

# Bonded particle models for discrete element simulation of porous granules

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The growing interest in granular materials used in mechanical applications, for example as crash absorbers in ship collisions, leads to an increased need for numerical models to simulate such granules. Since, in the case of an application as a crash absorber, the fracture behaviour of the granules is of particular interest, the numerical models must be able to simulate the breakage and predict, for example, the energy dissipation during fracture. For this purpose, a discrete element method is used together with a bonded particle model. Since the bond model mainly affects the fracture of particles, this work focuses on new models and their influence on the breaking behaviour of granules.

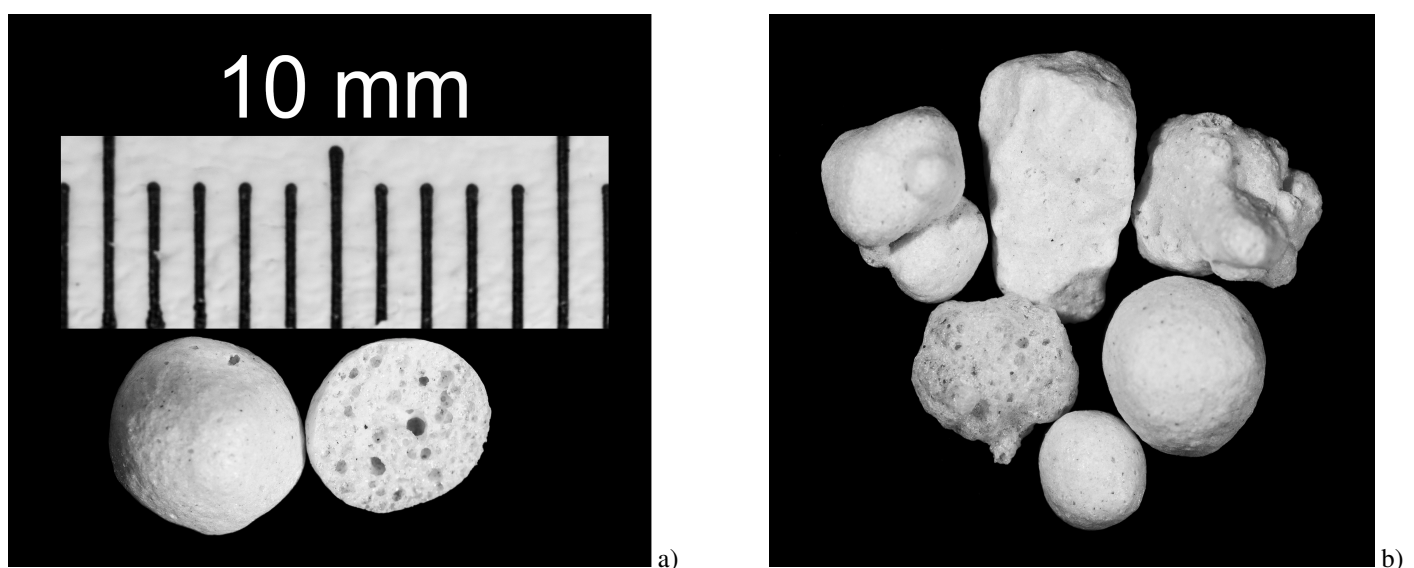
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## 1 Introduction

Functional particles are widely used in various applications, for example as building or carrier material [1] or as crash absorbers in the automotive, aircraft and marine industries [2]. The granular material investigated in this work is to be used to increase the collision safety of ships. For this purpose, as presented in [4], the double hull of a ship is filled with granules. This approach is based on the idea of transferring occurring collision loads from inner to outer hull and dissipating energy through crushing particles. Since collision experiments [5] in which both phenomena could be studied are very expensive, a way to numerically capture the crushing behaviour of the particles is investigated instead. For this purpose, simulations are performed using the discrete element method (DEM). To enable the computation of particle breakage, DEM is combined with a bonded particle approach [6]. As the breakage behaviour is crucial for load transfer between the hulls and energy dissipation, special attention is given to the bonded particle method and leading models. In the following sections, both the material used and the numerical method are described. Then, some simulation results are presented and discussed, concluding with a brief summary of the results in the last section.

## 2 Material and methods

Based on the results of experiments presented in [7], Poraver expanded glass is chosen for further numerical investigations. Poraver meets all the necessary requirements to be used as a filling material in marine applications [4] and dissipates energy

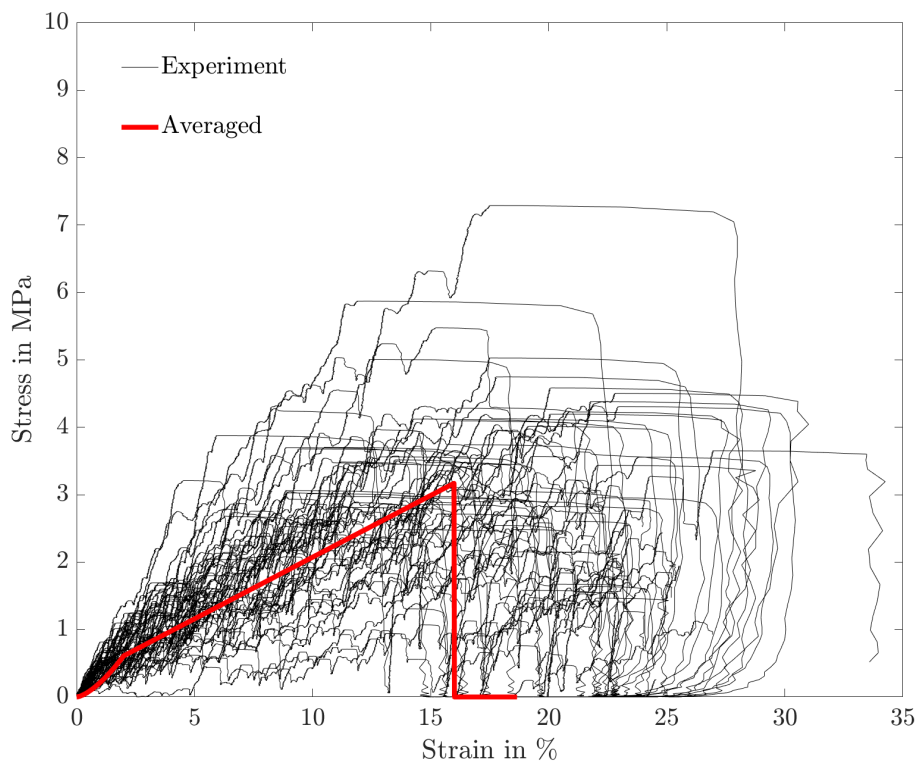


**Fig. 1:** Inner structure and shape of Poraver particles

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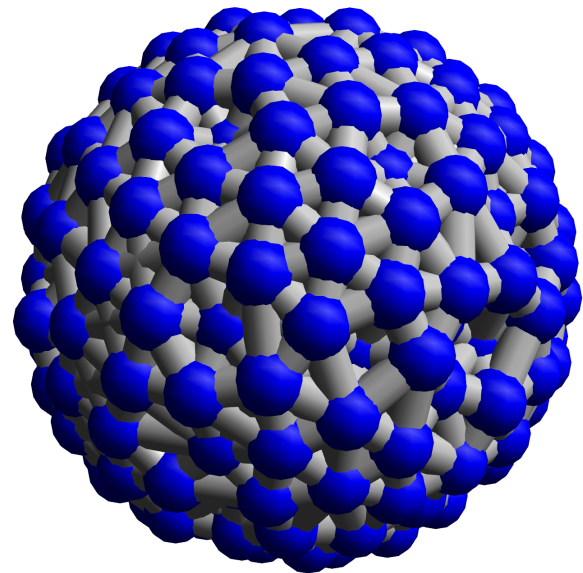


**Fig. 2:** Uniaxial pressure test results for a diameter fraction of 2.5 mm to 3.125 mm

while being crushed. However due to their porous structure and their variety in diameter and shape, as can be seen in Figure 1, the crushing behaviour of single particles differ from each other. For this reason the particles were divided into three diameter fractions to reduce the parameter scattering. Nevertheless a considerable amount of scattering remains as can be seen in the resulting stress strain curves for a diameter fraction of 2.5 mm to 3.125 mm as depicted in Figure 2.

Using a DEM to simulate the granular material gives the advantage of considering each granule separately and thus the breakage of individual particles. In the DEM the dynamic behaviour of quasi rigid bodies [8] is computed. Therefore the relevant neighborhood relations of all particles are ascertained in order to calculate the contact forces between the particles with a Hertz-Mindlin contact model [3]. Taking these forces into account, the Newtonian equations of motion are solved in translational and rotational direction with an explicit time integration scheme.

The simulations for this work are carried out with the open source code MUSEN [9]. In MUSEN, the DEM is extended by a bonded-particle method (BPM), which allows the computation of particle breakage in a numerically stable way. For BPM simulations each granule is modelled as an agglomerate, see Figure 3, composed of primary particles connected by solid bridges – also called bonds. Since the bonds are considered massless, no mass conservation problems occur when the agglomerates break into several parts. The breakage of the agglomerate is governed by the used bond model which predefines the stress-strain behaviour of the bond. The underlying bond model used in this work is a linear-elastic approach introduced by [6]. The corresponding breaking criterion of this first model is limited by a maximal stress as can be seen in Figure 4 which shows the stress-strain behaviour of a bond for different bond models, the first one is referred to as model 1. Model 2 represents an elastic perfectly plastic [10] material behaviour of the bonds. For this model, the stress increases linearly similar to model 1 until it reaches the yield stress, see Figure 4. From this the stress remains constant until a certain strain limit is reached, acting as breakage criterion.



**Fig. 3:** Agglomerate of primary particles (blue) and bonds (gray)

During the execution of the experiments, a creaking noise was noticeable without the occurring of visible cracks. This leads to the conclusion, that micro cracks appear inside the particles due to their porous texture. Since these micro cracks are mainly responsible for the energy dissipation capability of the granules, they need to be taken into account. In order to do this, a third model is developed. The stress-strain curve obtained with this model is shown in dark green in Figure 4. Similar to model 1 and 2 the stress first increases linearly until the yield strength is reached but instead of levelling out, the stress decreases again, corresponding to an occurring micro crack [11, 12]. This micro crack can be seen in Figure 5, which shows a sketch of Poraver material each bond has to represent, including its breaking pattern. Each stress drop corresponds to a crack, marked with a, b and c until the bond breaks which is marked with a d. All three described bond models are used to simulate single and multi particle compression tests to find the best approach.

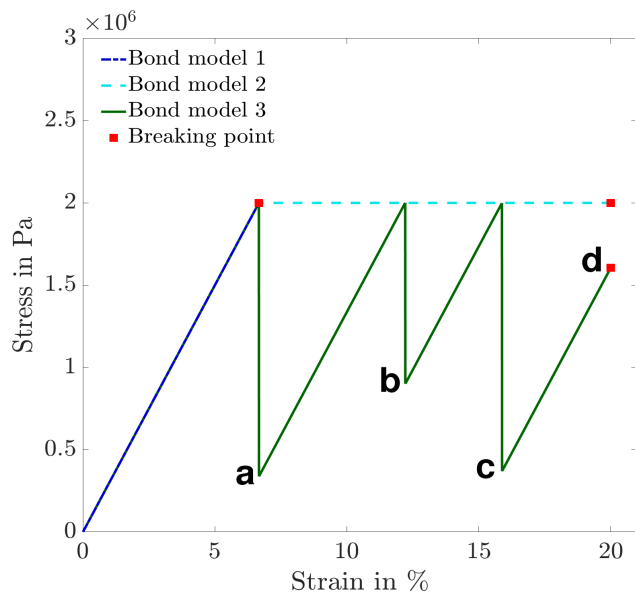


Fig. 4: Stress-strain curves for different bond models

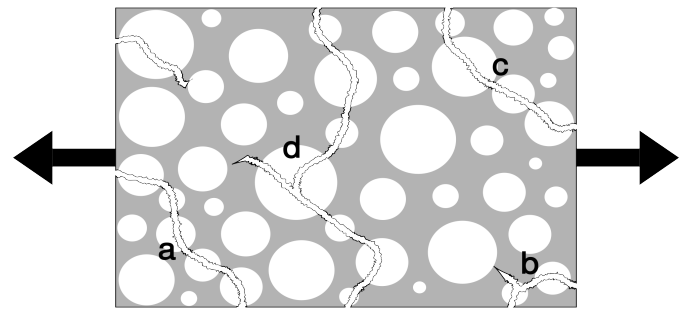


Fig. 5: Breaking pattern of a bond

### 3 Results and discussion

In accordance with the experiments, uniaxial compression tests are simulated with single particles. In this test, a particle is placed on a metal plate and crushed by a downward-moving metal punch, see Figure 6. From this, the crushing behaviour can be derived in form of a stress-strain curve, as depicted in Figure 2. The initial simulations are performed with spherical agglomerates and material parameters determined from experiments.

When simulating the same agglomerate with all three bond models, their influence on the fracture behaviour is clearly visible. Figure 7 shows the stress-strain curves derived from all three simulations together with a measure for the amount of broken bonds. In the results obtained from the simulation with Model 1, significant stress drops are visible, which can be attributed to the simultaneous breaking of a large number of bonds. In addition, the slope of the curve and thus the stiffness of the agglomerate is significantly higher compared to the average experimental results. In contrast, the stress drops in the curves representing the simulation results with models 2 and 3 are considerably lower. Moreover, the slope of the resulting stress-strain curve of the calculation with model 2 is similar and that with model 3 is almost the same compared to the slope of the average experimental results. This means that the stiffness of the agglomerate and thus its fracture behavior is very similar to that of the granules. This leads to the conclusion that bond model 3 is the most suitable one for the simulation of single particles.

Bond model 3 is therefore used to investigate various simulation parameters for their influence on the results. The most important influencing parameters are the Young's modulus of primary particles and bonds as well as the bonds yield strength,

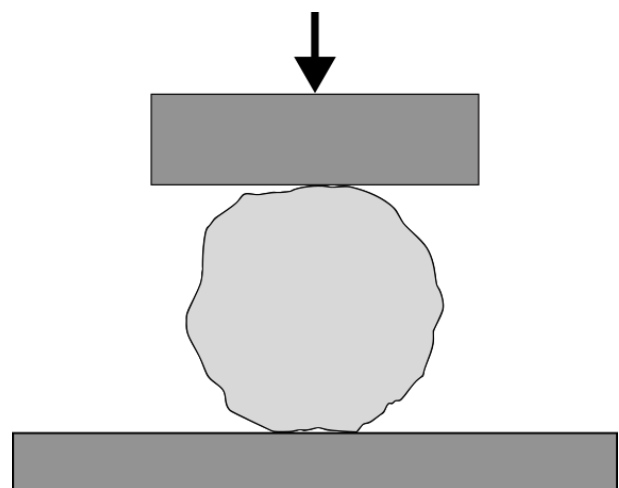
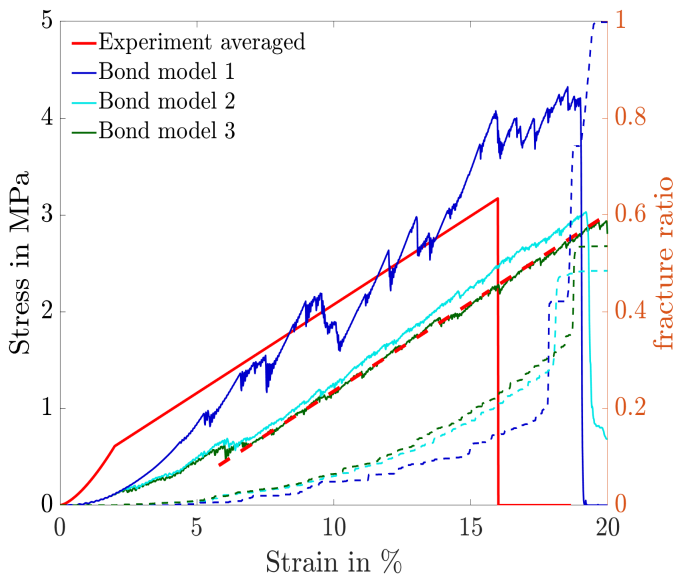
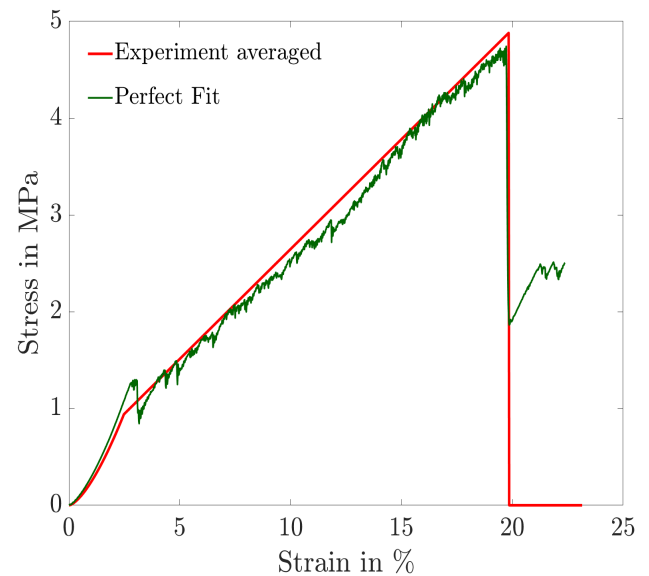


Fig. 6: Uniaxial compression test setup

since this parameter determines bond model 3. In addition, some geometrical parameters were investigated with the result that especially the shape of the agglomerate and its porosity have a great influence on the fracture behaviour of the agglomerates. The shape of the agglomerate is changed from spherical to slightly flattened at the top and bottom of the agglomerate, resulting in a kind of elliptical shape. This flattening changes the number of primary particles connected to the steel plates right from the beginning of the simulation, which affects the initial stiffness of the agglomerate and thus its Young's modulus. The porosity describes the packing density of the agglomerates. This means that if for example an agglomerate has a porosity of 0.3, that 30 % of the agglomerates volume is not filled while the remaining 70 % of the agglomerates volume consist of primary particles. Thus, the lower the porosity, the more densely packed the agglomerate and the stiffer it becomes. However, the porosity has no influence on the initial stiffness and thus the elastic modulus of the agglomerate. Taking all these findings into account and using a design of experiment approach, it is possible to generate an agglomerate that almost perfectly reproduces the behaviour of the average experimental curve, as can be seen in Figure 8. This agglomerate is slightly flattened, with a porosity of 0.42. The primary particles Young's modulus is 380 MPa, the bonds Young's modulus 580 MPa and the yield strength of the bond 6 MPa.



**Fig. 7:** Single particle uniaxial compression test simulated with all three bond models

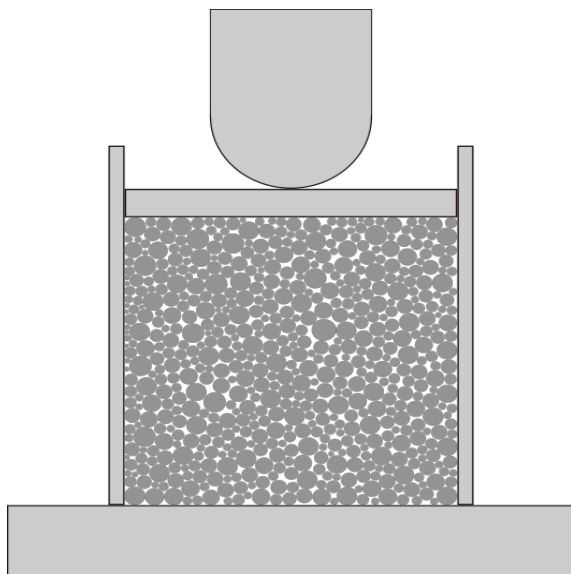


**Fig. 8:** Simulation results of a single particle uniaxial pressure test with optimised parameters

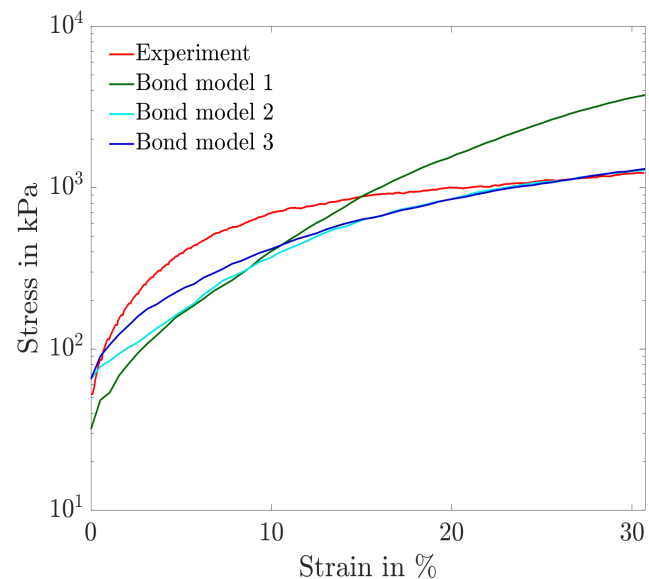
Based on the information gained by simulating single particles, multi particle simulations are carried out. Beside the material parameters derived from the single particle computations, information about the friction coefficient is needed. These information are determined through simulations of angle of repose experiments [13]. For these experiments a hollow cylinder is placed on a metal plate and filled with granules. The cylinder is then slowly moved upwards to eject the particles, which settle into a cone of a specific diameter and angle that depends on the sliding and rolling friction of the material. For the experiments the cylinder is loosely filled with 1182 Poraver particles and moved up with two different velocities of 1 mm/s and 20 mm/s. Both velocities as well as the number of particles and the filling height is used for the simulation setup. The simulation results lead to a rolling friction coefficient of 0.16, while a sliding friction coefficient of 0.87 is used, which is taken from [5]. With these parameters the average experimental cone height of 18.3 mm can be reproduced in the simulations.

In addition, multi particle uniaxial compression tests, also referred to as Oedometer tests, are carried out. In this experiment again a hollow steel cylinder is filled with granular material as can be seen in Figure 9, however this time a metal plate is driven downwards to crush the particles inside the cylinder. Since this experiment is closest to the overall goal of simulating collisions with particle filled double hulls it is the most important one, allowing the investigation of interacting particles under pressure. Again, to be certain that bond model 3 is also well suited for simulating multi particle interactions, simulations are performed using all three models. In order to make sure that the simulation is set up as good as possible, the number of particles as well as the weight of the probe is the same as in the experiment. Furthermore, in an attempt to cover the material parameter spread, several agglomerates of each diameter fraction are used in the simulation. These agglomerates are selected so that the averaged stress-strain curve of the agglomerates corresponds to that from the experiments and the standard deviation is as similar as possible compared to the experimental results. Figure 10 shows the resulting stress strain curves compared to experimental results. Therein the influence of the bond model is clearly visible. Bond model 1 leads to a less stiff behaviour up to a strain of 10 % and afterwards the particles in the simulation react much stiffer. Bond model 2 and 3 are similar from a strain of 15 % onward, however up to 15 % model 3 leads to a stiffer behaviour and thus gets closer to the experimental results.

The simulation results are not yet accurately displaying the initial stiffness of the Oedometer test. Nevertheless it is already a quite good result.



**Fig. 9:** Schematic sketch of the Oedometer test setup



**Fig. 10:** Oedometer simulation results with all three bond models compared to experimental data

## 4 Conclusion

Summarizing the presented results, it is possible to simulate the breakage of granules in an accurate way. Moreover it is evident, that the bond model is decisive for the results of the simulations of single particles as well as multi particles. For the single particles test parameter studies have been carried out leading to simulation results which accurately display the experimental results. However, even though the results of the oedometer test are as well already in good agreement with the experiments, further parameter studies are aspired to investigate the main influences on these multi particle simulations. Therefore parameter studies will be carried out with down scaled oedometer tests, which only containing 50 to 200 particles in order to reduce the computational time needed for each simulation. These simulations will give further insides in the parameters needed for accurate DEM simulations which can afterwards be used for coupled DEM-FEM simulations.

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