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Simulation of Coated Particles Breakage Using a low Fidelity DEM–BPM Model

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ABSTRACT

Previous studies have demonstrated that filling a ship's double hull cavity with lightweight glass particles, like Poraver significantly enhances its ability to withstand collisions. The energy absorption capability of such particles can be improved by coating them in a fluidised spray granulation process. In order to find the extent of this improvement, a numerical model needs to be developed. For that purpose, the discrete element method (DEM) with the bonded particle method (BPM) is employed using the open-source code MUSEN. This allows the breakage of particles to be simulated using a cluster of particles bonded to each other. Since a single particle in the experiment is represented with an agglomerate of several smaller particles in the simulation, it significantly adds to the computational costs and limits the scale of the simulations which can be performed. This paper explores the different fidelities of a DEM–BPM numerical model with its advantages and disadvantages in its depiction of a coated particle breakage.

1 | Introduction

The collisions of ships contribute to a significant number of maritime accidents. In China, for example, over the last two decades, 41% of maritime accidents were related to the collision of ships [1]. Any collision, whether big or small, leads to a negative impact on the structure of the vessel by reducing its ability to carry loads [2]. Consequently, any collision might be disastrous due to its environmental impact, such as oil leakage or loss of human life [3]. Therefore, improving the ship structure against collisions is important.

One way to overcome this problem is to insert granular media inside the cavity of a ship double hull [4]. This leads to two advantages. First, the granular media or particles absorb kinetic energy from the collision and dissipate it through breakage. Second, once the double hull is filled with particles, the whole structure behaves like a sandwich. This allows the transmission of loads from the outer to the inner hull. However, it must be noted that these particles must not negatively modify the existing properties of the structure. As a result, they must be lightweight, non-toxic, inflammable and hydrophobic. For that purpose, Poraver or lightweight glass particles were found to be suitable [5]. These glass particles can be further optimised in their mechanical properties by adding a layer of coating in a fluidised spray granulation process [6]. This coating layer has similar characteristics as that of Poraver itself. As a result, it does not negatively effect the existing ship structure; rather, it improves the dynamic behaviour of Poraver particles by preventing powder formation before a collision would take place. Thereby, the ability of particles to dissipate energy through breakage is not reduced in addition to the reduced difficulty in maintenance. However, the crushing behaviour is dependent on the type of coating material. A candelilla wax coating, for example, results in brittle or stiff compression behaviour, whereas the silicon coating is more soft and sponge-like. Consequently, a different stress–strain

relationship is produced depending on the type of coated particles used inside the double hull.

In order to study the effect of such coated particles inside the double hull, a numerical model needs to be developed. In that direction, discrete element method (DEM) extended with the bonded particle method (BPM) is used [7]. This method allows the modelling of particles as agglomerates which is a network of particles bonded or connected to each other. As compression is applied, the agglomerate undergoes breakage as the bonds between the particles are broken. However, this method requires definition of a significant number of material and geometrical parameters inside DEM and BPM which need to be reduced and optimised. Furthermore, only one particle in the real world is represented through an agglomerate. Thus, a large scale numerical simulation like the double hull would be impossible to carry out with a high-detail DEM model. Nevertheless, a simplified approach needs to be adopted to keep the computational costs as low as possible while maintaining accurate results. In this contribution a comparison between a high-fidelity (HF) and low-fidelity (LF) DEM–BPM model is made. The computational times and costs of these models along with their limitations in the generation of accurate results are discussed. Section 2 describes the different numerical models used for this task followed by the simulation results and their corresponding discussion in Section 3.

2 | Materials and Methods

As mentioned in the previous section, DEM and BPM are used to describe the mechanical behaviour of a coated particle. Each particle in DEM is a discrete quasi-rigid body [8]. In addition to the volume forces, if the particles come into contact with each other then a contact model, in this case Herz–Mindlin, is used to calculate the contact forces. Afterwards, the sum of all forces, including their normal and tangential components, is used to compute the velocity and displacement of each particle by the Newton–Euler equations using an explicit time integration scheme, in this case the Leap Frog method. In order to maintain the data structure for each particle, a Verlet list is used. However, this can be memory intensive, as described in the later sections, when the number of particles increases especially in high-compression areas where a large number of particles can come into contact with each other. In order to simulate the breakage of an agglomerate the BPM is used. In this method, the discrete particles are connected to each other using bonds or solid bridges. These objects are weightless and therefore mass conservation is fulfilled. The forces generated inside a bond are computed using a material model, such as elasticity or elastoplasticity. In this work, a microcracking model with elastoplasticity is used. It is particularly useful for particle breakage because it allows the modelling of small cracks and their corresponding energy dissipation [9]. Once the stress or strain inside a bond reaches a certain limit, it breaks and is removed from the simulation. To perform the DEM and BPM simulations, the open source code MUSEN is used [10]. This has two advantages. First, it allows the mesoscale modelling of the coated particle. If the actual microstructure of the coated particles is modelled, as shown in Figure 1, then a significant number of smaller particles would be required to model each pore of a different size. Additionally, several smaller particles would be needed to model the thin and continuous coating layer. The second advantage of the code is that it allows the speed of simulations by running them on a GPU.

TABLE 1 | Summary of the differences in structure between the HF and LF model.

	High fidelity (HF)	Low fidelity (LF)	Factor of reduction
Parameters	28	14	2.00
Bonds	8685	3180	2.73
Particles	2141	484	4.42

The microstructure depicted in Figure 1 is unique for each coated particle. Moreover, they have distinct shapes and it is very rare to find a perfectly spherical particle. Consequently, each particle compression exhibits a different stress–strain relationship [6]. However, they can be divided into fractions based on the diameter of particles. Nevertheless, variation in results remain. As mentioned above, MUSEN allows the mesoscale modelling of such microstructure. A cross section of a numerical model is depicted in Figure 2. As observed, the model is a simplified illustration of the actual microstructure. The smaller wax particles, diameter 0.1 mm, and the larger Poraver particles, diameter 0.25 mm, are depicted in red and blue, respectively. The smaller bonds between the wax particles themselves and Poraver particles and the larger bonds between Poraver particles are depicted in light red and blue, respectively. A large number of material and geometrical parameters need to be defined, each for wax and Poraver. A methodology for reduction of these parameters based on this model and using sensitivity analysis followed by optimisation with the particle swarm algorithm was performed in previous work [11]. Although the model is a mesoscale approximation of the actual microstructure, this detail of modelling in DEM, later referred to as the HF approach, significantly adds to the computational costs, as seen in the latter section.

In contrast to this approach, a LF representation of the same microstructure of a coated particle is depicted in Figure 3. This agglomerate has the same diameter of 2.28 mm as before. Furthermore, the size of Poraver particles are also the same. The difference arises from the fact that the smaller wax particles and bonds are ignored with the resulting space occupied by larger Poraver particles and bonds. A summary of the reduction of parameters is provided in Table 1. The number of parameters needed by MUSEN is halved. Also, both the number of bonds and particles are reduced by factors of 2.73× and 4.42×, respectively. To do a comparison between both approaches in terms of computational costs and time, two different setups are made. These are based on the experiments and the details have been discussed in previous work [6, 11]. They include the single particle compression test (SPT), where one agglomerate is compressed between steel plates and the multi-particle compression test (MPT), where more than one agglomerate, usually the number is equal to the number of particles in experiments are compressed inside a steel cylinder. The procedure of reducing the number of parameters for the LF model, followed by their optimisation is the same as mentioned above and similar to the previous contribution [11].

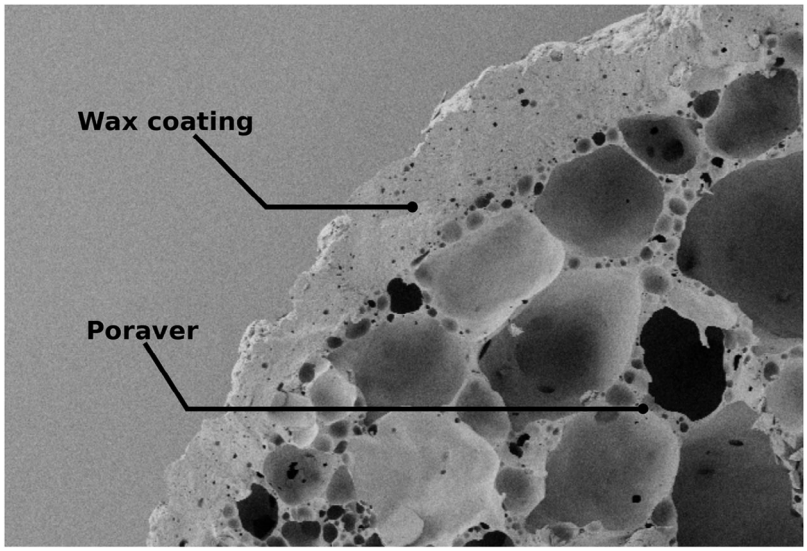

FIGURE 1 | Microstructure of a wax coated Poraver particle with 500× magnification.

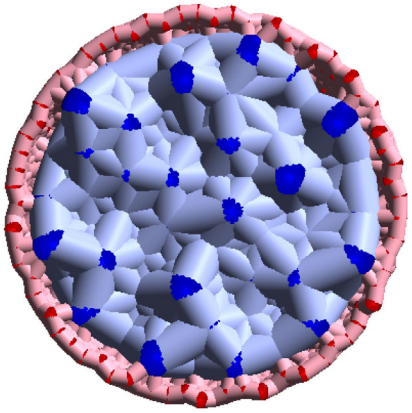

FIGURE 2 | Agglomerate consisting of primary particles of wax (red), wax-wax-Poraver bonds (light red), Poraver particles (blue) and Poraver–Poraver bonds (light blue). Referred to as HF.

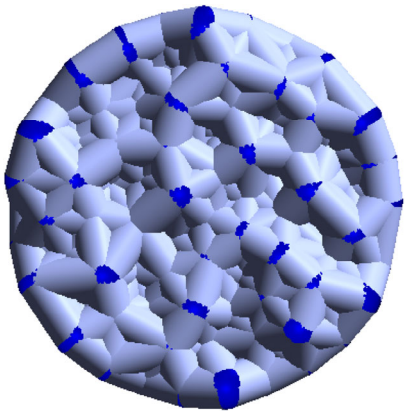

FIGURE 3 | Agglomerate consisting of primary particles of Poraver (blue) and Poraver–Poraver bonds (light blue). Referred to as LF.

3 | Results and Discussion

This section describes the differences in computational times and costs between the two levels of modelling of the coated particles using DEM and BPM based on the single and multi-particle compression test. First, the simulation results for SPT are compared, as illustrated in the force displacement plot in Figure 4. The red line represents the average curve generated based on the mean breakage force and displacement of the experimental diameter fraction 2.0–2.5 mm [6]. The result of the HF model is depicted in blue. The material properties of this model are optimised using the particle swarm algorithm around the experimental averaged curve and show a good agreement. The list of its optimised parameter set is given in previous work [11]. The bond model mentioned in Section 2 allows microcracking through breakage of bonds inside the agglomerate, which are depicted as small drops in value of force before a significant number of bonds are broken around 13 N at 0.3 mm of displacement. In contrast, the LF model has a reduced number of parameters, bonds and particles before the optimisation process, see Table 1. Nevertheless, they are reduced and optimised in a similar manner. A list of the optimised parameter set for a similar setup is given in Table 2. The result of the simulation is given in the green plot. It can be observed that the LF model exhibits a more or less similar force displacement curve behaviour in comparison to the HF model. Both models break around 13 N at 0.3 mm of displacement. The difference in force drop values occurs due to the randomness of the bond model [9], and the number and type of material properties of the bonds. Overall, it can be said that both numerical models successfully depict the average experimental curve.

TABLE 2 | Optimised set of parameters for a wax coated Poraver particle LF model with diameter 2.28 mm.

Young's modulus	MPa
Poraver bonds and particles	502
Breakage strain	—
Poraver – Poraver bonds	0.0033

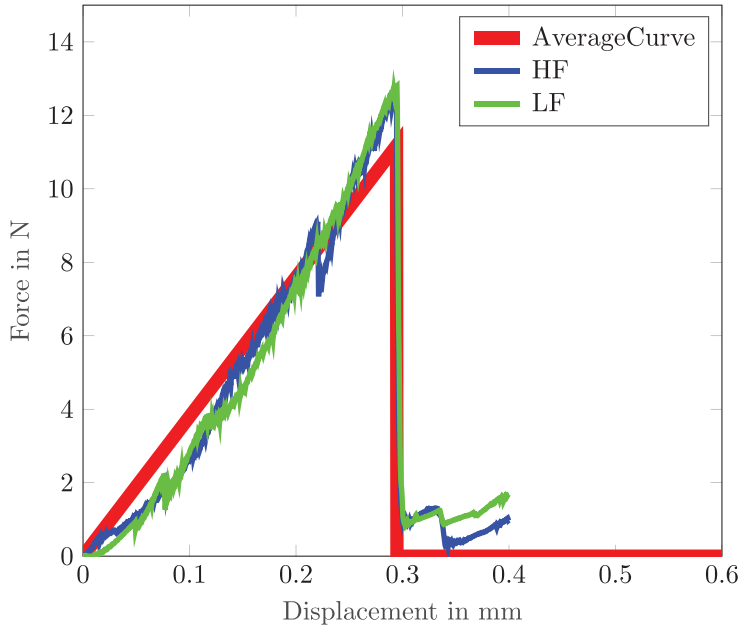

FIGURE 4 | Difference between average experimental and optimised simulation of HF and LF force-displacement curve for wax coated Poraver particles of diameter 2.0–2.5 mm.

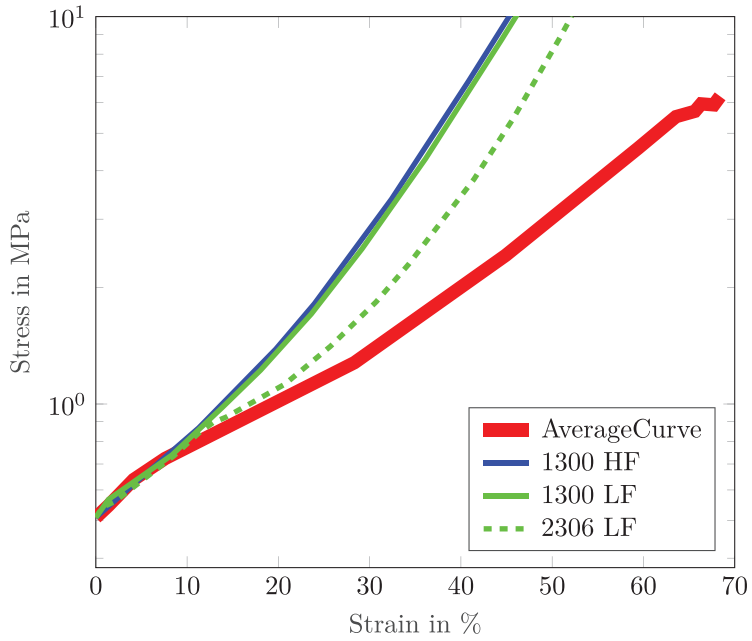

FIGURE 5 | Difference between average experimental and simulation of HF and LF stress–strain curve for wax coated Poraver particles with different number of agglomerates.

As mentioned in Section 1, the final goal of the numerical model is to simulate the double hull. For that purpose, its suitability needs to be checked when more than one agglomerate interact with each other. Namely, the multi-particle compression test. The stress–strain plots for this study are depicted in Figure 5. Similar to the compression of single particles, the average of the experimental curves is shown in red. In case of the MPT, variation in the experimental results is lesser [6]. Furthermore, less microcracking is observed as there are no significant drops in stress values. The average number of particles present inside the cylinder for these experiments was 2306. For the HF model, it was attempted to randomly generate inside the cylinder the same number of agglomerates. However, memory of the GPU, in this case Nvidia GeForce RTX 3090 with 24 GB of GDDR6X memory was not sufficient to start the simulation. As mentioned previously in Section 2, the Verlet list becomes too large and is not able to maintain data of all the particles and bonds present inside the simulation. Therefore, the simulation crashes before it even starts. Nevertheless, 1300 agglomerates are generated to check the suitability of the HF model, which is more than 50% of the original number. This time the simulation does not crash and results are depicted in the blue plot. To make the results comparable,

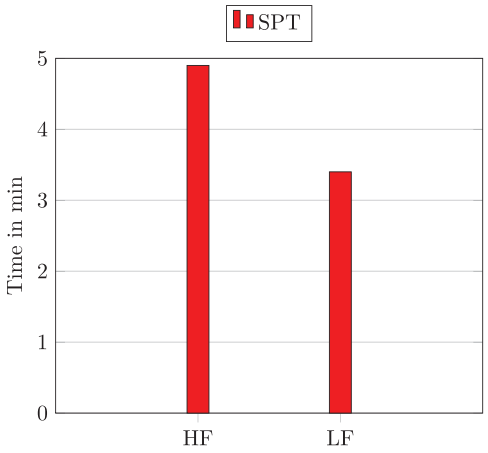

FIGURE 6 | Computational times for low and high fidelity DEM model for uniaxial compression of single particle.

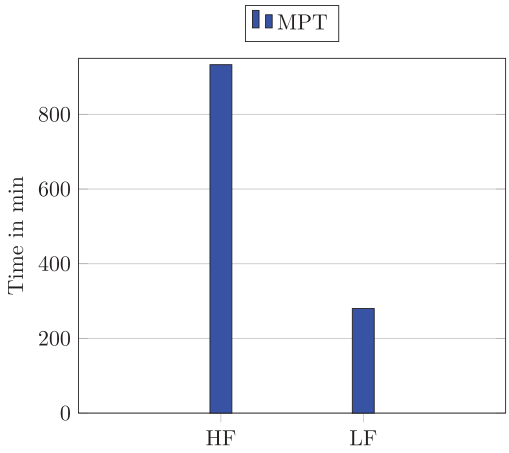

FIGURE 7 | Computational times for low and high fidelity DEM model for uniaxial compression of multi-particles.

stress and strain values are normalised. The model provides a reasonable approximation to the experimental curve till 8% of strain. However, beyond this region the magnitude of stress increases greatly. This can be attributed to not enough breakage happening inside the simulation to dissipate energy. Simply, the number of bonds are not enough. Moreover, at this point in the simulation, there is not enough space inside the cylinder for the particles to move around. Consequently, a significant number of particles are being compressed which cannot deform or break. To make a fair comparison between HF and LF model for the same number of agglomerates, a similar simulation is performed for LF model with 1300 agglomerates depicted by the green line. It is observed that even for a different set of material parameters, particles and number of bonds, the results are similar as before. Both the curves match closely for the same value of 8% strain. Again the problem arises due to the lack of number bonds and densification of the particles in the domain. The real advantage, however, is seen when the same number of agglomerates as particles in the experiments is used, as indicated by the green dashed line. The model is able to predict the stresses upto 20% of the strain which is 2× more than the previous results. More bonds are present in the simulation that can undergo breakage to dissipate before the particles are highly compressed and stress starts to increase exponentially. Although the LF model does not have have the features like the small wax particles near the circumference of the agglomerate, the model can still predict values of stress in an efficient manner.

Another important aspect regarding the comparison of the fidelity approaches are the computational times, shown on the *y*-axis in minutes for both setups, illustrated in Figures 6 and 7 for single and multi-particle compression tests, respectively. These results are based on GPU simulations, where Nvidia GeForce RTX 3090 with 24 GB of GDDR6X memory and 10496 CUDA cores were used. Figure 6 shows that for the LF model the speedup of simulation was by a factor 1.4×. This is understandable since the LF model has to solve for fewer particles and bonds, see Table 1. In case of the multi-particle compression test, the results are similar but the factor increased by a factor of 3.3. It must be noted that it is difficult to derive an exact relationship between the time it will take for a simulation to finish and the number of particles and bonds present in the setup. As mentioned in the previous section, the bonds are deleted from the simulation once they are broken. Additionally, the material properties for LF and HF are dissimilar, as mentioned above, which affects the number of bonds and at which timestep in the integration scheme they are broken. Thus, it is impossible to predict the exact factor value by which the simulations will become fast. Nevertheless, it does show that the computational times for LF are lower than the HF model. Also, if more agglomerates are added, the speedup factor will increase. In case of a future double hull simulation, the LF would provide a much faster result when compared to the HF model.

4 | Conclusion

This contribution uses the DEM extended with the BPM to predict the compression of the coated particles. This allows the modelling of particles as agglomerates that can undergo breakage as they are compressed. In addition, it allows the mesoscale modelling of the microstructure, which is advantageous because it is computationally faster and cheaper. For that purpose, two different numerical models are explored. The HF model includes both smaller particles as coating material and the larger Poraver particles, whereas the LF model only includes larger Poraver particles for the same agglomerate diameter. This results in significantly more particles, bonds and therefore parameters definition for the HF approach. Consequently, it is disadvantageous when the multi-particle simulations are performed. The HF approach is less efficient as there is not enough memory in the system to account for all the object data. As a result, the scale of the simulation has to be reduced leading, to results being valid for a small percentage of strain. In contrast, the LF approach is more efficient as it is less memory intensive and can perform simulation with the same number of agglomerates as particles in the experiment. The stress–strain results are also comparable to the experiments and the HF approach because the material properties for the particles and the bonds have been optimised to account for the coating material. Finally, a comparison of simulation times shows that the LF model is more than twice as fast as the HF model for the multi-particle compression test and the difference is expected to grow if the simulation is scaled up.

Although the LF approach is computationally efficient, it must be noted that the scale of these experiments is very small compared to the double hull. A complete simulation using DEM and BPM would be impossible to carry out based on the current hardware. Further simplification of the numerical model can be done; however, this will lead to inaccuracies in the results. A better solution to this problem would be to use a coupled partition approach where areas of small deformation are modelled as a continuum using the finite element method coupled with the DEM model in areas where large deformation takes place.

Acknowledgments

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