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RESEARCH ARTICLE

Numerical investigation of multi-particle interactions using the discrete element method

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Abstract

The numerical simulation of particles that can be used as crash absorbers, for example, in ship collisions, is of high interest, as experimental investigation is often associated with high costs. After extensive studies on the breakage of single-particles, the focus is now on the investigation of multi-particle simulation. Although many parameter studies have been carried out for single-particle compression tests, their results cannot be transferred to multi-particle compression tests. The influence of various simulation parameters differs greatly between single and multiple particles due to the interaction between individual granules. Therefore, it is necessary to repeat the parameter studies with respect to these interactions in order to gain a better insight into the bulk behaviour of granular materials, which can then be used for the simulation of particle-enhanced collisions.

1 | INTRODUCTION

The idea of filling the double hull of a ship with granular material to increase collision safety has already been investigated in several papers [1–4]. Nevertheless, there are a number of open questions regarding the numerical simulation of the filling material and its behaviour during a compression. Therefore, in addition to numerical simulations of single-particle compression tests, which can provide insights into the breakage of individual particles, the interaction of several particles being compressed is to be investigated in more detail. For this purpose, simulations are carried out with a discrete element method (DEM) [5]. In order to enable the fracturing of particles, the DEM is combined with a bonded particle method (BPM) [6]. To reduce the computational effort, multi-particle experiments with 200 particles are simulated and compared with experiments using the same number of particles. The simulations are performed with different simulation parameters such as time step size, compression velocity and coefficient of restitution to investigate their influence on the computational results. This contribution is structured as follows. First, the material and the numerical method used for the simulations are described. Afterwards, the simulation results including the influence of different parameters are presented and discussed, and lastly a short summary of the results is given.

2 | MATERIAL AND METHODS

The material considered in this work has been investigated experimentally in detail in Woitzik and Düster [7], among others. These experiments lead to the conclusion that Poraver expanded glass [8] is best suited for the given purpose [2].

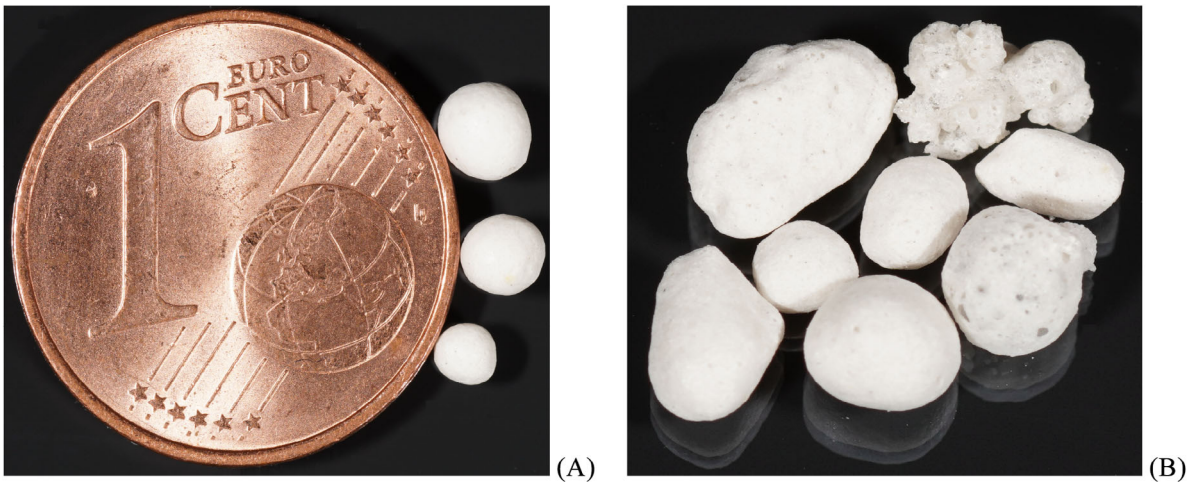

FIGURE 1 (A) Diameter distribution and (B) shape of Poraver particles.

With its chemical properties and internal structure, Poraver meets all the requirements necessary for use in a double hull of a vessel. These properties include environmental friendliness, non-combustibility, low weight and energy dissipation, to name but a few, Schöttelndreyer [1] lists all the necessary requirements. The Poraver particles used have a size from 2 to 4 mm, as can be seen in Figure 1A, and different shapes, visible in Figure 1B. This diversity leads to highly scattering material properties, as shown in Woitzik and Düster [7]. Overall, the shape and porosity themselves pose a challenge in the numerical simulation of the particles, and the scattering properties add to this.

To meet this challenge and take into account the differences in the particles, a DEM is used. The DEM has the advantage that it models individual particles instead of discretising the particle-filled space. Since each particle is treated individually, in addition to the existing volume forces, the forces arising from the contact of the particles must also be taken into account. These contact forces include normal and tangential components, which are calculated using a Hertz–Mindlin contact model [9]. After calculating all forces, the Newton–Euler equations are solved using an explicit leapfrog time integration scheme [10].

For the purposes of the simulations carried out in this work, the fracture of the particles is of particular interest. Therefore, the BPM [6] is used together with the DEM. A simulation tool that combines these two methods is the open source code MUSEN [11]. For the simulation, each particle is modelled as an agglomerate of primary particles (blue) connected by solid bonds (grey), as shown in Figure 2A. The particles connected by bonds add additional forces, which are computed using a linear elastic model introduced by Potyondy and Cundall [6]. In this model, the bonds may break due to the stress occurring inside the bond. If the stress in the bond exceeds a certain limit, the bond breaks, that is, it is deleted from the simulation, resulting in a crack in the agglomerate, as can be seen in Figure 2B. Initial investigations of the fracture behaviour of Poraver glass and its simulation showed promising but not yet satisfactory results. For this reason, a new bond model was developed that takes into account micro cracks [12, 13] that occur when particles break due to their porous nature. This bond model leads to very accurate results for single-particle compression tests as presented in Rotter et al. [13] and is therefore used to investigate simulations of multi-particle compression tests and the influence of different simulation parameters.

3 | RESULTS AND DISCUSSION

The aim of this work is to investigate the interaction of Poraver particles while they are crushed in a multi-particle compression test. In advance to the simulations, experiments have been carried out using a Zwick Roell material testing machine. In order to track small forces, an additional load cell was installed under which a hollow steel cylinder filled with particles and a steel stamp are placed. The particles are then crushed with a velocity of 0.5 mm/s. The experimental setup is shown in Figure 3. To simplify and speed up the simulations, 200 particles are used for the experiments and simulations. Figure 4 depicts the simulation setup for the compression tests containing 200 agglomerates. As in Figure 2, the primary particles

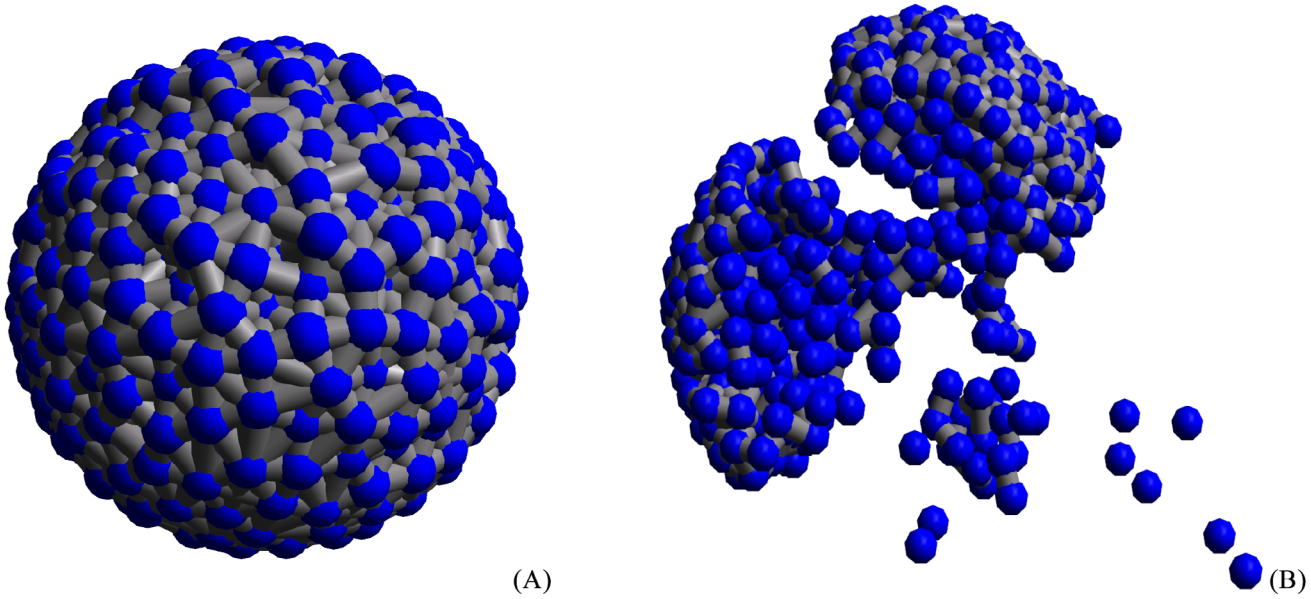

FIGURE 2 Simulation model of a Poraver particle (A) intact and (B) broken.

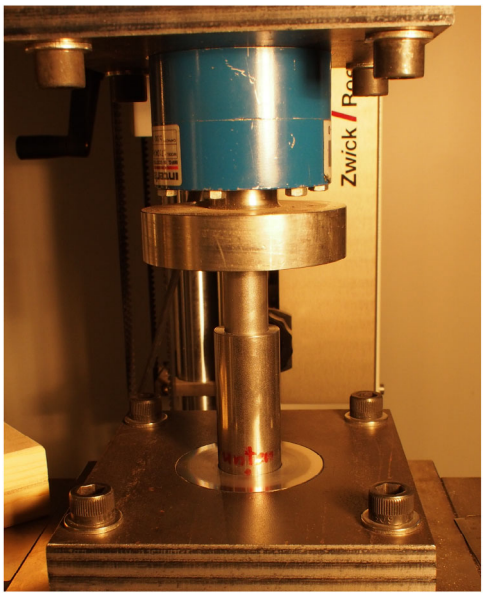

FIGURE 3 Experimental setup for multi-particle compression tests.

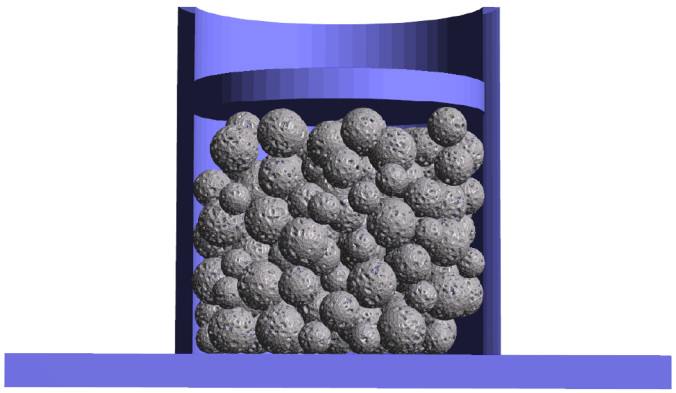

FIGURE 4 Simulation model for a multi-particle compression test.

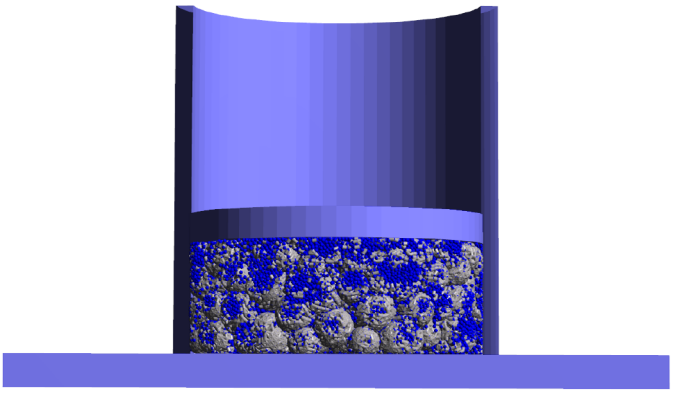

FIGURE 5 Multi-particle compression test simulation result after 40% of strain.

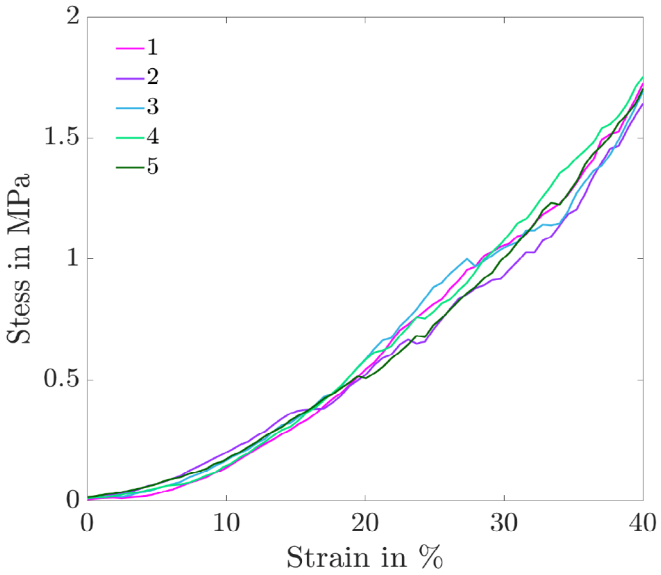

FIGURE 6 Influence of different particle arrangements inside the cylinder on the resulting stress–strain curves of multi-particle compression tests.

are coloured blue and the bonds grey. First, only intact agglomerates are visible and after 40% of strain, single primary particles can be seen which are no longer connected by bonds, see Figure 5.

The simulation setup as well as the computations used for the simulations are subjected to certain random processes. While the cylinder is filled with agglomerates, each agglomerate is placed randomly at a free place leading to different and not reproducible cylinder fillings. Moreover, the used bond model contains a random weakening factor, which leads to random residual stresses after each micro-crack. These two effects are investigated regarding the influence on the simulation results. Figure 6 shows the influence of the arrangement of the 200 agglomerates inside the cylinder. As can be seen, this has a considerable influence on the resulting stress–strain curve, leading to the conclusion that only one simulation setup should be used when investigating different simulation parameters. In comparison, Figure 7 shows the re-calculation of the same setup five times revealing the influence of the bond model. The curves only slightly differ from each other giving an idea of normally occurring variations of the simulation results which can be used to interpret the following results.

In addition to the presented statistical influences, some global simulation parameters are investigated. In Rotter, Dosta and Düster [13], the same parameters are investigated regarding their influence on single-particle compression tests, revealing no influence at all. However, this does not hold for multi-particle tests as can be seen in Figure 8 for the influence of the mass scaling. Since the mass has an influence on the time step size that has to be used to get a stable simulation, it is of high interest whether the scaling of the mass influences the interaction and with this the results of the compression simulation. In the stress–strain curves, there is no impact visible up to around 30% of strain. Afterwards, the curves differ

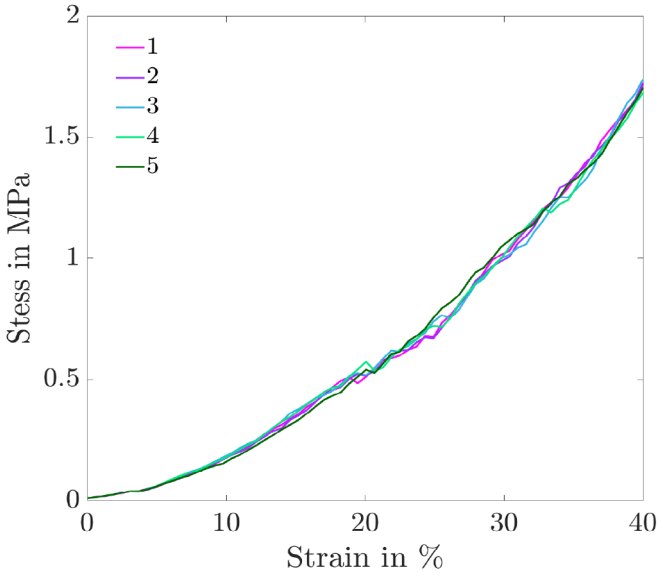

FIGURE 7 Influence of statistical phenomena due to the bond model on the resulting stress–strain curves of multi-particle compression tests.

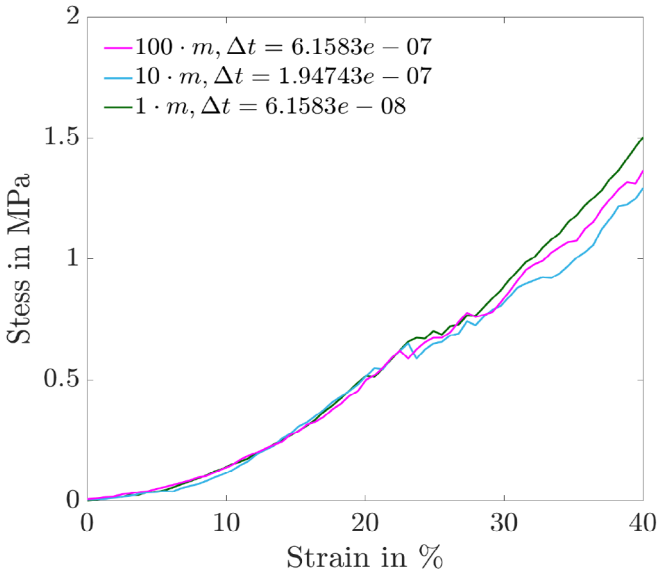

FIGURE 8 Influence of the mass scaling on the resulting stress-strain curves of multi-particle compression tests.

more than is explainable through the statistical distribution of the bond model. Nevertheless, since the differences are not severe, a mass scaling with a factor of 100 can be considered due to the massive reduction in computational time by a factor of 10.

Taking these results into account, additional simulations with different time step sizes are carried out. As the recommended time step size calculated according to Brown, Chen and Ooi [14] only gives a reference for a stable simulation, it says nothing about accuracy. Figure 9 shows the results of simulations with time step sizes from Δt = 5 e-6 s to Δt = 5 e-10 s. In the stress–strain curve, it can be seen that at a time step size of Δt =5 e-6 s an instability occurs, which immediately leads to forces so large that all particles flow out of the cylinder, leaving it empty. Moreover, a convergence for smaller time step sizes is visible. The differences between a time step size of Δt =5 e-9 s and Δt =5 e-10 s is in a range that can be related to the influence of the bond model. From these results, it is recommendable to use a time step size of Δt =5 e-9 s.

Further investigated parameters are the compression velocity and the restitution coefficient of the particles. These two parameters also show no influence on the stress–strain curves of single-particle compression tests [13]. In contrast to

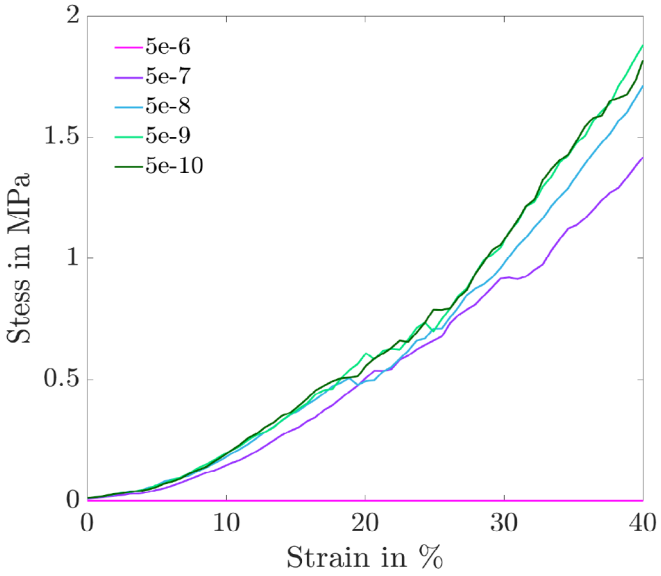

FIGURE 9 Influence of time step size on the resulting stress–strain curves of multi-particle compression tests.

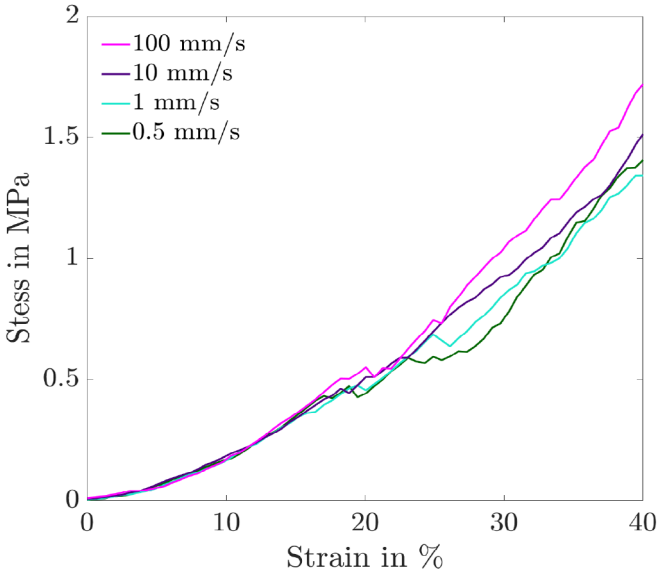

FIGURE 10 Influence of the compression velocity on the resulting stress–strain curves of multi-particle compression tests.

that, the compression velocity as well as the restitution coefficient show an influence on the results of multi-particle compression test simulations. Up to a strain of 20%, the velocities impact is negligible; however, when the particles are further compressed, the curves start to deviate for velocities between 100 and 0.5 mm/s. In Figure 10, it can be seen that higher velocities lead to a stiffer response of the particles. Moreover, a convergence towards smaller velocities is visible. Nevertheless, in order to save computational time, a compression velocity of 10 or even 100 mm/s can be used for preliminary parameter studies, even though the experimental velocity is much smaller with 0.5 mm/s. Therefore, for final simulations, a compression velocity of 1 mm/s or smaller should be used.

The restitution coefficient also shows an influence on the stress–strain response of the particles, see Figure 11. In the curves, a trend is visible showing a stiffer behaviour for smaller restitution coefficients. Smaller values indicate a more plastic and therefore harder contact while greater values lead to a softer contact. The influence of the restitution coefficient is detectable quite early in the simulation but rather small up to a strain of 40%. However the curves calculated with values between 0.6 and 0.1 only differ in a range which can also be explained by the influence of the bond models statistics. These values should, therefore, be investigated in more detail to gain a clear recommendation for a restitution coefficient.

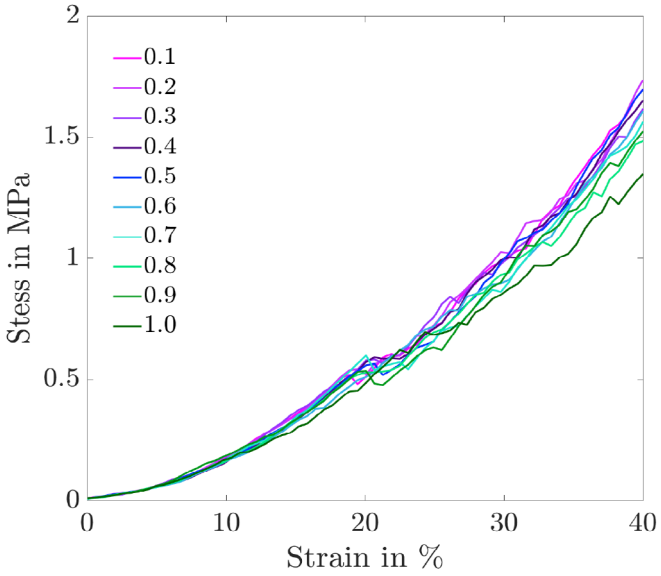

FIGURE 11 Influence of the restitution coefficient on the resulting stress–strain curves of multi-particle compression tests.

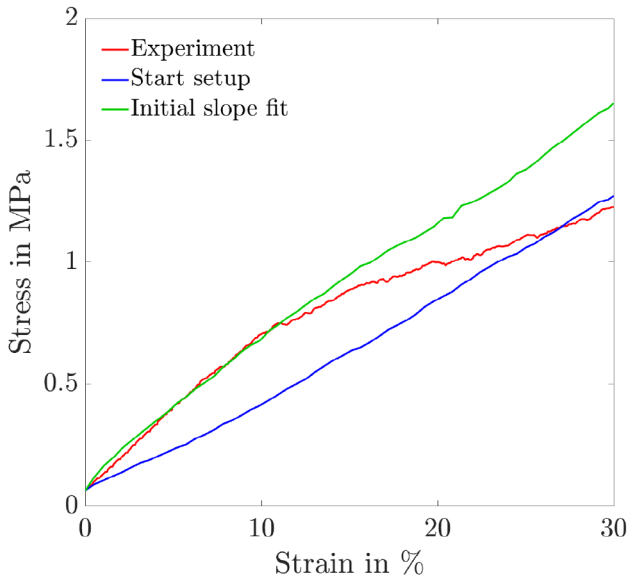

FIGURE 12 Comparison of different simulation results with averaged experimental results.

All parameters presented above show no influence on the initial slope of the curves. Nonetheless, it is possible and needed to influence the initial slope since the average stress–strain curves gained from experiments are much stiffer at the beginning. Figure 12 shows such an average curve in red compared to a curve computed with a start setup of parameters contained from experiments of single-particle compression tests and a result for which the simulation parameters have been modified to fit the initial slope in green. However, after 12% strain, the green curve is too stiff and overestimates the stress inside the cylinder. This result still shows room for improvement and the necessity of further parameter studies.

4 | CONCLUSION

To sum up the results, it is evident that we can not conclude anything from single-particle compression test simulations when investigating multi-particle compression simulations. Due to the interaction of the particles, each investigated parameter shows an influence on the stress–strain behaviour of a multi-particle setup. Moreover, it is of great importance

to reuse the same setup for parameter studies as the influence of different particle arrangements inside the cylinder can otherwise yield misleading results. The influence of the statistical scattering of the bond models is negligible. The gained results are promising but further parameter studies are necessary to get a better understanding of the interaction of the particles with regard to the material parameters and friction influence.

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