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Abstract

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Keywords

subjected, element, simulation, shear, behaviour, testing, fresh, direct, fouled, discrete, railway, ballast

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Behaviour of fresh and fouled railway ballast subjected to direct shear testing - A discrete element simulation

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Behaviour of fresh and fouled railway ballast subjected to direct shear testing - A discrete element simulation

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ABSTRACT

This paper presents the three-dimensional discrete element method (DEM) that was used to study the shear behaviour of fresh and coal fouled ballast in direct shear testing. The volumetric changes and stress-strain behaviour of fresh and fouled ballast were simulated and compared with the experimental results. ‘Clump logic’ in Particle Flow Code (PFC^{3D}) incorporated in a MATLAB Code was used to simulate irregular shaped particles in which groups of ten to twenty spherical balls were clumped together in appropriate sizes to simulate ballast particles. Fouled ballast with various Void Contaminant Index (VCI), ranging from 20%VCI to 70%VCI, were modelled by injecting a specified number of miniature spherical particles into the voids of fresh ballast. The DEM simulation captures the behaviour of fresh and fouled ballast as observed in the laboratory showing that the peak shear stress of the ballast assembly decreases and the dilation of fouled ballast increases with an increasing of VCI. Furthermore, the DEM also provides insight to the distribution of contact force chains and particle displacement vectors, which cannot be determined experimentally. These micromechanical observations clearly justify the formation of a shear band and the evolution of volumetric changes during shearing. The

reduced maximum contact force associated with increased particle contact area due to fouling explains the decreased breakage of fouled ballast. An acceptable agreement was found between the DEM model predictions and laboratory data.

1. Introduction

The ballast layer plays a crucial part in transmitting and distributing the wheel load from sleepers to the underlying sub-ballast and subgrade at a reduced and acceptable stress level (Selig and Waters, 1994). Upon repeated train loading, ballast becomes degraded and fouled by the progressive accumulation of fines within the ballast voids. In Australia, ballast degradation, infiltration of external fine particles such as coal into the ballast, as well as pumping (liquefaction) of soft subgrade, decreases the void ratio (fouling), seriously decreasing the shear strength and drainage capacity of the track (Dombrow et al. 2009; Indraratna et al. 2010b). Feldman and Nissen (2002) stated that in a Queensland freight line, coal fines account for 70%-95% of contaminants followed by 5%-30% of fouling due to ballast breakage. Given the prolonged droughts and hot climate in Queensland, tracks fouled by coal are often relatively dry, but in the event of rainfall the resulting poor drainage due to fouling adversely affects their performance (Indraratna et al. 2011a).

The behaviour of fresh and fouled ballast has been investigated in the past (e.g. Indraratna and Salim 2002; Suiker et al. 2005; Anderson and Fair 2008; Aursudkij et al. 2009; Huang et al. 2009a; Indraratna et al. 2009; Indraratna et al. 2010a; Tutumluer et al. 2007; Tutumluer et al. 2008). However, most of these studies were conducted in the laboratory and only limited attempts were made to study the effects of fouling numerically. Furthermore, due to the discrete nature of ballast material, continuum modelling through finite element or finite difference methods is no longer realistic. They are unable to provide any insight into micro-scale responses such as contact force chain developed among the particles and the associated displacement vectors when subjected to shear loads. The discrete element method (DEM) based on discrete particle mechanics introduced by Cundall and Strack (1979) has progressed rapidly over the years and can now model the more insightful micro-mechanical behaviour of granular materials that cannot be examined experimentally (e.g. Sitharam and Vinod 2005; Lobo-Guerrero and Vallejo 2006; Lu and McDowell 2006; Hossain et al. 2007; Sitharam and Vinod 2008; Sitharam

and Vinod 2009; Huang et al. 2009b; Thakur et al. 2010; Indraratna et al. 2010a; Wang and Gutierrez 2010; O’Sullivan et al. 2008; O’Sullivan and Cui 2009; O’Sullivan 2011), among others. The use of DEM to predict the stress-strain response of fouled ballast has been very limited in literature. Huang et al. (2009a, b) conducted an experimental and DEM study, but they did not analyse the volumetric change of ballast in relation to various levels of fouling. This current study is an attempt to apply DEM to model both fresh and fouled ballast subjected to direct shear testing, to capture the volumetric change and corresponding stress-strain behaviour at various levels of fouling.

2. Experimental program

A series of large-scale direct shear tests on 300mm × 300mm × 200mm size specimens were conducted. To minimise the boundary effects, slightly smaller ballast with a maximum size particle (d_{100}) of 40mm were used rather than the d_{100} of 55-60mm used in typical Australian ballast gradations (Indraratna et al. 2011a). This gradation satisfied the size ratios discussed by Fagnoul and Bonnechere (1969), Marachi (1969), Indraratna et al. (1993, 2012). By sub-dividing the sample of ballast into small layers, predetermined amounts of coal fines (fouling material) were uniformly distributed into the void spaces to represent a given void contaminant index (VCI) as defined earlier by Indraratna et al. (2010b):

$$VCI = \frac{1+e_f}{e_b} \times \frac{G_{s,b}}{G_{s,f}} \times \frac{M_f}{M_b} \times 100 \quad (1)$$

where e_f = void ratio of fouling material, e_b = void ratio of fresh ballast, $G_{s,b}$ = specific gravity of ballast, $G_{s,f}$ = specific gravity of fouling material, M_f = dry mass of fouling material, M_b = dry mass of fresh ballast.

The main advantage of Equation (1) is that it can include different types of fouling materials such as coal, mud, or pulverised ballast by incorporating their respective specific gravity ratio, unlike the previous methods of fouling assessment (e.g. Selig and Waters, 1994; Feldman and

Nissen, 2002). The particle size distribution of fresh and fouled ballast at various values of VCI is shown in Figure 1.

Large scale direct shear tests were conducted for fresh and fouled ballast at various levels of fouling, ranging from 0% to 95% VCI, at relatively low normal stresses ranging from 15kPa to 75kPa, to represent typical track conditions under low confinement (Lackenby et al. 2007). Each specimen was subjected to a maximum horizontal displacement of $\Delta h=37\text{mm}$ (approximately 12.3% shear strain), which corresponds to the maximum movement allowed by the direct shear test apparatus. While the experimental results were discussed in detail elsewhere by Indraratna et al. (2011a), some of this data was used to compare with the current DEM analysis. The laboratory results show that the peak shear stress increased non-linearly, with an increase in normal stress, but then it decreased as the VCI increased. Indraratna et al. (2011a) attributed this to coal fines coating the surface of the ballast particles and thereby reducing the interlocking effect among the grains. In other words, the coal fines may act as a lubricant that facilitates the grains sliding and rolling over each other more easily, resulting in increased dilation.

3. Numerical simulation

Particle Flow Code (PFC^{3D}) has been developed based on the discrete element method (Cundall and Strack, 1979). The calculation cycle in PFC^{3D} is a time stepping algorithm that utilises two successive cycles to calculate the contact forces and displacement of particles using Newton's second law of motion. The contact and body forces arising from the relative displacement at each contact are then updated by applying the force-displacement relationship (Itasca, 2008). The modelling of irregular shaped particles, model preparation, and the relevant micro-mechanical input parameters for the DEM simulation are discussed below.

4. Modelling the ballast assembly in DEM

The entities representing the particles in PFC^{3D} are spheres. Due to insufficient interlocking and inevitable excessive rolling, spherical units are usually unable to model granular particles that are by nature, irregular or angular (Oda and Iwashita, 1999). Lim and McDowel (2005); Lu and

McDowel (2007); Ferrellec and McDowel (2008); Thakur et al. (2010) have attempted to model the complex shapes of particles in DEM by ‘clump logic’, i.e. a method of forming irregular particles by connecting and overlapping a number of spheres of different sizes, and by assigning the corresponding radii and coordinates (Itasca, 2008). The clump behaves like a rigid body where the internal contacts are ignored. In this study, to model typical ballast shapes, nine distinct particle shapes with sizes ranging from 9.5mm to 40mm were introduced. The typical particle shapes selected from real ballast aggregates were mimicked by assembling a number of spherical balls as described elsewhere by Indraratna et al. (2010a). The size of DEM particles was influenced by the largest dimension of each particle of ballast and its angularity. A sub-routine using MATLAB code was created to build particle templates. The data obtained from the sub-routine, including the radii and coordinates of spherical balls in a Cartesian system, were then exported to PFC^{3D}. An additional sub-routine was written in FISH language to build a library of nine representative ballast shapes. Figure 2 shows the images of particle shapes generated for the DEM simulation.

4.1 DEM simulation of direct shear test

A large scale shear box 300mm long \times 300mm wide \times 200mm high, and separated horizontally into two equal boxes, was simulated with rigid walls. A free loading plate that allowed the particles to be displaced vertically during shearing was placed on the top boundary. This plate was used to apply a normal load and monitor normal displacement during shearing. The DEM simulation of this direct shear box for both fresh and fouled ballast (VCI=40%), is shown in Figure 3. A total of 8281 spherical particles with sizes ranging from 9.5mm to 40mm were generated in order to simulate actual ballast gradation (Figure 1). Irregular shaped particles were generated by ‘clumping’ using the sub-routines developed by the Authors. Particles were generated in the shear box at random orientations to resemble experimental conditions. The void ratio of the assembly representing the initial condition of the test specimen was controlled at 0.82 (i.e. porosity of 45%), similar to the ballast samples tested in the laboratory. A set of micro-mechanical parameters adopted for DEM simulation of fresh ballast are given in Table 1. A linear contact model, following previous studies, was used for the numerical simulations (e.g. Thakur et al. 2010; Indraratna et al. 2010a; McDowel et al. 2006).

The assembly was then cycled to reach equilibrium through facilitating particles to form contact with each other while keeping the void ratio of the assembly constant. The normal stress applied was kept constant by adjusting the position and velocity of the top plate using a numerical servo-control mechanism (Itasca, 2008). Similar to laboratory conditions, the lower part of shear box was allowed to move horizontally at a velocity of 0.1×10^{-4} mm/time step, while the upper section was fixed (Figure 4). This relatively low shearing rate was not enough to unduly disturb the assembly, but still attain an acceptable convergence rate. Each simulation was sheared to a horizontal displacement of 40mm (i.e., the maximum horizontal displacement observed in the tests). During shearing, the displacement of the top plate was recorded to determine the associated change in volume, and a sub-routine was developed to capture the resultant forces generated at the walls in the upper section of the shear box.

4.2 Computational procedures

As shown in Figure 4, the shear force F_S can be calculated by considering the equilibrium of forces in a horizontal direction. The normal force F_N acting on the shear band is the sum of the applied normal load N , the weight of ballast in the upper box W_b and the weight of the top load plate W_p . Therefore, the shear force F_S and the normal force F_N acting on the horizontal shear plane can be calculated as follows:

$$F_S = \sum_{iw=1}^{N_{wall}} (N_{Y_{iw}} + S_{Y_{iw}}) \quad (2)$$

$$F_N = N + W_b + W_p \quad (3)$$

In the above, $N_{Y_{iw}}$ is the normal force acting on the left and right hand side walls of the upper box, and $S_{Y_{iw}}$ is the shear force acting on the upper box. The upper box has four walls and a top plate, hence the total wall number $N_{wall} = 5$. The length and width of the shear box are L and B , respectively. If the box is sheared at a velocity of v , then at any time t , the contacted shearing area of the shear band incorporating the shear displacement is $B(L-vt)$. The normal and shear stresses are now readily computed as:

$$\sigma_n = \frac{F_N}{L(B-vt)} \quad (4)$$

$$\tau_{zy} = \frac{F_s}{L(B-vt)} \quad (5)$$

where σ_n and τ_{zy} are the normal and shear stresses, respectively.

The bulk coefficient of friction is then calculated by:

$$\phi_b = \frac{\tau_{zy}}{\sigma_n} = \frac{F_s}{F_N} \quad (6)$$

4.3 Numerical results and discussion

4.3.1 Shear stress-strain and volumetric change analysis

DEM simulations were conducted to model fresh ballast subjected to three different normal stresses of 27kPa, 51kPa, and 75kPa. The shear stress and volumetric changes were monitored during shearing. Figure 5 shows the plots of shear stress, shear strain, and volumetric strain obtained by DEM, compared to the laboratory data reported earlier by Indraratna et al. (2011a). The predicted results at all normal stresses, agreed with the experiment results. The strain softening behaviour of ballast follows a similar trend with other rockfill aggregates of comparable sizes (e.g. Marsal, 1973; Indraratna et al. 1998; Charles and Watts, 1980). Volumetric dilation was also observed in all simulations, whereby the greater the normal stress (σ_n), the higher the peak stress and the smaller the dilation, as expected. The DEM analysis shows a noticeable discrepancy in stress-strain curves, i.e. markedly decreased stress and retarded dilation shown by the experimental data at a shear strain of 4-8% compared to the predicted line. This difference may be attributed to some particle degradation that could not be accurately captured in the DEM simulation. Indeed, owing to the breakage of ballast aggregates, the reduction in shear strength would also be accompanied by a decrease in dilation (i.e. increased compression of the assembly of smaller particles). Lackenby et al. (2007) also demonstrated that particle breakage would increase the compression of the granular assembly followed by increased in dilation upon further shearing, which is in agreement with the experimental data plotted in Figure 5. Similar behaviour is also observed in Figures 12-14 presented later for fouled ballast.

4.3.2 Contact force distribution and particle displacement

Figure 6 presents the distribution of contact force chains at various shearing stages for a DEM simulated test with a normal stress of 51kPa. Contact forces between particles were plotted as lines whose thickness is proportional to the magnitude of the force. Figure 6 also illustrates how the applied load was transmitted within the particle assembly. At its initial state ($\epsilon_s=0\%$), the contact forces were distributed uniformly throughout the assembly and transmitted vertically from the top to the bottom of the shear box when normal stress was applied, but as shearing progressed, the contact forces intensified from the bottom left to the top right corner, as shown in Figures 6 (b)-(d). At the end of shearing, Figure 6d shows the lowest contact force magnitude compared to Figures 6b and 6c. This can be attributed to a reduced coordination number (the average number of contacts per particle) associated with an increase in dilation of the ballast assembly, and the corresponding drop in shear strength (strain softening).

The evolution of displacement vectors at shear strains of 3% and 13% at an applied normal stress of 51kPa are presented in Figures 7a and 7b, respectively. At 3% shear strain (Figure 7a), while particles in the lower box displaced horizontally, particles in the upper box moved downwards causing densification (compression) of the granular assembly. On the other hand, at much higher shear strain (e.g. 13%), particles in the upper box tended to displace upwards (Figure 7b) causing dilation. These micro-mechanical observations clearly present the insightful evolution of volumetric changes during shearing within a granular medium, and the corresponding strain softening response where a continuum mechanics approach is unable to deliver the same level of clarity.

During the process of shear box testing, the shear plane usually propagates horizontally at low shear strains. However, at a relatively large shear strain $> 10\%$, the intensity of inter-particle contact forces as determined by DEM tend to be inclined to the direction of shear strain (Fig. 7c). The DEM analysis shows that during shearing the particles of ballast at the rear of shear box displaced downwards while particles at the front displaced upwards. Volumetric strain was not distributed uniformly within the ballast assembly because dilation tends to occur at the front of the shear box and compression at the back. This can be attributed to a contact force chain that forms in the shear band where the particles within the shear band are displaced and rotate more

than those outside the shear band (Cui and O’Sullivan, 2006 and Zhang and Thornton, 2007). In this aspect, our understanding of conventional shear plane propagation in relation to continuum mechanics is different to the micro-mechanical implications of potential shear banding governed by inter-particle movement, contact force distribution, and associated principal stress relationships. This disparity between continuum mechanics and micro-mechanics has been further elaborated on by Liu (2006), Wang et al. (2007) and O’Sullivan (2011).

4.3.3 Further validation of the DEM model

The same DEM model was validated by simulating the additional direct shear tests conducted at significantly higher normal stresses of 170kPa, 241kPa and 310kPa by Huang et al. (2009a). Figure 8 presents the comparisons of predicted and measured shear stress-strain behaviour of fresh ballast. A good agreement can be found between the DEM predictions and the experimental results. There was strain hardening at the highest normal stress of 310kPa, which was well predicted by the DEM simulation. At lower normal stresses, the experimental data of Huang et al. (2009a) indicated strain softening. Except for the lowest normal stress of 172kPa, where the DEM prediction tended to overestimate the shear stress, the strain softening behaviour for $\sigma_n = 241\text{kPa}$ shows an acceptable agreement between the numerical simulation and test data. As Lackenby et al. (2007) explained, particle breakage and associated load drop can be significant at low normal or confining stress levels, but for the laboratory data in particular, the drop in shear stress at a shear strain of 4-6% may be attributed to some degradation of the particles.

5. DEM simulation for fouled ballast

Huang et al. (2009b) and Huang and Tutumluer (2011) presented a method to simulate fouled ballast in DEM by reducing the inter-particle coefficient of friction. This method is capable of capturing the stress-strain behaviour of fouled ballast within a reasonable computational time frame, but it did not examine the volumetric changes (either dilation or compression) of ballast at varying levels of fouling. A few past studies, including Ni et al. (2000) and Lu and McDowell (2008), suggested that depending on the extent to which inter-particle friction was reduced, the granular assembly could undergo less dilation. The tendency to dilate is also a function of the

initial distribution of particle sizes, initial compacted density, degree of fouling, applied confining pressure, and the rate of particle breakage, among others. In this study, the extent of dilation for the type of ballast and gradation given was predominantly a function of normal stress and to a lesser extent, by the degree of fouling (Figure 9). For a level of fouling less than VCI=40%, the maximum dilation at a given normal stress was relatively unaffected, while dilation at higher levels of fouling increased slightly. This was not surprising because when compacted, coal fouling is relatively incompressible, but during shearing at high VCI, the coal fines that fill the voids may impede the grains of ballast from re-packing and thereby promote dilation. Apart from decreasing the pore space between the grains of ballast, compacted coal fouling may even dilate itself and force the ballast to segregate and dilate.

5.1 Proposed method for modelling fouled ballast in DEM

Fouling is caused by fine particles that accumulate in the voids of ballast. Therefore, fouled ballast should ideally be simulated in DEM by injecting various amounts of fine particles into the voids to represent different values of VCI (Figure 10a). Owing to fouling material between the individual rough and angular particles of ballast, the inter-particle friction angle is expected to decrease (Figure 10b). This reduction in the apparent angle of friction was evaluated experimentally and presented in Figure 11 showing increasing normal stress. This reduction of the inter-particle coefficient of friction (μ) in DEM was approximately determined based on the decrease in the apparent angle of friction of fouled ballast measured experimentally, as shown in Figure 11. In this DEM study, coal fines were simulated by 1.5mm spheres, which was similar to d_{50} of coal fines conducted in the laboratory, generated within the voids of fresh ballast.. The values of normal and shear stiffness (k_n and k_s) required for the DEM analysis are always difficult to determine correctly, so in order to obtain some acceptable values of k_n and k_s , a conventional shear box test (60mm \times 60mm \times 25mm) was conducted on compacted coal fouling with a density of 1280kg/m³. By varying the k_n and k_s values in the DEM simulation to match the shear stress-strain plots obtained for direct shear testing, $k_n=k_s=1.27 \times 10^4$ N/m was found to be appropriate. The relevant micro-mechanical parameters (k_n , k_s , μ) for varying the VCI are shown in Table 2, where the increased VCI is represented by an increased number of small spheres that mimic the fouling particles.

Large scale direct shear of fouled ballast at three different normal stresses of 15kPa, 27kPa, and 75kPa were simulated using DEM. Figures 12-14 show the comparisons between DEM simulation and experimental results where VCI=20%, 40%, and 70%, respectively. It is evident that the shear stress-strain curves predicted by DEM simulation generally agree with those measured experimentally. The DEM simulation also predicted that the ballast would soften under strain at all levels of fouling and dilate significantly when the shear strain exceeded 5%. As expected, the peak shear stress decreased with an increase in VCI at every level of applied normal stress. As mentioned earlier, coal fouling would reduce the inter-particle friction of fresh ballast by coating the surfaces of rough aggregates, causing a reduction in shear strength. All the samples were compressed at the beginning of the test, followed by significant dilation. This was expected from dense granular materials that normally indicate strain softening at high rates of dilation. At a relatively low applied normal stress (15kPa), dilation occurred almost from the beginning of shearing, whereas significantly less dilation occurred at the highest applied normal stress ($\sigma_n = 75kPa$).

Not surprisingly, there is some disparity in volumetric strains between the numerical predictions and laboratory data. This can be attributed to differences in particle angularity between the DEM simulation and laboratory observations, as well as particle degradation not considered in the current DEM analysis. McDowell et al. (2006) also observed similar differences in volumetric strain between DEM and experimental data for tri-axial testing. Irrespective of the efforts made in DEM to clump particles together to mimic irregular or angular ballast used in real rail tracks, accurate representations of the sharp corners of blasted aggregates and their surface roughness will always remain a key challenge to the DEM modeller. Dilation that depends on size and shape, and the nature of particle degradation depending on the applied stresses and shearing rates, will require further insight into micro-mechanical modelling to make further improvements in the DEM.

5.2 Distribution of Contact forces in fresh and fouled ballast

Figure 15 shows the evolution of chains of contact force in fresh and fouled ballast at VCIs ranging from 0% to 70%, at a normal stress of 51kPa. The maximum contact forces and number of contacts for each simulation in the assembly are shown in Figure 16. While the number of

contacts increases significantly with an increased VCI, the maximum value of contact forces decreases with an increasing VCI. When there are coal fines in the voids, the applied load does not only transmit through the large aggregate skeleton but also across the fine coal particles. This results in a reduced maximum contact force magnitude corresponding to a higher number of particle contacts. Consequently, a more uniform distribution of stress is expected in the fouled ballast, as reflected by the distribution of a more dense contact force. The greater the VCI, the more prominent will be the corresponding uniform distribution of contact forces over a larger number of contacts, a result that may reduce ballast breakage by diminishing the intensity of stress concentrated in the fouled ballast matrix. These micro-mechanical observations obtained from DEM clearly explain the reduced breakage of fouled ballast compared to fresh ballast as measured experimentally.

6. Conclusions

A series of DEM simulations that captured three-dimensional shaped ballast in direct shear tests, were conducted on fresh and fouled ballast at various levels of fouling, to study the volumetric change and corresponding stress-strain behaviour of this granular assembly. These irregularly shaped particles of ballast were simulated by overlapping spherical particles using the clump logic of PFC^{3D}. The coal fines were modelled by introducing a specified number of fine spherical particles into the ballast voids. The degree of fouling was defined by the Void Contaminant Index (VCI) that was varied from 20% to 70%. For a given normal stress (σ_n) and VCI, the DEM model captured the shear stress-strain response and volumetric changes observed in the laboratory experiments. As expected, the highest peak shear stress occurred in fresh ballast, but it decreased consistently with an increase in VCI for a given value of normal stress.

The DEM simulation indicated that coal fines would reduce the shear strength and increase the dilation of fouled ballast at relatively high levels of VCI (>60%). Dilation was highest at the lowest values of normal stress ($\sigma_n = 15kPa$). It was shown that the volumetric dilation predicted by DEM was somewhat higher than the dilation actually measured. This can be attributed to the inevitable variations in particle angularity between the DEM model and actual ballast, as well as any particle degradation that was not considered in the numerical analysis. The drop in peak shear stress and increased compression in the laboratory at shear strains of 5-7%

also supports the view that particle degradation can have a significant influence. Even with small quantities, the coal fines coat the grains of ballast and reduce the surface roughness (i.e. role of lubricant), while at increased VCI the coal fines inhibit the ballast from repacking by forming a compacted layer between the aggregates. Therefore, apart from a decrease in shear strength as a result of reduced inter-particle friction, coal fines at high VCI values can also increase the dilation of the fouled ballast, especially at low normal stresses. So by taking advantage of the DEM simulation technique, the internal distribution of contact forces and displacement of the particles could be examined. Such micro-mechanical observations enable us to insightfully appreciate the evolution of volumetric changes and corresponding shear strength during geotechnical laboratory processes, which is currently not possible through FEM and other continuum mechanic approaches. The more uniform contact force distributions attributed to increased overall particle contact area of fouled ballast justify the reduced breakage as observed in the laboratory. Although the current DEM analysis did not consider ballast breakage, the numerical predictions of stress-strain behaviour at various levels of fouling and normal levels of stress were in acceptable agreement with the experimental observations of direct shear test.

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8. Notation

B	width of the shear box
d_{100}	maximum particle size
e_b	void ratio of fresh ballast
e_f	void ratio of fouling material
F_N	normal force at the shear band

F_S	shear force at the shear band
$G_{s.b}$	specific gravity of ballast
$G_{s.f}$	specific gravity of fouling material
k_n	contact normal stiffness
k_{n-wall}	contact normal stiffness of wall-particle
k_s	contact shear stiffness
k_{s-wall}	contact shear stiffness of wall-particle
L	length of the shear box
M_f	dry mass of fouling material
M_b	dry mass of fresh ballast
N	applied normal load
$N_{Y_{iw}}$	normal force acting on the left and right side walls of the upper box
$S_{Y_{iw}}$	shear force acting on the upper box
v	shear velocity
VCI	Void Contamination Index
W_b	weight of ballast in upper box
W_p	weight of the top load plate
t	shearing time
ε_s	shear strain

μ inter-particle coefficient of friction

σ_n normal stress

τ_{zy} shear stress

ϕ_b bulk coefficient of friction

9. References

- Anderson, W. F. & Fair, P. (2008). Behavior of railroad ballast under monotonic and cyclic loading. *Journal of Geotechnical and Geoenvironmental Engineering*. 143(3): pp.316–327.
- Aursudkij, B., McDowell, G. R. & Collop, A. C. (2009). Cyclic loading of railway ballast under triaxial conditions and in a railway test facility. *Granular Matter*. 11: pp.391–401.
- Charles, J. A. & Watts, K. S. (1980). The influence of confining pressure on the shear strength of compacted rockfill. *Géotechnique*. 30(4): pp.353-367.
- Cui, L. & O'Sullivan, C. (2006). Exploring the macro- and micro-scale response of an idealised granular material in the direct shear apparatus. *Géotechnique*. 56(7): pp.455-468.
- Cundall, P. A. & Strack, O. D. L. (1979). A discrete numerical model for granular assemblies. *Géotechnique*. 29(1): pp.47-65.
- Dombrow, W., Huang, H. & Tutumluer, E. (2009). Comparison of coal dust fouled railroad ballast behavior- granite vs. limestone. *Bearing Capacity of Roads, Railways and Airfields, Proceedings of the 8th International Conference (BCR2A'09)*. Taylor & Francis Group.
- Fagnoul, A. & Bonnechere, F. (1969) Shear strength of porphyry materials. *Proceedings of the 7th International Conference on Soil Mechanics and Foundation Engineering*. Mexico.
- Feldman, F. & Nissen, D. (2002). Alternative testing method for the measurement of ballast fouling. *Conference on Railway Engineering*. RSTA, Wollongong.
- Ferrellec, J. F. & McDowell, G. R. (2008). A simple method to create complex particle shapes for DEM. *Geomechanics and Geoengineering*. 3(3): pp.211 — 216.
- Hossain, Z., Indraratna, B., Darve, F. & Thakur, P. K. (2007). DEM analysis of angular ballast breakage under cyclic loading. *Geomechanics and Geoengineering*. 2(3): pp.175-181.
- Huang, H., Tutumluer, E., & Dombrow, W. (2009a). Laboratory characterisation of fouled railroad ballast behavior. *88th Annual Meeting of the Transportation Research Board*. Washington, DC.

- 1 Huang, H., Tutumluer, E., Hashash, Y. M. A., & Ghaboussi, J. (2009b). Discrete element
2 modeling of aggregate behavior in fouled railroad ballast. *Geotechnical Special Publication 192*,
3 *ASCE*: pp.33-41.
- 4 Huang, H. & Tutumluer, E. (2011). Discrete Element Modeling for fouled railroad ballast.
5 *Construction and Building Materials*. 25: pp.3306-3312.
- 6 Indraratna, B., Wijewardena, L.S.S. & Balasubramaniam, A. S. (1993). Large-scale triaxial
7 testing of greywacke rockfill. *Géotechnique*: 42(1): pp.37-51.
- 8 Indraratna, B., Ionescu, D. & Christie, D. (1998). Shear behaviour of railway ballast based on
9 Large Scale Triaxial Testing. *Journal of Geotechnical and Geoenvironmental Engineering*,
10 *ASCE*. 124(5): 439-449.
- 11 Indraratna, B. & Salim, W. (2002). Modelling of particle breakage of coarse aggregates
12 incorporating strength and dilatancy. *Geotechnical Engineering, Proceedings of Institution of*
13 *Civil Engineers, UK*. 155(4): pp.243-252
- 14 Indraratna, B., Lackenby, J., & Christie, D. (2005). Effect of confining pressure on the
15 degradation of ballast under cyclic loading. *Géotechnique*. 55(4): pp.325–328.
- 16 Indraratna, B., Vinod, J. S. & Lackenby, J. (2009). Influence of particle breakage on the resilient
17 modulus of railway ballast. *Géotechnique*. 59(7): pp.643–646.
- 18 Indraratna, B., Thakur, P. K. & Vinod, J. S. (2010a). Experimental and numerical study of
19 railway ballast behavior under cyclic loading. *International Journal of Geomechanics, ASCE*.
20 10(4): pp.136-144.
- 21 Indraratna, B., Nimbalkar, S. & Tennakoon, N. (2010b). The behaviour of ballasted track
22 foundations: track drainage and geosynthetic reinforcement. *GeoFlorida 2010: Advances in*
23 *Analysis, Modeling & Design (GSP 199)*. Orlando, Florida.
- 24 Indraratna, B., Ngo, N. T., & Rujikiatkamjorn, C. (2011a). Behavior of geogrid-reinforced
25 ballast under various levels of fouling. *Geotextiles and Geomembranes*. 29(3): pp.313-322.

- 1 Indraratna, B., Hussaini, S. K. K. & Vinod, J. S. (2012). On the shear behaviour of of ballast-
2 geosynthetic interfaces. *Geotechnical Testing Journal*. 35(2): pp.1-8.
- 3 Itasca (2008). Particle flow code in three dimensions (PFC^{3D}). *Itasca Consulting Group, Inc.,*
4 *Minnesota*.
- 5 Lackenby, J., Indraratna, B., McDowell, G., & Christie, D. (2007). Effect of confining pressure
6 on ballast degradation and deformation under cyclic triaxial loading. *Géotechnique*. 57(6):
7 pp.527–536
- 8 Lim, W. L., & McDowell, G. R. (2005). Discrete element modelling of railway ballast. *Granular*
9 *Matter*. 7(1): pp.19-29.
- 10 Liu, S. H. (2006). Simulating a direct shear box test by DEM. *Canadian Geotechnical Journal*.
11 43(2): pp. 155-168.
- 12 Lobo-Guerrero, S, & Vallejo, L. E. (2006). Discrete element method analysis of railtrack ballast
13 degradation during cyclic loading. *Granular Matter*. 8(3-4): pp.195-204.
- 14 Lu, M., & McDowell, G. R. (2006). Discrete element modelling of ballast abrasion.
15 *Géotechnique*. 56(9): pp.651-655.
- 16 Lu, M., & McDowell, G. R. (2007). The importance of modelling ballast particle shape in the
17 discrete element method. *Granular Matter*. 9(1-2): pp.69-80.
- 18 Lu, M., & McDowell, G. R. (2008). Discrete element modelling of railway ballast under triaxial
19 conditions. *Geomechanics and Geoengineering: An International Journal*. 3(4): pp.257-270.
- 20 Marsal, R. J. (1973), Mechanical Properties of Rockfill. *In: Embankment Dam Engineering*.
21 Wiley, New York, pp. 109-200.
- 22 Marachi, N. D. (1969). Strength and deformation characteristics of rockfill materials. *PhD*
23 *Thesis*. University of California.

- 1 McDowell, G. R., Harireche, O., Konietzky, H., Brown, S. F., & Thom, N. H. (2006). Discrete
2 element modelling of geogrid-reinforced aggregates. *Geotechnical Engineering* 159(GE1):
3 pp.35-48.
- 4 Ni, Q., Powrie, W., Zhang, X., & Harkness, R. (2000). Effect of particle properties on soil
5 behaviour: 3-D numerical modelling of shearbox test. *Geotechnical Special Publication* 96,
6 *ASCE*: pp.58-70.
- 7 Oda, M., & Iwashita, K. (1999). *Mechanics of granular materials: An introduction*. Rotterdam:
8 A. A. Balkema.
- 9 O'Sullivan, C., Cui, L., & O'Neill, S. C. (2008). Discrete element analysis of the response of
10 granular materials during cyclic loading. *Soils and Foundations*. 48(4): pp:511-530
- 11 O'Sullivan C., & Cui, L. (2009). Micromechanics of granular material response during load
12 reversals: Combined DEM and experimental study. *Powder Technology*. 193: pp:289-302
- 13 O'Sullivan C. (2011). *Particulate Discrete Element Modelling: A Geomechanics Perspective*.
14 Spon Press, London.
- 15 Selig, E. T. & Waters, J. M. (1994). *Track geotechnology and substructure management*. Thomas
16 Telford, London.
- 17 Sitharam, T. G., & Vinod, J. S. (2005). Shear behavior of glass beads using DEM. *Proceedings*
18 *of the 5th International Conference on Micromechanics of Granular Media (Vol.1)*. Stuttgart,
19 Germany.
- 20 Sitharam, T. G., & Vinod, J. S. (2008). Numerical simulation of liquefaction and pore pressure
21 generation in granular materials using DEM. *International Journal of Geotechnical Engineering*.
22 2(2): pp.103-113.
- 23 Sitharam, T. G., & Vinod, J. S. (2009). Critical state behaviour of granular materials from
24 isotropic and rebounded paths: DEM simulations. *Granular Matter*. 11(1): pp.33-42.

- 1 Suiker, A. S. J., Selig, E. T., & Frenkel, R. (2005). Static and cyclic triaxial testing of ballast and
2 subballast. *Journal of Geotechnical and Geoenvironmental Engineering Computations*. 131(6):
3 pp.771–782.
- 4 Thakur, P. K., Vinod, J. S., & Indraratna, B. (2010). Effect of particle breakage on cyclic
5 densification of ballast: A DEM approach. *Materials Science and Engineering*. 10: pp.1-7.
- 6 Tutumluer, E., Huang, H., Hashash, Y., & Ghaboussi, J. (2007). Discrete element modeling of
7 railroad ballast settlement. *Proceedings of the AREMA 2007 Annual Conference*. Chicago, IL,
8 USA.
- 9 Tutumluer, E., Dombrow, W., & Huang, H. (2008). Laboratory characterization of coal dust
10 fouled ballast behavior. *Proceedings of the AREMA 2008 Annual Conference*. Salt Lake City,
11 UT, USA.
- 12 Wang, J., Dove, J. E., & Gutierrez, M. S. (2007). Discrete-continuum analysis of shear banding
13 in the direct shear test. *Géotechnique*. 57(6): pp. 513–526.
- 14
- 15 Zhang, L. & C. Thornton (2007). A numerical examination of the direct shear test.
16 *Géotechnique*. 57(4): pp.343–354.

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3 **10. List of Tables**

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6 specific VCI

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1 Table 1. Micro-mechanical parameters adopted for ballast and shear box boundary walls in
2 DEM

Micromechanical parameters	Values
Contact normal stiffness k_n (N/m)	0.52×10^8
Contact shear stiffness k_s (N/m)	0.52×10^8
Inter-particle coefficient of friction μ	0.8
Contact normal stiffness of wall-particle, k_{n-wall} (N/m)	1×10^8
Shear stiffness of wall of wall-particle, k_{s-wall} (N/m)	1×10^8
Particle density (kg/m^3)	2700

3
4 Table 2. Micro-mechanical parameters adopted for coal fines to simulate fouled ballast at a
5 specific VCI

VCI (%)	Contact normal stiffness, k_n (N/m)	Contact shear stiffness, k_s (N/m)	Inter-particle coefficient of friction of coal fine, μ	Number of added balls to simulate fouling	Inter-particle coefficient of friction of fouled ballast assembly
20	1.27×10^4	1.27×10^4	0.2	72,833	0.72
40	1.27×10^4	1.27×10^4	0.2	145,665	0.65
70	1.27×10^4	1.27×10^4	0.2	252,113	0.58

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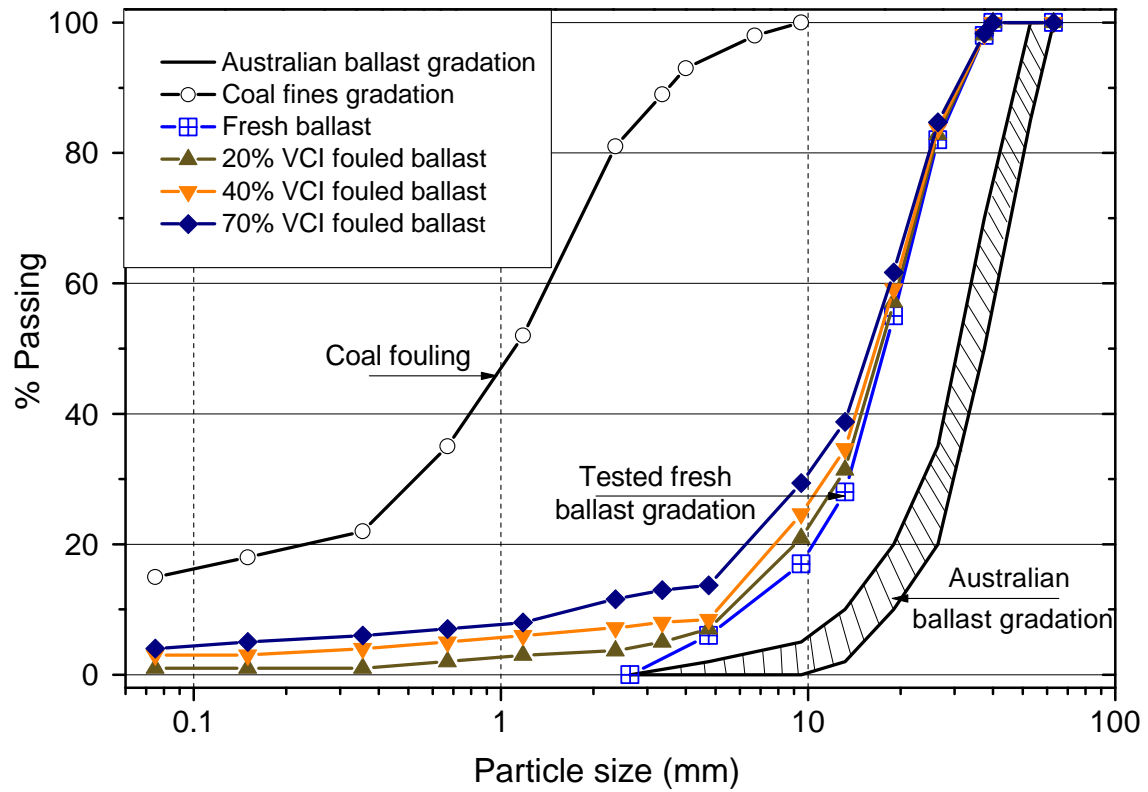
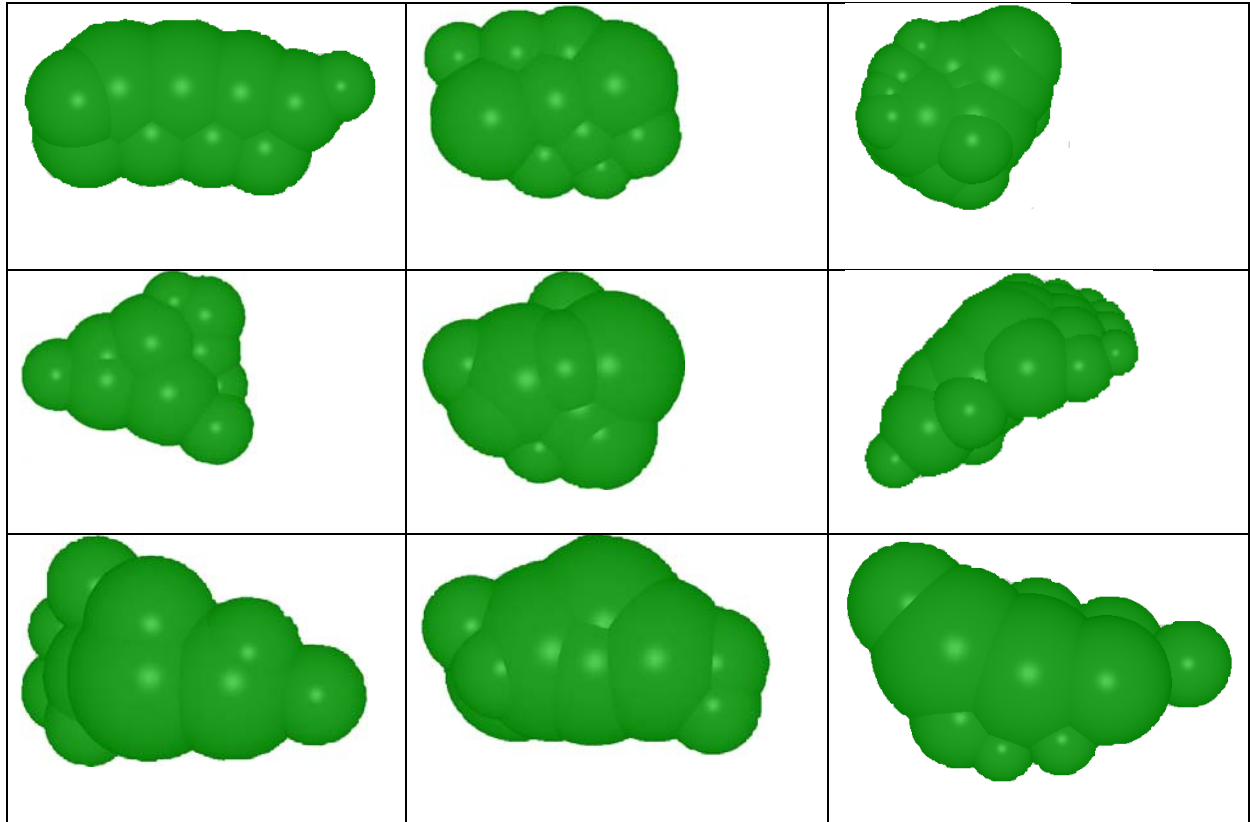


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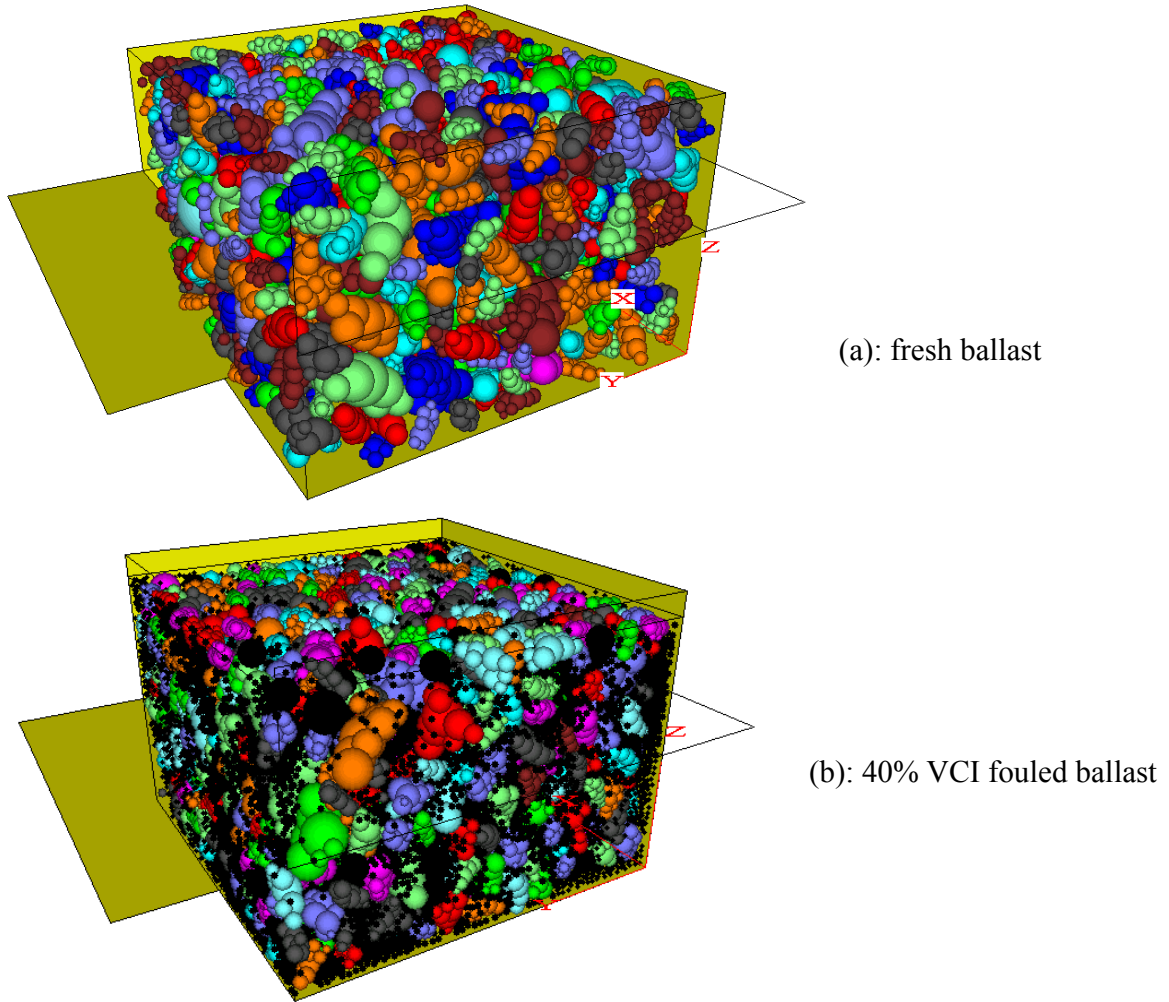


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2 Figure 2. Library of ballast particle shapes simulated in DEM

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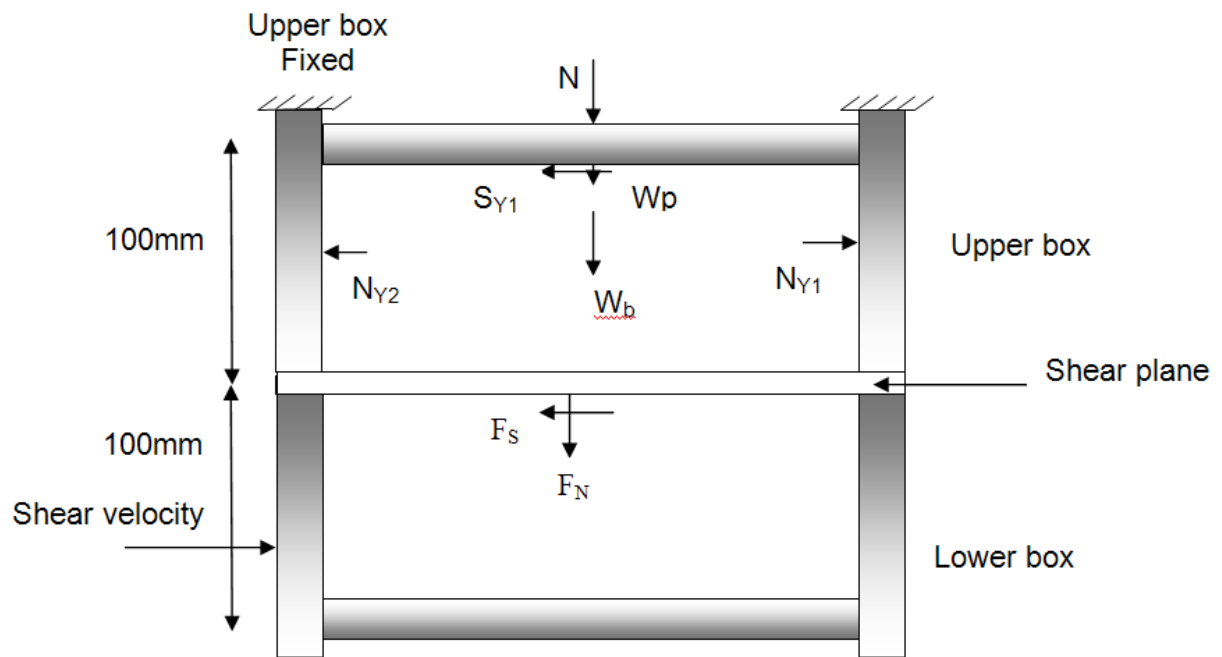
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4 Figure 3. Initial assembly of large-scale direct shear test with irregular shaped particles, (a) fresh
5 ballast and (b) 40%VCI fouled ballast



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2 Figure 4. Schematic diagram of forces acting in the direct shear box (not to scale)

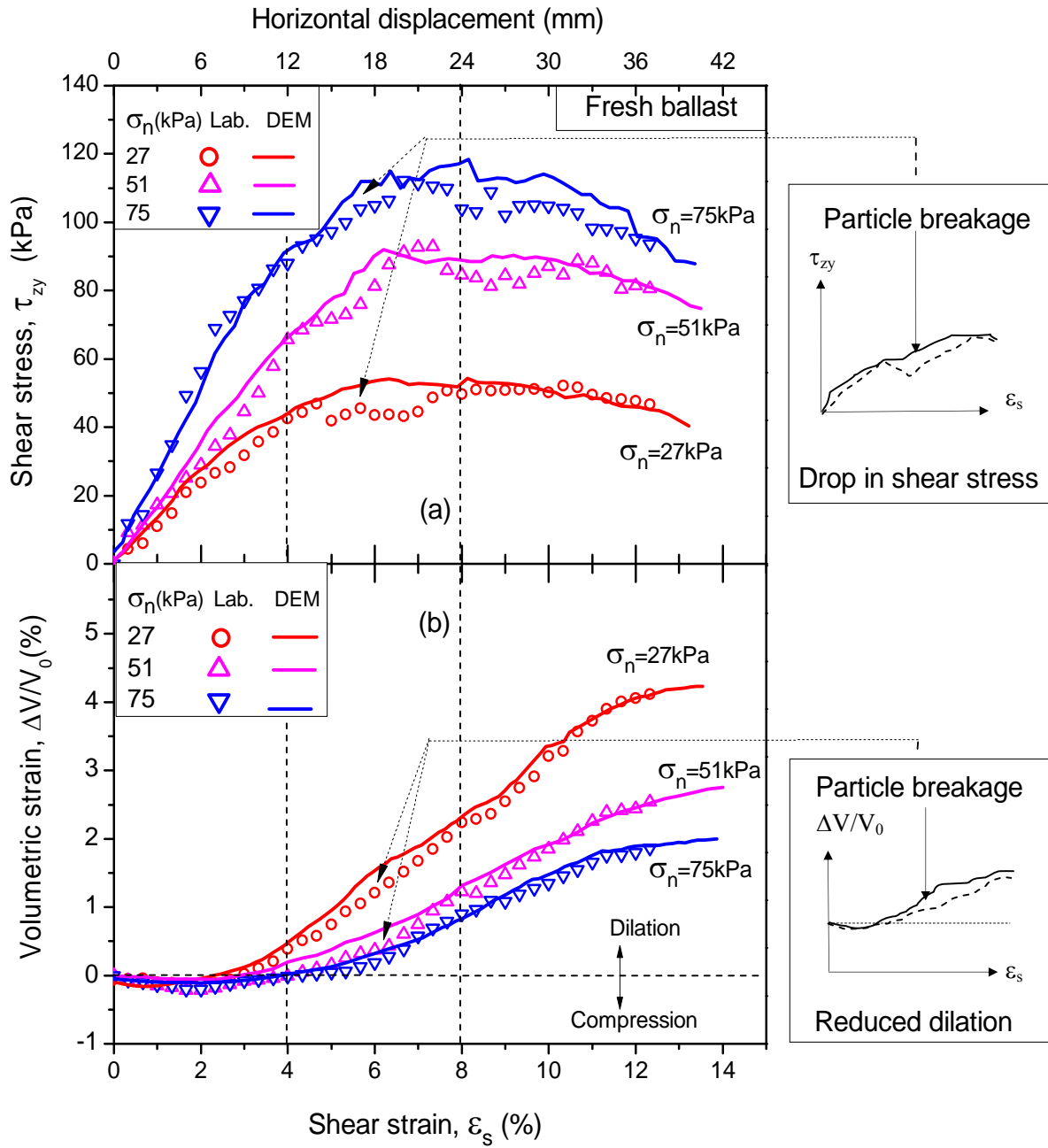
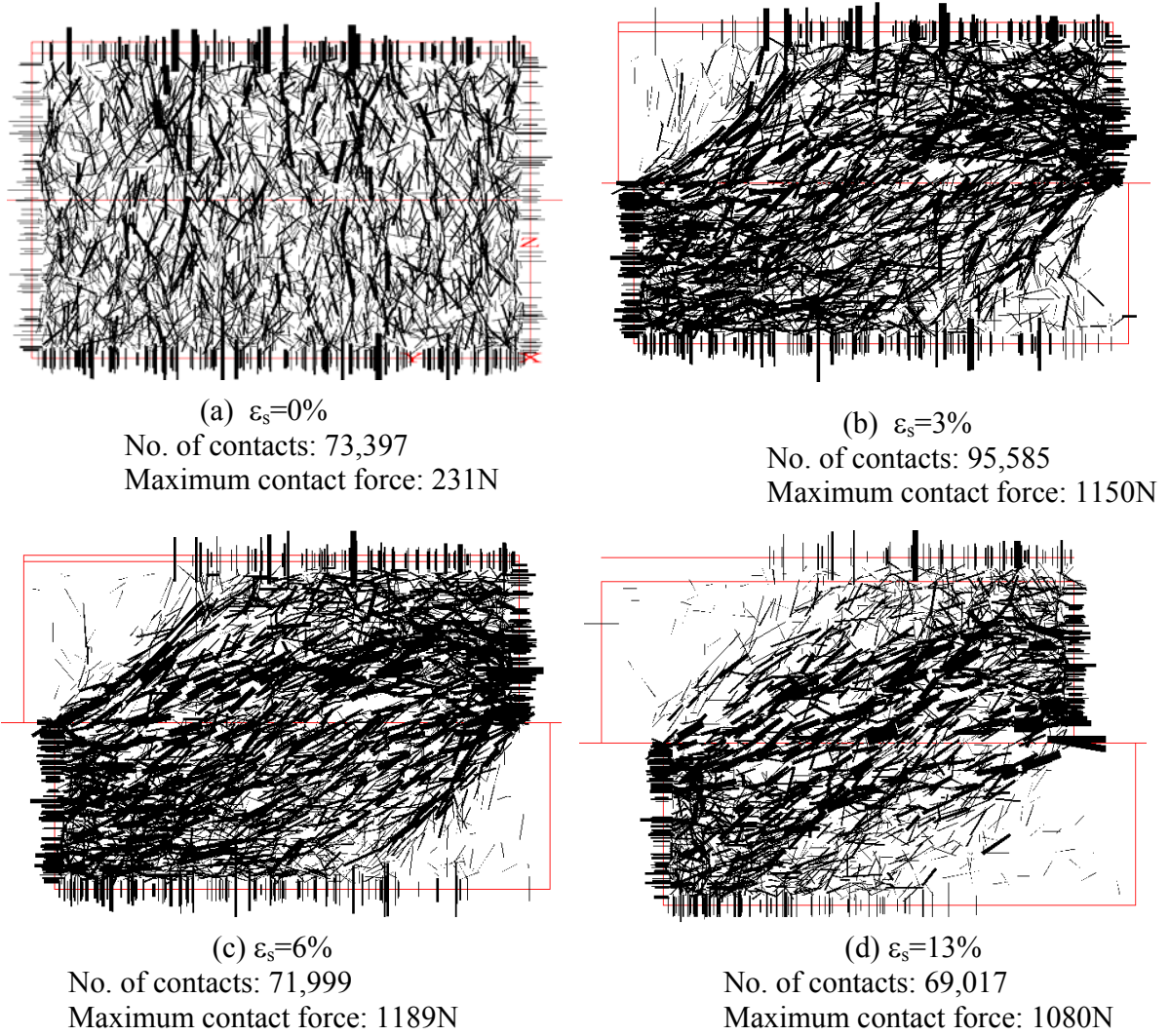
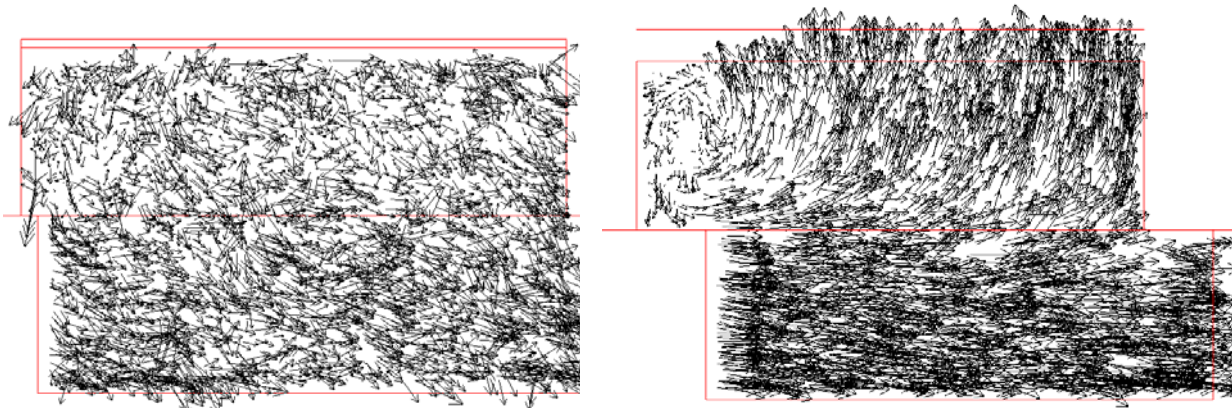


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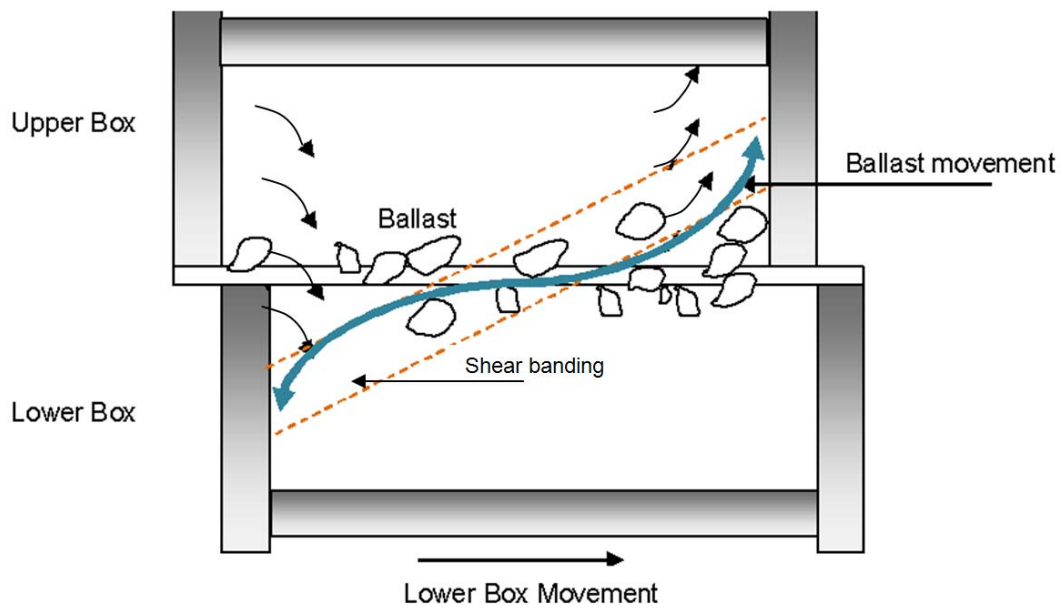


3 Figure 6. Distribution of contact forces in fresh ballast for a normal stress of 51kPa, (a) at shear
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(a)

(b)



(c)

Figure 7. Displacement vectors of particles in the shear box for a normal stress of 51kPa, (a) at a shear strain $\epsilon_s = 3\%$, (b) at a shear strain $\epsilon_s = 13\%$ and (c) a schematic diagram of the conceptual movement of ballast particles in direct shear testing

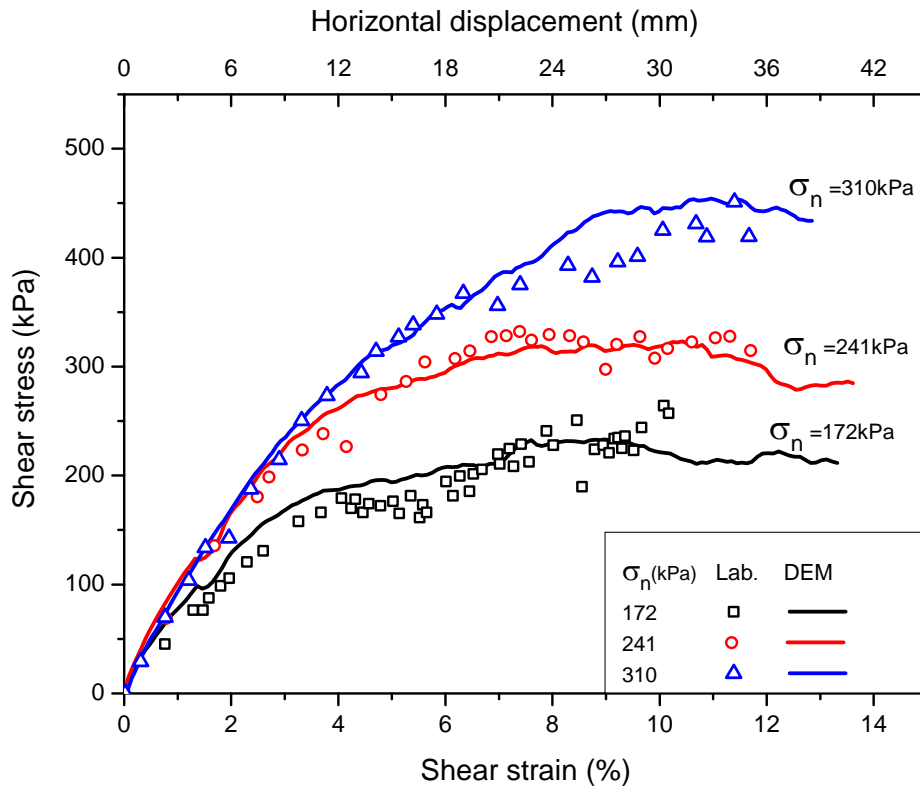


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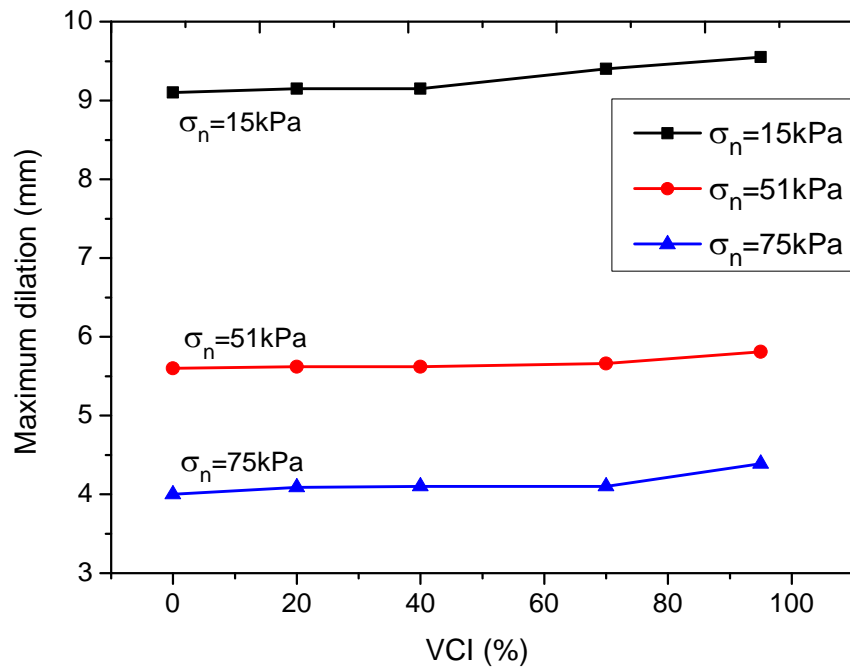
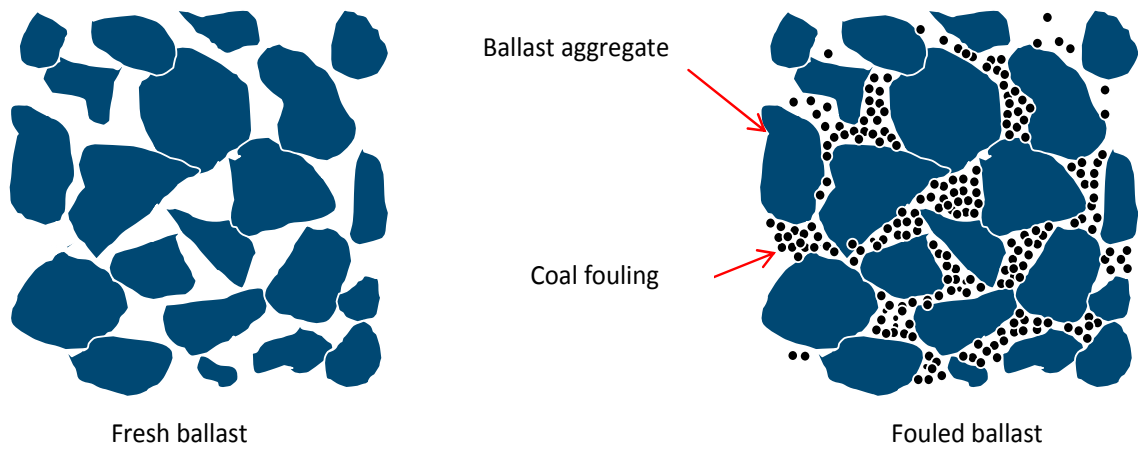
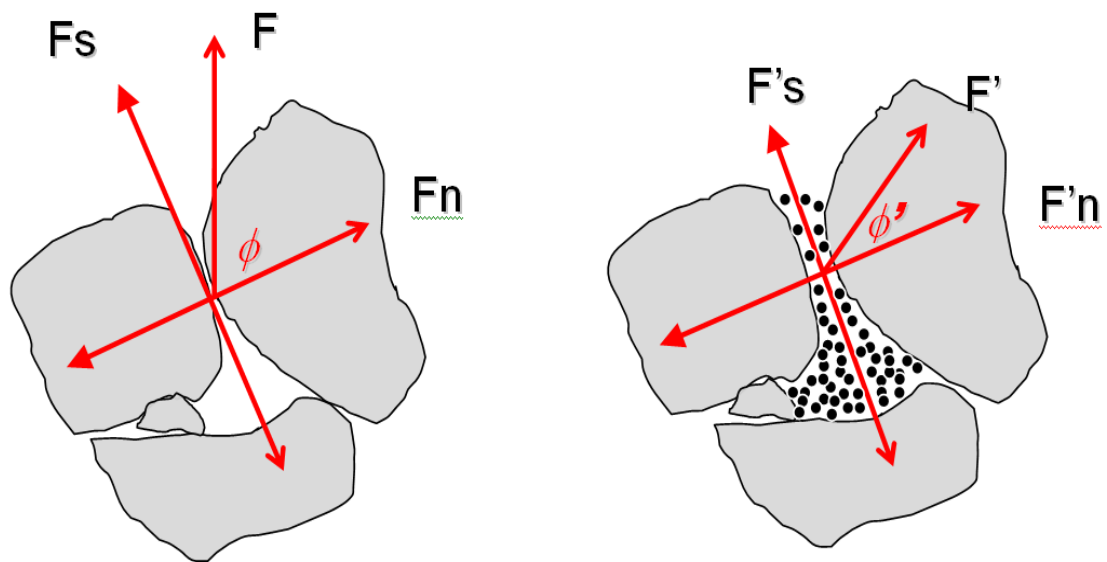


Figure 9. The variation in maximum dilation (at the end of shearing) of fouled ballast with various VCIs ranging from 0% to 95%, measured experimentally by the Authors



(a) small spherical balls added to simulate fouled ballast



Fresh ballast, inter-particle friction angle ϕ

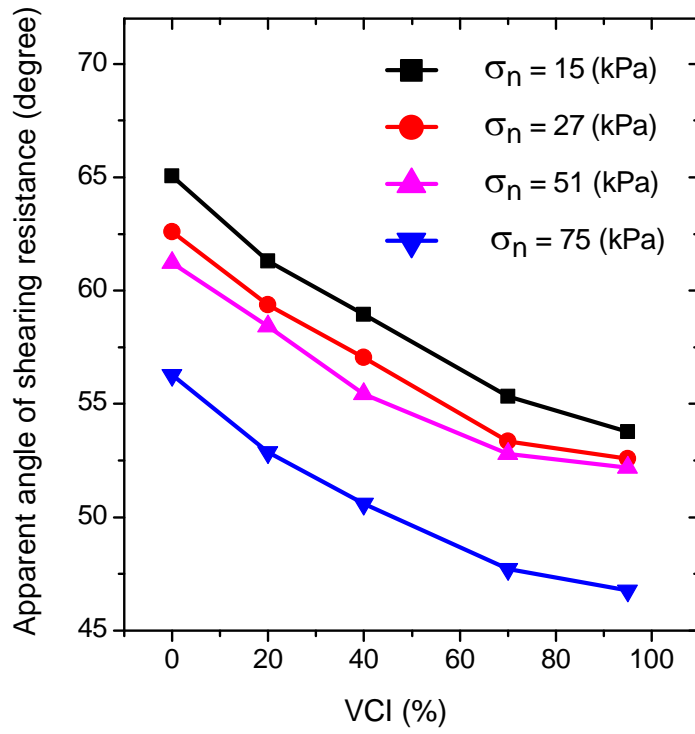
Fouled ballast, inter-particle friction angle ϕ'

(b) inter-particle coefficient of friction reduced to simulate fouled ballast

1

2 Figure 10. A combined method for modelling fouled ballast, (a) small spherical balls added to

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1
 2 Figure 11. Effect of VCI on the apparent angle of shearing resistance of fouled ballast, measured
 3 experimentally by the Authors

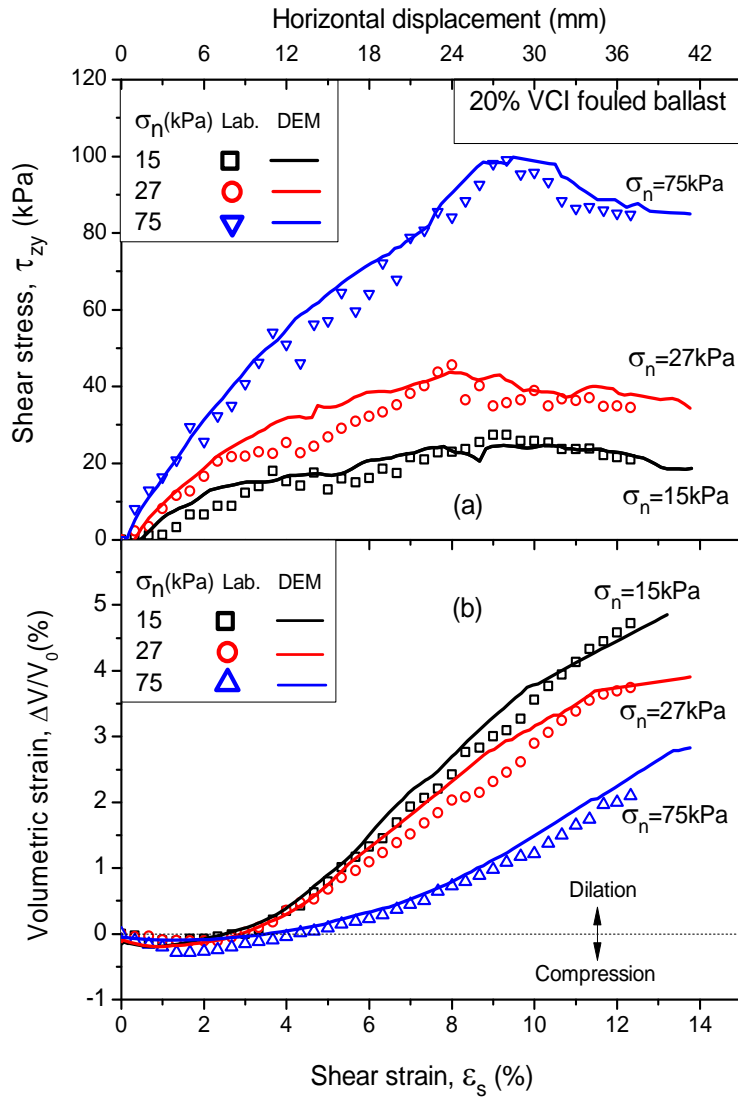
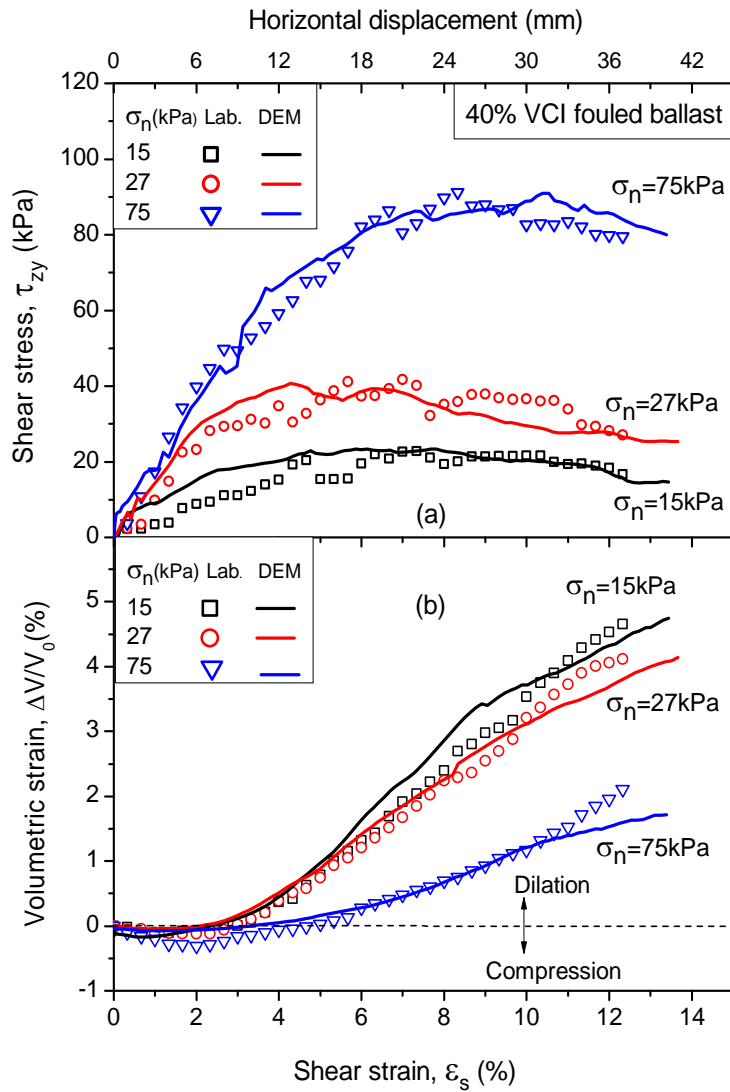
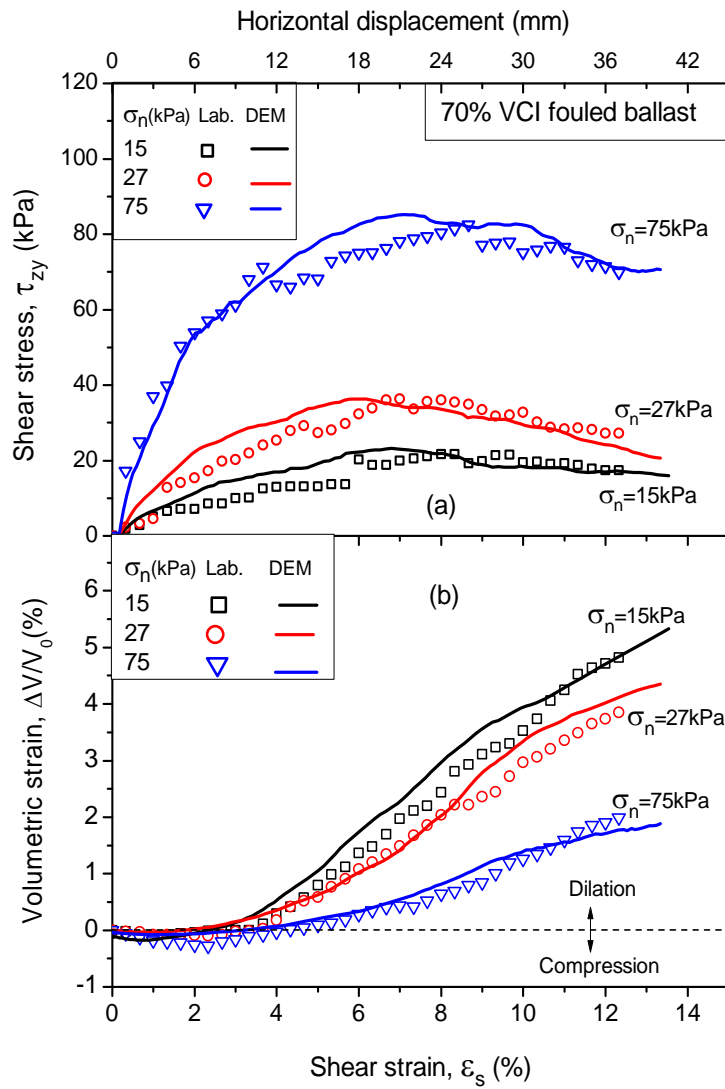


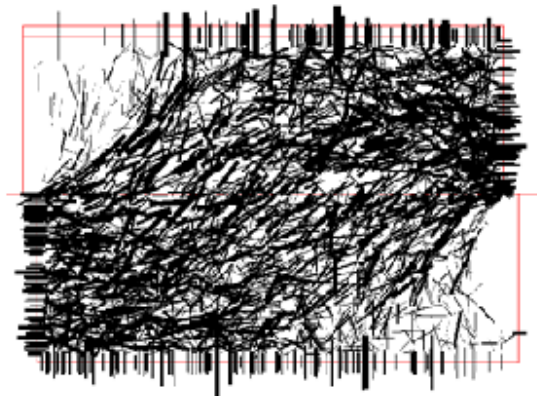
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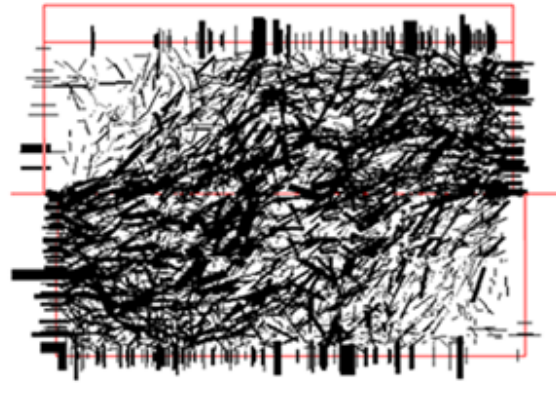
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2 Figure 13. Comparisons between the DEM simulation and experiment for 40%VCI fouled ballast
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4 volumetric strain versus shear strain



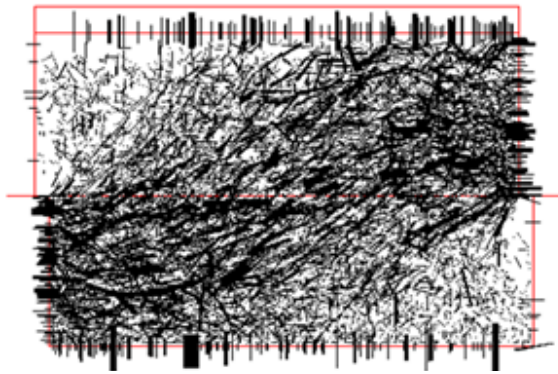
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2 Figure 14. Comparisons between the DEM simulation and experiment for 70%VCI fouled ballast
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4 volumetric strain versus shear strain



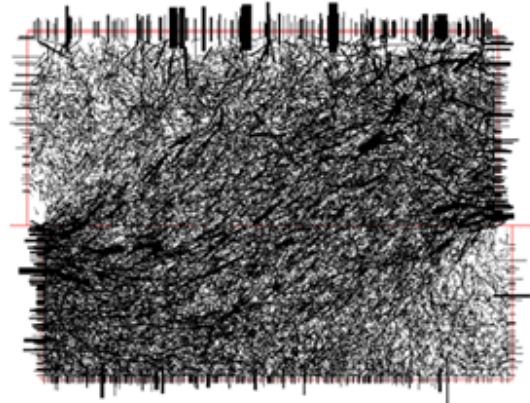
(a) VCI=0%
No. of contacts: 95,585
Maximum contact force: 1150(N)



(b) VCI=20%
No. of contacts: 285,445
Maximum contact force: 839(N)



(c) VCI=40%
No. of contacts: 519,818
Maximum contact force: 560(N)



(d) VCI=70%
No. of contacts: 936,450
Maximum contact force: 414(N)

1

2 Figure 15. Evolution of the distribution of contact forces in fresh and fouled ballast at various

3 VCIs (at 3% shear strain), (a) 0% VCI, (b) 20%VCI, (c) 40% VCI and (d) 70% VCI

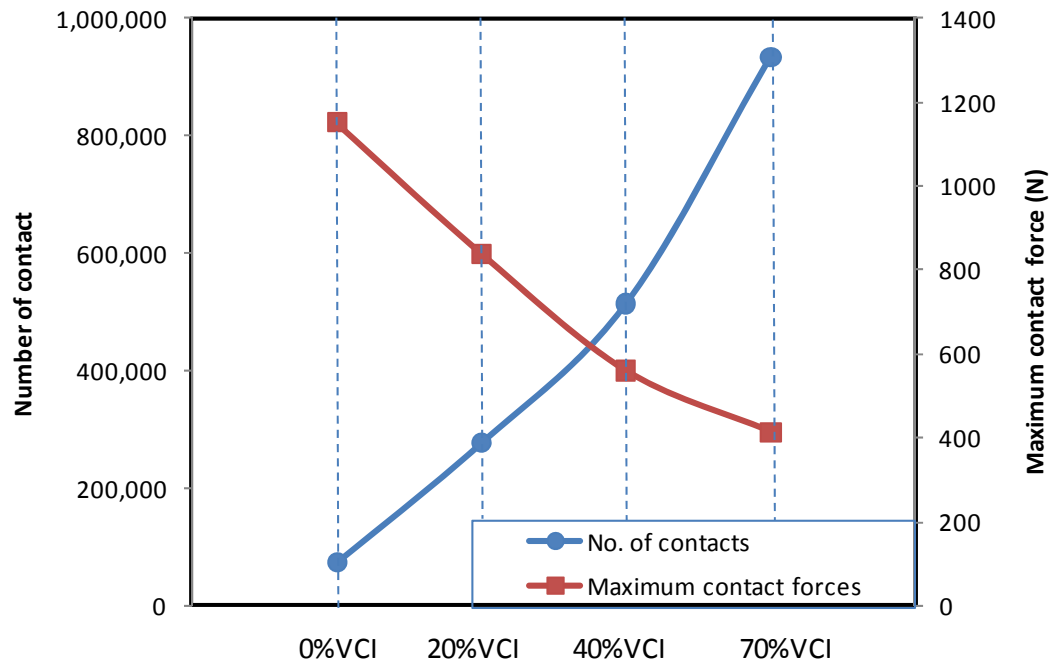


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