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Modelling particle kinetic behaviour considering asperity contact: formulation and DEM simulations

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23 **1. Introduction**

24 Upon contacting, particles behaviour is closely dependent on its physical characteristics, such
25 as the density, shape, size and surface at contact [1-3]. On the contact surface, the asperity, or
26 roughness, governs the particle response, mainly in the form of energy loss in a dynamic or
27 tribological process (e.g., the wheel rolling on the rail) [4-7]. The energy loss, at least a major
28 portion of it, is recognised of arising from the surface adhesion and frictional properties [6-8].
29 This means that the energy loss in itself is caused primarily by the surface deformation at
30 contact. According to Buckley [9], the deformation includes the elastic and plastic components.
31 The two components are related to the conditions of contact existed between the particles of
32 concern and, depending on the contact conditions, are subject to variation in magnitude. As a
33 result, the relationship between the surface asperity, deformation components, and energy loss
34 is still poorly understood [10-11]. Albeit there are experimental solutions (e.g. [3,9]) developed
35 to eliminate the lack of understanding, the test conditions are less than ideal, and the
36 corresponding results are not accurate enough. The reasons, as per Zappone et al. [12], were
37 the challenge to set up a well-defined rough surface and the difficulty to avoid environmental
38 noises (e.g., the surface chemistry characteristics) surrounding the particles in the test. These
39 difficulties can be resolved through mathematical tools which enable a virtual system free of
40 environmental disturbance.

41 In this study, a discrete element model (DEM) was developed to reproduce the system
42 and approximate particle kinetic behaviour in response to the surface asperity that the particle
43 is subjected to. The surface asperity characteristics were defined specifically to subject the
44 particle to a unique, exclusive rugged surface. On the rugged surface, the particle was assigned
45 a velocity and allowed to travel through. The model was used to gauge the particle trajectory
46 and velocity in travel so that the energy loss was recorded. The model was validated against
47 the analytical solution established in the same asperity conditions as for the DEM model. DEM

48 simulations were performed on some interesting case studies in order to gain a further insight
49 into the particle kinetic behaviour at micro-scale.

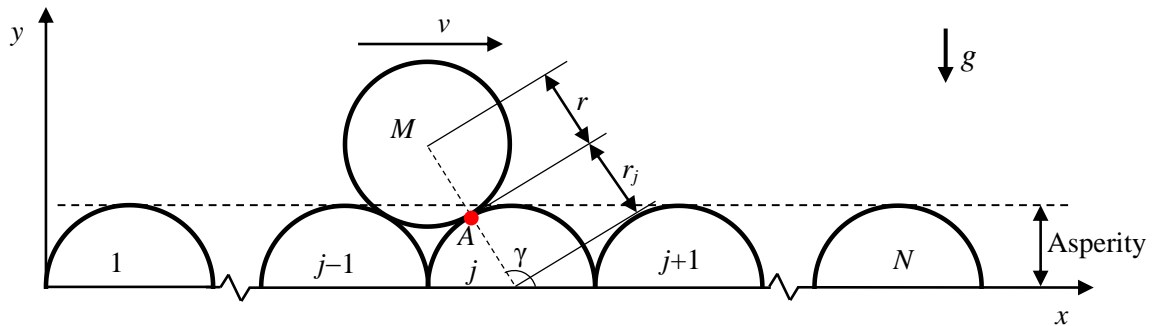
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51 **2. Model Development**

52 **2.1 Geometry**

53 The geometry used to develop the model is provided in Figure 1. An array of semicircular discs,
54 1 to N , are lined up at fixed positions in (x, y) plane, forming the asperity based on the substrate
55 of x -axis. The discs are equal in radius, r_j , where $j=1, 2, \dots, N$, and placed edge to edge with
56 individual centroids sitting on the x -axis. At time t , disc M moves at a velocity, v , in the x -
57 direction. Disc M measures r in radius and m in mass. The position of the moving disc in
58 relation to disc j is determined by the contact angle, γ , which measures the angle from the x -
59 axis to the centre-to-centre line drawn between discs M and j . Disc M is in contact with disc j
60 at point A . This model uses circular asperities (which are less angular than some surface
61 projections), but as suggested in past studies [13-15], this geometry defines a clear, continuous
62 and manageable asperity surface. This geometry facilitates: *i*) the expression of the asperity
63 surface (i.e. circular function), *ii*) the assessment of discs contacting condition, and *iii*) the
64 adaption of the geometry to the analytical model [16]. Similar circular, spaced asperities were
65 adopted in past studies [14-15,17-19]. The model geometry in the current study however differs
66 in the following aspects: *i*) the substrate being horizontal thus avoiding the angle of inclination,
67 *ii*) the substrate being fixed, and *iii*) the single disc moving through the asperity. In addition,
68 we assumed the following conditions: *i*) There is no sub-asperity at the particle surface; *ii*) the
69 discs and surface are smooth and, as per Gollin et al. [20], the energy loss is in the form of
70 collisional energy dissipation; and *iii*) the collisions are elasto-viscous. In this current study,
71 the collisional energy dissipation was determined using two approaches: the discrete element
72 simulation method and the analytical solution. The analytical results were used to verify the

73 simulation results. The two approaches and the method verification are presented in the
 74 following sections.

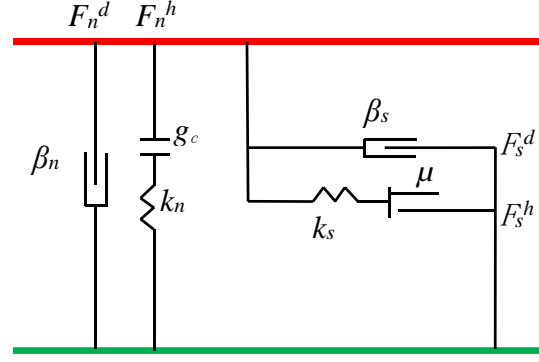


75
 76 Figure 1. The model geometry of disc M moving at velocity v on the asperity surface, a
 77 substrate comprised of an array of equal-size semi-discs 1 to N which are arranged, edge-to-
 78 edge, with respective centroids sitting on x -axis.

79

80 2.2 DEM model

81 The DEM model was developed to reproduce the mechanical responses of two or more discs
 82 at contact, e.g., point A in Figure 1. As per Cundall [21], the mechanical responses at contact
 83 can be represented by using a combination of simple mechanical elements, such as the spring,
 84 slider and dashpot. The combination is dependent on the materials to be examined and, as
 85 suggested in the past similar studies [17-19,22], is often governed by the Hertz Contact model
 86 [23]. The Hertz Contact model uses the least number of mechanical elements, as illustrated in
 87 Figure 2, but enables the mimicking of a wide range of distinct element based problems. The
 88 model is simple in concept and preferably applicable to represent the contacting occurred
 89 between the kinetic particles.



90

91 Figure 2. Diagram of the Hertz Contact model (adapted from ITASCA [24]), where F_n^h and F_s^h
 92 are respectively non-linear contact force at normal and shear direction; F_n^d and F_s^d are dashpot
 93 (viscous) forces at normal and shear direction, respectively; β_n and β_s are damping coefficients
 94 at normal and shear direction, respectively; k_n and k_s are stiffness at normal and shear direction,
 95 respectively; g_c is gap distance between the two bodies of interest; and μ is friction coefficient.

96

97 In the Hertz Contact model, the individual mechanical elements govern energy
 98 transformation occurred at particles contact. The energy transformation arises from three
 99 components: the elastic strain energy, E_s , stored in the spring elements, the slip energy, E_μ ,
 100 dissipated by frictional sliding, and the dashpot energy, E_β , being dissipated due to damping
 101 [25]. The energy is dissipated to other forms of energy, e.g., heat and sound. Owing to the no-
 102 friction contact as defined in Figure 1, the dashpot energy dissipation E_β is the only source of
 103 energy loss at contact. For the same reason, the moving disc M changes only its normal velocity
 104 component [26]. The energy loss E_β is expressed as:

$$E_\beta = -\sum F_n^d (\dot{\delta}_n \Delta t) \quad (1)$$

105 where δ_n is the relative normal displacement; Δt is the time step increment; F_n^d is the normal
 106 dashpot force at contact and, as per Itasca [24], is calculated as:

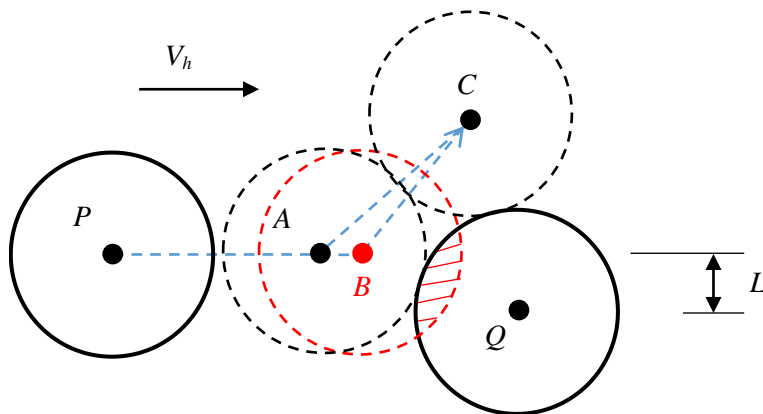
$$F_n^d = 2\dot{\delta}_n^2 \beta_n \sqrt{m_c k_n} \quad (2)$$

107 where β_n is the normal critical damping coefficient, k_n is the normal stiffness, and m_c is the
 108 mass of the system of interest and defined by:

$$m_c = \frac{m_1 m_2}{m_1 + m_2} \quad (3)$$

109 where m_1 and m_2 are the mass of discs 1 and 2 respectively.

110 In a DEM model, the particles are assumed to be non-deformable. Instead an overlap is
 111 allowed to develop at the point of contact in order to account for disc-to-disc interactions [25].
 112 This overlap likely influences the trajectory of the moving disc, as illustrated in Figure 3. Figure
 113 3 shows the potential overlap at the contact between moving disc P and stationary disc Q . The
 114 two discs collide at an eccentricity of L . DEM algorithm allows disc P to penetrate into disc Q ,
 115 creating a contact overlap as shaded between the two discs. As a result, the centroid of disc P
 116 passes on the trajectory of points A , B and C in DEM simulation, but in reality may not pass
 117 through point B . The influence to the trajectory of disc P may be negligible in one collision.
 118 However, where a continuously bumpy surface as in Figure 1 is of the choice and multiple
 119 collisions occur, the influences may accumulate, likely leading to noticeable trajectory
 120 deviation. The change in trajectory is supposed to affect the prediction of the contact angle γ
 121 which in turn brings possible inaccuracy to estimate of the energy loss of the moving disc. The
 122 overlap influence can be examined by cross checking the simulation results with the results
 123 obtained from an analytical solution.



124

125 Figure 3. The centroid of particle P travelling, at velocity v_h , in trajectory of A–B–C occurred
126 during an oblique collision with particle Q .

127

128 **2.3 Analytical solution**

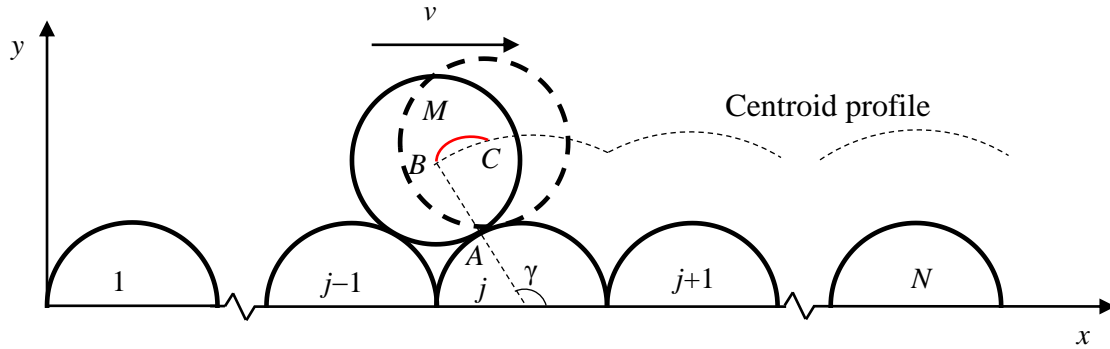
129 This section presents the analytical solution to the same problem of the disc travelling on
130 asperity surface as simulated by the DEM approach. The DEM adopts the Newton’s laws of
131 motion, and the analytical solution considers the restitution of material. According to [22,26],
132 both the Newton’s laws of motion and the restitution can be used to describe the dissipative
133 interaction of particles. As per Doménech-Carbó [4] and Ling [27], the restitution coefficient
134 quantifies the elastic energy restored at contact, which is recovered back to kinetic energy, and
135 the energy dissipation that results from plastic deformation. Upon surface colliding, no body
136 penetration (i.e., the overlap) between the discs of interest is allowed. Therefore, the analytical
137 method offers an accurate prediction of the disc trajectory and can be used to examine the
138 influences of overlap identified in the DEM simulation.

139

140 **2.3.1 Model description**

141 The geometry in Figure 1 was adapted to the geometry in Figure 4. The new element added is
142 the centroid profile where the centroid of disc M lies on. The profile was plotted based on the
143 radii of the discs so that the overlap issue was avoided. On the centroid profile, a sub-profile,
144 curve BC , was plotted to illustrate one disc bounce. Multiple bounces may occur depending on
145 the kinetic energy of the moving disc and the disc material properties assigned. The rest
146 conditions such as the surface asperity, velocity and radii remained the same as in Figure 1.
147 When disc M moved on the bumpy surface, the following conditions were assumed: *i*) Only
148 the point of contact was examined during the collision; and *ii*) Disc collision completed

149 instantaneously, so that the collision time was negligible. These conditions were used to
 150 simplify the model and to agree with the conditions assumed for the DEM approximation.



151
 152 Figure 4. The model geometry of disc M moving, with the consideration of bounces, at velocity
 153 v on the asperity surface which is comprised of an array of equal-size semi-discs 1 to N arranged,
 154 edge-to-edge, with centroids sitting on x -axis.

155

156 At a moment when disc M travels on the asperity surface, the disc takes one of three
 157 moves: rotating, sliding and bouncing. As there is no surface friction, the disc does not spin.
 158 Therefore the disc either slides or bounces on the surface, depending on the condition of contact
 159 between the moving disc and one of the base discs. The contact condition can be judged based
 160 on the centre-to-centre distance D_j^t measured at time t between discs M and j , which is
 161 expressed as

$$D_j^t = \sqrt{(x^t - x_j)^2 + (y^t - y_j)^2} \quad (4)$$

162 where (x_j, y_j) and (x^t, y^t) are the coordinates of the centres of discs j and M , respectively.
 163 Disc M is bouncing if $D_j^t > r + r_j$ or sliding if $D_j^t = r + r_j$. The condition $D_j^t < r + r_j$ is not
 164 allowed to avoid the surface overlap. For base disc j , the centre coordinate is expressed as:

$$x_j = r_j + 2 \sum_{i=1}^{j-1} r_i \quad (5)$$

$$y_j = 0 \quad (6)$$

165

166 **2.3.2 Trajectory of bouncing**

167 Upon a collision with disc j , disc M loses a portion of the normal velocity. The residual normal
 168 velocity drives the disc to bounce up and then falls under gravity, as of the profile BC shown
 169 in Figure 4. This bouncing process continues several times until the normal velocity vanishes.
 170 Assume disc M is in collision with disc j at time t . Meanwhile, the disc bounces up at velocity
 171 components (v_x^t, v_y^t) . If, at time step $t+\Delta t$, disc M is in the move of the first bounce, the
 172 corresponding velocity components become:

$$v_x^{t+\Delta t} = v_x^t \quad (7)$$

$$v_y^{t+\Delta t} = v_y^t + g \times \Delta t \quad (8)$$

173 The centr relocates to location $(x^{t+\Delta t}, y^{t+\Delta t})$ which are respectively expressed as:

$$x^{t+\Delta t} = x^t + v_x^t \times \Delta t \quad (9)$$

$$y^{t+\Delta t} = y^t + \frac{(v_y^{t+\Delta t} + v_y^t) \times \Delta t}{2} \quad (10)$$

174 Substitute Eqs. (9) and (10) to Eq. (4) to update discs centre-to-centre distance $D_j^{t+\Delta t}$. The

175 updated $D_j^{t+\Delta t}$ is then used to confirm the occurrence of the first bounce presented for disc M .

176 If $D_j^{t+\Delta t} > r + r_j$ the presumption is confirmed; if $D_j^{t+\Delta t} = r + r_j$, the disc is sliding; and if

177 $D_j^{t+\Delta t} < r + r_j$, disc M has performed two or more bounces in the time step increment Δt .

178 Where two or more bounces occur in the time step increment Δt , the time $t+\Delta t_0$ when
 179 the first bounce completes needs to be determined. As Δt is sufficiently small (and Δt_0 is further
 180 smaller), the horizontal and vertical velocities are assumed to be constant during the collision

181 period Δt_0 . Assuming a linear trajectory during $(t, t+\Delta t_0)$, the centre of disc M , $(x^{t+\Delta t_0}, y^{t+\Delta t_0})$,
 182 satisfies the translation condition:

$$y^{t+\Delta t_0} = y^t + \frac{v_y^{t+\Delta t_0}}{v_x^{t+\Delta t_0}} x^{t+\Delta t_0} - \frac{v_y^{t+\Delta t_0}}{v_x^{t+\Delta t_0}} x^t \quad (11)$$

183 At time $t+\Delta t_0$, discs M and j are in contact, leading to

$$(y^{t+\Delta t_0})^2 + (x^{t+\Delta t_0} - x_j)^2 = (r + r_j)^2 \quad (12)$$

184 Solving Eqs. (11) and (12) yields two roots $x^{t+\Delta t_0} = x_1$ and x_2 respectively as follow:

$$x^{t+\Delta t_0} = \begin{cases} x_1, & \text{if } |x_1 - x^t| < |x_2 - x^t| \\ x_2, & \text{if } |x_1 - x^t| > |x_2 - x^t| \end{cases} \quad (13)$$

185 The time increment Δt_0 is calculated as:

$$\Delta t_0 = \left| \frac{x^{t+\Delta t_0} - x^t}{v_x^t} \right| \quad (14)$$

186 During the time increment Δt_0 , the x -velocity component of disc M remains unchanged:

$$v_x^{t+\Delta t_0} = v_x^t \quad (15)$$

187 Disc M changes in elevation, the y -velocity component is updated as:

$$v_y^{t+\Delta t_0} = \lim_{\Delta t_0 \rightarrow 0} \frac{v_y^t}{|v_y^t|} \sqrt{(v_y^t)^2 - 2g(y^t - y^{t+\Delta t_0})} \quad (16)$$

188 The contact angle γ at $t+\Delta t_0$ becomes:

$$\gamma^{t+\Delta t_0} = \arctan \frac{y^{t+\Delta t_0} - y_j}{x^{t+\Delta t_0} - x_j} \quad (17)$$

189 The tangential and normal velocity components are calculated respectively as:

$$v_s^{t+\Delta t_0} = v_x^{t+\Delta t_0} \cos \gamma^{t+\Delta t_0} + v_y^{t+\Delta t_0} \sin \gamma^{t+\Delta t_0} \quad (18)$$

$$v_n^{t+\Delta t_0} = v_x^{t+\Delta t_0} \sin \gamma^{t+\Delta t_0} + v_y^{t+\Delta t_0} \cos \gamma^{t+\Delta t_0} \quad (19)$$

190 If the disc rebounds, the disc is subjected to damping and the normal velocity reduces to:

$$v_{n,r}^{t+\Delta t_0} = -\alpha_n v_n^{t+\Delta t_0} \quad (20)$$

191 where α_n is the material restitution coefficient. Kawaguchi et al. [28] expressed α_n as a
 192 function of damping coefficient β_n :

$$\alpha_n = e^{\frac{\beta_n \pi}{\sqrt{1-\beta_n^2}}} \quad (21)$$

193 Substituting Eq. (21) into Eq. (20) yields:

$$v_{n,r}^{t+\Delta t_0} = -e^{\frac{\beta_n \pi}{\sqrt{1-\beta_n^2}}} v_n^{t+\Delta t_0} \quad (22)$$

194 Transforming the tangential and normal velocity components to velocity components in (x, y)
 195 plane, we have:

$$v_x^{t+\Delta t_0} = v_s^{t+\Delta t_0} \cos \gamma - v_{n,d}^{t+\Delta t_0} \sin \gamma \quad (23)$$

$$v_y^{t+\Delta t_0} = v_s^{t+\Delta t_0} \sin \gamma - v_{n,d}^{t+\Delta t_0} \cos \gamma \quad (24)$$

196 The new velocity components drive the disc to rebound. At time step $t+\Delta t$, the velocity of disc
 197 M and the coordinate of the centre are determined respectively as:

$$v_x^{t+\Delta t} = v_x^{t+\Delta t_0} \quad (25)$$

$$v_y^{t+\Delta t} = v_y^{t+\Delta t_0} + g(\Delta t - \Delta t_0) \quad (26)$$

$$x^{t+\Delta t} = x^{t+\Delta t_0} + v_x^{t+\Delta t_0}(\Delta t - \Delta t_0) \quad (27)$$

$$y^{t+\Delta t} = y^{t+\Delta t_0} + v_y^{t+\Delta t_0}(\Delta t - \Delta t_0) \quad (28)$$

198 The coordinate of the discs centre is subject to the contact criterion (i.e. $D_j^{t+\Delta t}$ vs. $r + r_j$). If
 199 $D_j^{t+\Delta t} > r + r_j$, disc M is in the move of the second bounce. The algorithm proceeds to the next
 200 time step. Otherwise, Eqs. (11)–(28) are skipped and the current bounce completes, and the
 201 disc enters into the phase of sliding. The skipping is acceptable as the normal velocity at $t+\Delta t_0$
 202 is sufficiently small and in period $(t+\Delta t_0, t+\Delta t)$ the remaining bounces are relatively small in

203 scale and less in number, and are negligible. The neglected trivial bounces would influence the
 204 determination of kinetic energy loss of disc M and thus its trajectory. However, the influence
 205 is very small if not zero because time step increment Δt itself is a significantly small value, i.e.,
 206 $\times 10^{-4}$ s, and a smaller value for increment $\Delta t - \Delta t_0$, e.g., $\times 10^{-6}$ s, causes marginal changes to the
 207 trajectory.

208

209 2.3.3 Trajectory of sliding

210 Where the normal velocity of disc M dissipates completely at time $t + \Delta t_0$, the disc does not
 211 bounce but enters into sliding on the surface. Upon departure, the angular velocity is
 212 determined as:

$$\omega^{t+\Delta t_0} = \frac{v_s^{t+\Delta t_0}}{r + r_j} \quad (29)$$

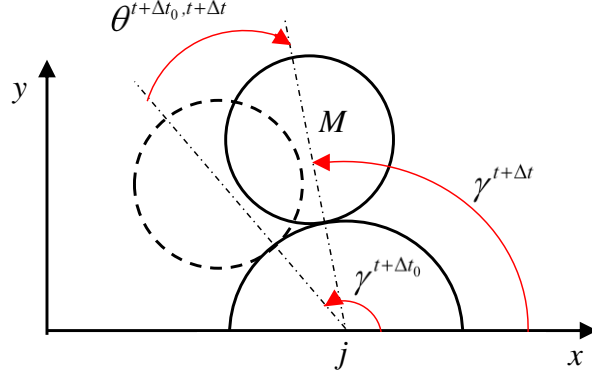
213 where the tangential velocity $v_s^{t+\Delta t_0}$ is determined in terms of Eq. (18). Meanwhile, the angular
 214 acceleration $\dot{\omega}^{t+\Delta t_0}$ is equal to:

$$\dot{\omega}^{t+\Delta t_0} = \frac{g \times \cos \gamma^{t+\Delta t_0}}{r + r_j} \quad (30)$$

215 The angle of rotation θ completed during the time increment $(\Delta t - \Delta t_0)$ is calculated as:

$$\theta^{t+\Delta t_0, t+\Delta t} = \omega^{t+\Delta t_0} \times (\Delta t - \Delta t_0) + 0.5 \times \dot{\omega}^{t+\Delta t_0} \times (\Delta t - \Delta t_0)^2 \quad (31)$$

216 Define angles θ and γ to be positive if they rotate in clockwise and anti-clockwise directions
 217 respectively, as shown in Figure 5.



218

219 Figure 5. The schematic of the change of the contact angle γ and rotation angle θ occurred at
 220 time increment $t+\Delta t_0$ to $t+\Delta t$ when the moving disc M slides on the base disc j .

221

222 At time step $t+\Delta t$, the contact angle is updated as:

$$\gamma^{t+\Delta t} = \gamma^{t+\Delta t_0} - \theta^{t+\Delta t_0, t+\Delta t} \quad (32)$$

223 The centre of disc M relocates to:

$$x^{t+\Delta t} = x^{t+\Delta t_0} + (r + r_j) \times (\cos(\gamma^{t+\Delta t_0} - \theta^{t+\Delta t_0, t+\Delta t}) - \cos \gamma^{t+\Delta t_0}) \quad (33)$$

$$y^{t+\Delta t} = y^{t+\Delta t_0} + (r + r_j) \times (\sin(\gamma^{t+\Delta t_0} - \theta^{t+\Delta t_0, t+\Delta t}) - \sin \gamma^{t+\Delta t_0}) \quad (34)$$

224 The angular velocity ω , tangential velocity v_s , x-velocity component v_x , and y-velocity
 225 component v_y , respectively, are updated as:

$$\omega^{t+\Delta t} = \frac{\omega^t}{|\omega^t|} \times \sqrt{(\omega^t)^2 - 2 \times g \times \frac{y^{t+\Delta t} - y^t}{(r + r_j)^2}} \quad (35)$$

$$v_s^{t+\Delta t} = \omega^{t+\Delta t} \times (r + r_j) \quad (36)$$

$$v_x^{t+\Delta t} = v_s^{t+\Delta t} \times \cos(\gamma^{t+\Delta t}) \quad (37)$$

$$v_y^{t+\Delta t} = v_s^{t+\Delta t} \times \sin(\gamma^{t+\Delta t}) \quad (38)$$

226

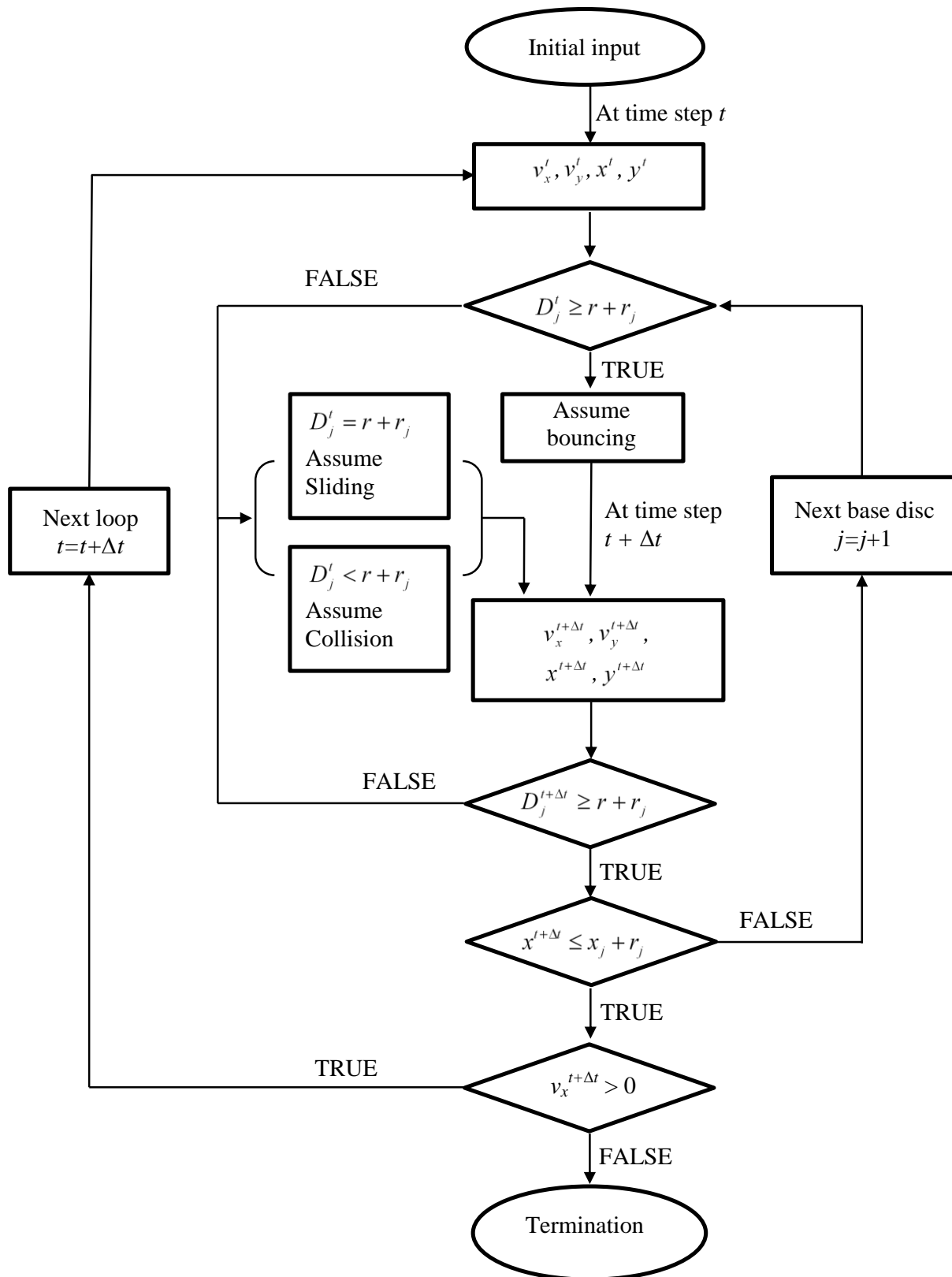
227 Eqs. (29)–(38) are used to calculate the trajectory of disc M performed during time step
 228 $(t+\Delta t_0, t+\Delta t)$. Continue the same algorithm at the next time increment $(t+\Delta t, t+2\Delta t)$ if disc M is

229 sliding in terms of the contact criterion of $D_j^{t+2\Delta t}$ vs. $r + r_j$. Otherwise, the algorithm
230 developed for bouncing, i.e. Eqs. (11)–(28), is used. An additional contact check is performed
231 between discs M and $j+1$. If, at time t , $x^t > x_j + r_j$, then disc M is in contact with disc $j+1$ and
232 disc $j+1$ becomes the current disc of interest in the algorithm.

233

234 **2.3.4 Model flowchart**

235 A flowchart of the model is presented in Figure 6. The initial input values include the velocity
236 components and the position of the centre of disc M . The position values are plugged in the
237 contact criterion of D_j^t vs. $r + r_j$ to determine the motion of the disc. Where in the motion of
238 bouncing, disc M is updated, using the corresponding algorithm, in respect to its centre
239 coordinate and velocity components. The new values are subject to the contact criterion again.
240 Where disc M is in the motion of sliding, the new values are plugged into the algorithm for
241 sliding, thus updating the centre position and disc velocity. And the new values flow to the
242 contact criterion again. In either motion, disc M is subject to the check of contact with the next
243 base disc $j+1$. If there is, disc $j+1$ becomes the current base disc, and a new loop runs. Before
244 the flowchart ends, the x -velocity component is checked. If the velocity component is not equal
245 to zero, the loop keeps on running. Otherwise, the program ends.



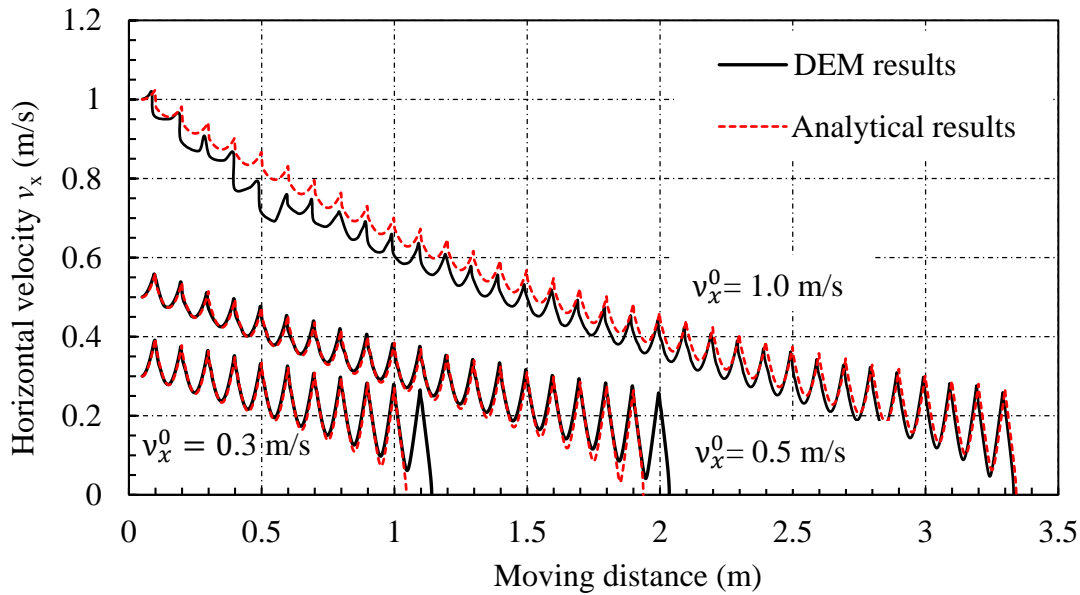
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247 Figure 6. Computer flowchart developed to guide the travel of the moving disc on a bumpy
 248 surface.

249

250 **3. DEM Validation**

251 The DEM model was validated against the analytical solution. Both approaches were applied
252 to the model shown in Figure 1. The models were established using the following properties.
253 The radii were 0.3 m for the moving disc and 0.05 m for the base disc. All discs had a density
254 of 2,000 kg/m³. In the DEM, the Hertz contact was used which adopted a Poisson's ratio of 0.3
255 and shear modulus of 100 GPa. The relatively large shear modulus was assumed to reduce the
256 influence of the contact overlap, enabling a simulation environment similar to that for the
257 analytical method. For both methods, a damping coefficient $\beta_n = 0.5$ was used to dissipate
258 energy at each collision. The moving disc was assigned three initial velocities $v_x^0 = 0.3, 0.5$ and
259 1.0 m/s respectively. The results of the horizontal velocity versus the distance for the disc
260 assigned the three initial velocities are provided in Figure 7.



261
262 Figure 7. The results of the horizontal velocity versus the distance obtained for the disc assigned
263 three different initial velocities v_x^0 to travel on the same substrate as specified on Figure 1
264 where the moving disc radius is $r = 0.3$ m, base discs radius is $r_j = 0.05$ m, and damping $\beta_n = 0.5$.
265

266 In Figure 7, all three curves exhibit a ‘saw-tooth’ mode. This mode is caused by the
267 bumpy surface: accelerating on down-slopes and decelerating on up-slopes. The horizontal
268 velocity of the disc goes down at the end of the travel, as a result of energy loss at collisions.
269 Excellent agreement is attained between the DEM results and the analytical solutions across
270 the three cases of different initial velocities. The pairs of curves exhibit agreed amplitudes,
271 frequencies, gradient and the final moving distances of the disc. This suggests that the DEM
272 simulation can capture the trajectory of the disc which travels at various initial velocities,
273 validating the capability of the DEM model to predict the loss of kinetic energy. In both the
274 numerical and analytical scenarios, the dissipation of energy is attributed to the asperity
275 collision along the substrate. At each collision, the velocity reduced at a gradient of 0.013 m/s
276 per disc or 0.25 m/s per meter. It is noted that the numerical predictions deviated from the exact
277 results at the early stage of travel if v_x^0 increased from 0.5 to 1.0 m/s. The velocity discrepancy
278 at the early stage arises from the conditions assumed for the DEM and analytical methods
279 respectively. As opposed to the analytical method, DEM assumes occurrence of
280 particle–surface overlaps in collisions. It means that part of kinetic energy is converted to the
281 elastic potential energy. Where the overlaps are relatively significant, i.e., at the early stage of
282 greater velocity, greater energy conversion occurs and the kinetic energy and the corresponding
283 velocity become less. The total mechanical energy however remains the same, which explains
284 that the curves eventually agree where the velocity reduces and the overlaps become less
285 significant.

286

287 **4. Simulation Results**

288 The validated DEM model was used to perform a parametric study. The study was focused on
289 the travel mode of the disc of interest where important material properties and surface asperity
290 characteristics were changed. The properties included the material damping, collision angle

291 and mixed asperities surface. In addition, the energy transformation associated with the disc
292 travel in each of the simulation cases was examined.

293

294 **4.1 Damping**

295 Damping influences the energy loss at collision. To gain an insight into the influence, the DEM
296 model was applied to the discs assigned two damping coefficients, $\beta_n = 0.1$ and 0.9 , respectively.

297 The moving disc was assigned an initial velocity of $v_x^0 = 0.5$ m/s. The rest conditions remained
298 the same as for the model used in the validation section. The simulation results, in the form of

299 the velocity versus the moving distance curves, are provided in Figure 8. As shown in Figure

300 8 (a) and (c), close agreement is obtained between the DEM and analytical results obtained for

301 the two cases $\beta_n = 0.1$ and 0.9 . In both cases, the moving discs travel through 19 base discs and

302 stops on the trough between the 19th and 20th discs. This agreement suggests that the damping

303 coefficient less likely influenced the mode of overall energy dissipation of the moving disc,

304 where the other conditions remained the same. However, the energy dissipation at each

305 collision can be different, as shown in Figure 8 (b) and (d). These two figures present the

306 velocity versus distance relationship for disc M travelling through the first three base discs.

307 When the damping coefficient was relatively small (Figure 8 (b)), two collisions, as represented

308 by the corresponding vertical short lines, and one bounce, as of the short horizontal short line,

309 occurred. When the damping coefficient increased as in Figure 8 (d), one collision (and no

310 bounce), as of the short vertical line, occurred. Disc M was in the motion of sliding for the rest

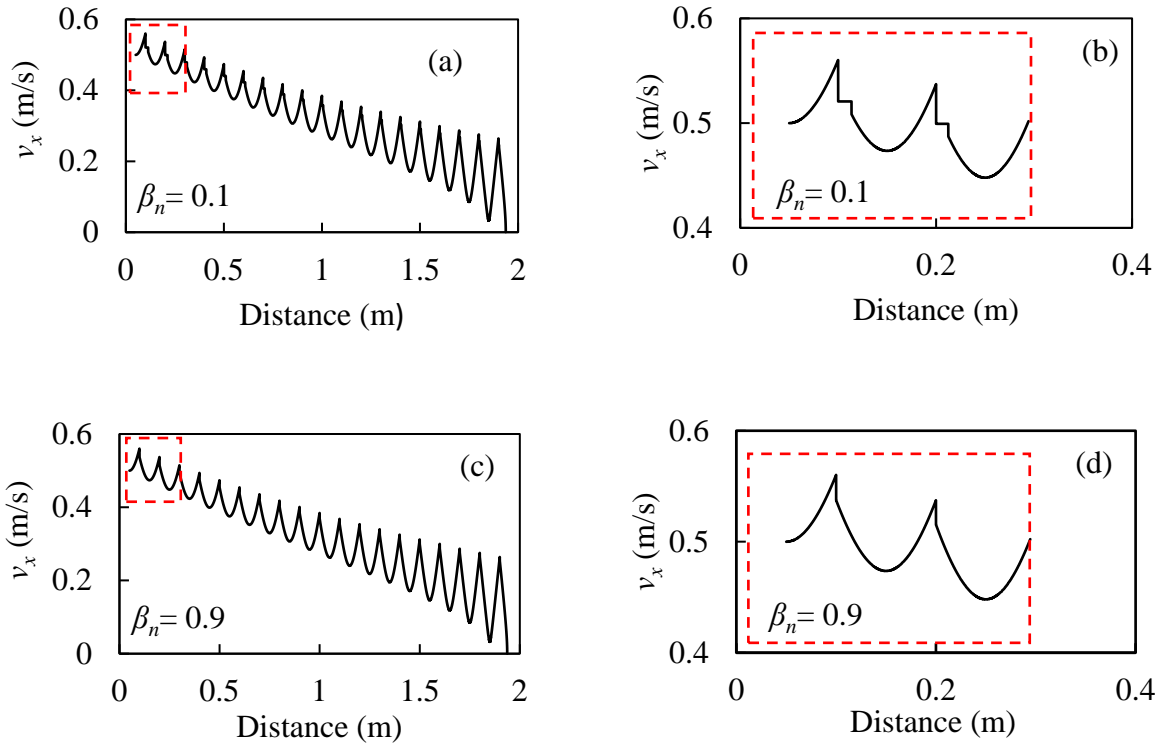
311 part of the travel on the same base disc. For both cases, the moving disc eventually lost the

312 normal velocity when it contacted the base asperity. For example, in Figure 1, the moving disc

313 finally slide at the surface of base disc $j+1$, no matter of the collisions number, and the only

314 change to the moving disc was its normal velocity. This explains that the damping coefficient

315 does not affect the actual trajectory of disc on the surface, and the energy dissipation is greatly
 316 influenced in a single collision (Figure 8 (b) and (d)).



317 Figure 8. The results of the horizontal velocity v_x versus the moving distance obtained for the
 318 disc traveling on the substrate model as specified on Figure 1 where the moving disc radius is
 319 $r = 0.3$ m and the base discs radius is $r_j = 0.05$ m, under different damping conditions: (a)
 320 damping $\beta_n = 0.1$, the complete travel profile; (b) $\beta_n = 0.1$, the travel profile through the first 3
 321 discs; (c) damping $\beta_n = 0.9$, the complete travel profile; and (d) $\beta_n = 0.9$, the travel profile
 322 through the first 3 discs.

323

324 4.2 Loss of energy at different damping conditions

325 To gain a further insight into the effect of damping on the travel mode of the disc, energy
 326 dissipation developed in different damping conditions was examined. The DEM model was
 327 applied to asperity surfaces assigned six different damping coefficients $\beta_n = 0.1, 0.2, 0.3, 0.4,$
 328 $0.5,$ and 0.9 respectively. The initial velocity of the disc was $v_x^0 = 0.5$ m/s, whereas the rest

329 conditions remained the same as in the validation study. In order to quantify the loss of energy
330 at each collision, we defined the following equation:

$$\Delta E_{\beta,j} = -(E_{m,j} - E_{m,j-1}) \quad (39)$$

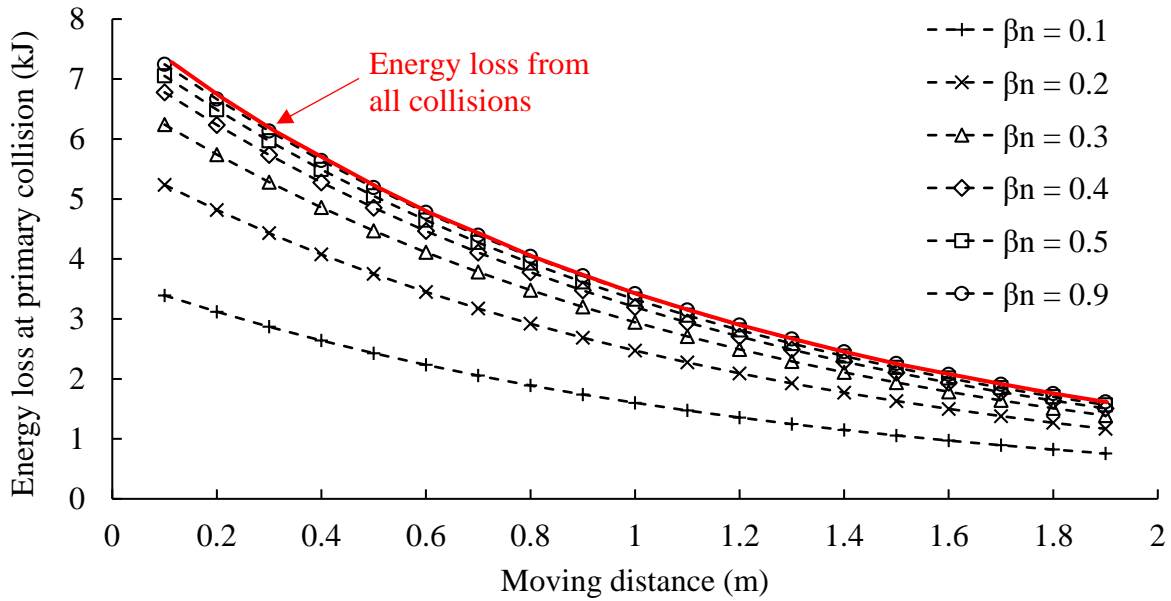
331 where $\Delta E_{\beta,j}$ is the energy dissipated at the base disc j ; $E_{m,j}$ and $E_{m,j-1}$ are the system mechanical
332 energy measured when the moving disc is in contact with base disc j and $j-1$, respectively. The
333 mechanical energy of the system can be calculated as:

$$E_m = E_k + E_s + U \quad (40)$$

334 where E_k , E_s and U are the kinetic energy, strain energy at contact, and gravity potential,
335 respectively, and are calculated using corresponding energy expressions. The gravity potential
336 takes the initial elevation as the reference. Energy dissipation at the first collision between the
337 moving disc and a new substrate asperity is of particular interest, because it denotes the primary
338 collision while the remaining bounces are categorised as secondary collisions.

339 The relationships of energy loss at each primary collision versus distance for the discs
340 assigned different damping coefficients are provided in Figure 9. In all cases, the energy
341 dissipation rate (i.e., the curve gradient) decreased with the distance. This is because the slower
342 the particle was moving, the less the kinetic energy was dissipated. However, the proportion of
343 energy dissipation was noticeably different between $\beta_n = 0.1$ and 0.9 in each collision. On a
344 lower damping coefficient (i.e., $\beta_n = 0.1$), multiple collisions occurred at each base substrate,
345 and the energy loss in the primary collision used only a proportion of the total energy which is
346 represented by the solid line in Figure 9. In comparison, when β_n increased to 0.9, the loss of
347 primary energy was nearly equal to the loss of total energy. Despite the variation of energy
348 dissipation in primary collisions, similar trendlines of the total energy loss were identified
349 across the cases examined. As explained in the model development section, the total energy
350 loss at each base disc is dependent on the normal velocity when the moving disc first contacts

351 a new base disc. Figure 9 also suggests that asperity-induced energy loss was velocity-
 352 dependent, which resulted in viscous behaviour.



353

354 Figure 9. The results of the energy loss at the primary collision versus the moving distance
 355 obtained for the disc traveling on the substrate model as specified on Figure 1 where the moving
 356 disc radius is $r = 0.3$ m and the base discs radius is $r_j = 0.05$ m, under different damping
 357 conditions.

358

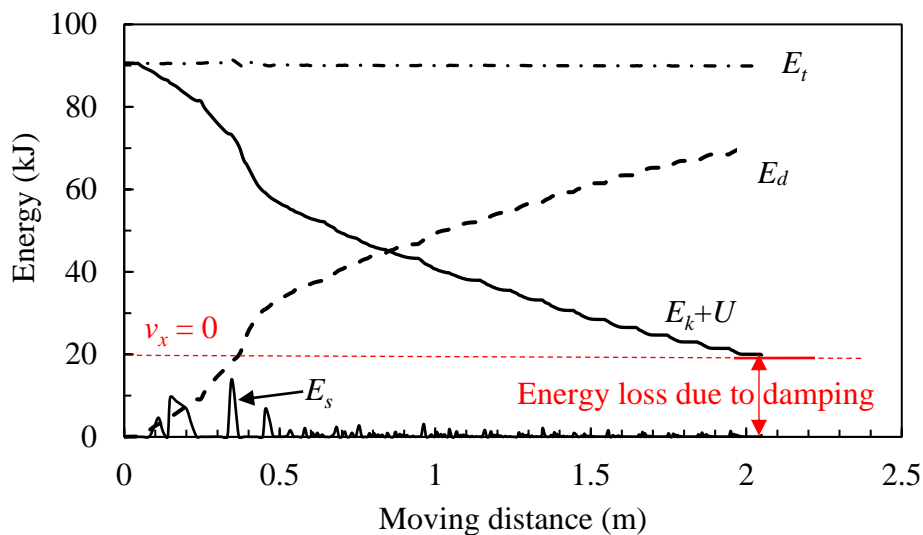
359 4.3 Energy transformation

360 This section further examines the energy transformation occurred when the disc moves on the
 361 asperity surface. The total energy of the system E_t contains two parts: the mechanical energy
 362 E_m and dashpot energy E_β . The relationship is expressed as:

$$E_t = E_m + E_\beta \quad (41)$$

363 Apply the above relationship to the case of $\beta_n = 0.9$ and $v_x^0 = 1.0$ m/s. The total energy and the
 364 energy components versus disc moving distance are plotted in Figure 10. At the initial position,
 365 the dashpot energy and strain energy were zero. Since the moving disc was placed at the crest
 366 of the base asperity, the sum of the gravity potential and kinetic energy was in peak. With an

367 increase in the moving distance, a portion of the kinetic energy and gravity potential was
 368 transformed to the strain energy, while the rest portion was dissipated at collisions, in the form
 369 of heat and sound. It is clear that the loss of kinetic energy was equal to the increase of dashpot
 370 energy, because the total energy was constant throughout the kinetic process. Where the
 371 horizontal velocity decreased to a small value to slide over the last disc, the moving disc
 372 bounced, back and forth, in the trough of the last two base discs until the kinetic energy was
 373 dissipated completely. Figure 10 also shows the contribution of contact overlap to the energy
 374 transformation, as captured by strain energy E_s . When the velocity reduced at the later stage of
 375 travel, the influence of contact overlap became less significant. The strain energy was nearly
 376 zero after the moving disc travels to 0.5 m.



377
 378 Figure 10. The results of the energy components and dissipation versus the moving distance
 379 obtained for the disc traveling on the substrate model as specified on Figure 1 where the moving
 380 disc radius is $r = 0.3$ m, initial velocity is $v_x^0 = 1.0$ m/s, base discs radius is $r_j = 0.05$ m, and
 381 damping is $\beta_n = 0.9$.

382

383 4.4 Surface asperity gap

384 The previous sections confirm that surface asperity can influence trajectory of moving object.
385 According to [16], however, the bumpy surface can be described as a collection of different
386 asperities (e.g., varying amplitudes). It is worth assessing characteristics of surface asperity
387 and examining how the characteristics influence travel of disc. For example, it is still not clear
388 about the relationship between the asperity amplitude parameters and energy dissipation, such
389 as whether it is linearly related to energy loss or not. In this section, the asperity properties,
390 including the average asperity and asperity variance, are evaluated against the energy loss.

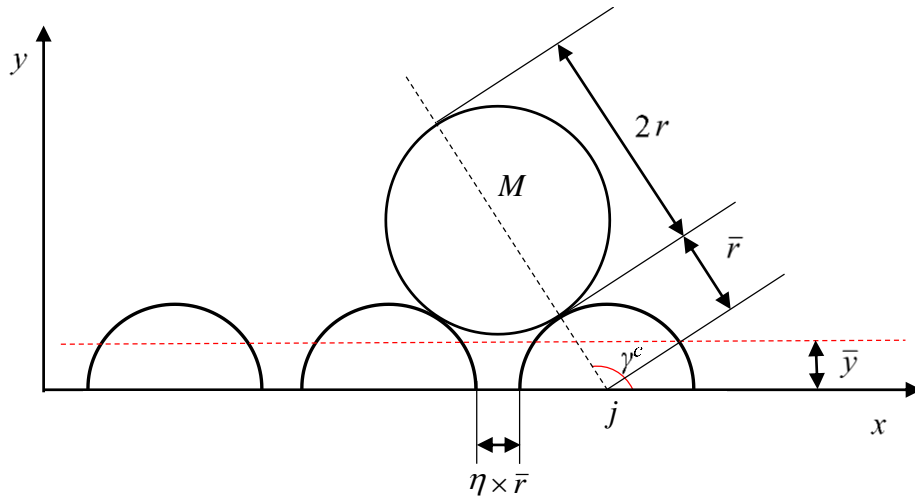
391 There are a number of different methods that can be used to constitute the roughness
392 degrees of the substrate. Gadelmawla et al. [29] suggested the use of asperity amplitude
393 parameters. Specifically, one of the basic properties used to describe a rough surface is R_a , the
394 average of the absolute values of the profile height deviation from the mean line that is recorded
395 with the elevation length. This method is complicated and subject to the determination of the
396 mean line. As a further step to the approach illustrated on Figure 1, a simplified approach was
397 developed in the current study. The concept was to constitute the surface asperity using a set
398 of discs with the same radius \bar{r} which were spaced per $\eta \times \bar{r}$ where η is the gap coefficient. In
399 this study, the radius \bar{r} ranged from 0.04 to 0.07 m, and η from 0 to 1. The model developed
400 based on the disc gaps is illustrated in Figure 11. The average asperity per distance, \bar{y} , is
401 expressed as:

$$\bar{y} = \frac{\int_0^{\bar{r} \times (1+0.5\eta)} y dy}{\bar{r} \times (1+0.5\eta)}, \quad y \in [0, \bar{r} \times (1+0.5\eta)] \quad (42)$$

402 The variance of the asperity is expressed as:

$$\text{Var}(y) = \frac{\int_0^{\bar{r} \times (1+0.5\eta)} (y - \bar{y})^2 dy}{\bar{r} \times (1+0.5\eta)}, \quad y \in [0, \bar{r} \times (1+0.5\eta)] \quad (43)$$

403

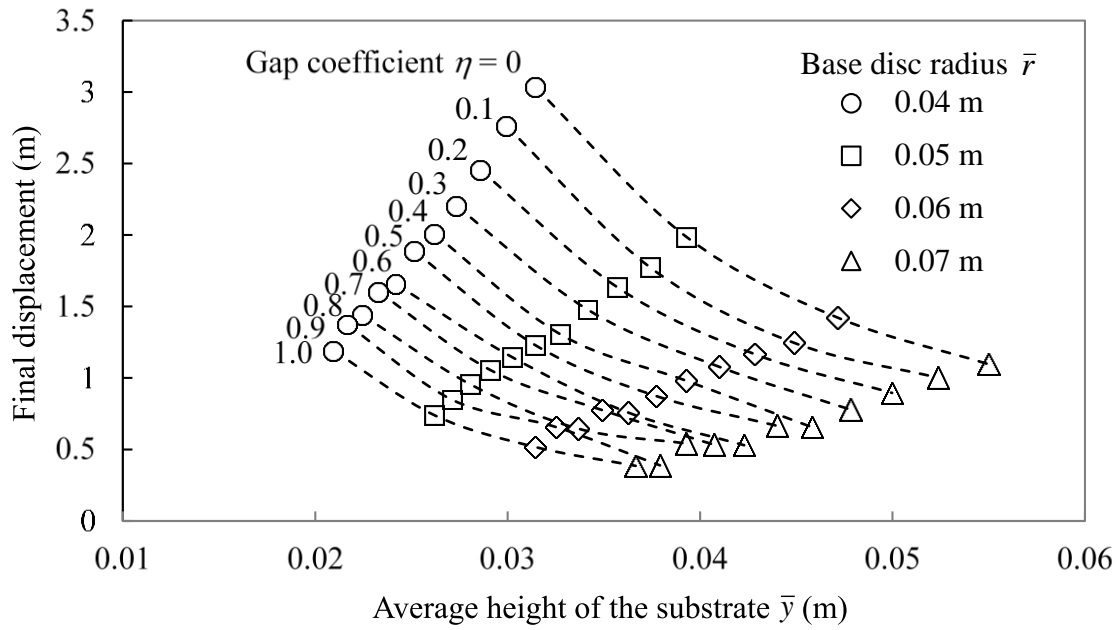


404

405 Figure 11. The asperity model developed based on gap coefficient η and average disc radius
 406 \bar{r} which determines \bar{y} , the average asperity per distance.

407

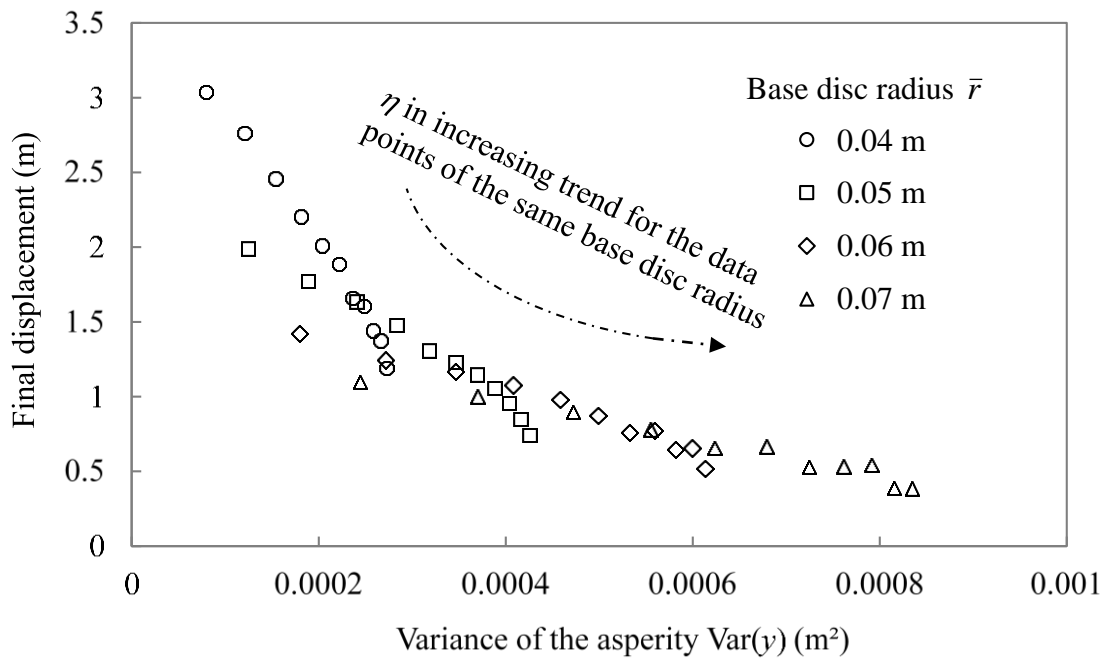
408 Simulations were performed based on the model shown in Figure 11. The simulations
 409 were focused on the disc travel distance versus asperity characteristics, including the average
 410 asperity elevation and asperity variance. These characteristics were examined by considering
 411 the base disc radii, disc gaps and asperity average elevation. The rest simulation conditions
 412 remained the same as in the validation section. A total of 44 simulations were performed to
 413 collect the disc travel distance information and were plotted against surface average height or
 414 height variance. The simulation results are provided in Figure 12 and Figure 13 respectively.



415

416 Figure 12. The results of the final displacement versus the average height of the substrate \bar{y}
 417 obtained for the disc traveling on the substrate model as specified on Figure 11 where the
 418 moving disc radius is $r = 0.3$ m, initial velocity is $v_x^0 = 1.0$ m/s, and damping is $\beta_n = 0.9$, with
 419 different base disc radii \bar{r} and gap coefficients η .

420



421

422 Figure 13. The results of the final displacement versus the variance of the asperity $\text{Var}(y)$
423 obtained for the disc traveling on the substrate model as specified on Figure 11 where the
424 moving disc radius is $r = 0.3$ m, initial velocity is $v_x^0 = 1.0$ m/s, and damping is $\beta_n = 0.9$, with
425 different base disc radii \bar{r} and gap coefficients η .

426

427 In Figure 12, the final displacement of the moving disc is plot per the base disc radius
428 \bar{r} and gap coefficient η . With the same gap coefficient, the asperity average height increased
429 with the disc radius, resulting in a decrease of in the final displacement. When the disc radius
430 remained constant, an increase in the gap ratio decreased the substrate height, which in turn
431 decreased the final displacement. However, the final displacement was independent on the
432 average height of the surface substrate, because the actual maximum displacement occurred at
433 an intermediate surface height (e.g., the case with $\bar{r} = 0.04$ m and $\eta = 0$). This indicates that
434 the average surface height was not linearly related to the trajectory of the disc. In comparison,
435 the surface-height variance provides better quantification of final displacement. It can be
436 identified that the lower the asperity-height variance was, the farther the object can travel.
437 Theoretically, the asperity gap helps refine surface asperity characteristics. However, there are
438 still some slight overlaps between different groups of radii as shown in Figure 12–13, and these
439 points inside the overlap area produce a reverse trend as opposed to the general relationship.
440 Hence, it is necessary to seek additional description of surface roughness which is discussed in
441 the following section.

442

443 **4.5 Collision angle**

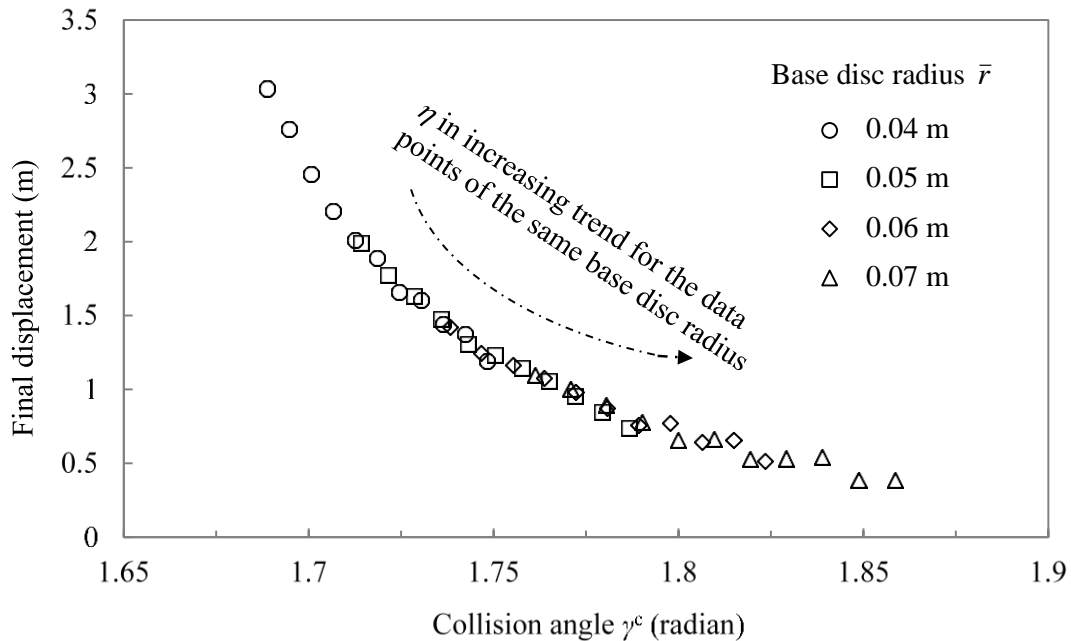
444 In this section, the collision angle γ^c is used to characterise surface roughness. At each
445 collision, the collision angle influences the loss of the normal velocity of the moving disc as
446 shown in Figure 8. The collision angle γ^c is different from the contact angle γ . The collision

447 angle γ^c is defined as the contacting angle when the moving disc collides a new base disc and,
 448 as shown in Figure 11, is calculated as:

$$\gamma^c = \arccos \frac{\bar{r} \times (1 + 0.5\eta)}{r + \bar{r}}, \quad \gamma^c \in \left[\frac{\pi}{2}, \pi \right] \quad (44)$$

449 It should be noted that there may be other collisions occurred between the moving disc and the
 450 base disc of interest. However, due to a relatively low horizontal velocity, the collision must
 451 happen in the middle of the two base discs where most of the kinetic energy is dissipated, as
 452 shown in Figure 9.

453 The final displacements are plotted against the collision angle γ^c as shown in Figure
 454 14. A monotonic relationship was observed: the smaller the collision angle was, the less
 455 distance the disc can move on the surface. The final displacement was entirely dependent on
 456 the collision angle. From this perspective, the collision angle was a parameter governing the
 457 surface roughness.



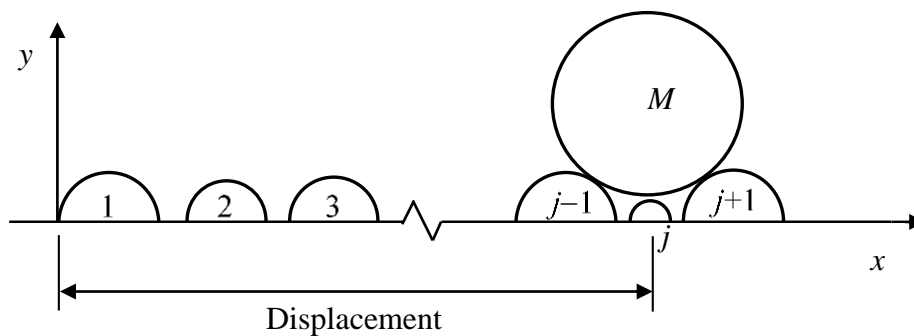
458
 459 Figure 14. The results of the final displacement versus the collision angle γ^c obtained for the
 460 disc traveling on the substrate model as specified on Figure 11 where the moving disc radius

461 is $r = 0.3$ m, initial velocity is $v_x^0 = 1.0$ m/s, and damping is $\beta_n = 0.9$, with different base disc
 462 radii \bar{r} and gap coefficients η .

463

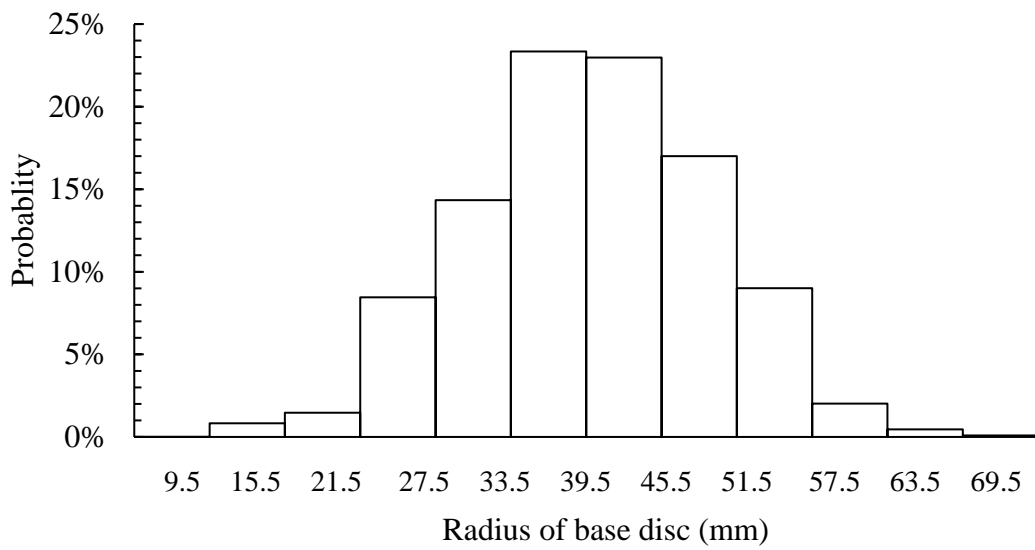
464 **4.6 Mixed asperities**

465 A surface of even asperity facilitates model development and simulation. However, a surface
 466 of mixed asperities often occurs. To account for the mixed asperities, the substrate was
 467 constituted with a group of discs of different radius r_j and gap coefficients η . The schematic is
 468 shown in Figure 15. The two governing parameters r_j and η were assumed to be independent
 469 and, as per Persson et al. [8], follows a normal distribution, $N(\mu, \sigma)$, where μ is the mean and
 470 σ is the standard deviation. The two distribution parameters are determined in terms of the disc
 471 travel distance expected. The distance travelled under the mixed asperities varies significantly,
 472 but, due to the presence of varying collision angles arising from the mixed asperities, is
 473 relatively less than that obtained in the even asperity cases. In order to properly measure the
 474 actual collision angle, a threshold distance of passing over 20 base discs was specified. To
 475 satisfy the distance, we iterated the distributions for the radii and gaps in terms of the initial
 476 velocity, and determined the corresponding distributions as $N(40, 10)$ and $N(20, 6.5)$
 477 respectively. The distribution details are provided in Figure 16 and Figure 17 respectively.



478

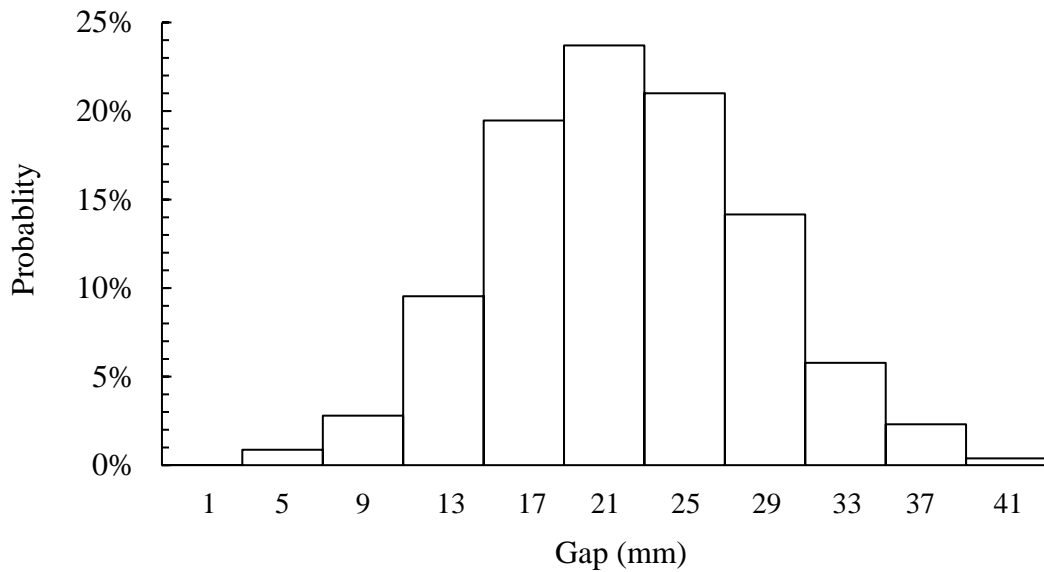
479 Figure 15. The asperity model developed based on mixed surface asperities which vary in the
 480 base discs diameter and gaps.



481

482 Figure 16. The normal distribution of base disc radii used for the model provided on Figure

483 15.



484

485 Figure 17. The normal distribution of base disc gaps used for the model provided on Figure

486 15.

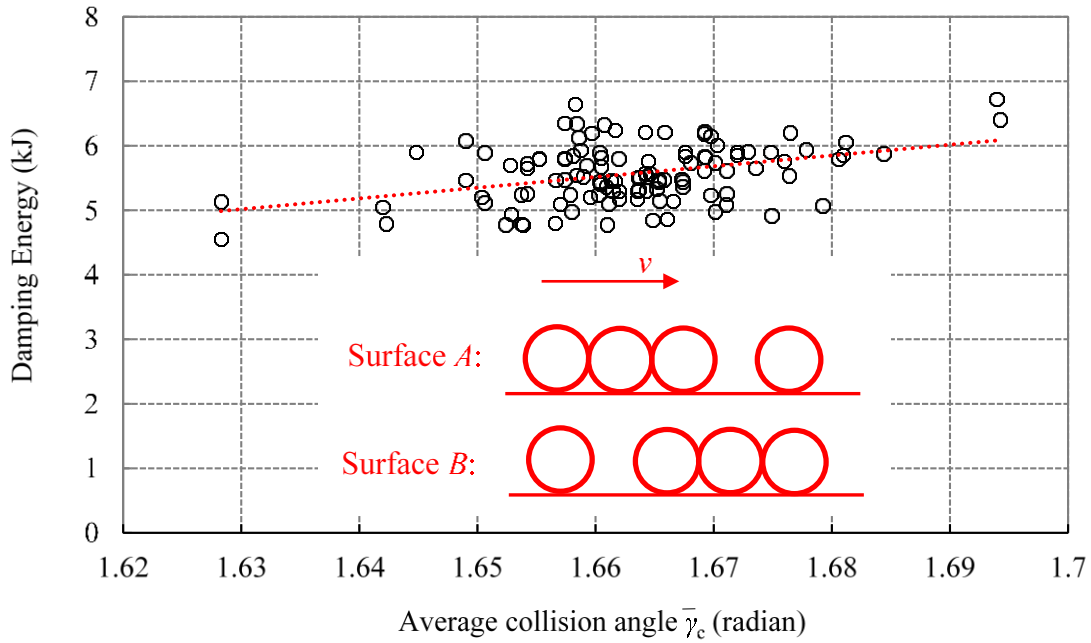
487

488 Additional efforts were made to gauge the actual collision angle. In the case of mixed

489 asperities, the actual collision angle cannot be determined before the disc rest, as opposed to

490 the even asperity case. For example, Figure 15 shows that the moving disc does not contact the
491 base disc j . Therefore the collision angle between the moving disc and the substrate j does not
492 have physical meaning. Also, due to the complexity of the substrate, the moving disc may
493 exhibit some significant jumps depending on its initial velocity. For these reasons, the actual
494 trajectory of the moving disc was gauged to attain the actual collision angles.

495 In order to validate the surface properties of energy dissipation for an actual bumpy
496 surface, a sufficient number of different surfaces where asperities are randomly distributed
497 need to be generated. This collection of substrates can be generated in *PFC2D* by using a
498 random number, called ‘seed’, which governs particles generation. Changing this ‘seed’ value
499 can generate different assemblies of the discs and thus the substrates which we followed to
500 reproduce a collection of surfaces of mixed asperities. We generated a total of 250 sample
501 surfaces and flew a disc, at an initial velocity $v_x^0 = 0.5$ m/s, through each of the surfaces. The
502 relationship between the dissipated energy and collision angle is presented in Figure 18. The
503 dissipated energy occurred at the 15th collision with respect to the actual average collision angle
504 was calculated. At the assigned velocity, the moving disc passed through more than 20 base
505 discs, but the number of the effective collisions as presented in Figure 18 was less, as some
506 base discs, e.g., the j th particle as shown in Figure 15, were of low elevation and not in contact
507 with the moving disc.



508

509 Figure 18. The results of the dissipated energy at the 15th collision versus the actual average
 510 collision angle $\bar{\gamma}^c$ obtained for the disc traveling on the substrate model as specified on Figure
 511 15 where the discs radius and gaps are randomly generated in a total of 250 samples.

512

513 In Figure 18, the average collision angle $\bar{\gamma}^c$ was calculated as the sum of the collision
 514 angles divided by the number of collisions. As can be seen, the dissipated energy increased
 515 with the increase of the average collision angle, which generated a linear distribution. However,
 516 the spread of data suggests a results variation. The variation arises from the varying surfaces
 517 tested, which influences the energy dissipation. For example, surfaces *A* and *B* may exhibit
 518 identical substrate properties, e.g., the same collision angle, average height and height variance,
 519 but differ in sequences of elements (e.g., the location of gap) and therefore yield different
 520 energy dissipation modes. With respect to the energy dissipation, the mode for the disc on the
 521 surface of mixed asperity differed from that on the surface of even asperity. On the even
 522 asperity surface, the kinetic energy was gradually damped at each collision, while on the mixed
 523 asperity surface the kinetic energy was dissipated in a fluctuating pattern, greater or less,

524 depending on the gaps and discs size to collide with. Sometimes significant energy was
525 dissipated completely simply because of collisions with the next relatively larger gap or disc
526 on the surface. These odd asperities often bring up a relatively greater collision angle and those
527 posing the maximum collision angle are worth further examining.

528

529 **4.7 Maximum collision angle**

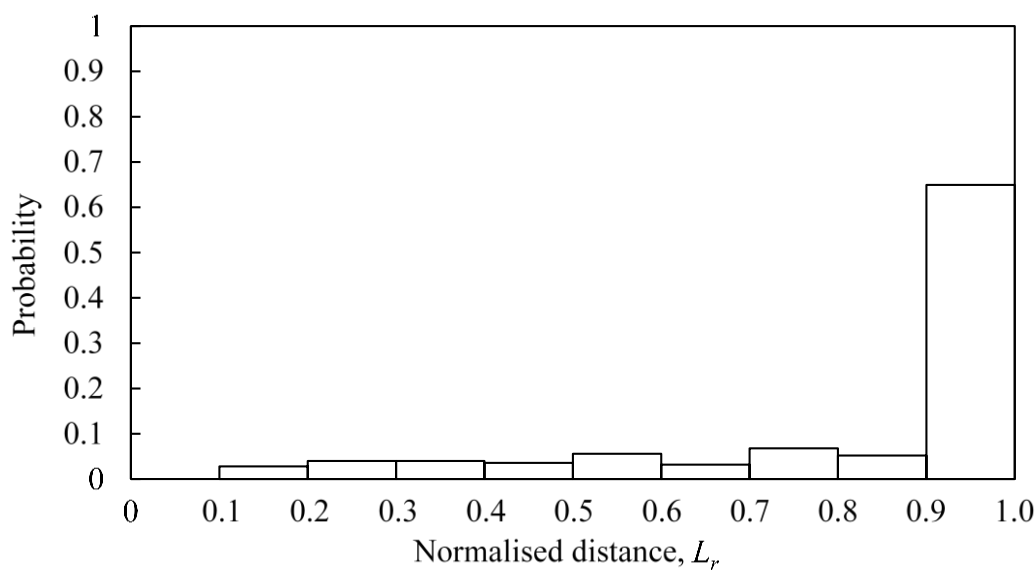
530 Theoretically, the moving disc can rest at any trough on a bumpy surface, but the simulations
531 suggest that the disc often rests at the trough where the maximum collision angle occurs. The
532 probability of the coincidence can be obtained by examining the relationship between the at-
533 rest distance and the location of trough that the maximum collision angle occurs. The location
534 of trough is represented by the normalised distance, L_r , which is expressed as:

$$L_r = \frac{S_{r,\max}}{S_{\text{stop}}}, L_r \in [0,1] \quad (45)$$

535 where $S_{r,\max}$ is the position corresponding to the maximum collision angle, and S_{stop} is the total
536 moving distance. If $L_r = 1$, the position for the maximum collision angle coincides with the
537 total distance. Otherwise, the maximum collision angle occurs before the disc is at rest.

538 Of the 250 surfaces tested, the probability for L_r is plotted in Figure 19. Approximate
539 65% surfaces had the discs rest at the troughs of the maximum collision angle, suggesting
540 occurrences of instant stop. The discs in the remaining tests passed through the troughs of the
541 maximum collision angle and travelled farther. The additional distances the discs travelled was
542 independent on the locations of the troughs of the maximum collision angle, due to the even
543 probability for $L_r = 0$ to 0.9. The probability distribution is explained in terms of at least three
544 factors: *i*) the kinetic energy to overcome the collision angle, *ii*) the locations where the
545 maximum collision angle occur, and *iii*) the initial velocity of the disc. Greatest kinetic energy
546 is required to pass by the trough of the maximum collision angle. This trough prohibits the disc
547 to move farther if the energy fails to meet the threshold required to pass by. The threshold

548 applies to a greater number of discs than those raised by less ‘tough troughs, and therefore
 549 builds to greater occurrences of discs at rest. The kinetic energy has not been dissipated
 550 significantly at the early stage of travel and likely enables the disc to pass over the trough of
 551 the maximum collision angle that occurs. The opposite takes place at the mid- to late stages of
 552 travel where the energy has been dissipated down to a lower level. Meanwhile the initial
 553 velocity should fall into a range so that the kinetic energy is properly loaded and dissipated
 554 over the mixed asperities.

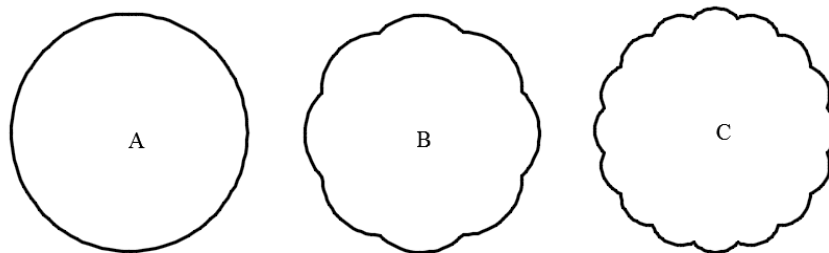


555
 556 Figure 19. The probability for the normalised distance L_r obtained for the disc that travels on
 557 the substrate model as specified on Figure 15 where the discs radius and gaps are randomly
 558 generated in a total of 250 samples.

559
 560 **4.8 Asperity and sub-asperity mixed surface**

561 In sections 4.1–4.7, we have examined the trajectory of the moving disc travelling on an
 562 asperity surface. However, on a real surface, there are sub-asperities affixed over the primary
 563 surface which influences the trajectory and energy loss of the moving disc. To account for the
 564 surface sub-asperities, we constituted a surface mixed with primary and sub-asperities. To
 565 attain the mixed surface, clumps of discs were used. The clump models are provided in Figure

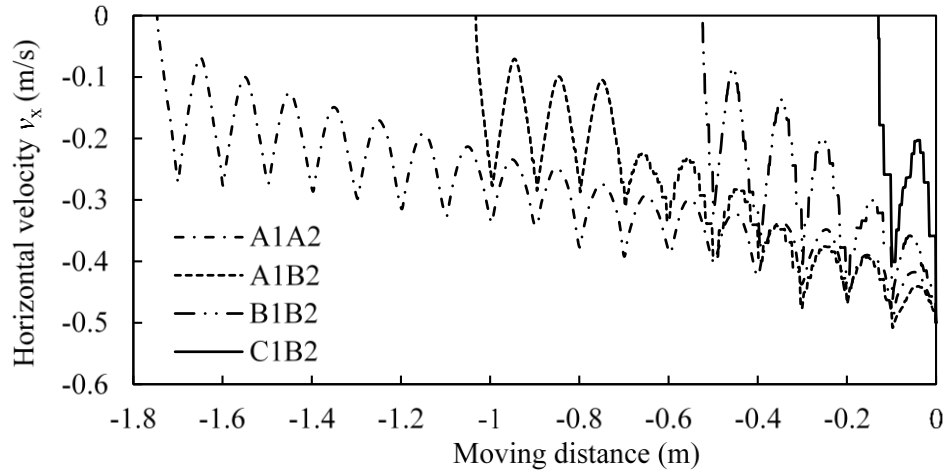
566 20. Clump *A* was spherical. Clumps *B* and *C* exhibited different sub-asperities. The sub-
567 asperities were formed by affixing a set of discs together, each disc sharing a section of the
568 circular perimeter. The equivalent radius of clumps *B* and *C* was equal to the radius of clump
569 *A*. If travelling on the asperity and sub-asperity mixed surface, the moving disc is subjected to
570 greater collisions than on the asperity surface, and the additional collisions are expected to
571 cause greater energy loss in a shorter distance. Similar asperity and sub-asperity mixed surface
572 can occur to the moving disc, which prompts the importance of simulations.



573
574 Figure 20. The clumps used to represent primary and sub-asperities: clump *A* has primary
575 asperity, clump *B* combines primary asperity and 8 equal sub-asperities, and clump *C* combines
576 primary asperity and 16 equal sub-asperities.

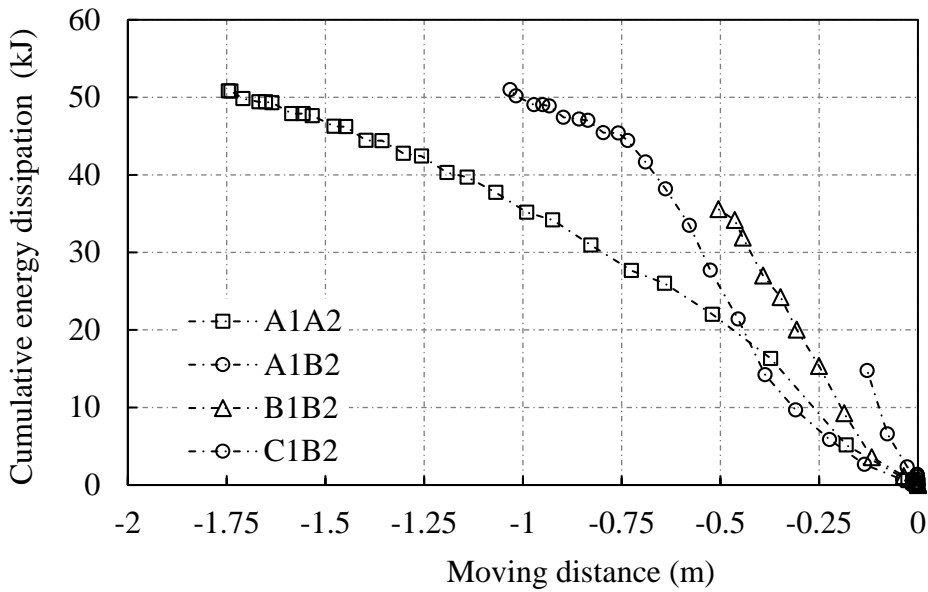
577
578 Clumps *A*, *B* and *C* were paired to reproduce the moving disc and base discs. Use
579 number ‘1’ to denote the moving disc and number ‘2’ to the base discs for the substrate. For
580 example, the combination *A1B2* represents the model of the clump *A*-based disc moving on the
581 clump *B*-based substrate. In simulations, we designed four combinations: *A1A2*, *A1B2*, *B1B2*
582 and *C1B2*, in the order of increasing number of asperities. The moving disc of the last three
583 models was initially placed in the trough of interest, thus enabling a stable start. The properties
584 of the clumps, such as the damping coefficient, density, volume and contact stiffness, remained
585 the same as in the validation case. The moving disc was assigned an initial horizontal velocity
586 of $v_x^0 = 0.5$ m/s. Note that, for a clump of discs, the discs collided eccentrically, leading to a

587 residual rolling velocity. In the simulations, rolling was restricted for the last three models to
 588 create the same condition with the first model. The simulation results are provided in Figure
 589 21. The figure shows the relationship between the horizontal velocity and moving distance
 590 captured for the four models.



591
 592 Figure 21. The results of the horizontal velocity v_x versus the moving distance obtained for the
 593 disc traveling on the substrate model as specified on Figure 1 where the moving and base discs
 594 use clumps defined on Figure 20, the moving disc is assigned an initial velocity $v_x^0 = 0.5$ m/s,
 595 and the damping is $\beta_n = 0.9$.

596
 597 In Figure 21, when the number of the surface sub-asperities increased, the moving disc
 598 travelled a shorter distance. For example, model *C1B2* travelled around one-tenth of the
 599 distance attained by model *A1A2*. It is suggested that the sub-asperity exhibited a significant
 600 effect on the final displacement. At the surface of a primary asperity, the sub-asperities
 601 increased the number of effective collisions. At the same distance, greater energy was
 602 dissipated in model *C1B2* than in the other models of fewer sub-asperities. In addition, the sub-
 603 asperities on the base discs caused a lower collision angle and thus greater energy dissipation.



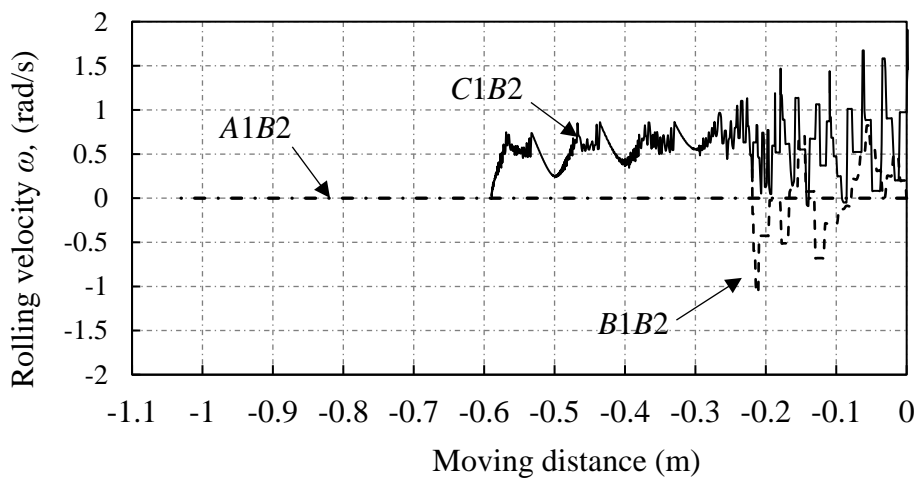
604

605 Figure 22. The results of the cumulative energy dissipation versus the moving distance obtained
 606 for the disc traveling on the substrate model as specified on Figure 1 where the moving and
 607 base discs use clumps defined on Figure 20, the moving disc is assigned an initial velocity v_x^0
 608 $=0.5$ m/s, and the damping is $\beta_n = 0.9$.

609

610 The simulations performed in this study suggested that surface asperity-induced friction
 611 can be considered as a larger number of individual collisions, and that these collisions cause
 612 the dissipation of kinetic energy. One of the major differences between the two conceptions
 613 (the friction vs. the collision) is that the collision-induced energy loss is velocity-dependent, as
 614 shown in Figure 8, while the friction conception assumes that the friction force is independent
 615 on the velocity of the moving object. The collision conception agrees with earlier studies
 616 performed at an atomic level [19,30-31]. In these studies, the friction force experienced
 617 velocity-dependent viscous behaviour. Research on atomic- or molecular-scale friction [30,32-
 618 33] also identified a sawtooth friction behaviour at the nanoscale, which is in further support
 619 of the current simulation results. This means that the surface of interest contains a large number
 620 of asperities and sub-asperities, and that the collisions at individual asperities and sub-asperities
 621 cause the surface friction attained at the macroscale.

622 Where the sub-asperity surface occurs, the moving disc rotates due to the eccentric force
623 acting on the disc. In this section, the rotation of the moving disc is examined. We designed
624 three models: *A1B2*, *B1B2* and *C1B2*, where the moving disc was assigned clumps *A*, *B* and *C*
625 respectively, and the substrate surface used clump *B* throughout. The relationship between the
626 rolling velocity and the sliding distance is plotted in Figure 23. Define the anti-clockwise
627 rolling to be positive. The moving disc in model *C1B2* travelled a longer distance than the
628 distance obtained in model *B1B2*, which was different from the results if the rolling was
629 restricted. As shown in Figure 21, the moving disc in model *B1B2* travelled much farther than
630 the disc in model *C1B2*. This can be explained from the perspective of a collision impact. For
631 model *B1B2*, the collision sometimes induced a negative angular velocity, and rotation at this
632 direction prohibited its movement at the surface. The translational velocity at the contact point
633 was therefore reduced, and the moving disc was finally at rest.



634
635 Figure 23. The results of the rolling velocity versus the moving distance obtained for the disc
636 traveling on the substrate model as specified on Figure 1 where the moving and base discs use
637 clumps defined on Figure 20, the moving disc is assigned an initial velocity $v_x^0 = 0.5$ m/s, and
638 the damping is $\beta_n = 0.9$.
639

640 **5. Conclusions**

641 This paper models the trajectory of a disc moving on a bumpy surface and examines the energy
642 dissipation at collisions. An analytical model based on a single-contact collision conception
643 was developed. The model was able to capture the trajectory of the moving disc. The analytical
644 model was established and applied to validate a DEM model. The DEM model was applied to
645 examine the effects of important surface asperity properties on the kinetic behaviour of the
646 moving disc. The properties included the material damping, average asperity height, height
647 variance, gaps, collision angle and sub-asperities. The energy loss associated with the property
648 characteristics was also examined. The simulations arrived at the following conclusions.

649 Upon contacting, the moving disc bounced on an asperity surface several times and
650 then slide on the same asperity surface. The first collision between the moving disc and the
651 base disc consumed a major portion of the energy, while the energy dissipated at other bounces
652 was marginal. The actual collision angle was in a monotonic relationship with the maximum
653 distance of the moving disc. The collision angle outweighed the other surface properties, such
654 as the average asperity height and surface-height variance, in respect to characterising surface
655 roughness.

656 The surface sub-asperities accelerated the loss of kinetic energy. If the sub-asperities
657 were of high density, the surface can dissipate a high level of kinetic energy. Sub-asperity-
658 induced rolling decreased translational velocity and thus restricted the motion of the disc. The
659 energy dissipation of the moving disc was positively proportional to the velocity of the disc.
660 The conception of asperity-induced energy loss reflected the effects of collisions and provided
661 an understanding of surface friction at microscale.

662

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668

669 **Notations**

670	D_j^t	relative distance between the moving disc and base disc at time step t
671	E_m	system mechanical energy
672	E_t	total energy
673	E_k	kinetic energy
674	E_β	dashpot energy loss
675	F_n^d, F_s^d	normal and dashpot force
676	F_n^h, F_s^h	nonlinear normal and shear contact force
677	g	gravity acceleration
678	k_n	normal stiffness
679	L_r	relative distance of the collision angle
680	m_1, m_2	mass of the bodies 1 and 2
681	m_c	mass of the system
682	r	radius of the moving disc
683	r_j	radius of base disc j
684	\bar{r}	average radius of the base disc
685	$S_{\gamma, \max}$	distance where the maximum collision angle occurs
686	S_{stop}	total moving distance
687	t	time step

688	Δt ,	time step increment
689	Δt_0	time step increment at bounce
690	v	velocity
691	v_n	normal velocity before collision
692	v_s	tangential velocity before collision
693	$v_{n,r}$	normal velocity after collision
694	x^t, y^t	centre position of the moving disc at time step t
695	U	gravity potential
696	α_n	restitution coefficient
697	β_n	damping coefficient
698	γ	contact angle
699	γ^c	collision angle
700	$\bar{\gamma}^c$	average collision angle
701	$\dot{\delta}_n$	relative normal translational velocity
702	ω	angular velocity
703	θ	rotation angle
704	η	disc gap coefficient
705	μ	mean of normal distribution
706	σ	standard deviation of normal distribution

707

708 **Ethical Statement**

709 Disclosure of potential conflicts of interest: The authors declare that they have no conflict of
710 interest.

711

712 Research involving Human Participants and/or Animals: This article does not contain any
713 studies with human participants or animals performed by any of the authors.

714

715 Informed consent: Informed consent was obtained from all individual participants included in
716 the study.

717

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