesiveness and particle inertia $Ad = 3\gamma/(\rho_pv^2r_i)$, where $\gamma$ is the adhesive coefficient of restitution describing the ratio between relative velocity after collision (subscript f) and the effective coefficient of restitution describing the ratio between particle adhesiveness and particle inertia $Ad = 3\gamma/(\rho_pv^2r_i) \cdot (1 + \beta^2)/((1 + \beta^2)\beta)$ [29], and the effective coefficient of restitution as function of the elasticity parameter at various adhesive parameters $Ad = \gamma/(\rho_pv^2R)$ for a coefficient of restitution $e = 0.3$.

5.2. Binary Adhesive Collision

Binary particle collisions are encountered in most problems being solved using the DEM method. Therefore it is important that the model proposed for reduced particle stiffness simulations yields similar results for particle collisions. This is investigated in the following with figure 6 giving an overview of the head-on particle-particle collision being simulated to validate the proposed model. By varying the elasticity parameter $\lambda$ and the adhesiveness parameter $Ad$, the particles either stick, rebound, or separate. The effective coefficient of restitution $e_{\text{eff}}$ is defined as the ratio between adhesive forces in the contact region and the effective coefficient of restitution $e$. The effective coefficient of restitution $e_{\text{eff}}$ of an adhesive collision process is generally lower than that of a non-adhesive collision $e$. 

Figure 5: Comparison to experiment by Dahneke [27] with PSL spheres colliding with a plane wall of polished quartz. Collision properties are $d_p = 1.27 \mu$m, $E = 271$ MPa, $\gamma = 0.11$ J/m², $\rho_p = 1026$ kg/m³ and $e = 0.86$ (fitted to experimental data at high velocities), see Krijt et al. [28] and supplementary online material for collision properties. When a reduced particle stiffness is introduced in the simulations, the surface energy density is modified using the criterion proposed in (24).

Figure 6: Overview of the different stages of a particle-particle collision: (a) Particles approaching each other; (b) Just prior to contact the particles are still unaffected and move with velocity $v$; (c) particles reach maximum normal overlap $\delta_n$; (d) Particles begin to separate; (e1-e2) Depending on the strength of the adhesive force the particles will either remain in contact (e1) or separate completely (e2).

Figure 7: Numerical simulations showing head-on particle-particle adhesive collisions by the non-modified model showing the effective coefficient of restitution as function of the elasticity parameter at various adhesive parameters $Ad = \gamma/(\rho_pv^2R)$ for a coefficient of restitution $e = 0.3$. 

Effect of adhesiveness on the collision, the coefficient of restitution $e$ decreases as the adhesiveness parameter and increases with increasing adhesiveness parameter. As the results show, decreasing the particle stiffness does, in most cases, result in a
different effective coefficient of restitution. The exception is at sufficiently low elasticity parameters, where the particle stay attached upon collision. Furthermore, the figure shows that as long as \( e_{eff}/e \approx 1 \), corresponding to high elasticity parameters, the elasticity parameter can be reduced with only small changes in effective coefficient of restitution as the collision behaves as non-adhesive.

Figure 8 shows how using the criterion in (24) makes the effective coefficient of restitution independent of changes in elasticity parameter from a base value \( \lambda = 10^6 \). As figure 8 shows, the effective coefficient of restitution \( e_{eff}/e \) retains the values from \( \lambda = 10^6 \) in figure 7 when the elasticity parameter is changed at various adhesiveness values. Even though the stiffness of particles undergoing binary particle-particle collisions can be greatly reduced, studies by Kobayashi et al. [9] and Gu et al. [8] show that collisions involving larger agglomerates behave differently when the particle stiffness is reduced beyond a certain point. In this study, this phenomenon is addressed in the following section where particle deposition on both a clean surface and a surface with an initial layer of particles is investigated.

5.3. Deposition on a Plane Surface

Most problems being solved using DEM involve particles colliding with a plane surface. This case is different from the previous head-on particle collisions as particles may roll on the surface or other particles and eventually come to rest due to adhesive rolling resistance torque described by equation (21). Therefore, this section is focused on the validity of the proposed model for particles with reduced stiffness colliding with a plane surface. Figure 9 gives an overview of the oblique angle particle-wall collision process investigated.

![Figure 8: Numerical simulation showing head-on particle-particle adhesive collisions showing how the effective coefficient of restitution remains constant when the particle stiffness is reduced (or increased) when the surface energy density is changed using the criterion proposed in (24). Again, results are shown for coefficient of restitution \( e = 0.3 \).](image)

![Figure 9: Overview of the different stages of the particle-wall collision: (a) The particle moving towards the wall; (b) Just prior to contact the particle is still unaffected by the wall and moves with velocity \( v \) at an angle \( \psi \) to the wall while affected by an external fluid/gravity force \( F_{ext} \); (c)-(d) Particle in contact with the wall. If the particle stay in contact with the wall, the normal equilibrium is established here; (e1-e3) The particle will either rebound and move away from the surface (e1), stay at the surface but keep rolling with a constant angular velocity \( \omega \) ≠ 0 (e2) or stay in place as a result of adhesiveness with shifted centre of contact and centre of mass \( \omega = 0 \) (e3), see figure 2(b).](image)

![Figure 10: The three possible outcomes of an adhesive collision with a plane wall and the effect of increasing/decreasing adhesiveness parameter \( Ad = 3\gamma/(\rho p v^2\sin^2(\psi)r_p) \) and coefficient of restitution \( e \). The particle is affected by a constant external force \( F_{ext} \) parallel to the wall (see figure 9) and the yield force is given by \( F_{yield} = 4F_{cu0}(\Delta\gamma/\gamma)/12 \).](image)

As the figure shows, three possible outcomes are expected as collision parameters are varied: rebound behaviour, particle deposition followed by rolling motion and particle deposition where the particle rolls a certain distance before coming to a halt. For most DEM simulations of particulate deposition, it is important that the outcome (rebound, rolling or sticking) remains the same when the particle stiffness is reduced. Simulations of particles colliding with a wall at oblique angles \( \psi \in [0;\pi/2] \) were done. The three possible outcomes are located as shown in the dimensionless map in figure 10, where elasticity and adhesiveness parameter are modified to account for the collision angle \( \psi \) so that: \( \lambda = E/(\rho p v^2\sin^2(\psi)) \) and \( Ad = 3\gamma/(\rho p v^2\sin^2(\psi)r_p) \).

A high elasticity parameter, high coefficient of restitution or low adhesiveness parameter will all inherently cause the particles to rebound. When the particles stay attached
to predict collisions of adhesive micron-sized particles for which the adhesive model by Johnson-Kendall-Roberts (JKR) model is applicable. The following conclusions can be drawn:

- When using the simplified JKR model (equation (8)), the particle Young’s modulus can be reduced from $E$ to $E_{mod}$ as long as the surface energy density is reduced as well using $\gamma_{mod} = \gamma (E_{mod}/E)^{2/5}$. That way, the border between sticking and rebounding behaviour remains the same when the particle stiffness is reduced.

- To use the rolling resistance model by Dominik and Tielens [2, 3], Krijt et al. [4] (equation (18) to (22)) for reduced particle stiffness simulations, only the term $(a/a_0)^{3/2}$ should be changed to use modified values. That way, the border between rolling and sticking remains the same. As a natural result of the reduced particle stiffness, the particles will travel a longer distance before the equilibrium condition is reached.

6.2. Discussion on computational time and limitations

As the particle stiffness is reduced, the time step size can be greatly increased. Figure 13 shows the velocity during a collision of a small PSL sphere impacting a polished quartz surface, corresponding to the experiment by Dahneke [27]. As the figure shows, the separation velocity is unaffected by a change in particle stiffness when the surface energy density is modified using (24). However, the particle collision process now takes place over significantly longer time periods. When resolving a collision over fixed number of time steps (Silbert et al. [30] suggests $\Delta t_{col}/\delta t \approx 50$), the time step size can now be greatly increased. By looking at how the collision time $\Delta t_{col}$ scales with a reductions in particles stiffness, it is found that $\Delta t_{col,mod} = \Delta t_{col}(E/E_{mod})^{2/5}$, see figure 13. This criterion can be used to estimate the possible speed-up for adhesive DEM simulations when introducing a reduced particle stiffness.

As a consequence of a reduced particle stiffness, the critical force required to separate two agglomerated particles is reduced as well. This fact is important when simulating particles in flow or magnetic fields where local external forces on particles can be strong. A such example could be a strong shear flow field. Therefore, care should be taken when introducing reduced particle stiffness to make sure that the critical force $F_C = 3\pi R \gamma_{mod}$ still remains significantly higher than typical external forces trying to separate the particles. Additionally, it should be noted that for collisions involving many particles with a local volume fraction approaching the closed-pack solution, the adhesive behaviour might be changed slightly if the particle stiffness is reduced too much, $E_{mod}/E < 10^{-3}$ [8, 9].
zero-overlap is found by isolating $\delta$. Next, expressions for the contact radius at $t = 0$ are found. The contact radius at zero-overlap is found by isolating $a$ in (10) with $\delta_n = 0$:

$$a^4 - 2R\delta_n a^2 - \frac{4\pi \gamma}{E} R^2 a + R^2 \delta_n^2 = 0 \quad (A.2)$$

The two real roots are:

$$a_1 = 0 \quad (A.3)$$

$$a_2 = \left( \frac{4\pi \gamma R^2}{E} \right)^{1/3} \quad (A.4)$$

Here we are interested in the non-zero root $a_2$, which is the lower limit of the integrals in (A.1):

$$a(\delta_n = 0) = \left( \frac{4\pi \gamma R^2}{E} \right)^{1/3} \quad (A.5)$$

The upper limits for $a$ at $\delta_n = \delta_n,0$ and $a$ at $\delta_n = \delta_n,0,mod$ are the equilibrium contact radius given directly by (7):

$$a(\delta_n = \delta_n,0) = \left( \frac{9\pi \gamma R^2}{E} \right)^{1/3} \quad (A.6)$$

$$a(\delta_n = \delta_n,0,mod) = \left( \frac{9\pi \gamma_{mod} R^2}{E_{mod}} \right)^{1/3} \quad (A.7)$$

Next, we look for an expression for $d\delta_n$. First, we derive an expression for $\delta_n(a)$ using (10). We obtain two solutions:

$$\delta_{n,1} = \frac{Ea^2 + 2R\sqrt{E\gamma a\pi}}{ER} \quad (A.8)$$

$$\delta_{n,2} = \frac{Ea^2 - 2R\sqrt{E\gamma a\pi}}{ER} \quad (A.9)$$

Here only the solution in (A.9) fulfills the criteria in (A.5) and (A.6). Next, we find the derivative $d\delta_n/da$ using (A.9) and isolate for $d\delta_n$:

$$d\delta_n = \left( \frac{2a}{R} - \frac{2\sqrt{\gamma \pi}}{\sqrt{EA}} \right) da \quad (A.10)$$

Carrying out the integral in (A.1) with the limits given by (A.5), (A.6) and (A.7) and inserting the expression for $d\delta_n$ from (A.10), we obtain:

$$\frac{\gamma^{5/3}}{E^{3/3}} = \frac{\gamma_{mod}^{5/3}}{E_{mod}^{3/3}} \quad (A.11)$$

which reduces to the expression in (24).

**References**


Nomenclature

Ad  adhesiveness parameter (-)
\( A_H \)  effective Hamaker constant (J)
a  contact radius (m)
d  particle diameter (m)
\( D_{\text{min}} \)  minimum separation distance (m)
E  (no subscripts) effective Young’s modulus (Pa)
\( E_i, E_j \)  Young’s modulus for particle i, j (Pa)
e  coefficient of restitution (-)
F  force (N)
\( F_C \)  critical force (N)
I  particle moment of inertia (kg m^2)
k  spring constant (N m^{-1})
k_r  rolling stiffness (N)
M  particle torque (Nm)
m  (no subscripts) effective particle mass (kg)
m_i, m_j  particle mass for particle i, j (kg)
n  normal unit vector (-)
R  effective particle radius (m)
r  particle radius (m)
r_i, r_j  particle radius for particle i, j (m)
S  damping force coefficient (kg s^{-2})
t  time (s)
v  relative velocity (m s^{-1})
v_L  relative rolling velocity (m s^{-1})
v_S  slip velocity (m s^{-1})
x  particle position (m)

Greek letters

\( \beta \)  coefficient used for damping force (-)
\( \Delta \gamma/\gamma \)  adhesion hysteresis value (-)
\( \Delta t_{\text{col}} \)  time period for oscillations or collision (s)
\( \delta t \)  collision time step size (s)
\( \delta s_t \)  tangential displacement (m)
\( \delta \)  normal overlap (m)
\( \gamma \)  surface energy density (J m^{-2})
\( \lambda \)  elasticity parameter (-)
\( \lambda_T \)  Tabor parameter (-)
\( \mu_s \)  sliding friction coefficient (-)
\( \nu \)  Poisson’s ratio (-)
\( \phi \)  adhesiveness parameter (-)
\( \rho_p \)  particle density (kg m^{-3})
\( \psi \)  collision angle (-)
\( \omega \)  particle angular velocity (s^{-1})
\( \xi \)  rolling displacement (m)

Subscripts

0  equilibrium condition
ad  adhesive
crit  critical
con  contact
damp  damping
eff  effective
ext  external
f  final
mod  modified values
i  particle i
j  particle j
n  normal direction
r  rolling resistance
t  tangential direction
vdW  van der Waals

Acronyms

DEM  Discrete Element Modelling
DMT  Derjaguin-Muller-Toporov model
JKR  Johnson-Kendall-Roberts model