DEM modelling of swelling of grains

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Abstract. Swelling of grains due to water absorption is ubiquitous in many natural materials and industrial products. Hence, a thorough understanding of grain swelling is of great scientific importance. An experimental investigation can only provide limited information, whereas great insight could be gained from numerical modelling, rigorous numerical models for describing particle swelling are essential. Thus, the objective of this study is to develop and validate a discrete element method (DEM) model for swelling of grains. A first order kinetic model was introduced to describe the swelling of a single grain, and subsequently implemented into the DEM code LIGGGHTS. Model validation was performed by comparing the time evolution of the expansion of a packed bed made of super absorbent polymer (SAP) particles obtained numerically and experimentally. It was demonstrated that the developed model can accurately predict the bed expansion. The validated model was then used to investigate the effect of material properties on the swelling behaviour using rice and SAP as the model materials. It is shown that the swelling depends significantly on material properties, as expected; the expansion of the powder bed made of rice is much lower than that of SAP. The developed model could be further advanced to study consequences of swelling phenomena in granular materials, such as segregation and heat generation.

1 Introduction

The expansion of a solid due to water absorption is commonly known as swelling and is caused by restoration of the equilibrium in chemical potential between the absorbing solid and the absorbed fluid [1]. This phenomenon is observed in a variety of natural and industrial materials. For example, rice can increase its volume by about 40% during soaking [2] and a single super absorbent polymer particle can increase its radius by about 600% [3]. Many reseaerchers experimentally investigated water absorption of biological materials during isothermal soaking [4, 5] and a few studies also were performed to examine swelling associated with the water uptake [2, 6–9]. For instance, Perez *et al.* [2] investigated hygroscopic swelling in rice kernels and proposed a theoretical model to describe the variation of moisture absorption in the radial direction. Their model was successfully validated using the finite element method (FEM), and employed to investigate the effect of soaking temperature on infiltration of water and swelling of a single grain. They found that the rate of moisture absorption, water uptake and swelling of the kernel increase with the temperature. Although the FEM work provided some insights into the volume expansion of a rice kernel due to water absorption, it focused mainly on a single grain. As the swelling phenomenon usually involves a large quantity of grains, it is useful to investigate the bulk behaviour of swelling granular systems.

For this purpose, a DEM model that can link the swelling of single grains with the deformation of the granular system is worth pursuing. However, only a few attempts were made to develop DEM models for analysing swelling of granular materials. For example, a grain-scale model was proposed by Sweijen *at al.* [3], in which DEM was coupled with a pore finite volume (PFV) method to model the swelling of super absorbent polymers (SAPs) under fully saturated conditions. Although their theoretical model and simulations well reproduced the expansion of the granular bed observed experimentally, the deformation (i.e. height) of the granular media after swelling for over two minutes was somehow overestimated. The authors attributed this issue to some real phenomena, such as limited water availability inside the bed due to clogging or heterogeneous swelling of the particle, which their model was not able to capture. Their model was further adapted to take irregular particle shape and water uptake on the surface into account [10]. Applying their model to other materials requires experimental determination of the maximum amount of water that the material can absorb, the swelling rate of a single grain, and the diffusion coefficient. It is also unclear whether the model is applicable to describe the swelling of biological materials. Further efforts in developing robust DEM for such applications are hence required.

Hence, the objective of this study is to develop a generic DEM model for swelling of granular materials. A first order kinetic model is proposed and evaluated to predict

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the volume change of a single particle. The model is then implemented into DEM and validated at the macroscale using published experimental data. Furthermore, using the validated DEM model, a preliminary analysis of the effect of material properties on the macroscopic swelling of granular materials is performed.

2 Swelling of a single particle

For swelling of single particles, the overall trend of volume change with time during isothermal soaking appears to be similar for different materials. As an example, Figure 1 shows the volume change with time for a rice kernel [8] and a SAP particle [3]. At a given external condition, the particle increases its volume (V) from the initial volume (V_0) to the equilibrium volume (V_{eq}) with certain kinetics. Both the kinetics and the equilibrium volume are dependent on the material properties and the external conditions.
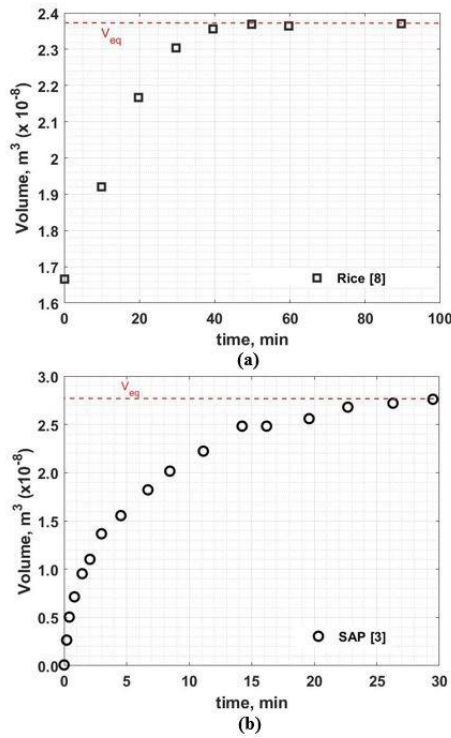
Fig. 1 Swelling of a single grain of (a) rice [8] and (b) SAP [3].

Thus, in order to develop a generic model to describe this generic behaviour, a dimensionless swelling parameter V' was introduced and defined as follows:

$$V' = \frac{V - V_0}{V_{eq} - V_0} \qquad (1)$$

The swelling behaviours can be approximated using a first order kinetics equation, i.e.

$$V' = 1 - exp(-kt) \qquad (2)$$

where t is the soaking time and k is a kinetic parameter. As stated above, the kinetic parameter depends on several variables related to material properties, i.e.

chemical composition and particle size, and external conditions, such as temperature or confining pressure. Due to the limited data available to fully evaluate the dependence of k on these variables, in this work this parameter was found by fitting experimental data at a given temperature. The quality of the fitting, obtained by employing Eq. (2) to forecast the volume of a kernel of rice [8] and SAP [3] during soaking, is shown in Fig. 2.
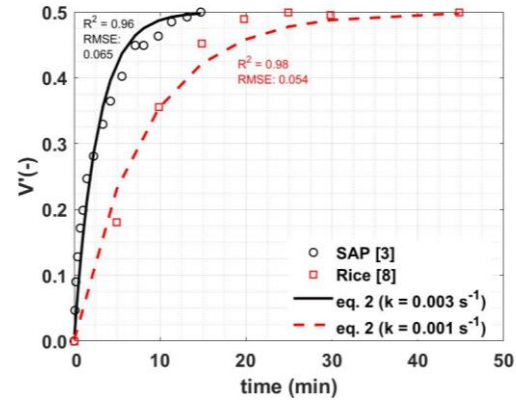

Fig. 2 Time evolution of the dimensionless swelling parameter (V') and fitting with Eq. (2) for a single grain of rice [8] and SAP [3].

3 DEM model

The model as described above was implemented into a DEM code, LIGGGHTS [11], and validated on the macroscale using experimental data for SAP reported in Ref. [3]. The Hertz-Mindlin theory was used for contact modelling. Only spherical particles were considered and buoyancy forces were neglected.

To validate the model, simulations were performed with the same initial configuration used by Sweijen *et al.* [3] in their experiments and simulations. 800 particles, with particle size distribution shown in Fig. 3, were generated and settled at the bottom of a box of size $10^{-2} \times 10^{-2} \times 10^{-1}$ m^3. The swelling of SAP particles was simulated for approximately 22 minutes. The kinetic parameter k (Eq. 2), material properties and material interactions employed in the simulation are listed in Table 1.
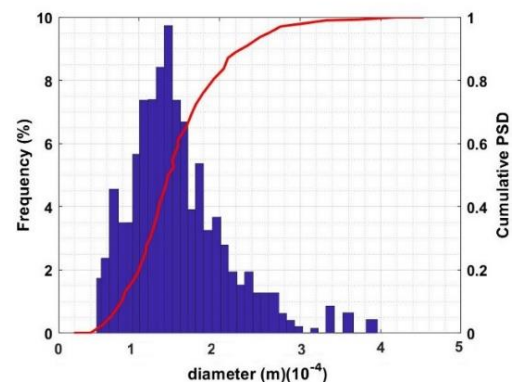
**Fig. 3** Particle size distribution of dry SAP as reported in Ref [3].

Table 1 DEM parameters and material properties

|	**SAP**	**Rice**	**Wall**
Kinetic parameter k (s^{-1})	0.003	0.001	-
Density ρ $(\frac{kg}{m^3})$	1,600 [3]	1,400 [8]	-
Young modulus E (Pa)	2.13x10^4 [3]	5.01x10^8 [8]	2.50x10^7
Poisson ratio ν (-)	0.50 [3]	0.28 [8]	0.25
Friction coefficient (-)	0.096 [3]	0.249 [12]	-
time step (s)	5.0x10^{-7}	5.0x10^{-7}	-

4 Model validation

The initial configuration of the system is shown in Fig. 4, while Fig. 5 shows snapshots at different swelling times. Validation of the model was performed by comparing the rise of the top surface of the granular bed with time with the literature data [3], as shown in Fig. 6. Initially, having just one layer of SAP at the bottom of the container, the height of the bed was $7.8\ 10^{-4}$m which correspond to the diameter of the largest particle. As shown in Fig. 6, after about 22 min of swelling, the height of the SAP bed of particles rose to $7.25\ 10^{-2}$m which is a rise of ~9,200%. At first sight, the latter value seems unrealistic, but this is due to an increase in radius of ~600%, which results in fewer particles per layer.

The results also show that the final height predicted by the model is in good agreement with the experimental data. The same is true for the initial and final swelling rates, as the slopes of the dashed curve, from 0 to 4 min and after 13 min, are consistent with the experimental data points. However, the height is slightly overestimated between 4 to 13 min of soaking, meaning that the swelling rate during this time period is not in good agreement with the experimental data. This could be related to the assumption of a kinetic parameter (k) that is independent of the particle radius. Being a diffusion-controlled phenomenon, the swelling rate of each grain is affected by the initial size [13]. The same outcome was obtained by Sweijen *et al.* [3] in their simulations. However, the overestimation obtained by employing a first order kinetic model presented in this study is lower than that obtained by their theoretical model. The latter observation suggests that the model employed in this work can better predict the overall behaviour of swelling granular media.
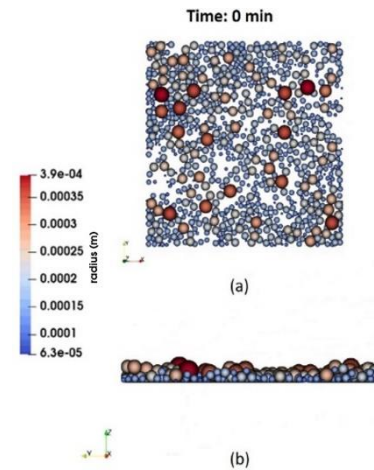
Fig. 4 Initial configuration, (a) top and (b) lateral views, of the system.
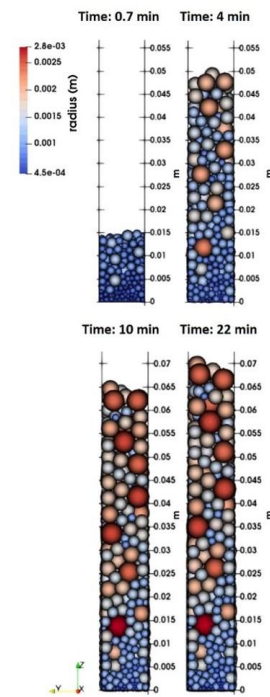

Fig. 5 Particle profiles at different swelling time.
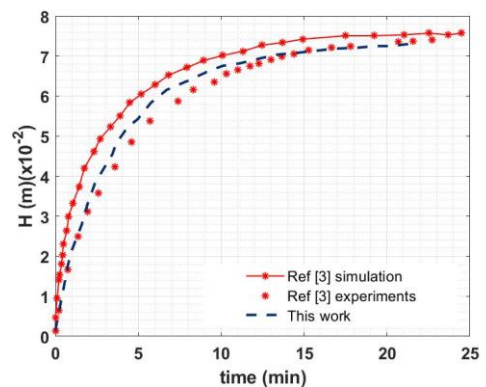
Fig. 6 Time evolutions of the height (H) of the bed of SAP.

5 The effect of material properties on the swelling behaviour

Using the validated DEM model, numerical analysis of the effect of material properties on the swelling behaviour of granular media was performed with the same initial configuration as described in the previous section, while the particle properties were changed to those of rice, as shown in Table 1. The swelling was simulated for about 12 minutes. Time evolution of the height of the bed obtained with rice was compared to that with SAP, as shown in Fig. 7. The swelling kinetic parameter of a single grain of rice ($k = 0.001$ s^{-1}) is lower compared to SAP ($k = 0.003$ s^{-1}). Furthermore, the maximum amount of water which can be absorbed by the material is less for rice. Hence, when using rice properties, instead of SAP, the expectation is to obtain a less significant bed expansion for a given swelling time. This is confirmed by the DEM analysis. As shown in the insertion in Fig. 7, after about 12 min of swelling, the bed of particles having rice properties increased its height by about 7% from its initial value, which is insignificant compared to the 8,600% change obtained for SAP. However, as shown in Fig. 1, the polymeric material can reach its equilibrium volume after around 25 min of soaking, while rice kernels require about 50 min to reach equilibrium. Therefore, the expansion of rice can be significant and cannot be overlooked over extended time periods.
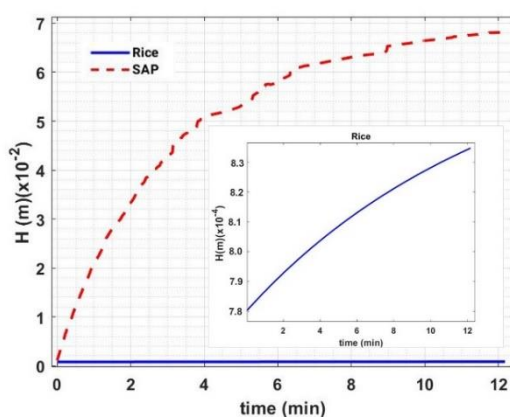
Fig. 7 Comparison of the expansion of the bed of particles with rice and SAP properties.

6 Conclusion

A DEM model for swelling was developed by considering a first order kinetic model to predict the swelling of a single particle. It was shown that the model can accurately reproduce the experimental observations. The DEM analysis performed by comparing the bed expansion for SAP and rice showed that the material properties play a significant role in swelling; After about 12 minutes of swelling, the height of the bed of particles with rice properties increased by about 7%, while the height increase for SAP was much more significant, as it increased by about 8,600%, even though the value of the kinetic parameter only triples. The developed model can be applied to study consequences of swelling phenomena in granular materials, such as segregation, or heat generation. Future research should investigate, and eventually include, the effects of temperature and initial particle size on the swelling rate.

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