Modelling and measuring of cohesion in wet granular materials

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Abstract

Using a Cohesive Discrete Element Method (CDEM), three-dimensional simulations have been performed to investigate the internal tensile stress and the tensile strength and shear strength of fine, cohesive granular materials. Interparticle cohesion is taken into account by modelling liquid bridges in pendular state. The influence of surface roughness is considered by a minimum separation distance of the particles with respect to liquid bridges. Agglomerates of mono-sized spheres have been formed to measure the stress caused by liquid bridges. A good general agreement with Rumpf’s equation is demonstrable, and divergences may be explained by the existence of stretched bridges. Spheres and more complex particle shapes have been used for shear and tensile test simulations. Applying negative loads, the yield loci in the tensile range could be measured successfully. A comparison with experimental ring shear tests on glass beads demonstrates a good agreement.

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1. Introduction

The cohesive properties of powder materials predominantly determine their flowability. Thus, parameters such as cohesion, unconfined yield strength, and tensile strength are important information for reliable design of bulk storage and handling equipment. These parameters are linked by the powder’s failure criterion that can be represented, e.g., by the yield locus, the conical failure surface in the principal stress space, or the Roscoe failure surface, respectively [1,2].

During the past hundred years, many methods and devices have been developed to determine the flow properties of powder materials [3]. In particular, shear testers are well investigated, and for some applications, such as silo design, it is well understood how shear test results can be interpreted and used.

However, shear testers fail if the desired range of normal loads is too small, and important properties, such as the cohesion $\tau(\sigma = 0)$ and the tensile strength $\sigma(\tau = 0)$ can only be obtained by extrapolation. Theoretically, the extrapolation could be validated against the tensile strength obtained from tensile tests with split cell testers and watch-glass testers [4–10]. Unfortunately, attempts to apply these techniques have not been very successful so far [8].

There are mainly two conceivable explanations for this apparent lack of success. Firstly, at present, no sample can be used twice, in a shear test as well as a tensile test. Therefore, it is difficult to ensure identical micro-structural conditions. Secondly, the design and operation of shear and tensile testers are very different. Schubert and Wibowo [7,9] have shown that even for one type of tensile tester, the tensile strength varies with the height of the sample. In consequence, it is also difficult to confirm any theories trying to estimate cohesive properties.

In a first step to understand this subject, the above outlined problems should be eliminated. Experimentally, this probably could be done with a special tester in a space lab on microgravity conditions. In this paper, however, the results of less-expensive computer simulations are presented. For this, a Cohesive Discrete Element Method (CDEM) is used (Section 2).
In Section 3, the influence of microscopic parameters, such as liquid bridge volume and surface roughness is shown by means of the simulation of wet static sphere assemblies. On the macroscopic level, the internal tensile stress is compared with Rumpf’s model [11].

More complex particle shapes are used in Section 4 for the simulation of slow deformation processes, namely, direct shear tests and tensile tests. In particular, it is focused on the tensile range of the yield loci, as it could be simulated directly.

2. Simulation method

2.1. CDEM model

The three-dimensional Discrete Element Method is used to simulate wet static assemblies (Section 3) as well as their slow deformation (Section 4). The particles are represented either by spheres or by penetrated primary spheres forming rigid bodies (Fig. 1). Although the particles are rigid with regard to the overall shape, contacts are assumed elastic.

The contact model considers normal and tangential forces. To describe the elastic deformation in the normal direction, the Hertzian law for spheres is used. The accompanying energy dissipation is modelled by means of a viscous damping law depending linearly on the relative normal velocity as well as on the deformation, i.e., the overlap of sphere caps. A linear spring law, which is cut off at the Coulomb friction force, describes the elastic deformation in tangential direction. The nature of the corresponding damping law in this direction is the same as that in the normal direction [12].

The rolling resistance due to the deformation on the microscopic contact scale is neglected. However, on the mesoscopic particle scale, free rolling is prevented in all directions when particles consist at least of three sphere segments not lying on a straight line. This makes the application of additional elements such as torsion contact springs [13] unnecessary.

Additionally, for modelling cohesive particle systems, forces emerging from attractive potentials can be incorporated. In the presented work here, the model of pendular liquid bridges has been used. Other models, such as the Van der Waals potential, have not been considered, as they contribute forces being approximately a decade smaller than liquid bridge forces [14].

2.2. Pendular liquid bridges

Much attention has been given to the subject of single liquid bridges between spherical objects [15–20]. The exact curvature can only be solved numerically. For the purpose of DEM simulations, such an algorithm is too time consuming. Fortunately, Lian et al. [21] have shown that the difference between the numerical solution of the exact shape and a toroidal approximation amounts to less than 10%. Considering the error of experimental results due to uncertainties of surface tension, wetting angle, liquid bridge volume, and particle roughness, this approximation is sufficiently accurate.

The resulting force of a toroidal liquid bridge can be calculated either on the three-phase contact area (boundary method) or on the gorge of the bridge [15] (neck or gorge method). The gorge method appears to be more accurate, and it is therefore used in the presented model. The force consists of a contribution of the capillary pressure $\Delta p$ as well as the surface tension $\gamma$:

$$F_{LB} = \pi R_1^2 \Delta p + 2 \pi R_2 \gamma.$$  \hspace{1cm} (1)

With the capillary (Laplace) pressure

$$\Delta p = \gamma \left( \frac{1}{R_1} - \frac{1}{R_2} \right)$$  \hspace{1cm} (2)

Eq. (1) can be rewritten as

$$F_{LB} = \pi \gamma R_2 \left( \frac{R_2}{R_1} + 1 \right)$$  \hspace{1cm} (3)

Herein, $R_1$ and $R_2$ are the principal radii of the liquid meniscus.

Because the surface curvature is assumed to exhibit a toroidal shape, the liquid volume $V_{LB}$ can be solved analytically as it depends on $R_1$ and $R_2$, as well as the half-filling angle $\beta$ and the wetting angle $\delta$ (Fig. 2). Unfortunately, the half-filling angle $\beta$ cannot be calculated explicitly. Therefore, to calculate $\beta$ as function of a given volume and the separation distance $a$, an iteration algorithm is applied. Typical curves are shown in Fig. 3.

A minimum separation $a_{\min}$ can be applied to take the surface roughness $a_r$ of particles into account.

$$a_r = \frac{a_{\min}}{2}.$$  \hspace{1cm} (4)

As suggested by Pietsch [22], this model causes liquid bridges to be prestretched even if body contacts exist (Fig. 4).

---

Fig. 1. Principle of CDEM Model. The particle shape may vary from simple spheres to complex shapes formed of sphere segments.
The critical separation distance $a_c$ is used as a failure criterion that can be found empirically by solving the exact curvature numerically [21].

$$a_c = \left(1 + \frac{1}{2} \theta^2\right)^{1/3} V_{LB}$$  \hspace{1cm} (5)

2.3. Scaling

The time steps in DEM depend mainly on stiffness and mass of the particles because they are governed by the equation of harmonic oscillation. For realistic material parameters of fine-particle systems, the simulation time steps take values that are not practicable for simulation of several thousands of particles, due to the limitation of current computational power. Therefore, in Discrete Element Simulations, it is very common to scale down the stiffness of particles by some decades. Although it can change the dynamic behaviour of particle systems dramatically, it is believed to be acceptable for low loaded dry systems. Unfortunately, in case of compressive stresses above 1 kPa, the contact deformations can become unrealistic. Consequently, this will cause higher coordination numbers and solid fractions than a real particle system would exhibit. Hence, the micro-mechanical fabric, as well as the internal stress state, is likely to become distorted.

Therefore, the way of scaling up the mass seems an alternative pragmatic procedure, although the advantage and justification are not as obvious as for the case mentioned above. Considering a simple mass oscillator with a mass $m$ and a stiffness $c$ of its spring, the time step $\Delta t$ needs to be a sufficient small fraction of the oscillation period. When the mass is scaled by a factor $f$, the scaled time step will be scaled by the square root of this factor. Unfortunately, in case of a constraint-driven system (e.g., direct shear process), more energy will be pumped into the system being deformed with the same velocity as a nonscaled system. Obviously, to keep the energy constant, the velocities have to be scaled down by the square root of the scale factor $f$. Therefore, the scaling advantage will be forfeited for a desired deformation.

However, as the deformation process is already slow enough to be considered quasi-static, the particle inertia will not have a significant influence on the stress state. This advantage is used in the present largely quasi-static situations. By scaling the particle mass by a factor of $10^3$ and $10^5$, the results presented here were obtained by applying a realistic Young’s modulus of 70 GPa for glass.

3. Stress state in wet particle systems

3.1. Generation process of wet agglomerates

For investigating the tensile stress in particle systems, agglomerates of mono-sized spherical particles have been
used. To obtain isotropic packings with respect to the spatial distribution of contact normal vectors, a gravity centre is used to attract 10,000 randomly moving particles. During this process, the particles are frictionless, but experience a global damping comparable to a surrounding viscous medium. Therefore, central sedimentation occurs with a velocity in the range of 0.01 m/s, forming spherical agglomerates as shown in Fig. 5.

Such assemblies are not supposed to be the densest random packing. Computer simulations based on central or uniaxial gravity consolidation usually produce loose random packings being comparable to poured, unvibrated packings. Densest packings are also possible but require special algorithms [23].

There are conjectures [23,24,26,27] that mono-sized sphere systems exhibit a void fraction within the limits of $\varepsilon = 0.4$ for loose random packings and $\varepsilon = 0.3634$ or $\varepsilon = 0.364$ for dense random packings.

The agglomerates presented here show a void fraction of $\varepsilon = 0.375$, which lies slightly closer to the proposed limit of dense random packings.

Post-genetic, the liquid bridges have been added to all body contacts, as it would take place during a capillary condensation when the relative humidity of the surrounding air is increased. The volume of the liquid bridges was small enough to avoid the contact of distinct bridges and hence to guarantee the pendular state. Thus, it was also ensured that the saturation defined as

$$S = \frac{V_L}{V_V} \approx \frac{1 - \varepsilon}{\varepsilon^2} \frac{3V_{LB}}{d^3}$$

was smaller than the limit of $S \approx 30\%$, marking approximately the transition from the pendular state to the funicular state [17].

Finally, the central gravity has been removed to allow the relaxation to a static equilibrium without body forces or external forces.

### 3.2. Contact deformation

A particle system in pendular state is characterized by a web of tensile forces resulting from distinct liquid bridges. Performing the transition from the microscale to the macroscale, these forces contribute a tensile stress to the internal stress state. In case of the static wet particle system investigated here, no external stresses are present. Hence, the tensile stress component is solely compensated by the elastic deformation of the particles.

For the contact of two wet spheres, the equilibrium of liquid bridge force and elastic force is reached at

$$a_{LB} = k \left( \frac{\pi \gamma R_2}{R_2} \left( \frac{R_2}{R_1} + 1 \right) \right)^{\frac{1}{2}}$$

(see Appendix A).
However, in an assembly, the particles form a coupled system preventing the majority of contacts from this equilibrium deformation of an isolated particle pair. Nevertheless, this deformation is very distinguishable in Figs. 6 and 7, as it belongs to the class with the largest relative frequency.

3.3. The wet coordination number

Suzuki [25] compared as much as 10 models describing the coordination number of body contacts (dry coordination number) as a function of the void fraction. Nevertheless, there are signs that the dry coordination number is rather independent on the void fraction and remains almost constant in the range $k = 6–7$ [26–28]. This agrees with the dry coordination numbers generated by the CDEM simulations presented here. However, the dry coordination number can be different from the wet coordination number, as the liquid bridges can be stretched between non-touching particles (Fig. 8). The amount of stretched liquid bridges is strongly history dependent. The generation process used here formed up to 18% of stretched liquid bridges for the upper range of the investigated liquid bridge volumes (Fig. 7). According to Eq. (5), the number of stretched bridges will reduce with decreasing liquid bridge volume.

This effect is shown in Fig. 9, where sphere agglomerates with various surface roughnesses have been used for simulation of drying processes. A constant coordination number can be observed for higher liquid bridge volumes. With proceeding drying process, the bridges start tearing apart. The beginning is indicated by the curve bend and depends on the surface roughness, as it prestretches the bridges. Further drying reduces the coordination number exponentially, until the dry coordination number ($k = 6.6$) is almost reached. At this point, nearly all stretched bridges have vanished, and all other bridges are prestretched due to surface roughness, apart from the case $\alpha_r/r = 0$. In the latter, unrealistic case, liquid bridges can only disappear if the liquid bridge volume is reduced to zero. Therefore, the wet coordination number converges towards the dry coordination number. In case of rough particles, almost all bridges break simultaneously, which is indicated by a sudden decay of the wet coordination number below the dry coordination number.

3.4. Tensile stress

In contrast to experimental measurements, a CDEM simulation provides the deformation-free access to the internal stress components. The stress tensor resulting from liquid bridge forces can be measured by [12,35]:

$$\sigma_{ij} = \frac{M}{2V} \left( d_i F_{LB,j} + d_j F_{LB,j} \right).$$

(8)

For the assumptions of:

- mono-sized spheres,
- a geometrical isotropic packing,
- isotropic distributed contact directions, and
- a unique cohesive force for all contacts.

Eq. (8) transforms into:

$$\sigma_t = \frac{1 - \varepsilon}{\pi} k \frac{F_t}{d^2}$$

(9)

(see Appendix B) where $F_t$ is the cohesive contact force, $\varepsilon$ the porosity, $k$ the coordination number of liquid bridge contacts (wet coordination number), and $d$ is the particle diameter. This is exactly the equation that Rumpf [11] derived for the above given assumptions.\(^1\)

For the sake of complicity, the related tensile stresses measured in the simulation and calculated from Rumpf’s model Eq. (9) are plotted in Fig. 10. The values are divided by the wet coordination number to avoid the influence of its variation. As shown in Appendix B, Eq. (8) will deliver exactly the same results as Rumpf’s Eq. (9) when the given assumptions are met. Hence, a difference between the simulated and the predicted stresses will emerge if one or more of these conditions are hurt. The investigation of the microstructure reveals that the assembly meets the condi-

\(^1\) In this paper, Rumpf corrected a more often referenced equation presented in Ref. [33]. Later, Molerus [34] deduced the same result by an equivalent derivation.
4. Deformation of wet particle systems

4.1. Generation process of specimens

Similar to the generation process of wet agglomerates (Section 3.1), nonspherical particles (see Appendix C) are attracted by a gravity centre to fill a column made by periodic boundaries. After the filling procedure, the gravity centre is switched off, and the upper and lower walls are moved towards each other until the cubic space is filled entirely as shown in Fig. 11. Liquid bridges and the Coulomb friction can be applied pre- or post-genetic to obtain different packing structures and densities.

In contrast to real shear testers and simulations of Jenike shear cells [29], this model eliminates the influence of sidewalls. Furthermore, the same data set that is used for shear tests can be subjected to a tensile test simulation. This ensures identical conditions for the comparison of the two tests.

4.2. Tensile test

In order to obtain the tensile strength of wet assemblies, a model as shown in Fig. 11 has been used. The bottom and lid are moved apart with a constant velocity while the stresses are recorded.

During this process, the sample has to satisfy the quasi-static equilibrium of the internal stress state and the external load. Neglecting the small contribution of friction and damping, the internal stress is determined by the attractive forces of the liquid bridges and the repulsive forces of the

Fig. 9. Decline of coordination number of liquid bridge contacts in a simulated drying process of agglomerates. Parameter is the surface roughness $a/r$ of particles.

Fig. 10. Measured tensile stress of simulated agglomerates (dots) in comparison to Rumpf’s equation.

Fig. 11. Deformation of wet particle systems
elastic contacts. Therefore, the applied external load is balanced by a relaxation of the elastic particle contact deformations.

This has been discussed by Schubert et al. [30] and is shown in Fig. 12 for a single contact of a pair of spheres. The curves start at the equilibrium deformation when no external force is applied. The liquid bridge force is considered constant for the range of the elastic contact deformation. To pull the spheres apart, an increasing external tensile force is needed. This force, represented by the solid line in Fig. 12, has to balance the sum of the internal forces, $F_H + F_{LB}$. The tensile process is stable as long as an elastic contact deformation exists that can relax in order to maintain the quasi-static equilibrium. Hence, the tensile strength is reached in the moment when the elastic contact deformation vanishes. The further application of the corresponding external force will result in an unstable fracture process, as the tensile force of a liquid bridge decreases with increasing separation distance (Fig. 3).

Although this principle also applies to the microscale of an assembly of particles, this process will appear slightly different on the macroscale. Applying an external tensile stress will cause the stretched bridges to break first. This causes the internal tensile stress to reduce. During the further deformation process, elastic contacts relax, and liquid bridges stretch. Ultimately, the initial deformation area narrows to a small fracture zone in which the entire extension of the assembly concentrates.

This process is shown in Fig. 13. The external load and the stress contributions of the liquid bridges (internal tensile stress $\sigma_{LB}$) as well as the elastic normal contacts (internal repulsive stress $\sigma_r$) are plotted.

The internal stresses are measured in the simulation by means of Eq. (8). Because this equation is applied to a finite volume element, it becomes increasingly difficult to measure the stresses as the deformation range narrows to a small fracture zone. In particular, it affects the result of the elastic normal stress that appears to be increasing after the tensile strength has been reached. The increase is caused by the influence of increasing elastic contacts in the immediate neighbourhood of the fracture zone.

In contrast to a single contact of a pair of spheres, the tensile strength is approximately reached when the assembly is stretched by the critical separation distance for the bridges. However, due to the distribution of contact direc-
tions and contact distances, the stress of elastic contacts has not vanished entirely when the tensile strength is reached.

Hence, the internal elastic contacts reduce the external load needed for the failure of the sample. It now becomes obvious that the internal tensile stress of a static wet particle system, predicted approximately by Rumpf’s model (Eq. 9), does not represent the tensile strength. If Eq. 9 is misused for comparison with tensile tests [31], it will appear to overpredict the measured tensile strength.

4.3. Direct shear tests

For the simulation of a direct shear process, again a sample as shown in Fig. 11 is used. The two plane walls are moved in opposite planar directions with a constant velocity. The applied normal load is held constant to maintain a chosen normal stress. For this purpose, the walls are controlled in normal direction by a servo algorithm. Because gravity can be switched off and the applied wall loads may be negative, shear tests in the range of normal tensile stresses can also be simulated.

4.3.1. Pre-shear test

The yield locus (curve of incipient failure) of a cohesive material depends on the bulk density. In order to measure a yield locus, the bulk densities of all shear specimens need to be equal. In real experiments, this is achieved by means of pre-shear tests on underconsolidated specimens with a definite pre-shear load. In this case, each specimen is expected to reach the same steady state characterized by a constant density and a constant shear stress.

To simulate the pre-shear test, an underconsolidated assembly has been generated. Fig. 14 shows the typical stress–strain curves that increase until the steady state of the shear stress is reached. Near the steady state, a scattering can be observed. This effect also emerges in real shear tests when the particles are large compared to the shear area. The simulation reveals the origin of the scattering. The approach to the steady state is accompanied by the formation of a narrow shear band in which the entire relative movement of particles occurs. This shear localisation increases the prob-
ability of temporary stable force chains bridging the shear band. Because of a temporary stable force chain, the shear stress increases and the entire assembly is deformed until the force chain fails. The influence of a single force chain is more significant when less particles are situated in the shear area.

4.3.2. Shear test

In contrast to real shear tests, the density in a simulation is strongly influenced by the generation process. Once an assembly has been formed, this data set can be used for all shear simulations of a yield locus. This automatically ensures a constant density and makes pre-shear tests redundant.

Fig. 15 shows the typical stress–strain curve for overconsolidated samples. At the peak of the shear stress, the microstructure of the sample exhibits the most significant response to the external load. The horizontal velocity shown in Fig. 16 demonstrates a gradient over the entire sample height. However, the gradient is not constant, but a larger gradient can be found in the lower section of the sample. In this section, the sample also has its largest dilatation. This causes the liquid bridges to rupture preferably in this area as it is indicated by plotting only the weakest (most stretched) bridges in Fig. 16. The weakest bridges are inclined in shear direction. However, due to the small long-range effect of liquid bridges, the frequency distribution of all liquid bridges remains constant for all directions. On the other hand, the largest elastic normal contact forces are inclined against the shear direction. They are responsible for the inclination of the major principal stress on the macroscopic level.

When failure occurred and the steady state is approached, the shear process will localise in a narrow band. Hence, the sample is divided in two parts that slide solid-like one over another. In contrast to a Jenike shear cell or an annular shear cell, the location of the shear band is not forced by the design of the shear cell. The shear bands emerge on the weakest area of the assembly and travel if a consolidation in this area occurs.
Due to the reduction of the stress state, the strong aligned structures of particle forces disappear and become more amorphous.

4.4. Yield loci

A yield locus is constructed by the pairs of shear and normal stresses belonging to the points of incipient failure. For instance, the shear and the normal stress at the peak in Fig. 15 deliver one point on the yield locus. Fig. 17 shows the yield loci of two different assemblies. The steeper line marked by squares belongs to an assembly of particles consisting of four sphere segments in a tetrahedral arrangement. The two other lines marked by rhombi and triangles belong to a wetted and a dry assembly of particles consisting of three sphere segments in a triangular arrangement.

As indicated by the larger gradient of the graph, the assembly of tetrahedrons exhibits a higher bulk friction than the assembly of triangles. The curve for the dry assembly passes through the origin, as no cohesive forces are present.

Applying a tensile load to the cohesive assemblies, shear tests with negative normal stresses could be simulated. For small tensile load, the yield locus appears to be the straight extension of the graph for positive loads. The tensile load can be increased until the tensile strength, measured by means of a tensile test simulation, is almost reached. As the tensile load increases further, the yield locus bends sharply until it meets the point of tensile strength on the axis of normal stress. Due to the high bulk friction, this is less pronounced for the system of tetrahedrons.

In Fig. 18, the yield locus of wet polydisperse glass spheres measured with an annular shear cell of Schulze[32] is shown. For the use in CDEM simulations, a polydisperse sphere assembly has been modelled. The size distributions of both the experimental and the numerical assembly are shown in Appendix C (Fig. C1). They exhibit a similar mean value $d_m$ and standard deviation $\sigma$.

The saturation of the experimental specimens has been measured by means of a standard drying procedure. From this, the required size of the liquid bridges in the simulations was calculated. The Coulomb friction ($\mu=0.3$) and the surface roughness ($a_r=0.05$) were estimated. Although the curved graph of the measured yield locus was not reproduced by the simulation with spheres, a good agreement of the simulated and the measured yield locus can be found in Fig. 18. However, using nonspherical particles in a simulation curved yield loci as shown in Fig. 17 can be principally produced. This leads to the conjecture that a small nonsphericity of the glass beads is responsible for the curvature of the yield locus.

5. Conclusion

A Cohesive Discrete Element Method has been used to simulate tensile stresses in wet particle systems. Only pendular liquid bridges were considered so far. It has been shown that for certain conditions, Rumpf’s equation is identical to the more general equation used for stress measurements in simulations. Hence, a good general agreement was found for the tensile stress in agglomerates consisting of mono-sized, spherical particles. The surface roughness appears to be a rather important parameter, as it prestretches the liquid bridges, and thus it has a large influence on the stresses in wet particle systems. Differences in simulated and predicted stresses arise from the presence of stretched liquid
bridges contributing less tensile stress. These stretched bridges are caused by the geometrical packing structure.

By means of simulated tensile tests, it could be shown that even when the tensile strength is reached, still elastic body contacts exist, supporting the external tensile load. This explains why, in the simulations presented here, the tensile strength is about 50% smaller than the internal tensile stress.

For comparison with tensile test simulations, shear tests were performed, including the range of negative normal stresses. For a small tensile load, the yield locus appears to be the straight extension of the graphs for positive loads. The tensile load can be increased almost up to the value of the tensile strength. In the vicinity of this load, the yield loci bend sharply to meet the point of tensile strength.

In the future, more simulations need to be performed to achieve a higher resolution of the tensile range. Particular attention has to be paid to the servo algorithm for controlling the load. The walls need to respond quick enough to the high frequent oscillations in order to avoid local stress peaks.

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Appendix A. Static equilibrium of a wet sphere contact

The resulting force from Hertzian pressure for equal spheres with a radius \( r \) (for different materials and radii, see relevant text books) may be written as

\[
F_H = \left( \frac{a}{k} \right)^{\frac{3}{2}}
\]

where

\[
k^3 = \frac{9(1 - \nu^2)^2}{2\pi Y^2}
\]

the stress tensor reads

\[
\sigma_{ij} = 3k \frac{1 - \nu}{\pi d^3} d_i F_{LB} \delta_{ij}
\]

After contraction, the trace of the stress tensor is obtained

\[
\sigma = \frac{1}{3} \sigma_{ii} = \frac{1 - \nu}{\pi} k \frac{F_{LB}}{d^2}
\]

Hence, the hydrostatic tensile stress caused by liquid bridges becomes identical to Eq. (9)

\[
F_{LB} = k \left( \pi \gamma R_2 \left( \frac{R_2}{R_1} + 1 \right) \right)^{\frac{3}{2}}
\]

Appendix B. Derivation of Rumpf’s model from the stress tensor

To obtain a continuum mechanical stress tensor from assemblies of discrete particles, Eq. (8) can be utilized

\[
\sigma_{ij} = \frac{M}{2V} \left\langle d_i F_{LB_i} + d_j F_{LB_j} \right\rangle
\]

This equation has been derived, e.g., by Cundall and Strack [35]. Here, \( M \) denotes the number of contacts, \( V \) the volume of the assembly, \( d_i \) the branch vector connecting particle centres and \( F_{LB} \), the liquid bridge force vector.

When Eq. (B1) is applied to a particle system obeying Rumpf’s assumptions of isotropic packed mono-sized spheres, the sample volume can be expressed by the particle volume \( V_p \), the number of particles \( N \), and the porosity \( \epsilon \)

\[
V = \frac{V_p N}{1 - \epsilon} = \frac{\pi d^3 N}{6(1 - \epsilon)}
\]

Combining Eqs. (B1) and (B2), the stress tensor can be written as

\[
\sigma_{ij} = \frac{6M(1 - \epsilon)}{\pi d^3 N} \left\langle d_i F_{LB_i} + d_j F_{LB_j} \right\rangle
\]

In the particular case of liquid bridges between spheres, the force vector is collinear to the branch vector. Furthermore, it is assumed that liquid bridges only exist on body contacts of particles. Therefore, the length of the branch vector corresponds to the sphere diameter \( d \), and the liquid bridge force is equal for all contacts. Introducing the Kronecker delta \( \delta_{ij} \) as well as the coordination number

\[
k = \frac{2M}{N}
\]

the stress tensor reads

\[
\sigma_{ij} = 3k \frac{1 - \epsilon}{\pi d^3} d_i F_{LB} \delta_{ij}
\]

2 Further literature, as well as a derivation of the equation, can be found in Ref. [12].
## Appendix C. Simulation parameters

Table C1. Parameters used for simulations

<table>
<thead>
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<th>Purpose</th>
<th>Measurements on agglomerates</th>
<th>Shear and tensile tests</th>
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<td>macroscopic speed (shear cell)</td>
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## References

[1] W.-F. Chen, Constitutive equations for engineering materials, Plastici-
   city and Modeling, Studies in Applied Mechanics, vol. 2, Elsevier,
   1994, p. 37, part B.


   measuring the tensile strengths of powders, J. Sci. Instrum. 41
   (1964) 763 – 768.

   (1968) 1405 – 1420.

[6] W. Pietsch, E. Hoffmann, H. Rumpf, Tensile strength of moist agglom-


[8] A. Schweiger, I. Zimmermann, A new approach for the measurement


    strength of a powder bed by a swing method measuring instrument,

    Kraftübertragung an Kontaktpunkten, Chem. Eng. Technol. 42 (8)

[12] T. Gröger, Schüttgutmechanische Untersuchungen zur senkrechten
    Schlauchgurtförderung, Logisch, Magdeburg, 1999, ISBN-3-930385-
    21-X.

[13] M. Oda, K. Iwasita, Study on couple stress and shear band develop-
    ment in granular media based on numerical simulation analyses, Int.

[14] J.P.K. Seville, C.D. Willett, P.C. Knight, Interparticle forces in fluid-


[16] W. Pietsch, H. Rumpf, Haftkraft, Kapillardruck, Flüssigkeitsvolumen
    und Grenzwinkel einer Flüssigkeitsbrücke zwischen zwei Kugeln,

[17] H. Schubert, Kapillarität in porösen Feststoffen, Springer Verlag,


    bridges between two spherical bodies, Langmuir 16 (2000)
    9396 – 9405.

    677 – 692.

    bridge forces between two rigid spherical bodies, J. Colloid Interface

    736 – 737.

[23] E.M. Tory, W.S. Jodrey, Comments on some types of random pack-
    ing, in: M. Shahinpoor (Ed.), Advances in the Mechanics and the
    Germany, 1983.

    poor (Ed.), Advances in the Mechanics and the Flow of Granular
    pp. 1 – 18.


[26] J.L. Finney, Structure and properties of granular materials: guide-
    lines from modelling studies of liquids and amorphous solids, in: M.
    Shahinpoor (Ed.), Advances in the Mechanics and the Flow of
    Granular Materials, Trans. Tech. Pub., Clausthal-Zellerfeld, Ger-
    many, 1983.

[27] K. Gotoh, Random structure of particle assemblies and physicochem-
    ical properties of liquids, in: M. Shahinpoor (Ed.), Advances in the


