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Short Communication

Some important aspects of modelling clay platelet interactions using DEM

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ABSTRACT

The discrete element method (DEM) is a popular tool for simulating soils, however it has rarely been used for modelling clays. This is despite the behaviour of clays being much less well understood compared to sands. This paper aims to increase the use of DEM to investigate clays by highlighting some important issues concerning the implementation of particle interactions to any model. When using spheres as the elementary unit in DEM, it is shown how special attention is needed to ensure repeatable interactions between platelets, and also how the geometry of the platelets affect both the normal and tangential interactions.

1. Introduction

The discrete element method (DEM) is a well-known numerical tool for modelling and investigating the microscopic behaviour of granular materials, particularly coarse-grained soils. However, attempts to uncover the microscale mechanisms governing the behaviour of clays using DEM have been few and far between due to several issues presented by clay particles. Notably, clay particles possess shapes which are inefficient to model (compared to bulky and approximately spherical sand grains), and exhibit complex interactions requiring specialised contact laws. The majority of DEM software and simulations are concerned with the interactions between spheres and (planar) walls, which can be calculated efficiently. Simulating non-spherical particles in DEM is therefore typically achieved by using bonded or rigidly fixed groups of spheres; although it is also possible to model certain other convex shapes natively without the use of spheres.

Previous attempts at modelling clay particles discretely can be grouped accordingly into those using rigid groups of spheres (or disks) [1–4], and those using non-spherical shapes directly: e.g. using rods (2D) [5], blocks [6], disks [7] and ellipsoids [8]. Although visually appealing, using non-spherical shapes natively to model clay platelets generally means only one contact may exist between two platelets, which has several disadvantages. Firstly, it is difficult to implement a single contact law which can take into account the relative positions and orientations of two interacting platelets. Secondly, it does not permit categorically different interactions to be defined between different parts of the platelets (e.g., between edges and faces etc.). Thirdly, contact detection algorithms for non-spherical particles are more computationally expensive compared to spheres, so any improvement in computational time does not scale directly with the reduced number of discrete elements and contacts. For these reasons, it can be argued that using the sphere-based approach to model platelets currently remains the most viable option; and is also used by others studying colloidal platelets in non-geotechnical contexts [9]. Due to the shape of clay platelets (the high aspect ratio, and small thickness), this approach requires a large number of elementary spheres to model even a modest number of platelets. Simultaneously, due to the size of clay platelets (generally $<1\ \mu m$), a large number of platelets need to be modelled to represent even the smallest laboratory sample. This has traditionally restricted the use of DEM in simulating clays, however, increases in computational power with each passing year allows larger and more realistic DEM simulations to be performed.

In addition to accurately capturing particle shape, it is essential for any discrete simulation of clay to include realistic platelet interactions. Due to the very small clay particle size, the interactions between clay particles are controlled by electrical/chemical forces rather than purely mechanical forces. This typically requires specialised contact laws to be developed, another factor which has hindered the modelling of clay particles. Interactions between identical clay particles can be either attractive or repulsive at various distances, and depend highly on the clay mineral and environmental conditions. Additionally, for plate-like particles such as kaolinite, interactions between the 'edges' and/or 'faces' can be highly dissimilar. This phenomenon can be captured easily when using platelets made of spheres, by classifying 'edge' spheres and 'face' spheres separately, and using different contact laws depending on which constituent spheres are in contact (the various possible combinations of attractive/repulsive forces between both edges and faces leads to a range of different reported particle 'fabrics'). It is the purpose of

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this short paper to highlight some important considerations for ensuring realistic and repeatable particle interactions when modelling platelets using spheres. The discussion will focus on 'face-to-face' interactions between platelets, but applies equally to edge-to-face and edge-to-edge interactions. The DEM software used in this study is PFC 3D [10], but the principles will apply to DEM models using any software.

2. DEM implementation

When using the sphere method to model a clay such as kaolinite, individual clay platelets are modelled using flat, rigid arrays of spheres, such as that shown in Fig. 1(a). These platelets can rotate and translate as single entities, and no internal interactions occur between the spheres within any single platelet. In any DEM simulation, the user defines the contact law(s) used to calculate the force(s) acting between any two interacting bodies. This means that when modelling platelets (or indeed any particle shape) using rigid groups of spheres, many individual contacts may exist between the various possible pairs of spheres in two different platelets. For instance, for two platelets in 'face-to-face' contact, such as those shown in Fig. 1(b), many hundreds or thousands of individual sphere-to-sphere contacts may exist. Hence, the overall face-to-face interaction between two parallel platelets will depend on the individual contact law between constituent spheres, as well as the number of contacts (which in turn depends on the platelets' relative positions and orientations).

It is important to note that any contact law acting between spheres must therefore be calibrated in order to achieve the desired *platelet-to-platelet* interaction. In some of the previous examples of modelling clay platelets in DEM, only the sphere-to-sphere contact laws were given, which are not indicative of the actual platelet-to-platelet interactions.

To illustrate this point, consider Fig. 2 which shows a simplified case of two parallel platelets. In part (i), one can reasonably infer that the

a

b

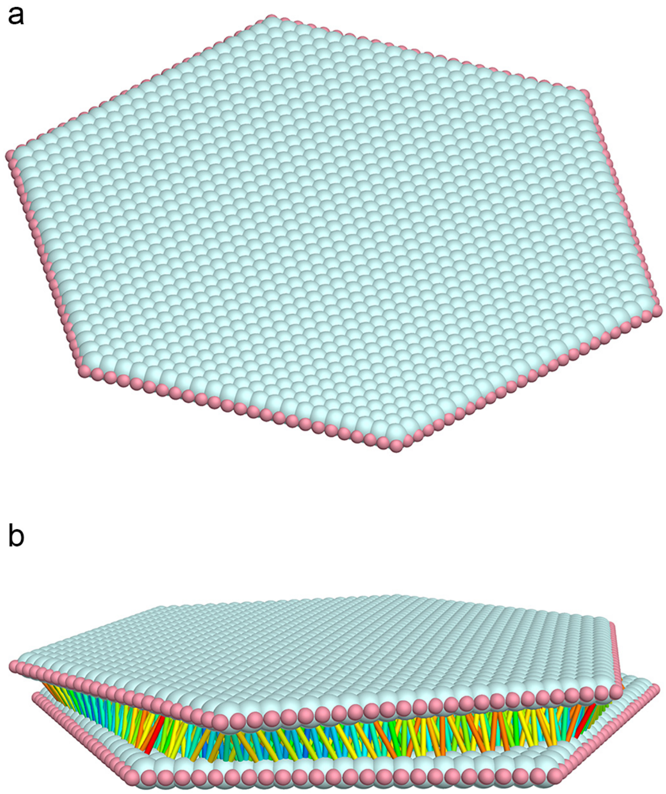

Fig. 1. Clay platelet constructed from spheres (a); multiple sphere-to-sphere contacts for single platelet-to-platelet contact (b).

macroscopic platelet-to-platelet normal interaction would correlate directly with the sphere-to-sphere interactions; however, in (ii) the net normal platelet interaction would be stronger, due to more micro contacts, and would involve smaller platelet separations.

3. Normal platelet interactions

For any large-scale DEM model, it is important that the specified platelet interactions are actually achieved and are repeatable. Much of the previous work modelling platelets using spheres [1–3] used regular, lattice-like particle spacing, as shown in Fig. 1, however this has significant implications regarding the repeatability of the platelet interactions. For example, considering parallel, face-to-face interaction—the net platelet normal force measured as a function of separation will highly depend on the platelets' initial approach and whether the spheres interlock. This was illustrated in Fig. 2, where the 2 schemes will exhibit significantly different macroscopic interactions. One may reasonably assume that under no constraints, two approaching platelets will naturally arrive in the 'interlocked' state as per (ii) in Fig. 2. Firstly, this emphasises the need to calibrate the sphere-to-sphere contact laws to achieve a given platelet interaction, especially given that clay platelets interact at 'long-range' without physically touching, and any interlocking directly affects the observed surface separation (and gives the possibility of negative separation which is unphysical). Of greater importance is that for hexagonally-spaced spheres the net platelet interactions will highly depend on whether the hexagonal lattices are aligned. These issues can be mitigated (but not removed) by increasing the density of spheres in the platelets.

To avoid these issues it is necessary (in the case of parallel platelets for example) that a consistent number of sphere-to-sphere contacts are formed per unit area of contact. This is easily achieved by giving each sphere a random internal displacement on the plane of the platelet (in addition to the high number of spheres in each platelet), as depicted in Fig. 3. Having a high density of spheres (so that they overlap each other) and randomly displacing them on the plane removes the regularity, and prevents the platelet as a whole from being able to penetrate into the voids of the opposing platelet. Although absent in past DEM models [1–3], a similar technique has occasionally been used by others modelling similar particles [4,9], although in those cases the platelets' motion was constrained and/or it was not sufficient to address the above issues. In the case here (Fig. 3), the spheres are given a (uniform) random translation within a square of width (0.4 x l), where l is the lattice spacing (the value 0.4 was chosen empirically to sufficiently remove the lattice).

To demonstrate the importance of removing the regular spacing, consider two platelets positioned as shown in Fig. 4(a). The larger platelet (left) is fixed and cannot move/rotate. The smaller platelet (right) is driven towards the larger platelet, either with a fixed velocity or via a force applied in the x-direction. During this strain- or load-controlled movement, the platelets remain parallel, but the smaller platelet is free to translate along the y,z axes, and to rotate about the x axis. The platelets are 0.04 μm thick, and have maximum diameters of 2, 1 μm, and consist of 5219, 1409 spheres.

The same contact law is used for *all* sphere-to-sphere contacts. In this case, the contact law shown in Fig. 4(b) is used, which consists of repulsion at large separations, as the spheres come in to range and begin to approach each other, followed by attraction at medium separation, and then stiff repulsion at small separations. This broadly represents the behaviour between two identically charged platelets in the presence of an electrolyte [11], implicitly accounting for the various electrical/chemical forces. However, it must be emphasised that any contact law may be used as seen fit, it is the purpose here only to demonstrate how to implement any chosen interaction (the analysis here applies equally even using a simple linear spring contact model).

Fig. 5 shows the results of driving the two platelets together at different rotations about the x axis (each plot shows 12 curves, with 15°

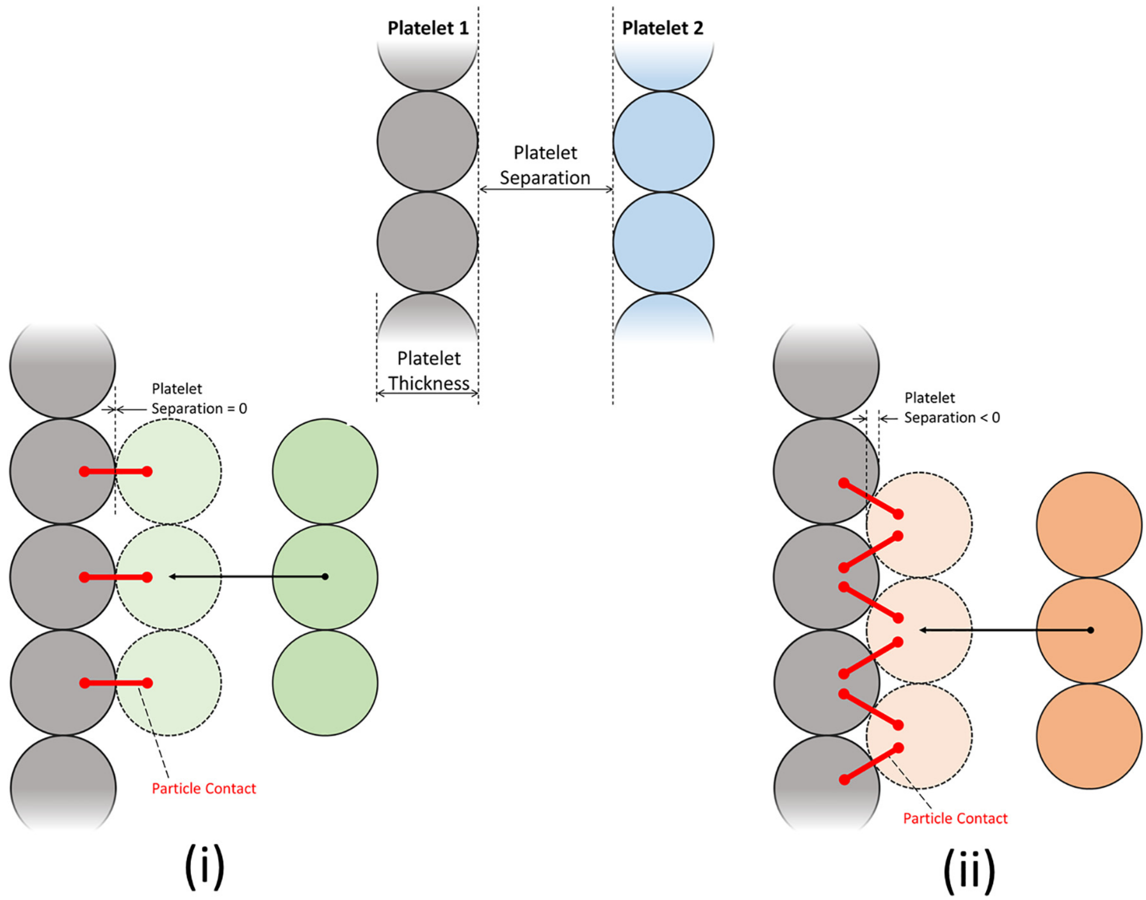

Fig. 2. Diagrams showing: separation measured between parallel platelets (top); close approach with fewest contacts (i); close approach with maximum contacts and interlocking (ii).

rotational increments). Fig. 5(a) shows the results using platelets with a regular, lattice arrangement of spheres, as shown in Fig. 1(a). Fig. 5 (b) gives the results using platelets with random internal displacement of the spheres, and corresponds to the platelet shown in Fig. 3. Clearly only with the internal displacements are the interactions between platelets repeatable, despite the contact law being identical in both cases. This is essential in order to achieve any particular desired *platelet-to-platelet* interaction, such as that shown in Fig. 5(b); where the

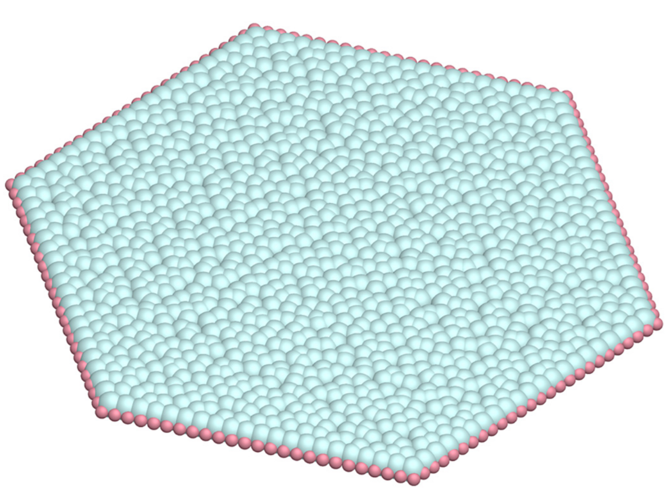

Fig. 3. Platelet made of spheres with random internal displacements.

peak repulsive/attractive forces, and the separation at which the normal force is zero (0.002 μm), are all clearly defined specific values.

4. Tangential platelet interactions

The other important aspect of any platelet-to-platelet interaction (e.g. face-to-face) is the tangential behaviour. There is a lack of available data compared to normal interactions; however, for two platelets being sheared over one another it seems reasonable to assume a linear/sublinear increase in tangential force with displacement, followed by a steady-state value as the particles being to slide (although again the actual platelet interaction assumed here is immaterial).

In previous attempts to simulate platelets, a variety of approaches have been used to account for tangential contact behaviour. In the work using the sphere method to model platelets, *sphere-to-sphere* contacts were usually given a linear elastic tangential stiffness, either with [3,4] or without [1,2] imposing a frictional limit (μ) on the shear force. In all cases, no demonstration or discussion of the *platelet-to-platelet* tangential behaviour was given. In the work using non-spherical shapes directly, in some cases a linear elastic model was used with a limiting coefficient of friction [6,12]; whilst in other models no mention is made of any tangential stiffness or inter-platelet friction used [7,8]. Thus it has often been unclear what actual tangential behaviour occurred between particles.

For any two platelets being sheared, the overall tangential response depends not only on the tangential sphere-to-sphere contact law, but also the normal contract law and the platelet geometry. It is essential therefore that the tangential sphere-to-sphere contact law is calibrated in order to achieve the desired tangential behaviour between platelets, particularly the inter-platelet coefficient of friction.

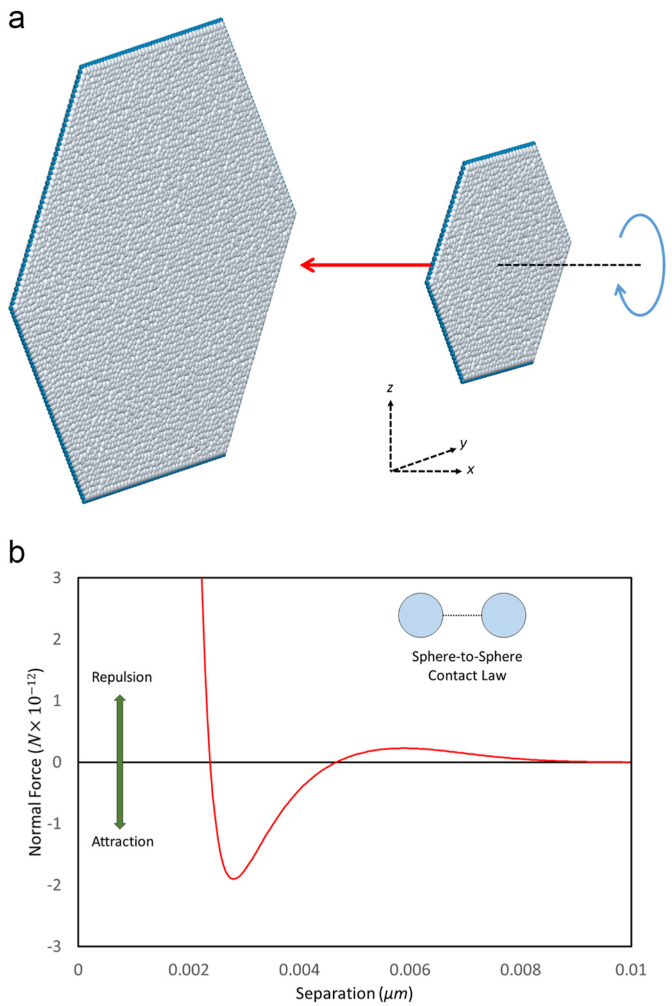

Fig. 4. Image of 2 parallel platelets being driven together (a); normal contact law used between spheres (b).

Considering face-to-face interactions again, the shear force as a function of shear displacement can be measured by shearing one platelet over another as shown in Fig. 6(a), using either strain- or load-control. Shearing the same platelets under increasing normal loads and taking the maximum tangential shear force allows the inter-platelet coefficient of friction to be obtained, for example as shown in Fig. 6(b). This figure shows the shear strength envelopes for two cases: with *no tangential contact law* between spheres; and with a simple linear tangential stiffness. With no tangential stiffness, only normal interactions occurs between the spheres, as illustrated in Fig. 7(a). The resistance to shearing arises from the geometry of the platelets, and is akin to the angle of dilation considered in Bolton's saw-tooth dilatancy model [13]. The high density of spheres used here, and the inability of the platelets to interlock results in a low coefficient of friction (less than ~0.01).

The presence of a tangential stiffness (with *no* limiting coefficient of friction) between contacting spheres shifts the shear strength envelope upwards, as shown in Fig. 6(b). It also increases the measured coefficient of friction, due to the fact that under greater normal loads, the platelets are closer, and sphere-to-sphere contacts experience greater tangential displacements—mobilising greater tangential forces, illustrated in Fig. 7(b). It should be noted that for both sets of results in Fig. 6(b), no coefficient of friction was defined in the models.

It goes without saying that it is essential to remove any regularity from the platelets to obtain repeatable tangential behaviour in any direction on the shear plane. Without doing so, any two platelets would exhibit significantly higher tangential forces when the lattices are aligned/interlocked, and lower forces otherwise.

Any particular macroscopic coefficient of friction between platelets can therefore be achieved by calibrating the sphere-to-sphere coefficient of friction. If for instance an *inter-platelet* friction coefficient of 0.2 is desired, using the same platelets and normal contact law as above, the simple linear tangential sphere-to-sphere contact law shown in Fig. 8(a) can be used. It is important to note that the sphere-to-sphere coefficient of friction (0.18) is lower than the resultant inter-platelet value (0.20). It is important that a suitably high tangential stiffness is used, which takes account of the expected shear displacements occurring between the sub-spheres (too low stiffness will not mobilise the full shear strengths). The maximum shear force for any sphere contact is calculated as $F_{S,max} = \mu F_N$, where F_N is the normal force. For simplicity in this instance, the maximum shear force is set to zero for tensile normal forces ($F_{S,max} = 0$ when $F_N < 0$). However it is straightforward to give tensile contacts a frictional shear strength by using an offset (e.g. $F_{S,max} = F_{S,0} + \mu F_n$). Using this tangential contact law gives the face-to-face tangential behaviour shown in Fig. 8(b), and the shear strength envelope shown in Fig. 8(c), in which the

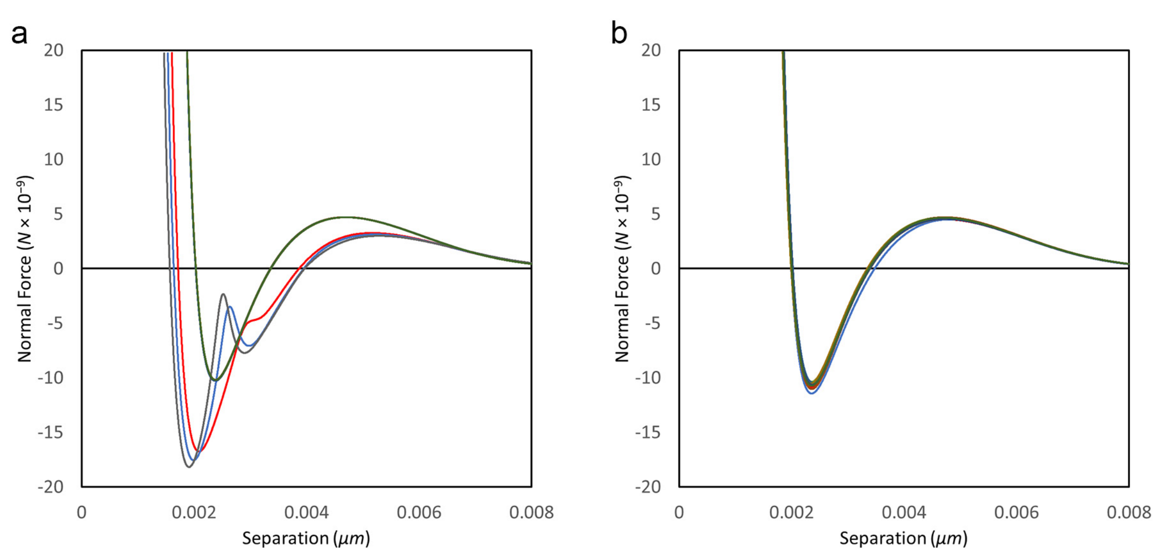

Fig. 5. Results from repeatedly driving two parallel platelets together: using regular lattice arrangement of spheres (a); with random internal displacements of spheres (b).

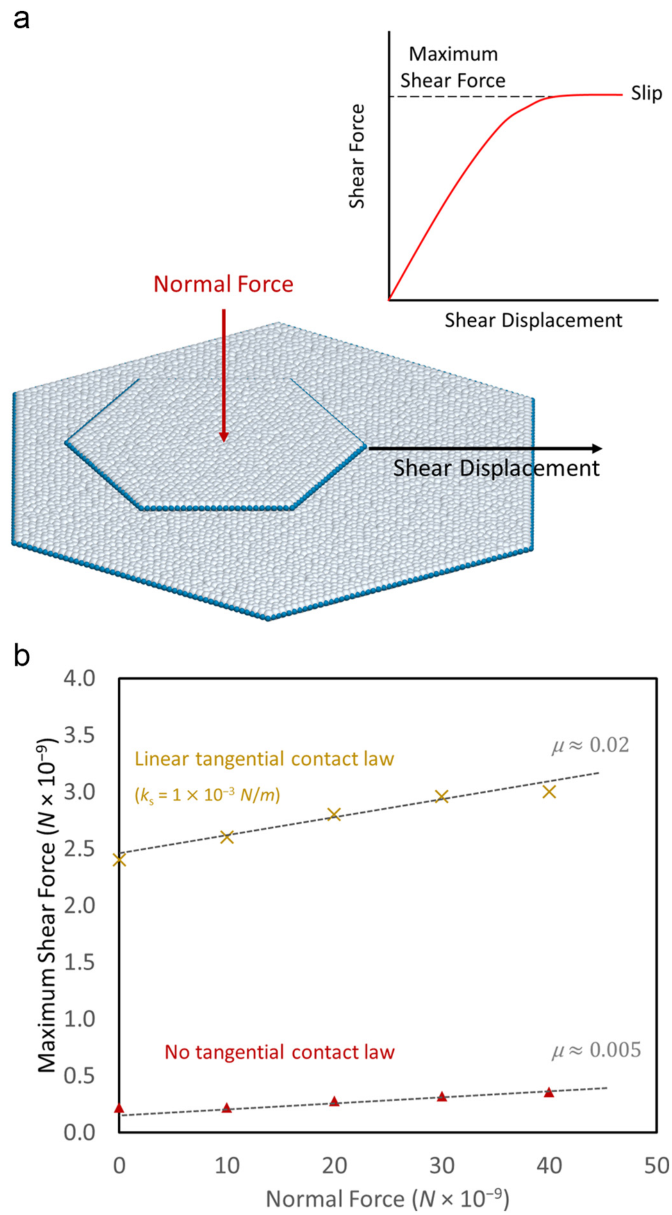

Fig. 6. Diagram of shearing procedure (a); failure envelopes showing approximate coefficient of friction (b).

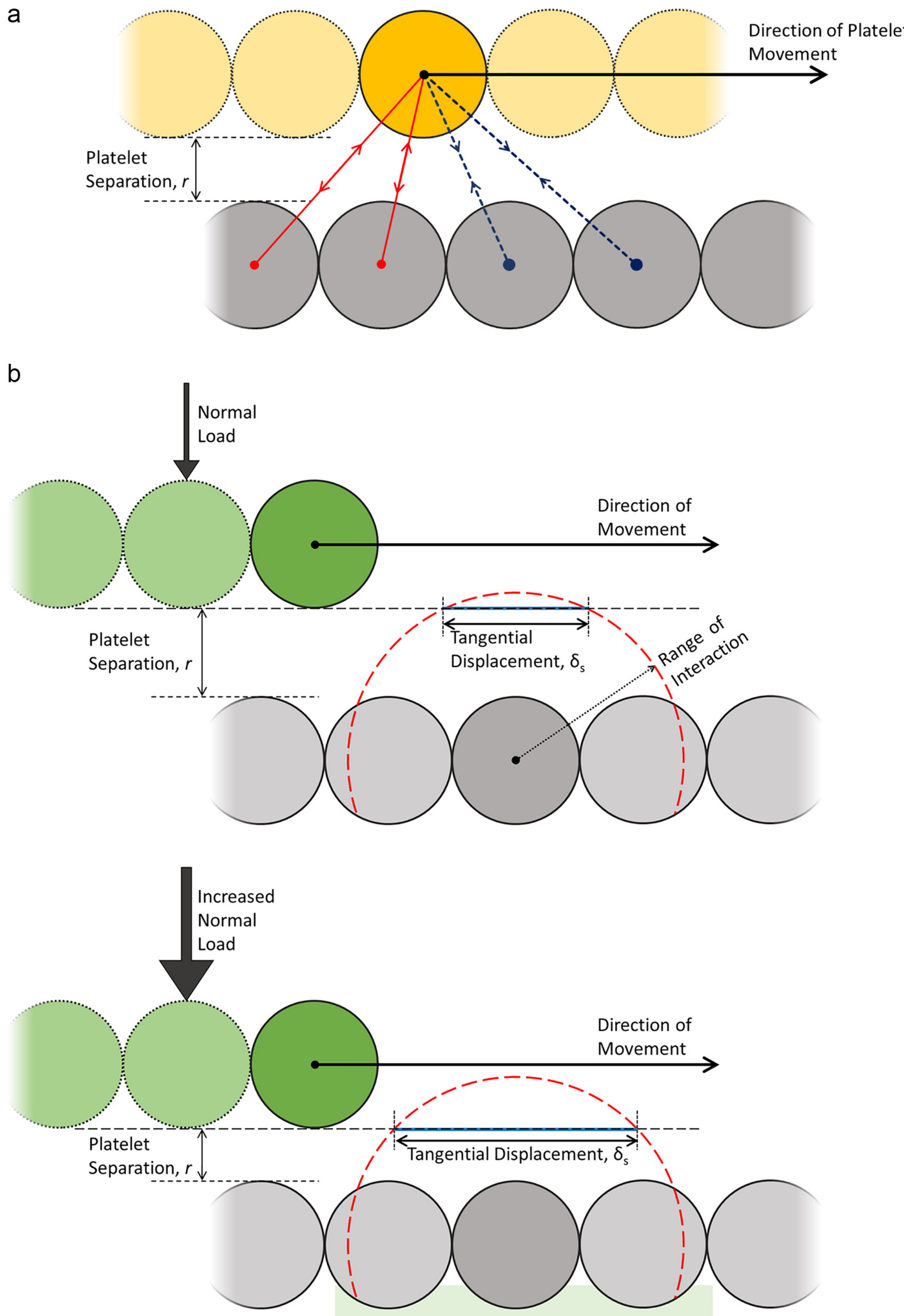

Fig. 7. Diagrams showing normal sphere-to-sphere contacts during shearing of platelets (a); and effect of increasing normal load, resulting in increased tangential displacements between spheres (b).

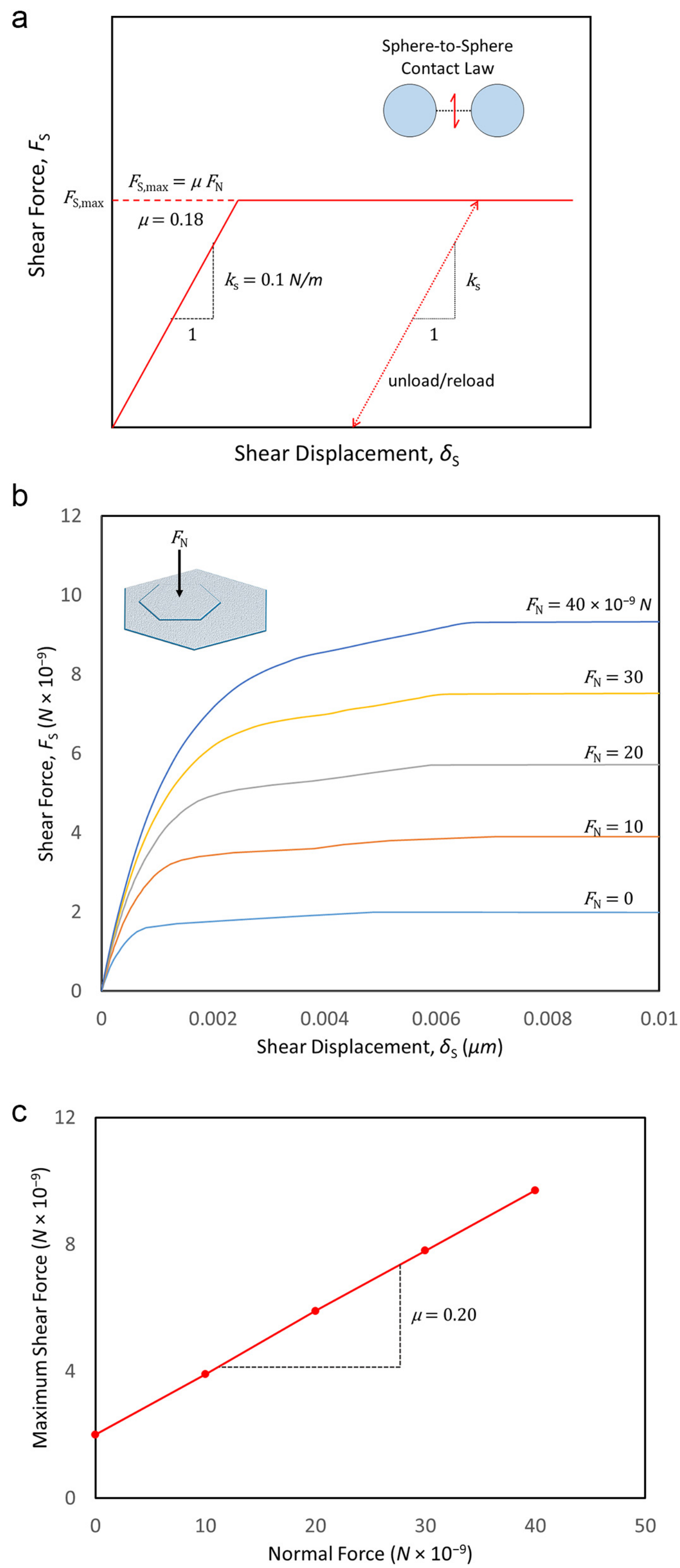

Fig. 8. Tangential contact law used between spheres (a); tangential platelet-platelet behaviour (b); shear strength envelope for platelet-platelet interactions (c).

macroscopic friction coefficient is 0.2. The shear strength under zero normal load can also be calibrated by applying an offset ($F_{S,0}$) to the maximum shear strength for individual contacts.

5. Conclusions

This work has sought to highlight some important issues that need to be considered when modelling clay platelets using DEM. Principally, it has been shown that when using elementary spheres to model platelets, care needs to be taken to ensure repeatability for any/all platelet interactions. This was demonstrated considering only *face-to-face* interactions, however it applies to *edge-to-face* and e*dge-to-edge* interactions equally. It was also shown how to properly implement an inter-platelet coefficient of friction, which will depend on both the tangential contact law, the normal attraction between platelets, and the platelet geometry. Although these issues are easily addressed by careful calibration of the sphere-to-sphere contact laws, they appear to have often been overlooked in previous work modelling clay platelets.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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