Shear dynamics simulations of high-disperse cohesive powder

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ABSTRACT

Continuum mechanical models and appropriate measuring methods were applied to describe the flow behaviour of cohesive powders. These methods were successfully applied for practical design of process apparatus, e.g. silos. In addition, studies on the particle mechanics give better physical understanding of essential constitutive functions of a powder "continuum". At present, by means of the discrete element method (DEM) (Cundall 1992) a method is available which allows one to consider in details the contact and adhesion forces within Newton's equations of motion for each particle in a dynamic system. Thereby the introduction of irreversible inelastic contact flattening by the model, "stiff particles with soft contacts", is essential to describe the increase of adhesion force. Therefore, the dynamic behaviour of cohesive powder flow can be "microscopically" investigated and understood. The contact model between high-disperse particles (about 1 mm) will be discussed. Using this, the results of steady-state flow, incipient yielding and consolidation of TiO_2 powder will be presented. Dynamic formation of the shear zone is also shown and compared with experiments in a Jenike shear cell (Jenike 1964).

Keywords cohesive powder, shear cell, DEM simulation, dissipative contact model

1 INTRODUCTION

Continuum-mechanical models and measurement methods on their base are used most often in the powder mechanics in order to describe the flow behaviour of a cohesive powder packing. These methods are successfully applied especially in the field of practical apparatus and machine design in process engineering, for example silos. In addition, the essential property functions of the powder "continuum" can be better described and understood with the help of particle mechanics (Tomas 2001).

The Discrete Element Method (DEM) (Cundall 1992) is a new strategy, which allows one to take into account the contact and adhesive forces into the equations of motion of the particles. In this context, the implementation of an irreversible inelastic contact flattening, which is an essential element and physical reason of the increase of the adhesive force, is of vital importance. This allows the dynamic behaviour of cohesive bulk materials to be studied and understood „microscopically".

In this paper, we first present and discuss a realistic and flexible microscopic model for contact laws with elastic, permanently plastic, and adhesion forces, as based on macroscopic observations from bulk-experiments (Tomas 2001, Tomas 2002). The model in a simplified form is applied to the Jenike shear test, in order to show that at least some qualitative agreement between numerical "experiment" and reality is possible with DEM.

2 CONTACT LAW

The yield limits of the cohesive powders can be derived from their physical basis. Hence, the concept „stiff particles with soft contacts" is convenient, which allows to explain by the elastic-plastic behaviour of a sphere contact with the unloading/reloading hysteresis (Tomas 2002, Walton 1986). Further, the non-linear adhesive normal force model (Fig. 1) is applied, which describes the instantaneous contact hardening in terms of a typical contact law. Next, the three flow behaviour parameters of a continuum (steady-state yield locus, instantaneous yield locus and consolidation yield locus) are formulated by means of this contact model (Tomas 2002).

We consider the contact of two mono-disperse isotropic and smooth spherical particles as the typical components of a particle packing under the static load F_N.

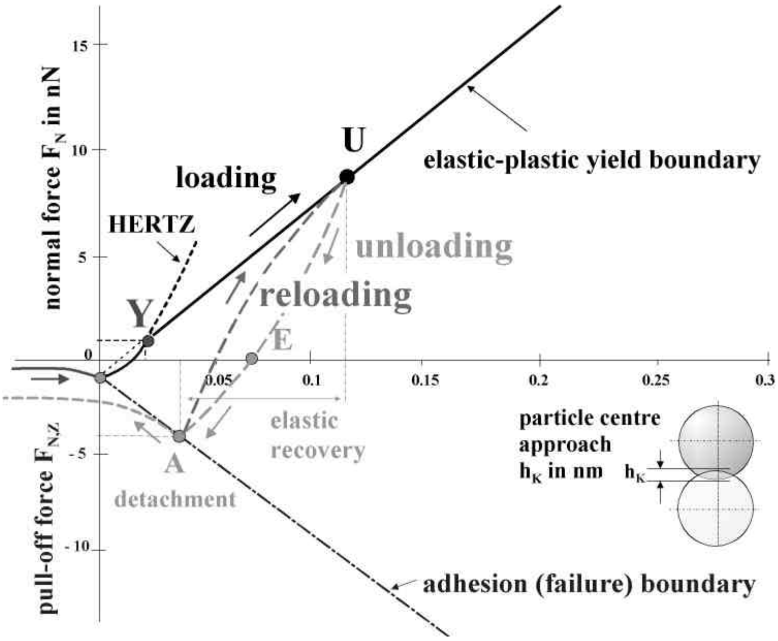

Fig. 1: Characteristic contact force as function of deformation for Titania Powder (d_{50}=610 nm, moisture X_W=0,4%) – non-linear elastic, linear plastic, adhesive, dissipative contact model

As the particles approach each other (Fig. 1, curve from –¥ to F_{H0}), the Van-der-Waals adhesive force is build up. Then we receive an elastic contact flattening described by Hertz (1882), as the effect of the created adhesive force F_{H0} itself or/and the effect of an additional static load F_N, for example the dead weight of a powder packing.

If the normal load F_N increases, the yield point *Y* in the Fig. 1 is reached, where the deformation merges into the linear plastic flow. The slope of this line is the measure for the elastic-plastic contact stiffness. Lower slope means plastically soft or compliant contact behaviour, and vice versa, the higher the slope, the stiffer is the contact behaviour. A confined plastic field is built in the circular contact centre after loading.

The unloading causes the elastic contribution to recover along the curve *U-E* in Fig. 1. Further unloading below the point *E* is only possible when a tension force is applied. The contact fails at point *A*. However, the contact could still be reloaded again along the curve *A-U*. The lens-shaped area between the reloading and unloading curves is the measure for the energy dissipation during one cycle (Tomas 2001). Therefore, our contact shows the typical hysteresis and in case of dynamic reloading/unloading cycles (oscillations) the damping as a response, which does not depend upon an applied velocity.

The adhesion boundary $F_{H,A}$ in the failure point *A* is the boundary stress function as well. Its slope corresponds to the stiffness in the tension force region. The higher the slope, the more compliant is the contact behaviour and the higher could be the adhesion force of the particle contact. A lower slope corresponds to a stiff contact with almost constant adhesion force.

3 THE MODEL SYSTEM

One possibility to gain insight about the material behavior of a granular packing is to perform elementary tests in the laboratory. Here, we chose as alternative the simulation with the discrete element model (D'Addetta 2002, Oda 2000, Kruyt 2001, Luding 2001).

The classical translational shear cell, developed by Jenike (1964), is modelled (Fig. 2). Considering a suitable CPU-time for a certain of particles one should imagine that we simulate here only a small two-dimensional (2D) element from the real shear cell. Fig. 2 shows the model for 2000 titanium dioxide particles with diameter of about (1±0,5) µm. The upper wall (shear lid) is stress controlled, i.e. when the reaction force F_N changes because of the particle reorganization, the height of the shear lid is changed as well. The normal stress $s=F_N/A$ is equal to $3\ kPa$ (A is equal to d_Z in the 2D case). The horizontal shear rate of the upper ring is preset. As the direct response, the corresponding values of the reaction force are obtained, which acts on the lateral walls. Furthermore, the corresponding shear stresses $t=F_S/A$ are calculated. The shear rate applied here is about 1-4 mm/min (similar to the one used in the Jenike shear cell in laboratory tests).

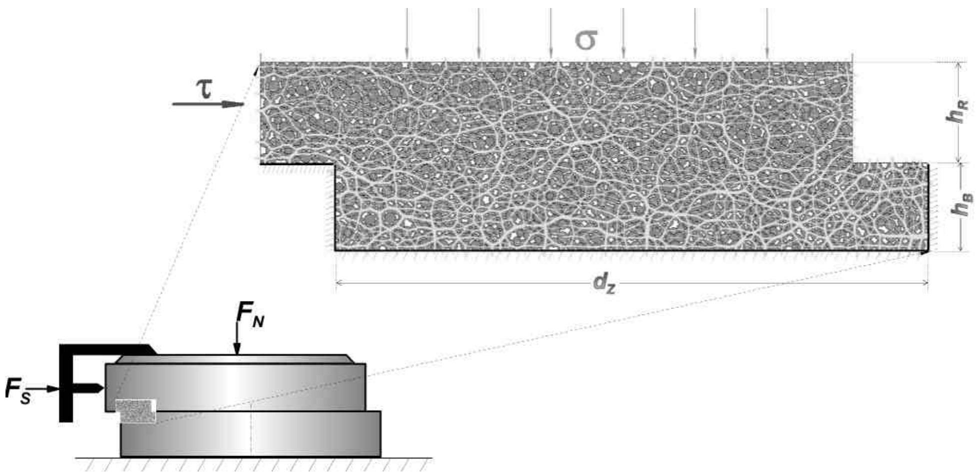

Fig. 2: The model system for the simulations
(lines in the particle system show the contact forces, with line thickness proportional to force)

4 SIMULATIONS AND RESULTS

Resulting forces acting on each particle, are determined by means of applying the force-displacement law for a particle contact in the particle system. These values are used then for the motion laws in order to update the whole system.

The first simulations are performed only with the linear adhesion contact law, which was implemented by the software (PFC2D, Itasca Inc.). A constant adhesion force of 1-10 mN (0,1-1% of average contact forces of loading) was used to approximate the load-history dependent pull-off force in Fig. 1. New results with the more general dissipative contact model for adhesive particles will be presented in a later paper.

Fig. 3 shows the force network during the shearing. The force lines run mostly from the upper left wall, where the shear force acts, to the lower right wall, where the corresponding resisting force acts. This correlates also sufficiently with the fact, that the orientation of the major principal stress s_1 is just as tilted in the shear direction.

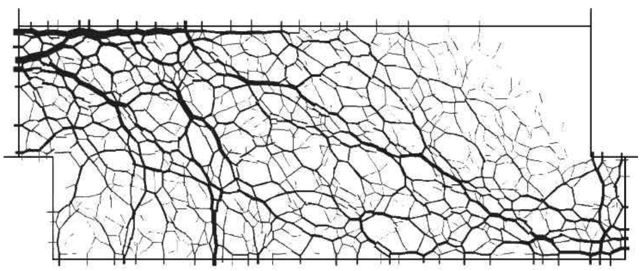

Fig. 3: Force distribution at the maximum value of shear stress

Fig. 4 presents the whole particle system after shearing both for the simulations (left) and the experiment (right). The shear zone and the angle γ, the so-called shear distortion are clearly recognised here. The angle γ is defined as a function of the shear displacement and the shear zone height.

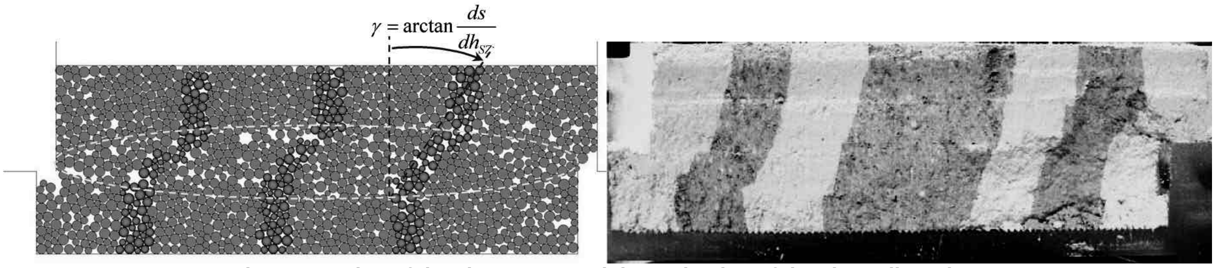

Fig. 4: Location of the shear zone and determination of the shear distortion.
Left: simulation, right: experiment

Fig. 5 shows the velocity vectors during the shearing. It is clearly shown that the motion takes place mostly in the upper ring, and the velocities in the upper ring are approximately equal to each other. Therefore, the stationary flow is reached at the end of the shear distortion.

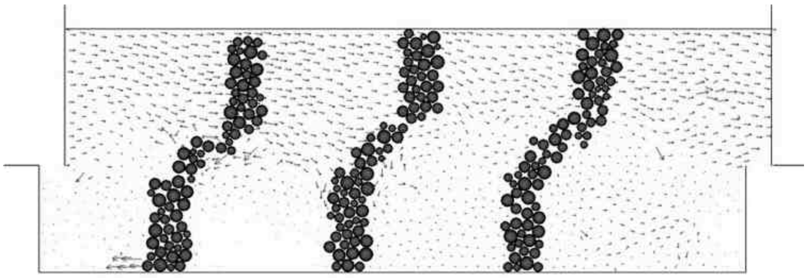

Fig. 5: Velocity vectors at the stationary flow

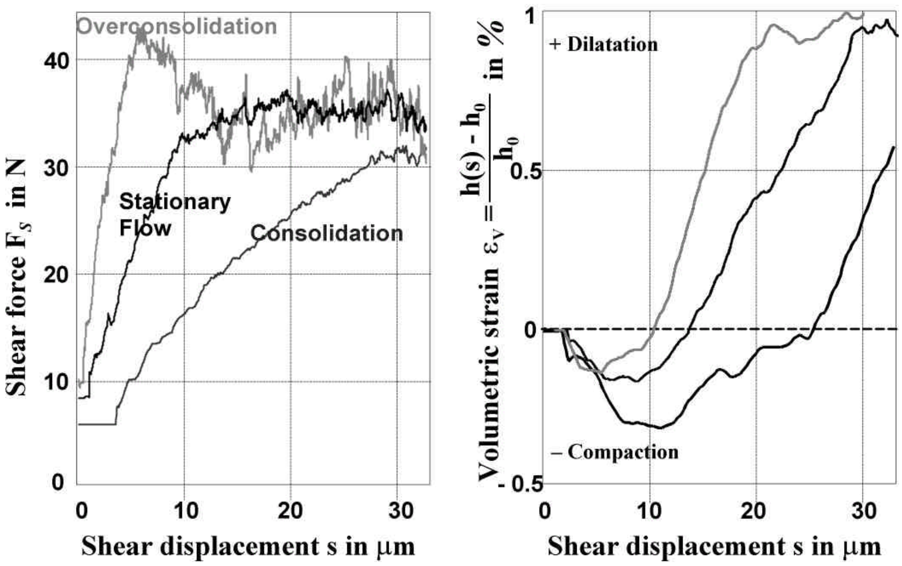

Fig. 6: Left: force-displacement diagram (stationary flow) and
Right: volumetric strain for three different porosity values

Fig. 6 shows the force-displacement diagram (left) and the volumetric strain (right) at the constant normal stress of s_N=*3 kPa* for three different values of porosity $e=1-r_b/r_s$ (where r_b is the bulk material density, and r_s – the solid density), i.e. three so-called preshear tests. The upper curve is obtained at a two-dimensional porosity of the particle system of $e_{2D}=0.16$ (it corresponds appr. $e_{3D}=0.46$ for three dimensions – see Deresiewicz 1958). The typical behaviour of the overconsolidated powder is observed in this case. The middle curve at $e_{2D}=0.18$ (e_{3D}~*0.50*) shows almost ideal stationary flow. The fluctuations of the shear force can be explained by means of the temporary and local shear-thickening and shear-thinning processes. The lower curve corresponds to $e_{2D}=0.20$ (e_{3D}~*0.54*) and shows the tendency of an underconsolidated material.

Taking into account the shear testing experiences, the good qualitative agreement is reached between the simulation results and the laboratory tests.

5 SUMMARY AND CONCLUSIONS

It is worth to notice here that the qualitative agreement of the simulations with experiments is reached. The future work includes the following problems to be solved: implementation of the general contact model for adhesive particles in the DEM-algorithm; measurements of particle contact deformation by means of the Particle Interaction Apparatus (based on Atomic Force Microscopy in cooperation with M.Kappl and H.-J. Butt (2002)), in order to calibrate the contact model; further simulations with increased number of particles and implemented adhesion force contact model (Jenike shear cell, vibrational shear cell); justification of the DEM-models by means of comparison of the simulations with laboratory measurements at the translational shear cell.

6 ACKNOWLEDGEMENT

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7 REFERENCES

CUNDALL, P. A, HART, R. D., (1992), *Numerical Modelling Of Discontinua*, 1st US Conference on DEM, Eng. Comput. 9, pp.101-113.

D'ADDETTA, G. A., KUN, F., RAMM, E., (2002), *On The Application Of A Discrete Model To The Fracture Process Of Cohesive Granular Materials*, Granular Matter 4 (2), pp.77-90.

DERESIEWICZ, H., (1958), *Mechanics of Granular Matter*, Advances in Applied Mechanics, Vol. 5, pp. 233–306.

HERTZ, H., (1882), *Über Die Berührung Fester Elastischer Körper*, J. Reine U. Angew. Math. 92 pp.156-171.

JENIKE, A.W., (1964), *Storage And Flow Of Solids*, Engineering. Exp. Station, Bull. No. 123, Univ. Utah.

KAPPL, M., BUTT, H.-J., (2002) *The Colloidal Probe Technique And Its Application To Adhesion Force Measurements*, Part. Part. Syst. Charact. 19, pp.129-143.

KRUYT, N. P., ROTHENBURG, L., (2001), *Statistics Of The Elastic Behavior Of Granular Materials*, Int. J. Of Solids And Structures 38, pp.4879-4899.

LUDING, S., LÄTZEL, M., VOLK, W., DIEBELS, S., HERRMANN, H.J., (2001), *From Discrete Element Simulations To A Continuum Model*, Comp. Meth. Appl. Mech. Engng. 191, pp.21-28.

ODA, M., IWASHITA, K., (2000), *Study On Couple Stress And Shear Band Development In Granular Media Based On Numerical Simulation Analyses*, Int. J. of Enginering Science 38, pp.1713-1740.

TOMAS, J., (2001), *Assessment Of Mechanical Properties Of Cohesive Particulate Solids – Part 1: Particle Contact Constitutive Model*, Particulate Science & Technology 19, 2, pp.95-110.

TOMAS, J., (2002), *Zur Mechanik Trockener Kohäsiver Schüttgüter*, Schüttgut 8, 6, pp. 522-537.

WALTON, O., (1986), *Stress Calculations For Assemblies Of Inelastic Spheres In Uniform Shear*, Acta Mechanica 63, pp.73-86.