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In many biomechanical applications, the collision of microscopic particles, under the influence of interparticle near-field forces, is an important step in an overall biophysical process. In this communication, expressions are derived relating the impact velocity needed for two small-scale particles to adhere as a function of particle sizes, material hardnesses, densities and interparticle near-field character.

1. Introduction

There are numerous applications in biomechanics where one step in an overall series of events is the collision and possible adhesion of small-scale particles (1–100 microns), under the influence of interparticle near-fields. For example, in study of atherosclerotic plaque growth, a predominant school of thought attributes the inception of atherosclerotic plaque growth to a relatively high concentration of microscale suspensions (low-density lipoprotein (LDL) particles) in the blood. Atherosclerotic plaque formation involves: (a) adhesion of monocytes (essentially larger suspensions) to the endothelial surface, which is controlled by the adhesion molecules stimulated by the excess LDL, oxygen content, and the intensity of blood flow; (b) penetration of the monocytes into the intima and subsequent tissue inflammation; and (c) rupture of the plaque accompanied by some degree of thrombus formation or even subsequent occlusive thrombosis. For an overall general introduction [Libby 2001a; 2001b; Libby et al. 2002; Libby and Aikawa 2002]. For extensive analyses addressing modeling and numerical procedures, see [Jou and Berger 1998; Berger and Jou 2000; Kaazempur-Mofrad and Ethier 2001; 2003; 2004; Younis et al. 2004; Stroud et al. 2002; Stroud et al. 2000]. For experimentally-oriented physiological flow studies of atherosclerotic carotid bifurcations and related systems, see [Bale-Glickman et al. 2003b; 2003a]. Notably, Bale-Glickman et al. [2003b; 2003a] have constructed flow models which replicate the lumen of plaques excised intact from patients with severe atherosclerosis, which have shown that the complex internal geometry of the diseased artery, combined with the pulsatile input flows, gives exceedingly complex flow patterns. They have shown that the flows are highly three-dimensional and chaotic, with details varying from cycle to cycle. In particular, the vorticity and streamline maps confirm the highly complex and three-dimensional nature of the flow. Despite the large body of work on the subject, the mechanisms in the initial stages of the disease involving the interparticle mechanics have not been extensively studied, although some simple semianalytical qualitative studies have been carried out recently [Zohdi et al. 2004; 2005c], focusing on particle-wall adhesion. Furthermore, particle-to-particle adhesion can play a significant role in the behavior of a thrombus, comprised of agglomerations of particles, ejected by a plaque rupture which can occur in later stages of the disease. The behavior, in

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particular the fragmentation of such a particulate-laden thrombus, as it moves downstream, is critical in determining the chances for stroke.

Another biological process where particle interaction and aggregation is important is the formation of certain types of kidney stones, which start as an agglomeration *seed* of particulate materials, for example combinations of calcium oxalate monohydrate, calcium oxalate dihydrate, uric acid, struvite or cystine [Kim 1982; Kahn et al. 1983; 1993; Kahn and Hackett 1984; Coleman and Saunders 1993; Pittomvils et al. 1994; Zohdi and Szeri 2005]. The mentioned examples are only a few of the many biomechanical applications, where the collision of microscale particles, under the influence of near-field forces, which play a considerable role at these scales, form an important step in an overall biophysical process. The objective of this communication is to shed light on some fundamental aspects of collision and adhesion of such particles, which are typically between 1–100 microns. In particular, we isolate and focus on a single aspect of particle adhesion, namely the determination of the impact velocity needed for two small-scale particles to adhere as a function of particle size, material hardness, density and interparticle near-field character. (We neglect fluid effects. This analysis is not meant to be a comprehensive or complete picture of the combined fluid-particle interaction problem.)

2. Analysis of a particle collision

We consider the scenario of two impacting particles, isolated from the group in Figure 1. The linear momentum exchange between two identical particles, i and j, each traveling with an initial velocity of v_o is opposite directions ($v_i(0) = v_o = -v_j(0)$). For the pair, along the line of impact

$$m_i v_i(0) + m_j v_j(0) = m_i v_i(\delta t) + m_j v_j(\delta t) = 0, \tag{1}$$

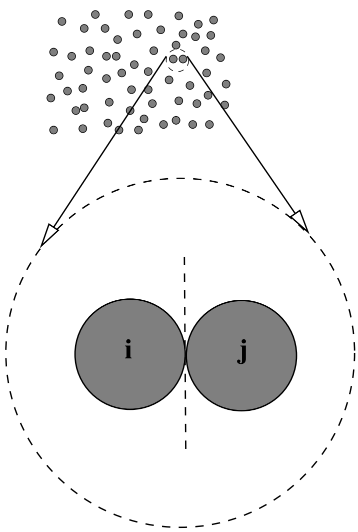

Figure 1. Isolating two particles undergoing a collision.

and for an individual

$$m_i v_i(0) + \underbrace{\int_0^{\delta t} I\,dt}_{\overline{I}\delta t} = m_i v_i(\delta t), \tag{2}$$

where $\overline{I}$ is the average impulse acting between particles. The impulse is

$$\overline{I} = \frac{m_i v_i(\delta t) - m_i v_i(0)}{\delta t}. \tag{3}$$

Recall the classical coefficient of restitution, defined as

$$e = \frac{v_j(\delta t) - v_i(\delta t)}{v_i(0) - v_j(0)}, \tag{4}$$

where $e = 1$ is a perfectly elastic (energy preserving) impact and where $e = 0$ is a perfectly plastic (full adhesion) impact.[1] The phenomenological parameter e depends on the severity of the impact velocity, and, implicitly, the pressure in the contact zone. See [Goldsmith 2001] for extensive experimental data or [Johnson 1985] for detailed analytical treatments. For the applications considered, involving particle bonding leading to agglomeration in such particulate media, it is advantageous to construct a coefficient of restitution relations that are pressure based, which idealize bonding as a limiting case as $e \to 0$. For example, empirically motivated relations involving the material's Vicker's hardness to determine whether two particles bond can be found in [Nesterenko et al. 1994]. See [Meyers 1994; Nesterenko 2001] for reviews on bonding criteria.

Specifically, the phenomenological material parameter e depends on $\overline{I}$, and thus implicitly on the impact velocity. An empirically derived condition for whether two surfaces will bond is if the magnitude of the surface pressure ($|P|$) exceeds or attains twice the Vicker's hardness $2H$, that is, if $|P| \geq 2H$. See [Meyers 1994; Nesterenko et al. 1994; 2001] for reviews.[2] We construct an ad hoc model for bonding by approximating the surface pressure as

$$|P| \approx \frac{|\overline{I}|}{a_c},$$

where a_c represents the apparent contact area. Clearly if $e = 1$, the impact is purely elastic with no adhesion, and thus there is no loss in energy, while if $e = 0$ there is a maximum loss in energy. Consistent with Nesterenko's experimental observations on bonding [Nesterenko et al. 1994; Nesterenko 2001], we shall follow the assumption that if the pressure exceeds twice the Vicker's hardness, the two surfaces will bond. Furthermore, we approximate e by a linear scaling with the pressure-to-hardness ratio [Zohdi 460]. Accordingly, a relatively simple constitutive relation for e, incorporating the pressure criteria ($|P| \geq 2H$), is

$$e = \frac{v_j(\delta t) - v_i(\delta t)}{v_i(0) - v_j(0)} = \max\left(\left(1 - \frac{|P|}{2H}\right), 0\right) = \max\left(\left(1 - \frac{m_i|v_i(\delta t) - v_i(0)|}{2Ha_c\delta t}\right), 0\right), \tag{5}$$

[1] The use of this relation for *charged* particles is valid, provided that we ignore the near-field contributions from particles other than the isolated pair. More general relations, which include the contributions from surrounding particles, can be found in [Zohdi 2005b; 2005a].

[2] The Vicker's hardness is correlated to the yield point for plastic deformation of the material by $H \approx 3\sigma_y$.

where we have used Equation (1), and where a_c is the contact area between two particles. We assume that the contact area is proportional to the cross-sectional area of the particle, $a_c \propto \pi b^2$, thus we can approximate a (proportional) contact area relationship of the form $a_c = k_1 \pi b^2$, where $0 \le k_1 \le 1$ and b is the particle radius. By setting $e = 0$ in Equation (5), we obtain

$$|v_i(\delta t) - v_i(0)| \ge \frac{3k_1 \delta t H}{2\rho b}, \tag{6}$$

where $m_i = \rho \frac{4}{3}\pi b^3$, ρ being the particle mass density. If we have identical adhering ($e = 0$) particles ($v_o = v_i(0) = -v_j(0)$), then $v_i(\delta t) = 0$. Also, the impact time, δt, is proportional to the size of the particles and the impact velocity, thus we approximate $\delta t = k_2 b / v_o$ (k_2 is dimensionless), and we have[3]

$$\frac{2v_o^2 \rho}{3Hk_1k_2} \ge 1 \Rightarrow v_o \ge \sqrt{\frac{3Hk_1k_2}{2\rho}} = k_3\sqrt{\frac{H}{\rho}}. \tag{7}$$

In other words, the critical velocity for two particles to adhere, based solely on mechanical pressure, is directly proportional to the material's hardness and inversely proportional to its density. Thus, hard, low-density, particles would require extremely high velocities in order to adhere.

3. Impact with near-fields present

Now consider the case where interparticle near-field (for example, electrostatic forces, van Der Waals, etc.) interaction is present. As before, for the pair, along the line of impact, we have

$$m_i v_i(0) + m_j v_j(0) = m_i v_i(\delta t) + m_j v_j(\delta t) = 0, \tag{8}$$

however, for an individual we have

$$m_i v_i(0) + \underbrace{\int_0^{\delta t} I\, dt}_{\overline{I}\delta t} + \underbrace{\int_0^{\delta t} E\, dt}_{\overline{E}\delta t} = m_i v_i(\delta t), \tag{9}$$

where $\overline{I}$ is the average impulse acting between the particles due to contact, and where $\overline{E}$ is the average impulse acting between the particles due to interparticle near-field interaction. The impulse is

$$\overline{I} = \frac{m_i v_i(\delta t) - m_i v_i(0)}{\delta t} - \overline{E}. \tag{10}$$

As before, we set $e = 0$ in Equation (5), using the same relations as before, and we now obtain ($v_o \stackrel{\text{def}}{=} v(0)$)

$$|P| = \frac{|\overline{I}|}{a_c} = \frac{1}{a_c}|-\overline{E} - \frac{mv_o}{\delta t}| \ge 2H. \tag{11}$$

Case 1: If the near-field is attractive between particles ($\overline{E} \ge 0$), we obtain

$$v_o \ge \left(2Ha_c - |\overline{E}|\right)\frac{\delta t}{m}. \tag{12}$$

[3] [Johnson 1985] for more detailed treatments of impact duration.

Case 2: If the near-field is repulsive between particles ($\overline{E} \leq 0$) and if $|\frac{mv_o}{\delta t}| \geq |\overline{E}|$, we obtain

$$v_o \geq \left(2Ha_c + |\overline{E}|\right) \frac{\delta t}{m}. \tag{13}$$

If the near-field is repulsive between particles ($\overline{E} \leq 0$) and if $|\frac{mv_o}{\delta t}| \leq |\overline{E}|$, we obtain *no adhesion.* If we utilize the previous assumptions in the "E-free" case,

(a) $a_c = k_1 \pi b^2$,

(b) $m_i = m_j = m = \rho \frac{4}{3} \pi b^3$ and

(c) $\delta t = k_2 b / v_o$,

the two cases become:

$$\textbf{Case 1}: \quad v_o^2 \geq \frac{3Hk_1k_2}{2\rho} - \underbrace{|\overline{E}| \frac{3k_2}{4\rho\pi b^2}}_{\geq 0} \tag{14}$$

and

$$\textbf{Case 2}: \quad v_o^2 \geq \frac{3Hk_1k_2}{2\rho} + \underbrace{|\overline{E}| \frac{3k_2}{4\rho\pi b^2}}_{\geq 0}. \tag{15}$$

In other words, the critical velocity for two particles to adhere is increased if the near-field is repulsive and decreased if the near-field is attractive. Essentially, the introduction of a near-field produces results which are deviations from the E-free term that first appeared in Equation (7):

$$\frac{3Hk_1k_2}{2\rho}.$$

Now consider $\overline{E}$ as a function of the separation distance, and hence b at the moment of contact. For example, consider a simple relation

$$\overline{E}(|r_i - r_j|) = \alpha |r_i - r_j|^{-\beta}, \tag{16}$$

where r_i is the position of the center of particle i, r_j is the position of the center of particle j and $0 < \beta < \infty$ and $-\infty < \alpha < \infty$. When $\alpha > 0$, then the resulting force between the particles is attractive, while if $\alpha < 0$, then the resulting force is repulsive. For direct central impact, at contact, this collapses to ($|r_i - r_j| = 2b$)

$$\overline{E}(b) = \alpha(2b)^{-\beta}. \tag{17}$$

We introduce the following (per unit mass^2) decomposition for the force imparted on particle i by particle j and vice-versa:

$$\alpha = \overline{\alpha} m_i m_j, \tag{18}$$

where $\overline{\alpha}$ has units of [Newton (meter)$^\beta$]$/kg^2$. The substitution of this near-field form into the equations for the two cases yields ($m_i = m_j = m$):

$$\textbf{Case 1}: \quad v_o^2 \geq \frac{3Hk_1k_2}{2\rho} - \underbrace{b^{(6-\beta)} \frac{4|\overline{\alpha}|\rho\pi k_2 2^{-\beta}}{3}}_{\geq 0} \tag{19}$$

and

$$\textbf{Case 2}: \quad v_o^2 \geq \frac{3Hk_1k_2}{2\rho} + \underbrace{b^{(6-\beta)}\,\frac{4|\overline{\alpha}|\rho\pi k_2 2^{-\beta}}{3}}_{\geq 0}. \tag{20}$$

Generally, if $\beta < 6$ then the critical velocity needed for adhesion decreases with increasing particle size, while, if the near-field is repulsive, the critical velocity increases with increasing particle size. For example, if $\beta = 2$, (similar to an electrostatic Coloumb-type character), then the critical velocity needed for adhesion decreases with increasing particle size, while the critical velocity increases with increasing particle size, if the near-field is repulsive. However, if $\beta \geq 6$, then the critical velocity needed for adhesion increases with increasing particle size, while the critical velocity decreases with increasing particle size, if the near-field is repulsive.

4. Summary

In summary, the objective of this communication was to investigate some fundamental aspects of the collision and adhesion of microscopic particles, such as those frequently encountered in biological applications. Basic relations were derived relating the impact velocity needed for two particles to adhere as a function of fundamental quantities such as the particle sizes, material hardnesses, densities and interparticle near-field character. The assumptions leading to the derivation of primary results, Equations (19) and (20), are easily replaceable with more accurate descriptions, if and when they become available; however, the overall structure can stay, more or less, intact. For example, one central assumption in the derivation of Equations (19) and (20) was the representation of the *charge per unit mass* (Equation (18)). This can be easily replaced with a *per surface area* relation or some other charge/particle-size metric, for example $\alpha_{ij} = f(b_i, b_j)$, where $f(b_i, b_j)$ is a function that correlates the particle sizes to the level of *near-field charge*.

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