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Using a deformable discrete-element technique to model the compaction behaviour of mixed ductile and brittle particulate systems

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Summary

The paper has illustrated the application of a combined discrete and finite element simulation of compaction of assemblies comprising both ductile and brittle particles. Through case studies, the results demonstrate the importance of using a fine mesh on the particle boundary, the effect of fragmentation and its impact on the form of the load compression curve and that the inclusion of ductile particles at about 25% by volume can be used to suppress any brittle failure mechanisms. The ability to extend the calculation to three dimensions has also been demonstrated. However, the computational cost is probably the only current limitation of three dimensional calculations. The task that can be completed in couple of days in two dimensions will require couple of months on the same computing platform.

The novelty of this approach is in its ability to predict material yield surfaces for the compaction of mixture of particles. The initial results are optimistic but there is a need for model improvement, principally through the ability to capture the random packing of irregular particles since this will eliminate a key problem in defining an initial density for the simulation.

The main advantage of this technology is in its ability to minimize the need for expensive tri-axial testing of samples to develop the yield surface history.

1. Introduction

Particulate systems are encountered widely in engineering. They exist in a range from submicron to hundreds of microns in shaped engineering products manufactured from ferrous, ceramic, hard metal or magnet powders. Similarly they occur in pharamaceutical, food and domestic products, all of which are pressed into a tablet form. In geological systems particulate systems occur at the micron scale, for example in clays, to several centimetres in the case of stone. At this scale, each discrete volume exhibits specific elastic and yielding behaviour. The particle may be very soft and ductile, or it may be very hard and brittle. Soils differ from engineering or tablet products since they are also likely to include a fluid phase, however the work in this paper will neglect this. Also from a design viewpoint, the emphasis of soil consolidation is to establish load bearing capability, or the extent of potential settlement. In engineering application, emphasis is placed on compaction processing such as pressing loads and the likelihood of defect occurrence within the forming cycle. Thus it is evident that particulate systems covering a wide size scale exist in engineering. The work that is described in this paper is generic to these systems.

Traditional finite element simulation of soil consolidation or particulate system compaction adopts a continuum framework. This was established initially for soils [1], but over the last decade it has been extended to engineering and tabletted products [2,3]. Thus material properties are assigned to the bulk that reflect its yielding under shear and normal stress, usually in a rate independent framework. Also it is essential to prescribe a friction model to account for the interaction between any rigid fixed or moving boundaries. Unlike solid materials, the yielding behaviour is characterised by a surface that evolves as the particulate assembly is compressed [1]. Similarly, friction between the particulate and rigid surfaces is influenced by a number of parameters [4] and within a Coulomb model framework, the coefficient may be expressed in terms of normal stress. To date these essential parameters can only be generated via experiments that are generally time consuming and costly to perform [5]. Also the results only apply to the particulate system that is under test, if there are changes in composition, then this will affect powder bulk properties and it is essential to repeat the test.

The ability to predict bulk material properties from particulate behaviour motivated the work described in this paper. This is important since it reduces the need to complete extensive experiments when different mixture compositions are explored. It may also be used to guide mixture selection in order to gain "good" consolidation or compaction behaviour or to demonstrate the impact of changes in inter particle friction through the addition of lubricant. Although linked micro-macro type models of compaction have been described in the literature [6], they are mainly based on simple geometry (spheres) and they do not appear to be capable of handling mixtures comprising particles that often exhibit different and complex yielding or friction behaviour. The strategy described below is more general. However in developing this strategy it has been necessary to test the approach through comparison with experimental data, drawn principally from the pharmaceutical sector.

The key objective of the work described in this paper was to explore the use of a combined finite and discrete element method to predict the yield surface. The discrete contribution tracks the kinematic behaviour of each particle and their interaction forces while the particle deformation response is computed via a finite element scheme that is applied to each particle. The latter captures the bulk and surface properties of each particle and the calculations for the assembly are coupled through the equations of mechanical equilibrium. Figure 1 compares the strategy with a traditional continuum analysis. [14]

Figure 1 compares the strategy with a traditional continuum analysis.

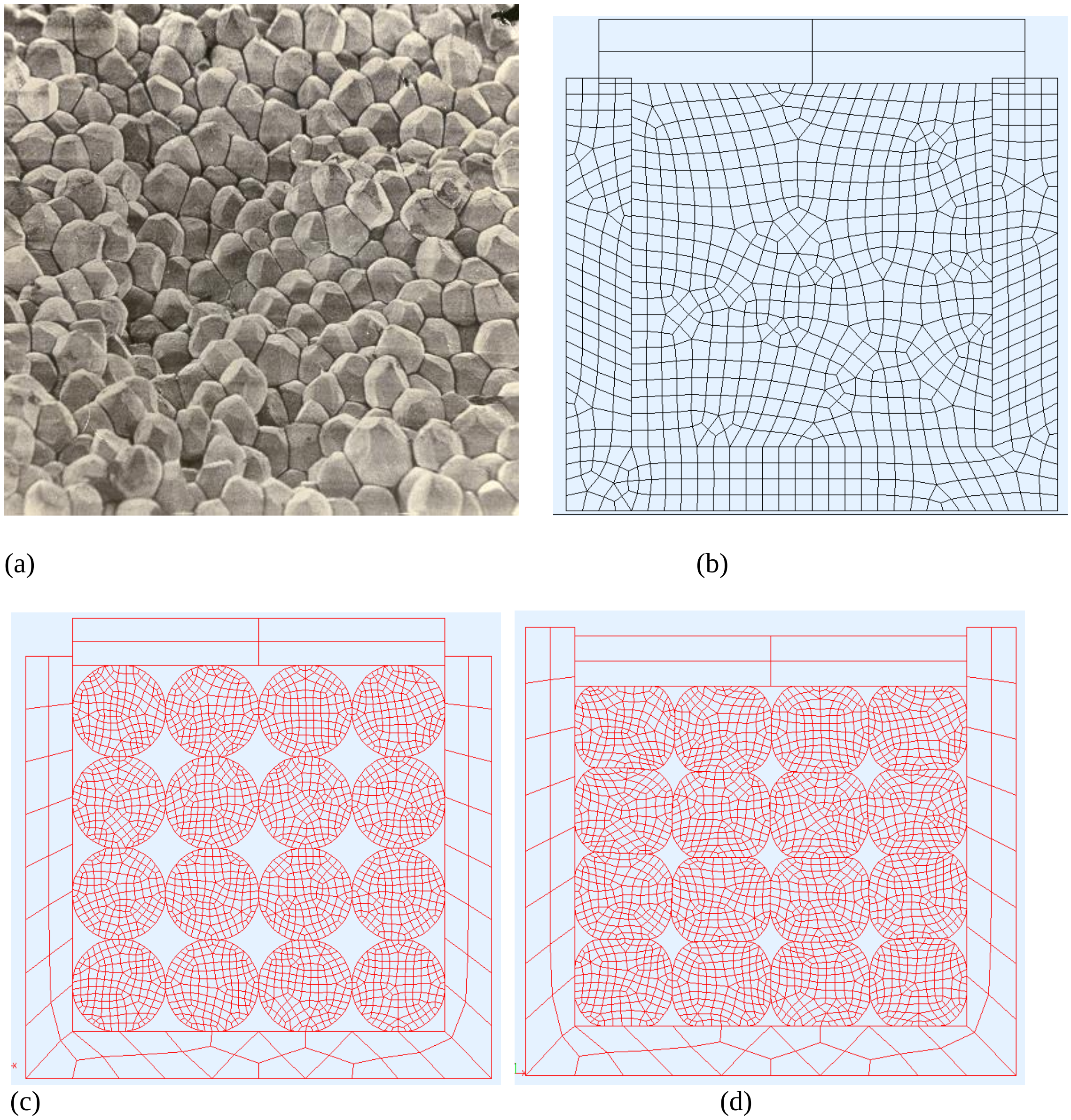


Figure 1:Powder compact (a) (Photograph given by Professor Ray Rowe and Dr. Ron Roberts of AstraZeneca), an equivalent continuum analysis mesh (b), and combined discrete/finite element mesh ((b) and (c)).

2. Relevant Literature

The discrete simulation technique was devised by Cundall and Strack in 1979 to explore interactions in rock systems [7]. In this work they developed a scheme that was referred to as the Distinct Element Method that has formed the basis for further developments. Generally in these developments, every particle is identified separately, with its own mass, moment of inertia and contact properties. The contacts can be deformable or rigid and normal and tangential springs and dashpots are used at each contact to represent contact compliance and energy absorption. The amount and rate of overlap between neighbouring elements are used to determine the contact forces at each instant in time. The total unbalanced forces and moment acting on each particle are computed based on local equilibrium of direct neighbours and are used to estimate accelerations of each particle which is in turn used to compute new displacements at the end of the current time step. This process is repeated until the unbalanced forces and moments are very small, thus approaching equilibrium incrementally.

Following a decade of development, Cundall and Hart [8] distinguished differences with existing continuum programs in the following way.

Discrete element programs should:

- allow finite displacements and rotations of discrete bodies, including complete detachment, and
- recognize new contacts automatically as the calculation progresses.

Without the first attribute a program cannot reproduce some important mechanisms in a discontinuous medium, and without the second, the program is limited to small numbers of bodies for which the interactions are known in advance. Dorby and Ng [9] also reported a comprehensive survey of the applicability of discrete element methods to various problems at that time (1989) where it is evident that the study of geological systems was the main focus. More recent work has included analysis of the deformation of the particle while retaining the spring and dashpot type models to account for kinematic behaviour [10-12]. However the deformation is restricted to a small value through the integration of a Hertzian contact representation. They are not capable of capturing large scale plastic deformation that is characteristic of compaction and consolidation. Most recently the compaction of an irregular packing of cylinders has been undertaken [13]. The aim of this work was to explore the impact of elastic material properties on the yield surface from which it was found that particle arrangement and interparticle friction had a significant impact.

In this paper, the discrete element simulation of an assembly of deformable particles has been performed. The novelty of this work is that each particle has been considered as a discrete element that is mapped by a finite element mesh. A continuum analysis with a von-Mises yield criterion is performed within ductile particles where as for brittle particles, a Rankine – brittle failure model is used. The commercial code ELFEN [14] has been used to undertake this analysis. Unlike preceding work, this is capable of accounting for the large plastic deformation of the particles as they come into contact or break during fracture.

Strategic Approach

Application of the discrete deformable element method focuses on the interaction between the two domains and the calculation of deformation within each domain. The interaction between particles determines the kinematic behaviour of the assembly, in that internal and external forces must balance. To achieve this, the boundary of each particle is mapped by an interface element forming a halo of finite thickness (t), see Figure 2.

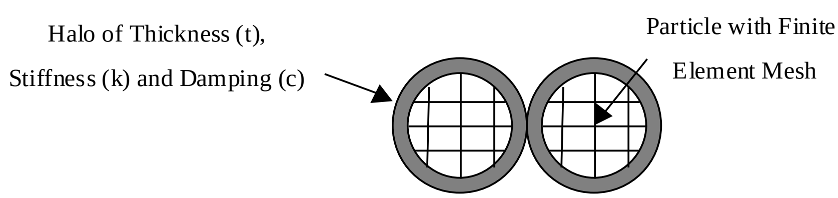


Figure 2 Schematic Representation of the Interaction Between two Particles

This interface has stiffness (k) and damping (c) properties assigned to it and these combined with penetration (x) and impact velocity (v) determine the contact force, i.e.

$$F = xk/(t-x) + cv/x \qquad (1)$$

The particle of mass (m) is given an acceleration (a)

$$a_t=-kx_t/m - P_v/m \qquad (2)$$

P_v is an external force. For the time increments $\Delta t_t = t - t_{last}$ and $\Delta t_{next} = t_{next} - t$ integration gives

$$v_{next}=v_t + 0.5a_t(\Delta t_t + \Delta t_{next}) \qquad (3)$$

$$x_{next}=x_t + v_{next}\, \Delta t_{next} \qquad (4)$$

Analysis of the failure of particles by either ductile or brittle mechanisms is based on a continuum model of the particle. Through application of continuum mechanics to one of the particles shown in Figure 2, it is possible to construct linearised equations of the form

$$[K]\{\delta\}=\{F\} \qquad (5)$$

Equation 5 represents the deformation of the continuum in response to an external force. The stiffness coefficient matrix [K] includes the ductile or brittle failure model for the particle as well as the contributions from particle interactions defined through contact algorithms that are capable of detecting new or developing contacts as they occur.

The final goal of this work is to explore the possibility of predicting yield surfaces for particulate systems that are subject to consolidation or compaction. Prior to this it is appropriate to demonstrate the capability of the technique and comparing this with practical observation, drawn principally from the pharmaceutical field. The work will be illustrated through four case studies. Within these simulations, three material types were considered and their properties are set out in Table 1.

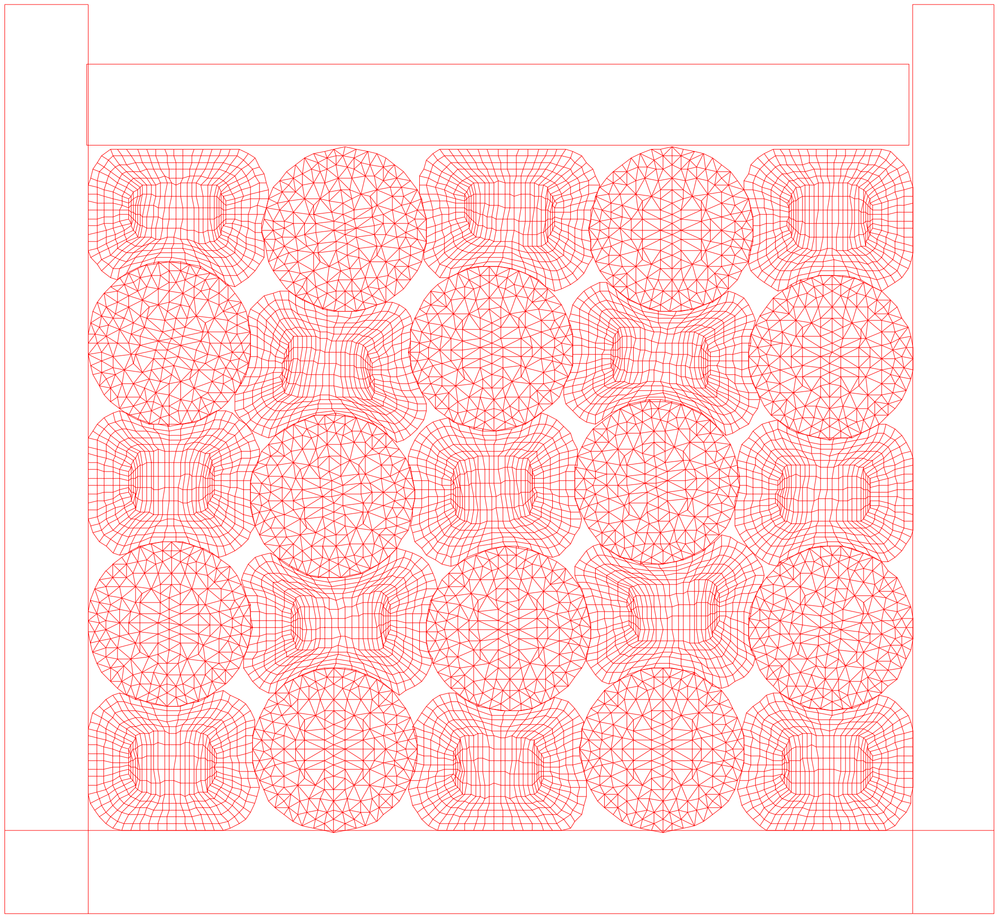
Soft Ductile Particle Properties	
Youngs' modulus	1.96e +05 N/mm^2
Poissons' ratio	0.33
Density	7.9e-03 kg/mm^3
Yield stress	50.0 N/mm^2
Hardening modulus	500.0 N/mm^2
Hard Ductile Particle Properties	
Youngs' modulus	2.0e+05 N/mm^2
Poissons' ratio	0.3
Density	7.9e-03 kg/mm^3
Yield stress	240 N/mm^2
Hardening modulus	500 N/mm^2
Brittle Particle Properties	
Youngs' modulus	5.0e+05 N/mm^2
Density	2.0e-06 kg/mm^3
Tensile strength	0.2 N/mm^2
Fracture energy	0.002 Nmm

Table 1 Particle Material Property Summary

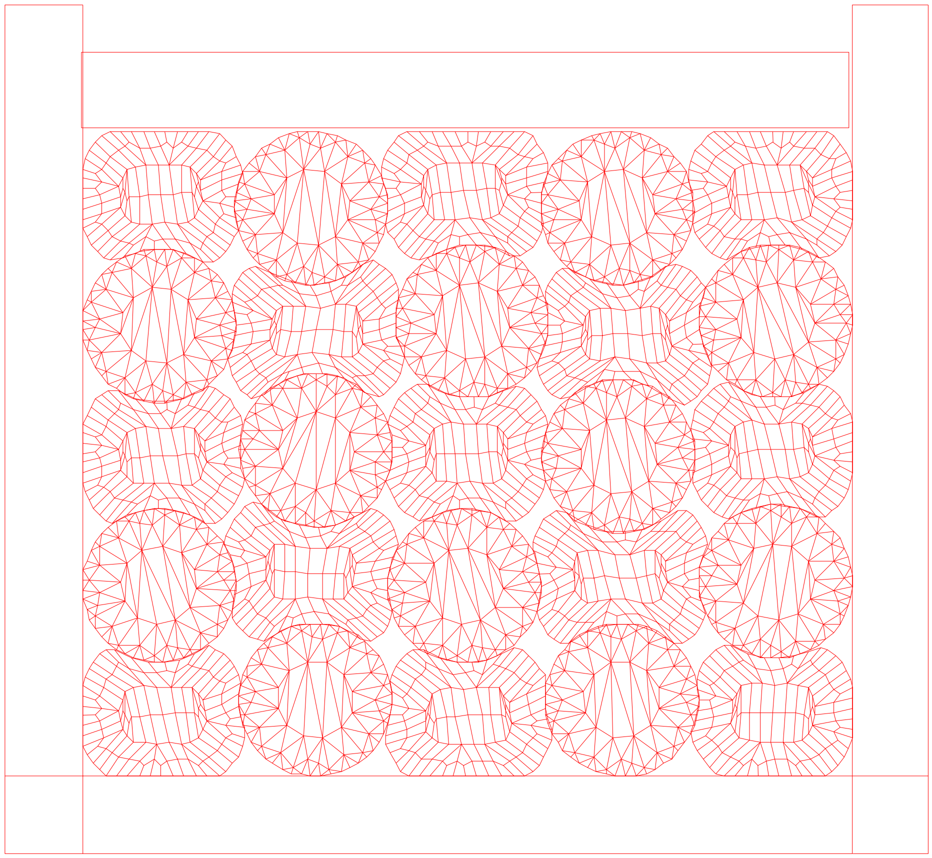
Performing such a complex nonlinear simulation that includes dynamic components in the particle kinematic model was found to be complex and initial scoping calculations were carried out to establish solution stability. For this purpose, the particle assembly shown in Figure 1 was used and the effect of contact parameters k, c and t in Figure 2 were explored. It was found that a stable solution could be obtained when node penetration (t) within the adjacent particle was limited to ~10% of the element size that maps the particle. Also it was found that a value of spring stiffness (k) that is proportional to the Youngs Modulus of the material offers a good basis for the choice of this parameter. Finally it was found that the damping parameter (c) had little impact on the solution result, rather it had a more significant impact on calculation duration.

Case Study 1 Mesh Sensitivity

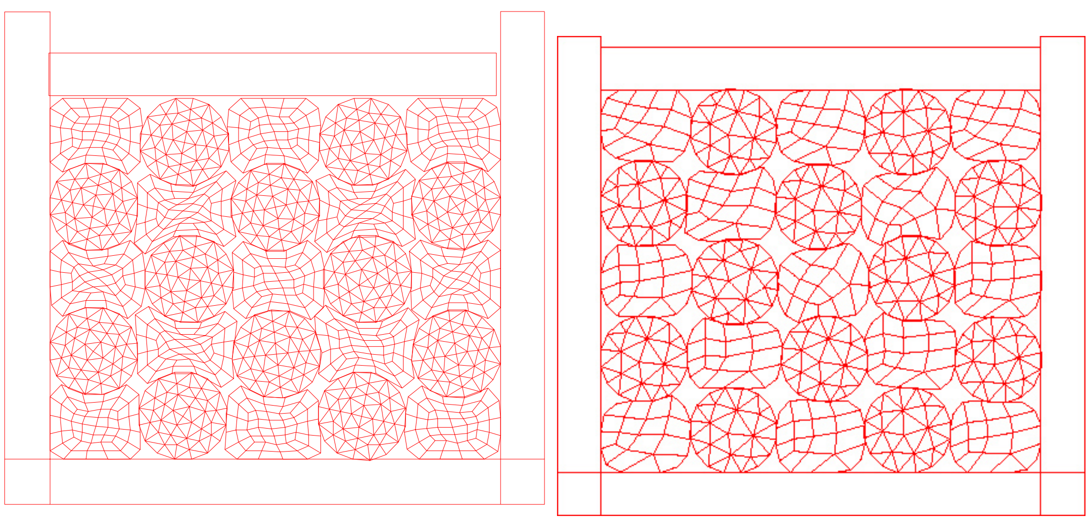
The first case study focuses on the impact of meshing within the particle domain, Figure 3 that shows a mixture of hard and soft ductile particles. It should be noted that each particle type in Figures 3a and 3b are all meshed identically to eliminate this effect from the analysis. In performing this simulation, load was applied through prescribed displacement of the top punch and the analysis displays particle shape towards the end of the compression process. It may be anticipated that such a problem should demonstrate a symmetrical result. However it is evident that this does not occur and that possibly the best results appears in Figure 3b. Through close examination of particle meshing the reason for this was traced to the discretisation in the contact zone. Contact can take place in three modes node-node, node-edge or edge-edge. The nature of this contact determines the local force application on the particle boundary and hence its deformation. Results were found to be more stable if a fine mesh was used at the particle surface while retaining a relatively coarse discretisation within the body (Figure 3b). Clearly this increases the computational cost.



(a) Very Fine Mesh



(b) Fine Mesh



(c) coarse mesh (d) Very coarse mesh

Figure 3 Mesh Sensitivity Results (Case study 1)

Discretisation effects will also have an impact on punch force evolution and this is displayed in Figure 4. When the results from the coarse and fine mesh are compared with the results from the very fine mesh, the maximum deviation remains within 10% and achieves a maximum deviation of 15% for the very coarse mesh. No firm conclusions may be drawn concerning the most appropriate mesh since no direct comparison with other data is readily available. However qualitative comparisons will be presented below to assist in assessing the usefulness of the approach.

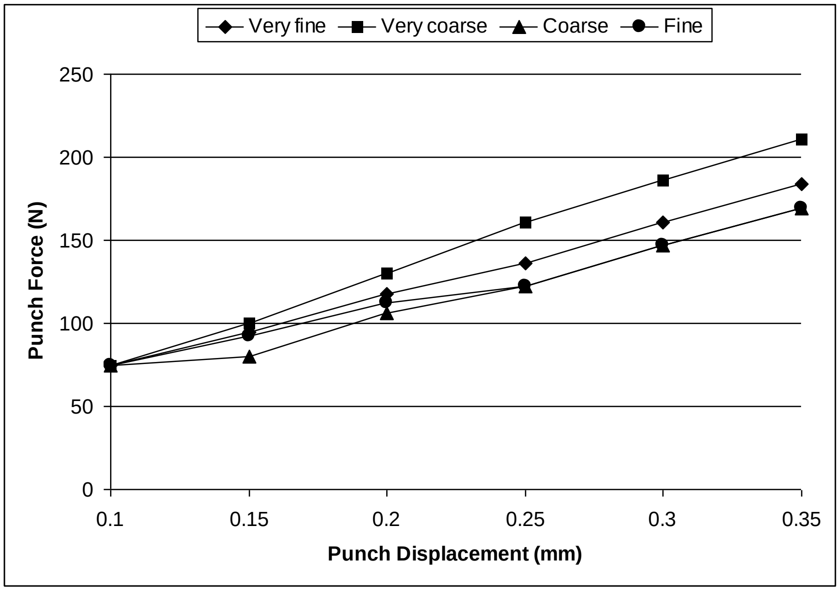


Figure 4 Particle Discretisation and its Impact on Punch Force Evolution

Case Study 2 Compression of a Mixture of Brittle and Ductile Particles

The purpose of this case study was to explore the compaction of a mixture of hard and soft ductile materials and to contrast this with the compaction of a mixture of hard ductile and brittle particles in which some fragmentation occurs.

The assembly used for this work comprised 16 particles as shown in Figures 5 and 7. The Figure 5 shows progressive compaction through stages of fracture and fragmentation. As indicated, fracture commences near to the moving punch since the load taken by the lower particles is reduced due to interaction with the fixed vertical surfaces. Also as fracture proceeds, the fragments infill the void space and are then subjected to further compression and ultimately these will fracture again. Experimental support for this mechanism is also shown in Figure 5 as a micrograph through a fractured tablet section. This tablet also comprises hard ductile and brittle components and there is clear evidence that the latter fragment and in fill the void space. The corresponding punch force evolution is shown in Figure 6. The figure shows a peak at about 0.147mm displacement and this corresponds to a point of particle fracture. The force then remains at a relatively low level as the particles rearrange in the voids and are then subjected to a further load increase at 0.17mm displacement.

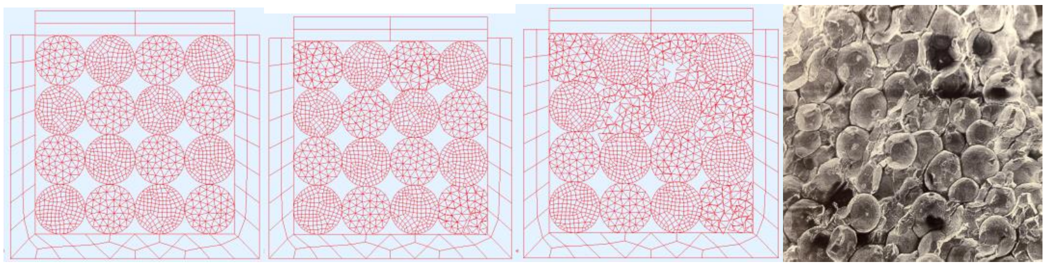


Figure 5: Brittle Fracture within an Assembly of Hard Ductile and Brittle Particles. The micrograph shows compaction and brittle failure in a pharmaceutical powder.

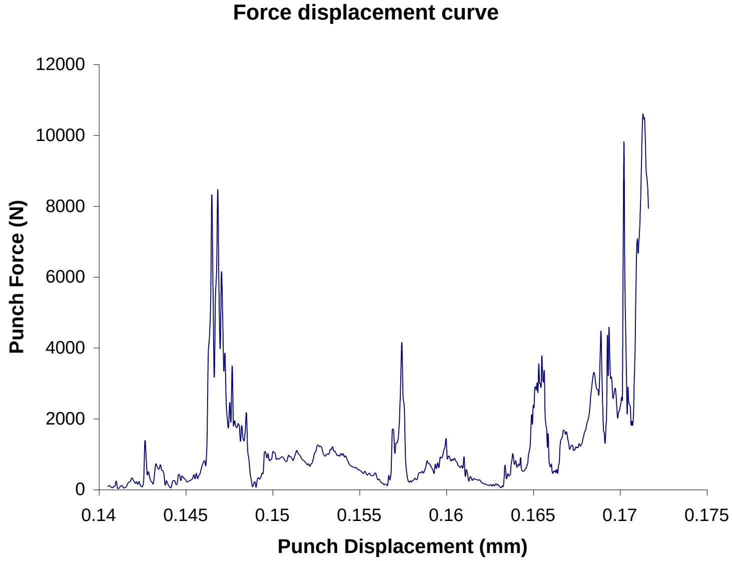


Figure 6 Punch Force Evolution During Compaction of a Mixture of Hard and Brittle Particles

The particle deformation during the compaction of a mixture of hard and soft ductile particles is shown in Figure 7. In this instance, the soft material extrudes about the harder counterpart, effectively isolating it from local high stress levels.

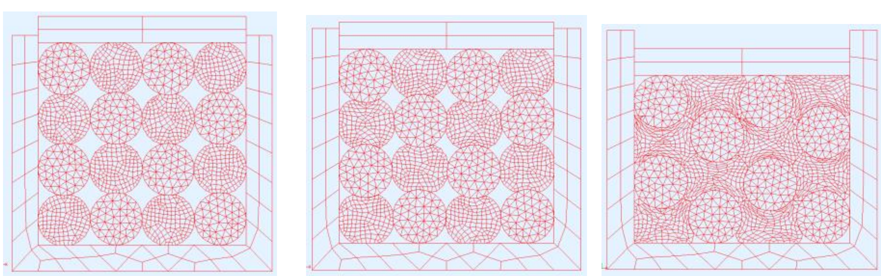


Figure 7 Deformation of Soft Ductile Material to Protect a Hard Particle System.

The corresponding punch force evolution is shown in Figure 8. This exhibits a form that corresponds to experimental observation through a rapid increase in punch force as the void space becomes completely closed. This contrasts with the trends shown in Figure 6 for brittle mixture, where for the range of compaction, there is no significant up turn, rather the force evolution is a consequence of particle rearrangement and localized contact buildup. Figure 8 also contrasts the results from the compression of a pure soft ductile system. Clearly the hard particles contribute to making the mixture stiffer since the softer particles are now forces to extrude between their harder counterparts.

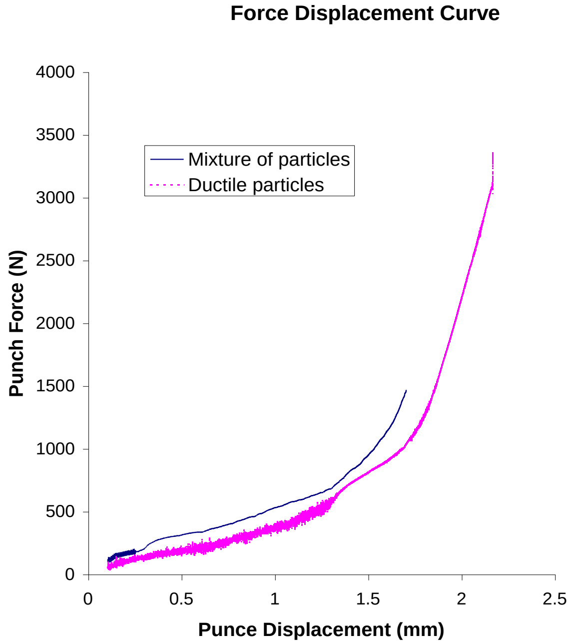


Figure 8 Compaction Force Evolution for a Mixture of Hard and Soft Ductile Particles

Case Study 3 Exploration of Mixture Proportions

Within this case study, the ability of the scheme to predict mixture ratio effects is explored. The case study focuses on a mixture of brittle and soft ductile powders and typical results in terms of deformed particles is shown in Figure 9. The major problem in this case study is the placement of the particles within the assembly. This is likely to affect the outcome considerably and ideally this effect should be minimized by performing the calculation with a very large number of particles. Computationally this is very demanding and was not attempted at this stage of the research. The problem will be particularly acute when simulating mixtures that include only a small percentage of a component are considered. Thus the results that are presented in Figures 9 and 10 can only be taken as indicative at this time.

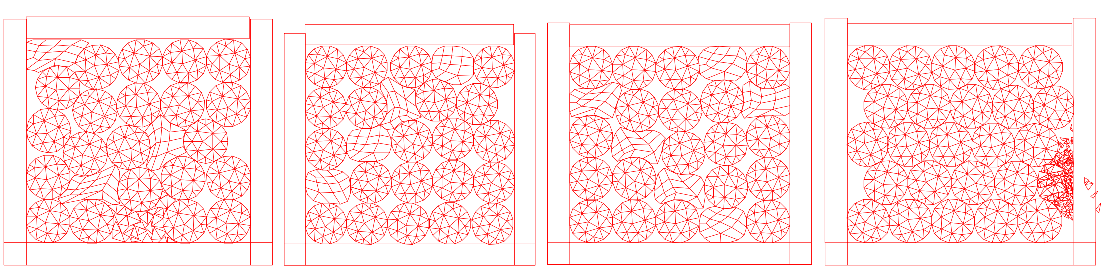


Figure 9 Compaction of Different Mixtures of Soft Ductile and Brittle Particles

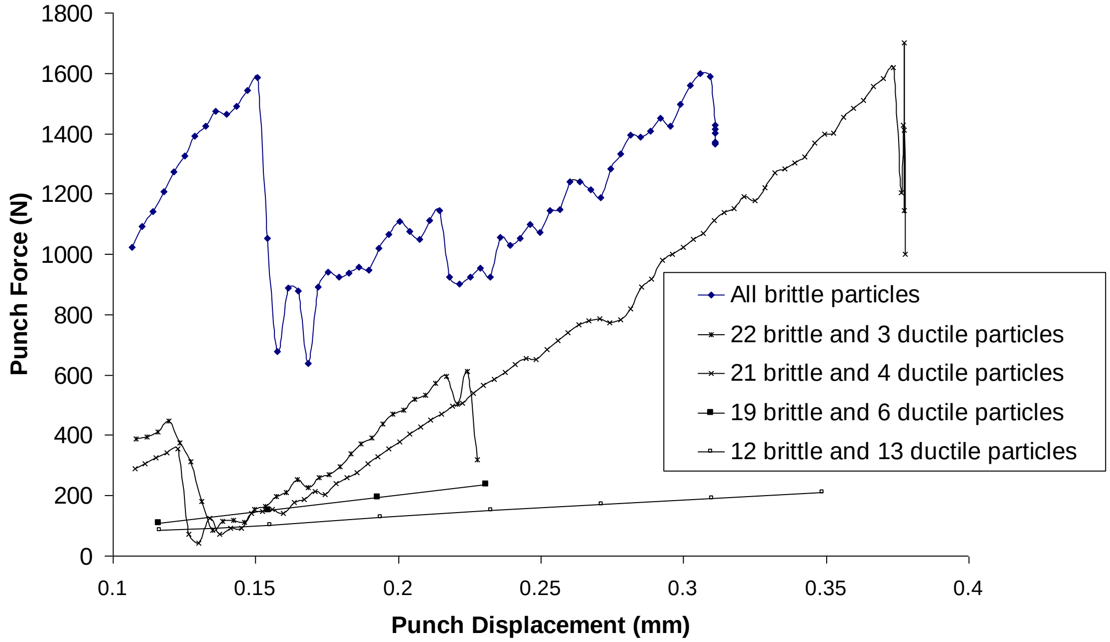


Figure 10 Punch Force Evolution for a Range of Mixtures

Figure 10 illustrates the punch force evolution for the range of mixtures. The extreme upper case reflects the pure brittle system where rapid decay in force level reflects particle fracture. This trend is present until the mixture achieves 6 ductile particles, representing 24% of the volume. Further increase in ductile particle content leads to a reduction in compaction force due to the soft nature of the particles and that extrude into the volume that is not occupied by their brittle partners.

Case Study 4 Simulation of Three Dimensional Particles

The simulation of three dimensional particles was undertaken for two reasons. The first was to quantify the computing demands in comparison with a two dimensional simulation. The second reason was to establish a more realistic initial density since the initial packing density. In the two dimensional simulation this was 78% of the solid material value whereas in a three dimensional simulation this falls to 52%. This now approaches a value that is practically realistic, for example, the fill density in a ferrous system is typically 48% of the solid value.

Figure 11 shows a pair of soft and hard ductile spherical particles of identical size that are subject to compression by a flat platen. The contact stress between the platen and the particle in the foreground are higher since it is the harder particle. The main result from this calculation is that the computing time in comparison with two dimensional analysis is about 20-30 times larger.Massive parallisation of the code and access to super computing facility is necessary to take this research forward.

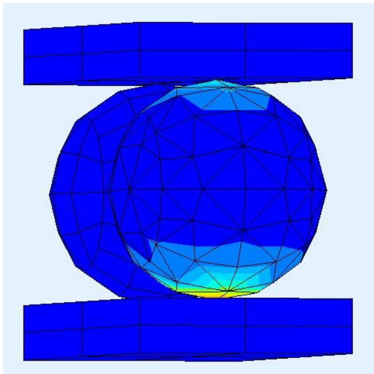


Figure 11 Example Three Dimensional Calculation for a Pair of Spheres Compressed Between Two Platens

The preceding case studies have illustrated the application of the technique to simulate the compaction of ductile and brittle particles and their combinations in mixtures. The results are plausible and in comparing with fracture micro sections they show qualitatively similar results. The simulation captures brittle failure and its impact on the punch force evolution. It has also illustrated how the introduction of a soft ductile component has a marked effect through eliminating the fracture of the brittle particle. Having illustrated the capability to capture compaction at the particle scale, the final section will focus on the opportunity to predict yield surface behaviour.

Yield Surfaces Prediction

Yield surface measurement for powder system is traditionally established using a triaxial test equipment. This is designed according to the particulate system that will be tested. In many metal powder systems, the stress level is high and currently pressures up to 800MPa are encountered. There are a number of variants of the triaxial test, but the most comprehensive has the ability to apply three components of load, so as to generate different stress paths (or stress probing scenarios). An example equipment is shown schematically in Figure 12. The top block is pressed down and through the relative motion with the remaining blocks it compresses the powder sample. The ratio between stress components is determined by the wedge slope and this is changed simply by using different wedge and block pairs. Practically the results from this test are obscured to some extent by the effect of friction that is present between the powder and block and between the blocks themselves. The ability to emulate this test will be explored through discrete simulation. If this is successful, then it has attraction in its ability to predict the impact of material properties and mixture ratio on the yield behaviour of the powder mass. It also has attraction since the friction that is intrinsic to the real experiment can be eliminated through the choice of model parameters.

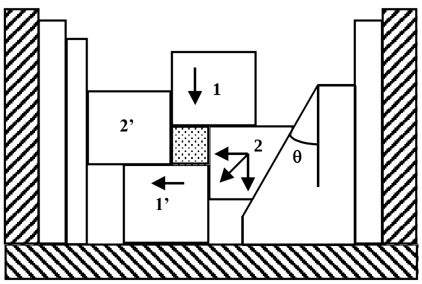


Figure 12 Schematic of a Triaxial Test Equipment

The model that was used to emulate the test is shown in Figure 13 where two stages in the loading path are displayed. Based on previous experience the particles are mapped by a large number of finite elements, particularly at the surface and in the simulation two punches were prescribed to move with different history in order to capture the different loading paths to achieve identical final density levels. The latter was chosen since yield surfaces are often plotted using density as the state variable.

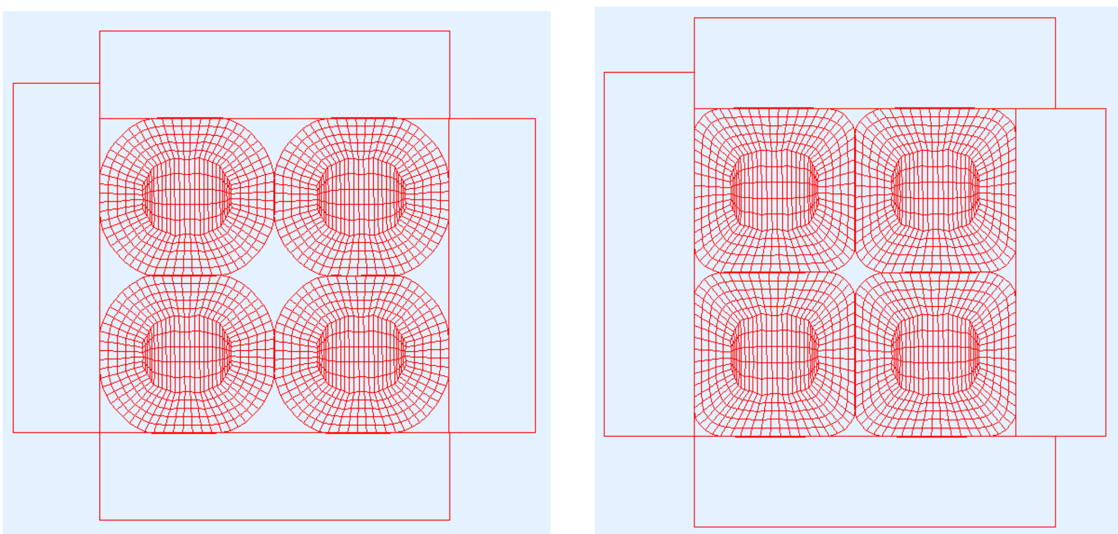


Figure 13 Triaxial Test Emulation Model

In this instance, due to the availability of experimental data, the simulation has been undertaken for iron powder. The particle size chosen is 0.5mm and the properties of the stock material are itemised in Table 2. The yield stress and hardening modulus has been obtained from data that was gathered during the conduct of the triaxial test. Within the scope of the work, a parametric study was also undertaken with different hardening modulii to highlight its effect. The effects of lubrication and other additives were ignored.

Youngs Modulus	1.96e+05 N/mm^2
Poisson Ratio	0.33
Density	7.9e-03 kg/mm^3
Yield Stress	50 N/mm^2
Hardening Modulus	500 N/mm^2

Table 2 Summary of Material Parameters for Iron Powder

In completing this study the major hurdle was the density at the initiation of compaction. For ferrous powders the initial density is about 48% of the solid value whereas the model shown in Figure 13, the ideal geometric void ratio is the ratio of the area of four circles with its circumscribing square. This ratio is 78%. However, after discretisation with the finite element mesh, this ratio became 0.74.

In discrete element simulation, the void ratio is gets automatically calculated based on the geometric deformation of each particle. To overcome this limitation, a mapping based on the concept of *degree of deformation* was assumed to relate the void ratio in 2D to the actual relative density in 3D. In both cases, whether 2D or 3D, initially the deformation in the particles was zero. And hence, the 2D geometric void ratio of 78% was considered equivalent to the 3D initial density of 48%. This assumption was perceived to be valid because in both cases the particles were tightly packed and the *degree of deformation* is zero. Similarly, the final 2D geometric void ratio is considered equivalent to the relative final density in the 3D case because in both cases the degree of deformation is similar. This way the results from a 2D numerical experiment were compared with 3D tria-axial testing experimental results.

In computing the stress state, it is essential to consider the normal (z-axis) component. Since the compression is two dimensional in the x-y plane this component was included using a plane strain model, the remaining components being derived from the punch forces and respective face area. The x and y components of stresses σ_x and σ_y are calculated by dividing the x and y components of punch forces by the actual punch length in x and y direction. σ_z is the average normal stress in the z direction. The average of σ_x, σ_y and σ_z gives the mean stress. The deviatoric stress is calculated by taking the half of the square root of sum of squares of difference of individual stress components (σ_x, σ_y and σ_z) and the mean stress. The yield surface – which is a locus of points in a deviatoric-mean stress plane, where the compact is likely to yield for a given density, was then plotted for different loading cases as shown in Figure 14.

The results shown in Figure 14 are for three hardening parameter settings used in the von-Mises simulation to model individual particle deformation. Predicted values that use no and half hardening (hardening modulus 250 N/mm^2) lie either side of the measured value that corresponds most closely to the compact density derived in the simulation. There are a number of reasons for the possible discrepancy between the measured and predicted values that use the full hardening modulus. The first is associated with the mapping principle and the fact that the ferrous particles are irregular and randomly packed. The second potential reason is that friction is present between the powder and its containment. Each of these requires consideration and to do so requires model refinement and software development to capture true particle shape and random packing.

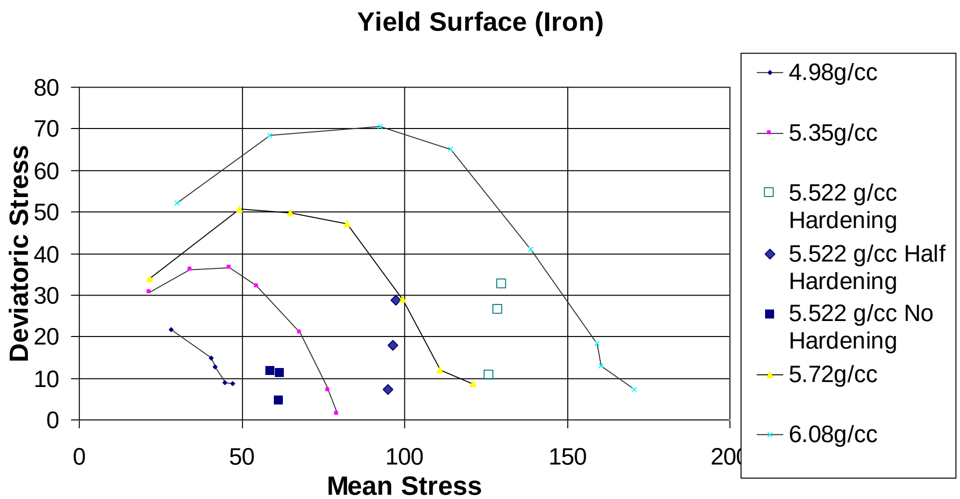
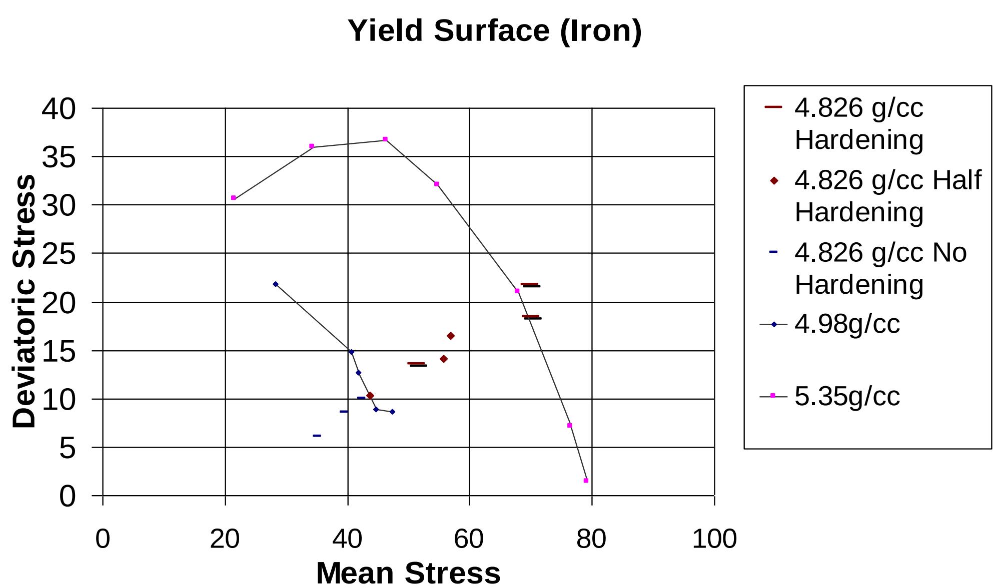


Figure 14 Predicted and Measured Yield Surface for a Ferrous Powder for different values of hardening modulus.



Conclusion

The paper has illustrated the application of a combined discrete and finite element simulation of compaction of assemblies comprising both ductile and brittle particles. The discrete part of the calculation accounts for kinematic behaviour and the finite element analysis accounts for the yield or failure of the individual particles. The importance of particle meshing on the particle periphery has been illustrated through case studies. These have also illustrated the effect of fragmentation and its impact on the form of the load compression curve and that the inclusion of ductile particles at about 25% by volume can be used to suppress any brittle failure mechanisms. The ability to extend the calculation to three dimensions has also been demonstrated. This has confirmed the requirement of super-computing techniques necessary to undertake this analysis.

The principles to predict material yield surfaces have also been explored. The results from this are positive, but there is a need for model improvement, principally through the ability to capture the random packing of irregular particles since this will eliminate a key problem in defining an initial density for the simulation.

Acknowledgements

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