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META-MODELLING OF PARTICLE BREAKAGE CHARACTERISTICS IN DEM SIMULATION

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Particle breakage plays an important role in determination of the physical and mechanical properties of granular materials. Limited by the unrepeatability and high expense of direct laboratory particle breakage tests, numerical methods (e.g., Discrete Element Method (DEM)) are often used to investigate the mechanism of particle breakage and corresponding soil macro-mechanical responses. However, the computational efforts of these numerical methods can be prohibitively expensive subjected to the situations, where a larger number of disk or sphere elements are used to approximately represent the soil matrix, or an accurate and high resolution prediction, where selection of micro input parameters needs thousands of trials. To address this difficulty, this study combines the Hermit Stochastic Response Surface (HSRS) with DEM analysis to predict the single particle breakage responses. The DEM analysis of particle breakage is first performed using PFC3D software with a set of predefined empirical input parameters. With this preliminary analysis, a fourth-order HSRS is established to predict the responses of single particle breakage. It is found that the fourth-order HSRS can predict the breakage characteristics of DEM simulation reasonably well. With the aid of HSRS, the calibration of micro input parameters can be accomplished with relative ease. It shows that DEM analysis using the parameters calibrated from HSRS can characterize the particle breakage behavior more realistically compared with that based on the conventional empirical parameters.

Keywords: Meta-modelling, Discrete Element Method, Particle Breakage Characteristics, Hermit Stochastic Response Surface

1 Introduction

Engineering properties of granular materials (such as volume change, stress-strain and strength behavior) are significantly affected by particle breakage, which results in changes of stress imposed on the particle (Bono and Mcdowell 2014). Therefore, it is pivotal to investigate the mechanism of particle breakage. In past two decades, many particle breakage tests have been conducted to reveal the relationship between individual particle breakage and macro mechanical responses of granular materials. Nakata et al. (1999) carried out an individual particle crushing test and triaxial compression tests with crushable sand particles, indicating that individual particle crushing strength in triaxial sand samples follows Weibull's distribution. Nakata et al. (2001) further examined this relationship with the consideration of particle size and soil grading. These studies provide valuable insights to facilitate the understanding of macro-mechanical behavior of crushable soil. However, it offers little information about fundamental micro-mechanical principles of individual particle breakage due to its limitation on tracking the particle internal stress-strain/force chain evolution in micro scale. Moreover, direct laboratory tests have high standards for particle breakage test apparatus.

Due to the above limitations of direct laboratory tests, DEM (Cundall and Strack, 1979) has drawn more and more attentions in recent years because it allows for the effective observation of particle breakage characteristics in a micro scale. Wang et al. (2013) investigated the effect of particle breakage on the shear failure behavior of granular soils using a Bonded Particle Model (BPM) in DEM, where a linear parallel bond was set among the contact spheres in an agglomerate to simulate the crushable sand particles. Wang et al. (2017) also used the BPM to model the single-particle crushing test of ballast stones. Note that the computational burden of DEM analysis shall increase significantly with the number of disk or sphere elements used in the analysis. Therefore, most of DEM studies only focus on small scale problems where only a small number of disks or spheres can be used to represent the natural soil matrix. In addition, for more accurate and reliable analyses, selection of suitable micro input parameters is a time-consuming task because it involves many trial-and-error procedures which need repeated DEM simulations. In order to reduce the computational efforts, one possible way is to employ the surrogate model to approximately represent the relationship between the input parameters of DEM analysis and the output responses concerned. Surrogate models have many successful applications in approximating the numerical analysis models, such as finite element model, limit equilibrium analysis model, and finite difference model (Li et al. 2011, 2016). Although some attempts have been made to use surrogate model to predict the stress-strain and volumetric strain-strain responses for granular soils under DEM formwork (Ellis et al. 1995, Li et al. 2017), the particle breakage is not taken into account therein.

This study employs the Hermit Stochastic Response Surface (HSRS) to predict the particle break characteristics (such as breakage displacement and force). This paper starts with a brief review of direct laboratory test of single particle crushing, followed by the development of numerical model for particle breakage simulation using DEM. Then, the HSRS is applied to predicting the particle breakage responses. Finally, the performance of HSRS is demonstrated with the single quartz sand particle crushing example and the micro contact model parameters are calibrated based on the HSRS to simulate the single quartz sand particle breakage behavior.

2 Single Particle Crushing Test

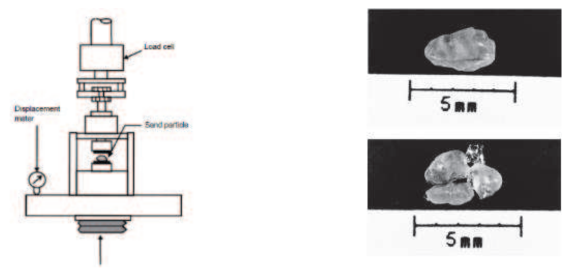
Particle crushing is a common phenomenon when the stress exerted on a soil particle exceeds its strength. Determination of this particle crushing strength needs sophisticate and specific apparatus. Consider, for example, Fig. 1(a) shows the schematic diagram of particle crushing test apparatus used by Nakata et al. (1999). The crushing test is conducted by fixing the soil particle between upper and lower hardened platens and then moving the lower platen at a constant rate of displacement to press the particle. In that experiment, the removable hardened platens has a diameter of 30 mm and the load-measuring capacity is 500 N with a resolution of 0.01N. During the test, a load rate of 0.1mm/min is used to crush the particle, and the force and displacement are measured at a certain time interval. The strength of particle breakage then can be obtained at the peak force. Fig. 1(b) also gives the photographs of quartz sand particle before and after the single-particle crushing test.

3 Particle Crushing Simulation Using DEM

Although the laboratory test of particle crushing using aforementioned apparatus can provide accurate strength of particle breakage, it is expensive to perform the test and difficult to control the experimental conditions. Therefore, studying particle crushing using DEM become more attractive due to its low cost and easy-to-control of loading conditions. More importantly, DEM makes it possible to track the micro-mechanical evolution of stress/strain occurred within the single particle during the crushing process. There are two commonly-used approaches for

Table 1 DEM simulation parameters in the single particle crushing test

Parameter properties	Parameter Values
Density of ball (kg/m^3)	2650
Normal and shear stiffness of ball (N/m)	1.48×10^7
Friction coefficient of ball	0.50
Normal and shear parallel bond stiffness (N/m^3)	5.00×10^{14}
Normal and shear parallel bond strength (N/m^2)	5.00×10^8
Ratio of parallel bond radius to ball radius	0.50

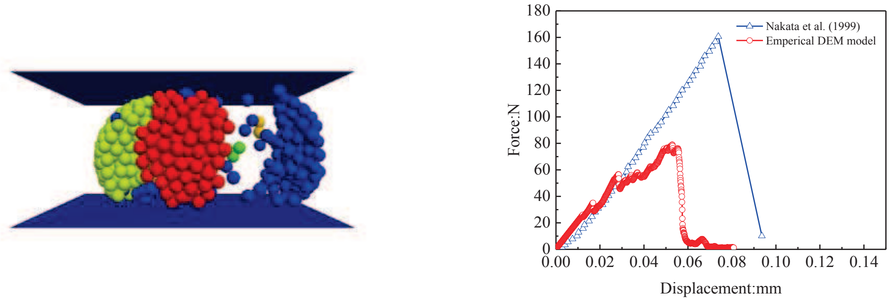


(a) (b)

Fig.1 (a) Particle-crushing apparatus; (b) quartz sand particle before and after the single-particle crushing test (after Nakata et al. 1999)

simulating particle breakage under the DEM framework. One approach simulates the particle breakage by replacing the original disks or spheres with several smaller ones (Zhou et al. 2014), some of which can be crushed by replacing them with even smaller elements once the stress applied to them reaches their strength that follows an empirical distribution. The second approach uses numerous smaller disks or spheres to form a porous agglomerate to represent the original particle. During the simulation, these elements are bonded together by BPM method to simulate the particle internal fabric and structure. The bond is deleted if the stress exceeds its strength. The second approach is more straightforward because it can, realistically, simulate the breakage process and does not need sophisticated algorithms to describe the fractal breakage phenomenon (Wang et al. 2017).

This study employs the second approach to simulate the single quartz sand particle crushing. Similar to Wang et al. (2013), the quartz sand particle is modelled with a 2.0 mm agglomerate constituted by 558 elementary balls. The diameter of elementary ball is 0.2 mm. All the elementary balls filling in agglomerate first balance down to make the agglomerate reach quasi-static state. The linear parallel bond contact model is applied to all contacts existing among the elementary balls within the agglomerate while the contact model between loading platen and particles is taken as the linear contact model. The loading platen is modelled by the top and bottom walls, which move towards each other at a constant velocity to form the pressure load. During the loading process, the force and displacement of walls are recorded until the particle is fractured into several small fragments. The micro input parameters of DEM simulation are summarized in Table 1, which follows McDowell et al. (2002) and Wang et al. (2013). Fig. 2(a) shows the numerical particle breakage contour. Compared with Fig. 1(b), it is observed that the DEM analysis can, realistically, reflect the particle crushing characteristics. Fig. 2(b) also compares the force-displacement curve obtained from laboratory test and that from DEM analysis. The two curves agree well with each other in term of the shape and trend, while, for the peak breakage strength obtained from the DEM analysis is lower than that from the laboratory tests. This might be resulted from the inappropriate selection of micro input parameters (such as strength parameters)



(a) (b)

Fig. 2 (a) Particle breakage contour; (b) Quartz sand particle breakage force-displacement curve

needed in the parallel bond model. Choosing suitable parameters in DEM analysis relies on a procedure of trial and error, which needs repeated simulations of the original BPM particle crushing model. In addition, there are more than one model parameters to be determined. Hence, determination of a set of ideal parameters through trial and error is time-consuming and sometimes ineffective, particular for a large number of unknown parameters. In this study, the Hermit Stochastic Response Surface (HSRS) is adopted to build the relationship between the particle breakage characteristics and unknown parameters of concern, which is detailed in the following.

4 Breakage characteristics prediction using HSRS

This section employs the HSRS to predict the particle breakage characteristics. HSRS can be treated as a mathematical function formed by a number of Hermite polynomials with explicit forms, which can be expressed as,

$$
\begin{aligned}
F(\boldsymbol{U}) = a_0 &+ \sum_{i_1=1}^{n} a_{i_1}\Gamma_1(U_{i_1}) + \sum_{i_1=1}^{n}\sum_{i_2=1}^{i_1} a_{i_1 i_2}\Gamma_2(U_{i_1},U_{i_2}) + \sum_{i_1=1}^{n}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3}\Gamma_3(U_{i_1},U_{i_2},U_{i3}) \\
&+\cdots+\sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2}\cdots\sum_{i_n=1}^{i_{n-1}} a_{i_1 i_2,\cdots,i_n}\Gamma_n(U_{i_1},U_{i_2},\cdots,U_{i_n})
\end{aligned}
\tag{1}
$$

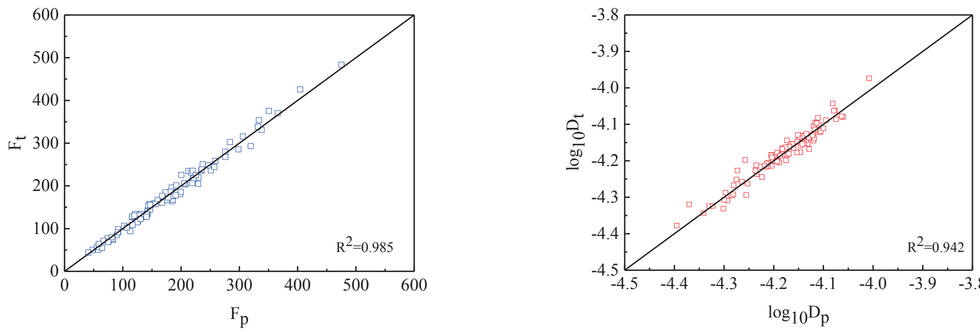
Where $F(\boldsymbol{U})$ is the response of interested; $a_{i_1 i_2,\ldots,i_n}$ are the unknown coefficients to be estimated; n is the number of uncertain parameters in the model; $\boldsymbol{U} = \left(U_{i_1}, U_{i_2} \ldots, U_{i_n}\right)$ is the vector of independent standard normal variables; $\Gamma_n\left(U_{i_1}, U_{i_2} \ldots, U_{i_n}\right)$ is multidimensional Hermite polynomials of the order of n. Herein, the particle breakage responses (i.e., peak force and its corresponding displacement) are concerned as target responses. The micro input parameters that have considerable effects on the particle strength (such as stiffness of parallel bond, strength of parallel bond and the ratio of parallel bond radius to ball radius) are treated as uncertain random variables in the HSRS. Table 2 summarizes the typical ranges of linear parallel bond contact parameters used in DEM simulation of particle crushing. These parameters are assumed to be independent and follow uniform distribution, which should be first transformed into independent standard normal variables for the construction of HSRS. To solve the unknown coefficients in the HSRS, a certain number of collocation points are chosen as the training samples. In this study, 105 collocation points are selected through Latin Hypercube Sampling in initial sample space to construct a fourth-order HSRS. BPM crushing model is then performed 105 times with the 105 collocation points as the input micro bond parameters to calculate the peak force of particle breakage and its corresponding displacement. With the results of initial samples, HRSR is established between the peak force F, the logarithm of breakage displacement D and the three

Table 2 Typical ranges of linear parallel bond parameters in DEM simulation of single particle crushing

Parallel bond parameters	Ranges of parameter value
Normal and shear parallel bond stiffness (N/m^3)	4.00×10^{14}-10.00×10^{14}
Normal and shear parallel bond strength (N/m^2)	4.00×10^{14}-10.00×10^{14}
Ratio of parallel bond radius to ball radius	0.40-0.80

Table 3 Calibrated linear parallel bond parameters in the single particle crushing simulation

Linear parallel bond parameters	Values
Normal and shear parallel bond stiffness (N/m^3)	4.98×10^{14}
Normal and shear parallel bond strength (N/m^2)	9.27×10^{8}
Ratio of parallel bond radius to ball radius	0.47



(a) (b)

Fig.3 Comparison of particle breakage characteristics between DEM simulation and HSRS prediction: (a) breakage force *F*; (b) the logarithm of breakage displacement *D*

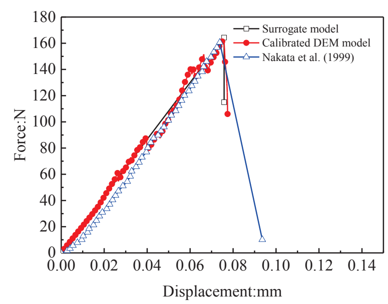


Fig.4 Force-displacement curves based on the calibrated parameters and the laboratory test

undetermined micro parameters. Interested readers are referred to Li et al. (2011) for the more details on the construction of HSRS.

Fig. 3 shows the fitting accuracy between DEM simulations results (F_t, $log_{10}D_t$) and predictions of fourth-order HSRS (F_p, $log_{10}D_p$) calculated based on 100 extra random samples drawn from the distribution of micro input parameters. It indicates that the fourth-order HSRS can predict the particle breakage responses reasonably well. The procedure of trial and error for selection of suitable micro parameters is then performed based on the HSRS. With the aid of HSRS, a set of linear parallel bond parameters are obtained by trial and error procedures and are shown in Table 3. To validate the reliability of the selected parameters, DEM analysis is performed again using the new micro parameters. The force-displacement curve of DEM analysis is plotted in Fig. 4. The result obtained from the HSRS using the new set of micro parameters given in Table 3 is consistent with that obtained from the laboratory test result by Nakata et al.

(1999). It is found that the DEM analysis can predict the peak breakage strength much more accurately using the micro parameters calibrated through HSRS compared with that (see shown Fig. 2(b) using empirical values. With the parameters calibrated from HSRS, the HSRS also provides reasonably accurate estimates of particle breakage responses.

5 Conclusion

This study combines the Hermit Stochastic Response Surface (HSRS) with DEM analysis to predict the particle break responses. The DEM analysis of quartz particle breakage using BPM method is first performed using DEM commercial software PFC3D. To reduce the computation efforts and construct an explicit relationship between the breakage responses and micro bond parameters, a fourth-order HSRS is established and validated. With the aid of HSRS, selection of micro input parameters becomes an effortless task. It is shown that DEM analysis using the parameters calibrated from HSRS provides the particle breakage behavior more realistically compared with that using empirical parameters. It should be noted that although only a single particle breakage example is used to illustrate the effectiveness and advantages of HSRS in prediction of DEM responses, the application of surrogate models in large scale problems is promising.

Acknowledgments

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