II International Conference on Particle-based Methods - Fundamentals and Applications
PARTICLES 2011
E. Oñate and D.R.J. Owen (Eds)

BREAKAGE OF NEEDLE-SHAPED PARTICLES IN A COMBINATION OF COMPRESSIVE AND SHEARING STRESS FIELD

ZDENĚK GROF*, **FRANTIŠEK ŠTĚPÁNEK*** **AND PAVOL RAJNIAK**†

*Department of Chemical Engineering, Institute of Chemical Technology, Prague
Technicka 5, 166 28 Praha 6, Czech Republic
e-mail: zdenek.grof@vscht.cz, www.vscht.cz/

†Merck & Co., Inc., West Point, PA, USA

Key words: Granular Materials, DEM, FEM, Contact Problems

Abstract. *In-silico* experiments of needle-shaped particles breakage during shearing have been carried out using DEM simulation. Results of preliminary studies with variation of individual particle strength, compaction ratio, and shearing rate are presented.

1 INTRODUCTION

Needle-shaped crystals are a common occurrence in many pharmaceutical and fine chemical processes. Even if the particle size distribution (PSD) obtained in a crystallisation step can be controlled, further fluid-solid separation steps such as filtration, filter washing, drying and subsequent solid handling can often lead to uncontrolled changes in the PSD due to breakage. Population balance modelling is a common method able to describe PSD changes, however two material- and stress-field specific functions are needed: the breakage kernel (selection function) and the daughter distribution function (breakage function). There are several alternative methodologies for determination of these two functions: (i) experimental, (ii) theoretical, or (iii) computational by detailed mechanistic modelling of the breakage of single particles.

Our previous work [1] we have developed a DEM framework for detailed numerical simulation of needle-shaped crystals movement and breakage. A randomly-packed bed of elongated particles with a given PSD has been formed by letting the particles to settle down by gravity. The bed of particles has been subjected to uni-axial stress by compressing it by two parallel planes. The PSD and all breakage events have been recorded during the compression. In a follow-up work [2], results from these computational (*in-silico*) experiments were used to identify both the breakage kernel and the daughter distribution functions.

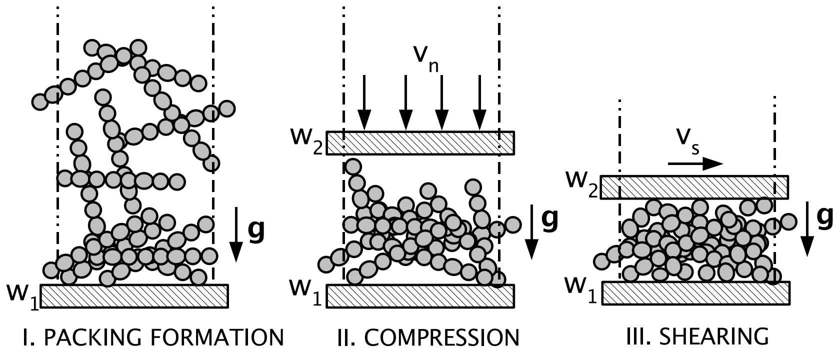

Figure 1: Scheme of the computational experiment

Our current objective is to extend our methodology [1, 2] which has been so far verified for uni-axial compression to more general stress fields.

2 METHODOLOGY

A methodology based on the discrete element method [3] modified to treat non-spherical particles by the multi-element model [4] has been used to simulate the movement and breakage of individual needle-shaped particles. The magnitude and the location of contact forces at each particle determine the load on the particle. Particles are treated as loaded beams in order to calculate bending and shear stresses along the particle. When a set threshold value anywhere along a particle is exceeded the particle breaks into two daughter particles at the point of maximum stress. A full description of the algorithm has been given in our earlier work [1]. Although only normal contact forces among elements of different particles are considered, the particles are not completely frictionless because of theirs geometry. They are represented as a compound of overlaid spherical elements, particle roughness is thus caused by gaps between elements. The set-up of computational experiment is illustrated in Fig 1.

Systems of two sizes have been generated for the simulation of shear induced particle breakage. Smaller systems containing initially 100 particles composed of 20 discrete elements (length = 20) were used for relatively fast simulations aimed to test wide range of model parameters. Selected set of parameter values has then been used in simulations with larger systems of 500, 20-elements long particles. Packing have been generated in the simulation box by letting particles to settle-down on the flat boundary by the gravitation force in the z-axis direction. Periodic boundary conditions were imposed in the x- and y-axis directions to avoid the influence of walls. During the next step, another boundary wall has been placed above the simulation box and the packing has been gradually compressed between the two walls. Particles whose loading exceeded a set threshold were allowed to break. In such a way a group of particle systems of different compression ratio has been obtained, cf. Fig 2

Position of particles near the top and near the bottom of the packing has been frozen.

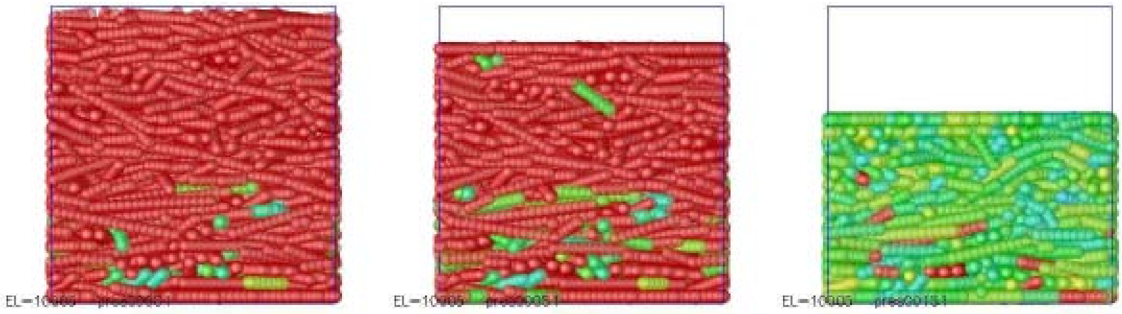

Figure 2: Illustration of the compression step. Particles are coloured according to their length.

The lower layer of particles was then forced to move at a specific velocity in the x-th axis direction while the top layer was held still. Particles in between then experience a shearing stress in a similar way as material in the ring shear device. Again, the particles whose loading exceeds a set threshold break into two parts.

3 RESULTS AND DISCUSSION

To find out the effect of the shearing rate on fragmentation of particles in the layer, simulations with different shear rate v_s were carried out. The configuration reached after the layer moved the length 3.15 times the simulation box width is shown in Fig 3. Starting from the same configuration (cf. Fig 2b), lower layer moved at two different speeds. From visual observation it is apparent that more breakage occurred at faster speed (Fig 3a) than at the 50 times slower one (Fig 3b). The breakage takes place mostly in the lower half of the layer in both cases.

Particle size distribution and number mean particle size evolution during shearing is shown in Fig 4. Here the larger and smaller systems are compared. One can see that results for both systems are comparable suggesting that for the computations one can use relatively low number of particles and smaller computational box. Regarding the velocity effect, the fragmentation is lower at slower velocities which is consistent with what one would expect: more careful (slower) particle displacement leaves more time for particle layer rearrangements and thus there is lower chance of local stress built-up and exceeding particle mechanical strength. If the shearing rate is much slower then the rate of layer rearrangements, then the shearing is in a pseudo-steady state and fragmentation does not depend on shearing rate anymore. Even in the pseudo-steady state regime the breakage can still occur if some particles get jammed during their displacement. As we would like to restrict ourselves to situations where the dynamical effects can be neglected, we aim to set the shearing velocity so low to be in the pseudo-steady state regime. It can be seen from results in Fig 4, that the substantial fragmentation occurs at the largest velocity, while there is less fragmentation and lower dependence on shearing velocity at remaining slower velocities.

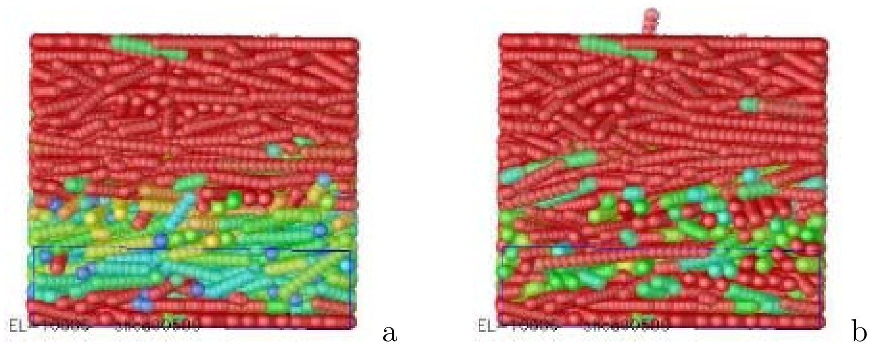

Figure 3: Illustration of the shearing step: (a) fast shearing, (b) slow shearing. Initial configuration, cf. Fig 2b

The simulation is stopped when the shearing distance reaches 6.25 and 12.5 times computation box width in larger and smaller system, respectively. Based on results, this length is sufficient as most of fragmentation occur at the beginning and no more or little fragmentation take place later as all jammed particles broke down and can be freely shifted.

Results investigating the effect of particle strength are introduced in Fig 5. Systems of three different particle strengths at two different compaction ratios are compared. It can be seen that there are small differences between particles of strength 30 and 40 at the lower compaction (88% of the initial particle height). The size of particles further decreases as expected during shearing. It is interesting to observe that the change of size distribution during shearing is smaller for weakest particles (20) than for stronger particles (40). The explanation is that the weakest particles have already broken more during compaction and short particles are less likely to get jammed and break during shearing.

4 CONCLUSIONS

A preliminary study has been made to investigate the possibility to use *in-silico* experiments to study breakage of needle-shaped particles under shearing stress. Our objective is to use these results in identifying breakage kernels and the daughter distribution functions. We have demonstrated that the simulation of shearing induced breakage is feasible even for modestly sized systems. There are two regimes in respect to the shearing velocity: The breakage depends on shearing velocity at high velocities. However, breakage is velocity independent when the shearing velocity is low enough. More simulations will be necessary to identify the transition between these regimes.

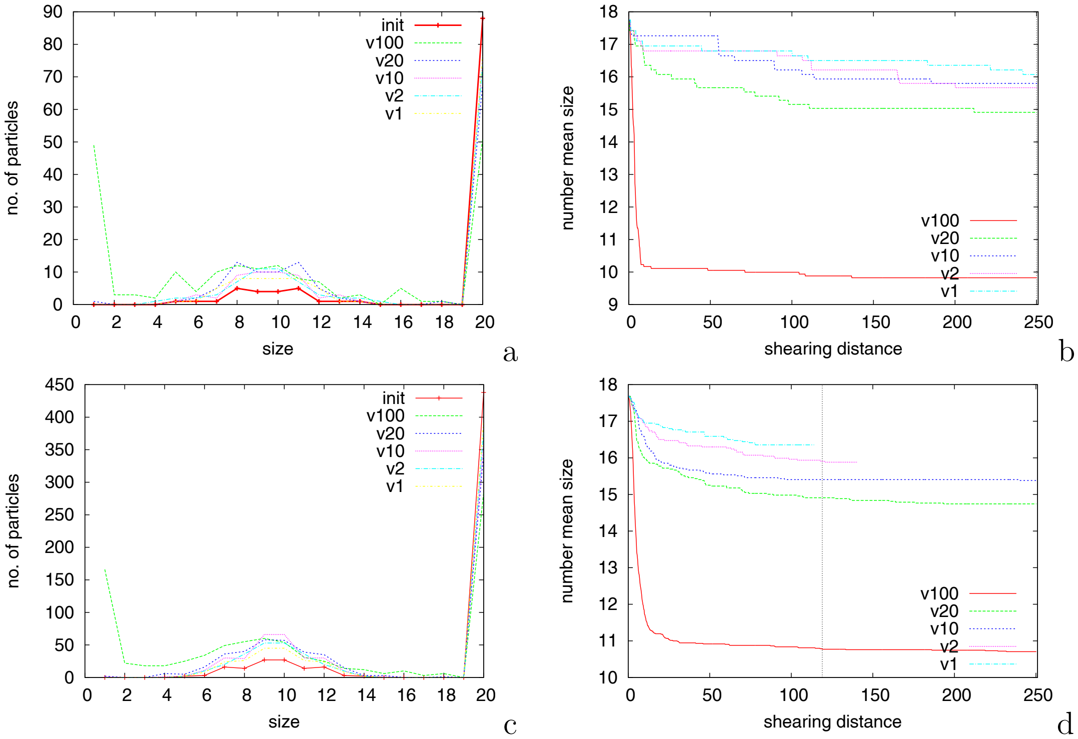

Figure 4: Effect of shearing velocity: Initial and final particle size distribution at different shearing velocities. Number average particle length evolution during shearing. Plots a) and b) are for smaller system, while plots c) and d) are for larger system. Shearing distance is dimensionless, with the unit length corresponding to the diameter of single element. Shearing velocity is also denoted in dimensionless units.

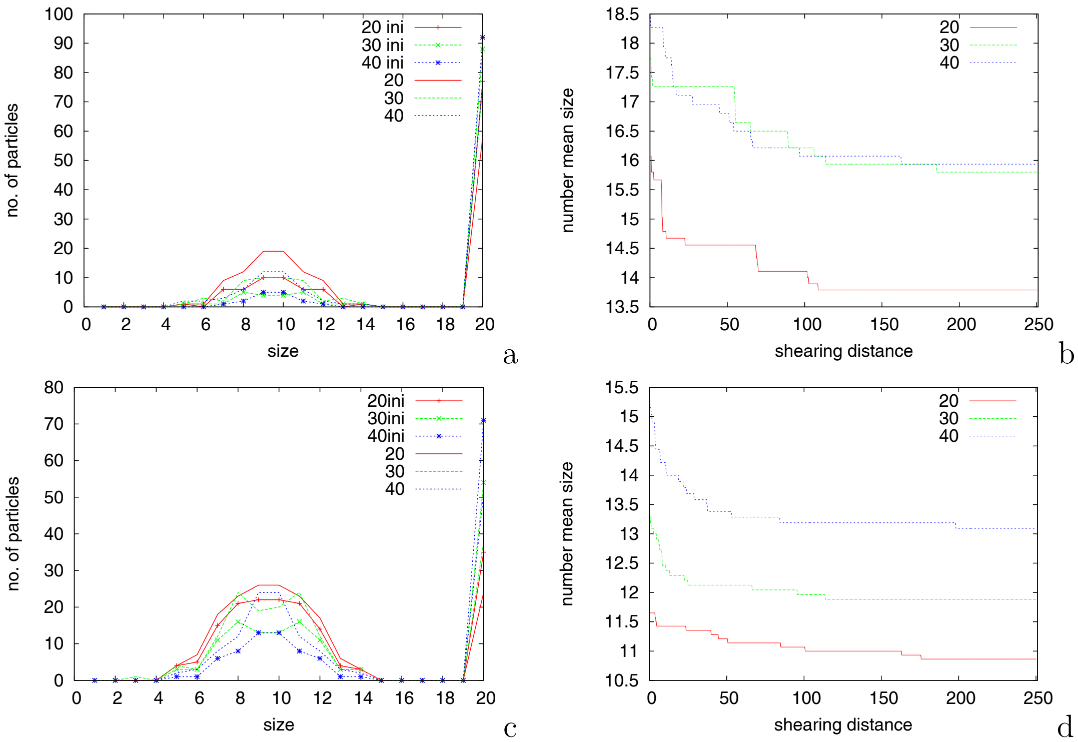

Figure 5: Effect of particle strength: Initial and final particle size distribution with particle strength of 20, 30 and 40 kPa. Number average particle length evolution during shearing. Plots a) and b) are for low compaction ratio (88%). Plots c) and d) are for higher compaction ratio (76%). Shearing distance is dimensionless, with the unit length corresponding to the diameter of single element.

ACKNOWLEDGEMENT

Funding from Czech Ministry of Education through grant MSM6046137306 is acknowledged.

REFERENCES

[1] Grof, Z., Kohout, M. and Štěpánek, F. Multi-scale simulation of needle-shaped particle breakage under uni-axial compaction. *Chem. Eng. Sci.* (2007) **62**:1418–1429.

[2] Grof, Z., Schoellhammer, C.M., Rajniak, P. and Štěpánek, F. Computer and experimental investigation of needle-shaped crystal breakage. *Int. J. Pharmaceutics* (2011) **407**:12–20.

[3] Cundall, P.A. and Strack, O.D.L. A discrete numerical model for granular assemblies. *Géotechnique* (1979) **29**:47–65.

[4] Favier, J.F., Abbaspour-Fard, M.H., Kremmer, M. and Raji, A.O. Shape representation of axi-symmetrical, non-spherical particles in discrete element simulation using multi-element model particles. *Eng. Comput.* (1999) **16**:467–480.