Final report (OTKA NN 107737)
Project title: Anisometric granular materials (2013-2017)
PI: Tamás Börzsönyi

This collaborative project focused on the flow and packing of granular materials consisting of anisometric grains. The project was realized according to the research plan with an extension of 8 months. This extension enabled us to proceed further than planned.

We successfully studied all 3 subjects listed in the research plan:

(1) ordering and alignment of anisometric granular materials in shear flows,
(2) flow and jamming phenomena in hopper flows,
(3) geometry of shear zones.

All three directions resulted in interesting new observations which merited to be published in highly ranked scientific journals (*Phys. Rev. Lett.*, *Soft Matter*, *New J. Phys.*, *Phys. Rev E*). As an application, we used our numerical model to solve an actual problem (improving the stability of railway tracks), which was documented in 2 publications.

(4) In addition to the planned activities, we were able to explore new segregation phenomena, namely we presented the first experimental demonstration of shear induced segregation in a binary granular mixture, where the two components differed only in the surface friction of the grains (published in *Soft Matter*). We classify this as an extension of the activities (1) and (3).

Here we give a detailed description of the results for all 4 subjects.

1. Ordering and alignment of anisometric granular materials in shear flows:

Extensive X-ray CT investigations were carried out using the tomograph provided by the German collaboration partner and optical measurements were done in the Wigner RCP to study how the ordering and the packing density changes in a granular material under shear. Using the cylindrical split bottom shear cell (see Fig. 1a), we have shown that shearing a random system results in an initial expansion of the material by about 10-15%. At the same time orientational ordering of the anisometric (elongated or flat) particles starts, leading to a compaction of the material. The corresponding density increase is about 5%, thus it can only partially compensate the initial dilation (see Fig 1b). Materials consisting of spherical particles undergo positional ordering due to the applied shear (see Fig 1c).

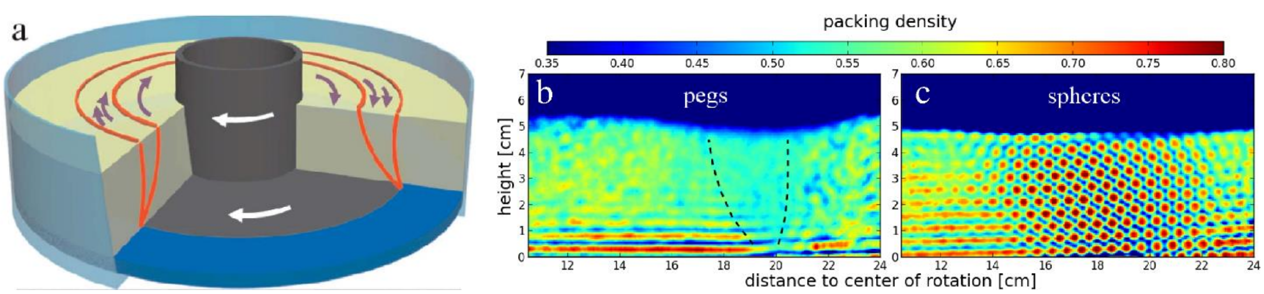

Fig. 1. (a) Cylindrical split bottom shear cell, (b) vertical cut of the averaged density profile, shear induced dilation is observed for pegs in the deformation zone, (c) shear induced ordering of uniform spheres.

In this ordered state, the grains form chain like structures (parallel to the streamlines), which we characterized by the pair-distribution functions. These results were published in a paper [Soft Matter **10**, 5157 (2014)], and other details were presented in two talks at conferences (Cambridge and Madrid).

We have discovered a new type of secondary flow in a system of sheared rods (Fig. 2), which leads to unexpected heaping in flows generated in the circular split bottom shear cell. Important parts of these measurements were done using the X-ray CT apparatus provided by the German collaboration partner. The velocity field characterizing the secondary flow which was determined from multiple tomograms is shown in Fig. 2(b) together with a sample tomogram. We have shown that the secondary flow is connected to a symmetry breaking in the system, which is a result of the peculiar alignment of the rods due to the shear flow. We have also shown, that the same phenomenon is taking place for the case of oblate particles (lentil like grains). The results were published in two papers [Soft Matter **11**, 2570 (2015), New J. Phys. **18**, 113006 (2016)], and a talk was given on this subject at the yearly Statistical Physics Meeting of the Hungarian Academy of Sciences.

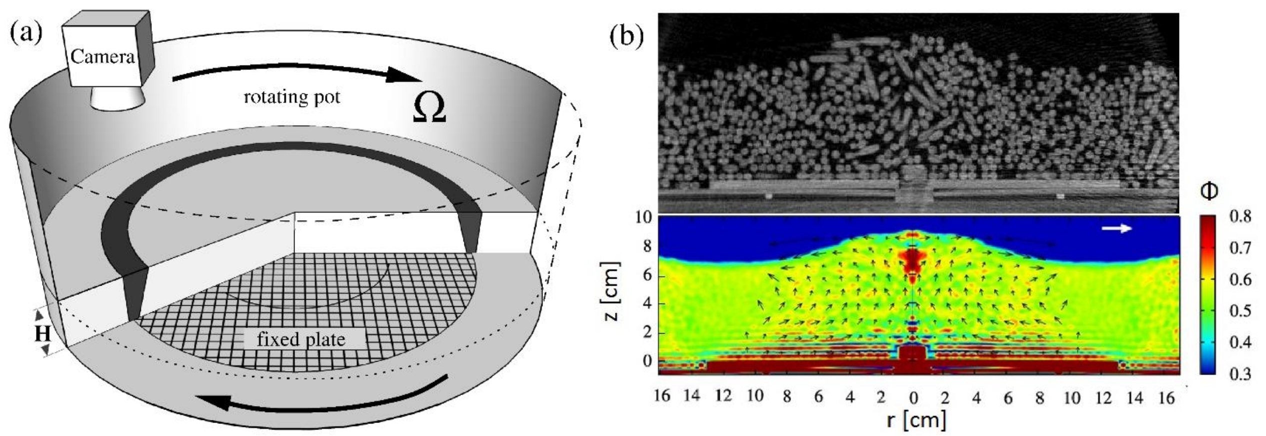

Fig. 2. (a) Cylindrical split bottom geometry - in this case the container is rotated and the middle part is standing, (b) central vertical cut of a sample tomogram and the averaged density profile together with the velocity field characterizing the secondary flow.

2. Flow and jamming phenomena in hopper flows:

Experiments were performed to compare the flow and clogging of spherical and non-spherical grains in a hopper.

- X-ray CT measurements were performed to determine the 3D arrangements of grains in a clogged hopper. In these measurements the hopper orifice was relatively small and clogging events were frequent. Consequently the displacement of grains between subsequent clogging events was small enough, thus we were able to determine the flow field (white lines in Fig. 3). We found, that similarly to simple shear flows the average direction of elongated grains was not parallel to the flow lines. Comparing the evolution of the orientational distribution in the two geometries, we detected an average angle closer to the flow lines, and a smaller order parameter in the hopper flow. These results were summarized in a paper [New J. Phys. **18**, 093017 (2016)]. Two invited talks were also given: (i) at the ZCAM Workshop on Flow and clogging in bottlenecks: simulations and experiments

(Zaragoza, 2014) and (ii) at the XXXVI Dynamics Days Europe (Corfu, 2016). A further conference presentation will take place (Powders and Grains, Montpellier, France, July 2017), and the corresponding manuscript has already been accepted to the conference proceedings [Powders and Grains, AIP Conf. Proc. (2017)].

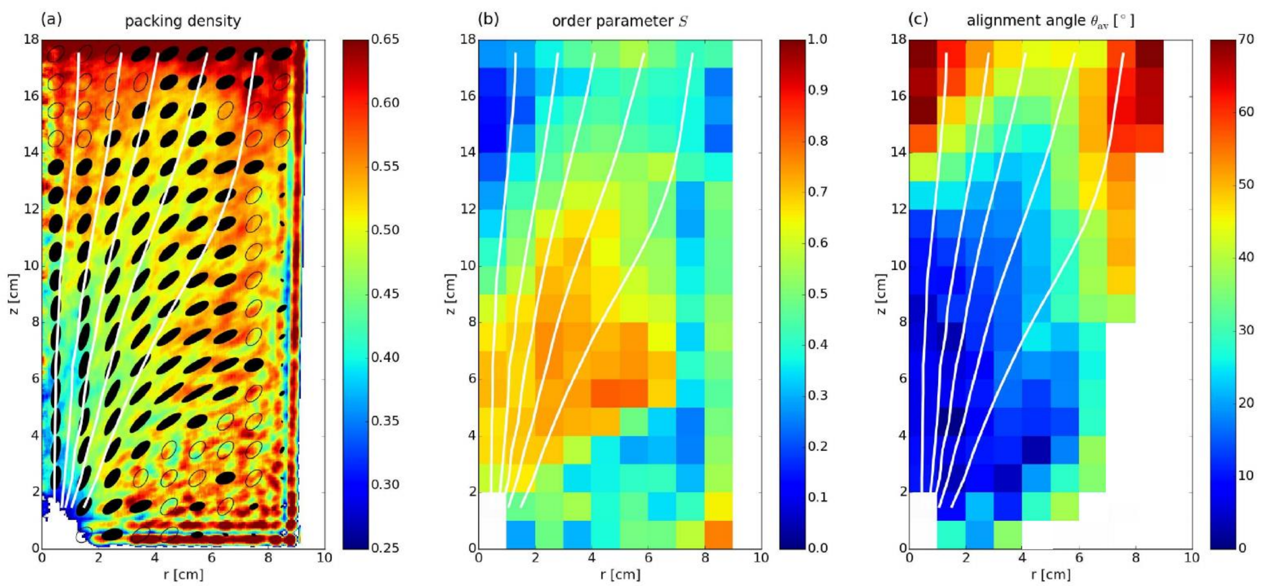

Fig. 3. (a) Packing density, (b) order parameter and (c) alignment angle of elongated grains in a 3-dimensional hopper. The orientation of elongated grains (represented by ellipses) is almost parallel to the streamlines (white lines). Density is lower in regions with higher shear rates.

- A second set of experiments was performed with slightly larger hopper orifice. We analyzed the effect of grain shape on the clogging probabilities. We found that an increasing aspect ratio Q of the grains leads to lower flow rates and higher clogging probabilities compared to spherical grains (Fig. 4). On the other hand, the number of grains forming the clog is larger for elongated grains of comparable volumes, since the long axis of these blocking grains is preferentially aligned towards the center of the orifice [Soft Matter **13**, 402 (2017)].

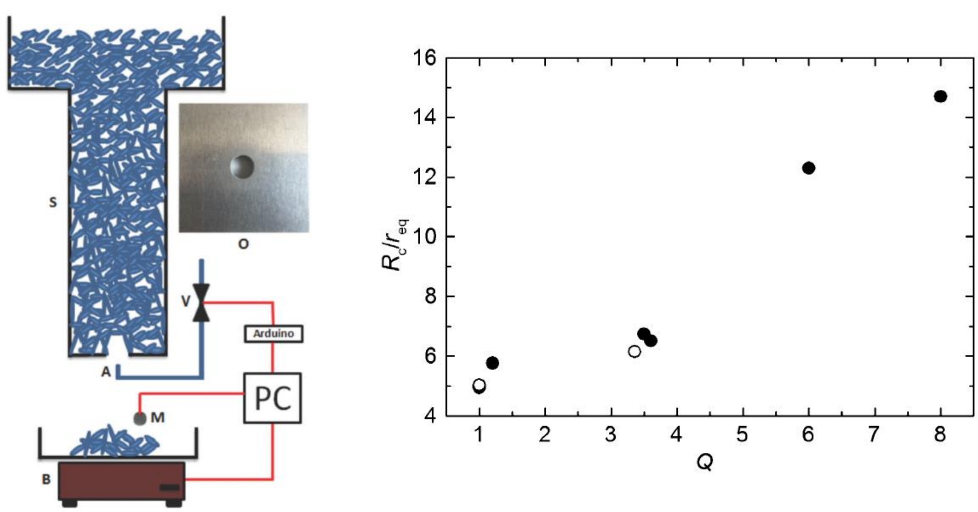

Fig. 4. Measurement of clogging probabilities in a 3-dimensional hopper. The critical radius (R_c) above which practically no clogging happens increases with grain elongation Q, thus the probability of clogging increases with grain elongation.

- Numerical simulations were performed to model arching in 3D hoppers. The average shape of the clogged dome for spheres is almost a hemisphere but individual samples have large holes in the structure indicating a blocked state composed of two-dimensional force chains rather than three-dimensional objects. For long particles the clogged configurations display large variations, and in certain cases the empty region reaches a height of 5 hole diameters. These structures involve vertical walls consisting of horizontally placed stable stacking of particles. These results will be presented at Powders and Grains, (Montpellier, France, June 2017), the conference proceedings paper has already been accepted [Powders and Grains, AIP Conf. Proc. (2017)].

3. Geometry of shear zones:

We have investigated the development of multiple shear zones in granular materials in collaboration with a German and an Iranian research group. The granular material was sheared in a modified Couette geometry (Fig. 5a-b). The resulting displacement profiles were fitted by a mesoscopic model developed by ourselves. We have shown that there is one single relevant parameter in the system, the ratio of the effective frictions near the wall and in the bulk. All the experimental results can be described by adjusting only this parameter. These results were published in a paper [Phys.Rev. Lett. 111, 148301 (2013)].

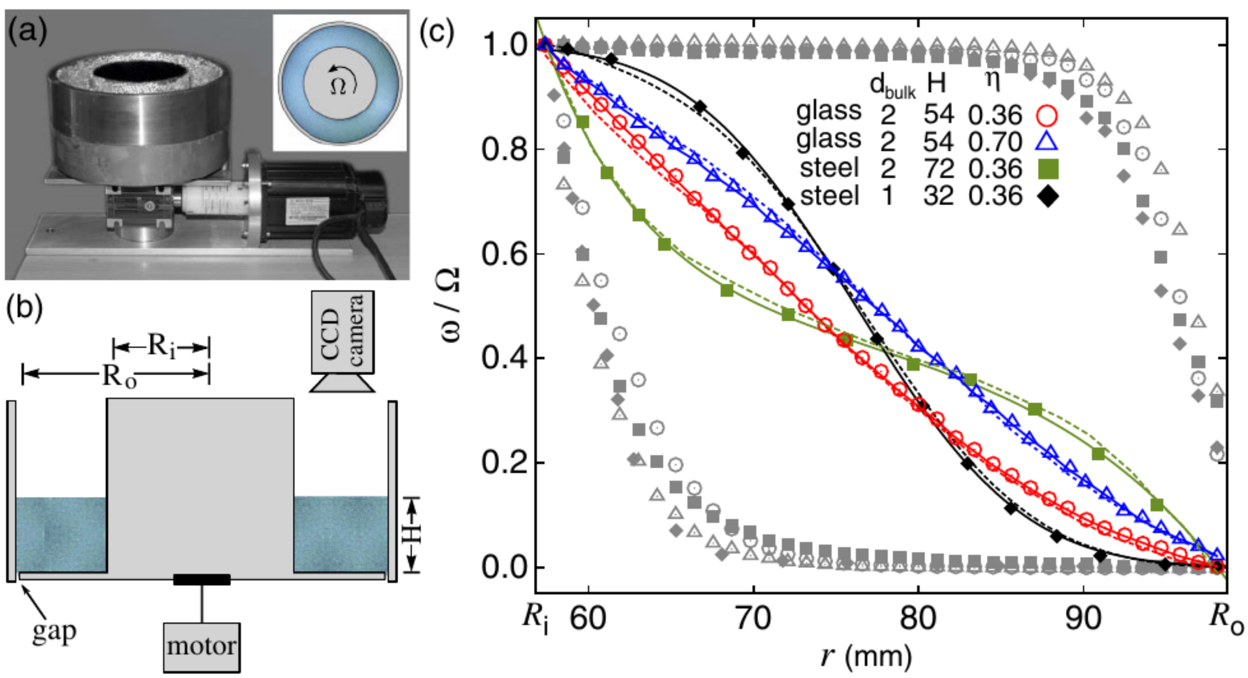

Fig. 5. A mesoscopic model accurately reproduces the experimental deformation profiles.

In connection with this study we have made other numerical investigations regarding the stability of railway tracks. This work was initiated by a railway building company, approaching us with a problem related to rail beds: The continuously welded rails built according to the actual Hungarian standards - which involves gluing part of the stones of the track ballast together - may fail in some conditions and the stones slip out of the track ballast.

We have investigated this problem by means of discrete element simulations. We have shown that gluing the stones of the track ballast together has the required force resistance but is sensitive to disturbances thus the system is vulnerable to failure. We have also suggested a new method to increase the radial resistance of the tracks in curves by using sleepers with rough bottom. The idea came from the previous study (see Phys. Rev. Lett. above), where we found that the deformation of the granular material strongly depends on the internal friction observed near the walls. The company made prototypes of the proposed sleeper, which were measured in real track conditions showing even better results than expected from the simulations. These results were published in the most prestigious railway journal of Europe (Der Eisenbahningenieur). This study was also invited for publication in the first issue of the Hungarian journal called Innorail (unfortunately, in the latter, for technical reasons the OTKA reference did not came out in the printed version). The results were also presented in two talks, at the meeting of the committee responsible for new Hungarian railway standards (invited), and the 2013 International Innorail Conference.

The formation and evolution of wide shear zones was investigated experimentally and numerically for quasistatic granular flows in split bottom shear cells. Shearing an initially random sample, the zone width was found to significantly decrease in the first stage of the process (Fig. 6b). The characteristic shear strain associated with this decrease is about unity and it is systematically increasing with shape anisotropy, i.e. when the grain shape changes from spherical to irregular (e.g. sand) and becomes elongated (pegs). The strongly decreasing tendency of the zone width is followed by a slight increase which is more pronounced for rod like particles than for grains with smaller anisotropy (beads or irregular particles). Results were published in a paper [Phys. Rev. E **90**, 032205 (2014)], and presented in two talks (Montpellier and Erlangen) and a poster (Easton, USA) at international conferences as well as in a talk at the yearly Statistical Physics Meeting of the Hungarian Academy of Sciences.

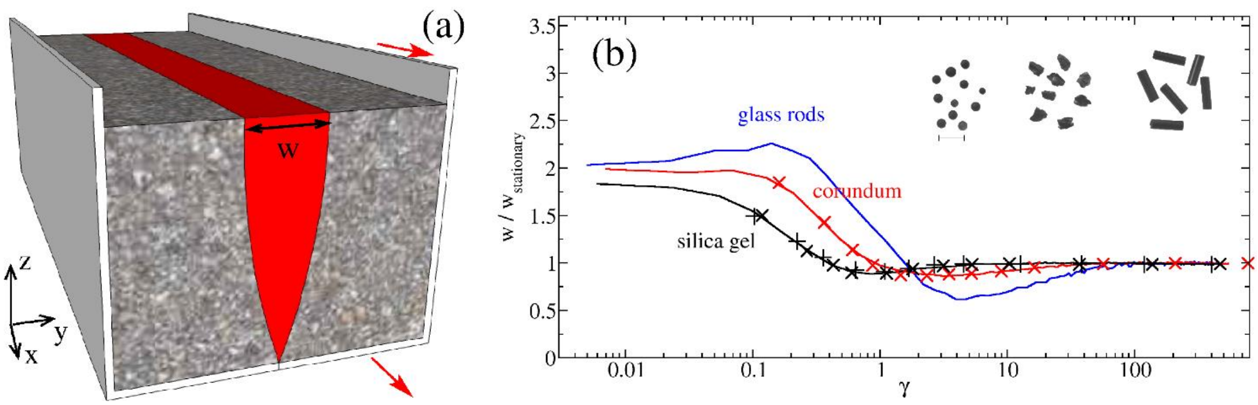

Fig. 6. Evolution of the width of the shear zone for spherical silica gel beads, corundum particles with irregular shape and glass rods as a function of the applied strain. The experiments were started with random grain configurations.

The mesoscopic model presented in publications [Phys.Rev. Lett. 111, 148301 (2013), Phys. Rev. E **90**, 032205 (2014)] has an interesting form in the case of simple shear geometry, where it is identical to another statistical physical model, the Bak-Sneppen model of evolution, which allowed us to measure critical exponents in discrete element simulations of granular materials. This work was done by a batchelor student Sára Lévay, who won the university TDK with rector prize as well as the national OTDK.

The study of transients in the simple shear geometry resulted in a refereed conference paper [Powders and Grains, AIP Conf. Proc. (2017)] where we have showed that a simple shear rate diffusion equation can describe the transient of a simple shear geometry with rough walls but fails for the case of smooth walls.

4. Segregation in binary mixtures:

We have detected experimentally that a mixture of sand particles with irregular shape and spherical glass beads of approximately the same size segregate in a shear flow. Segregation due to size and density differences are often observed, but in this case in principle these effects are excluded. Other two possibilities are shape and surface friction effects. To simplify the phenomenon we have prepared a mixture of two types of spherical grains which differ only in surface friction, by applying special surface treatment to plastic beads. This mixture segregated in shear flow, smooth particles sank to the bottom of the shear zone (see Fig. 7), just like glass beads in the sand - glass beads experiments. We have also performed numerical calculations using the discrete element method and

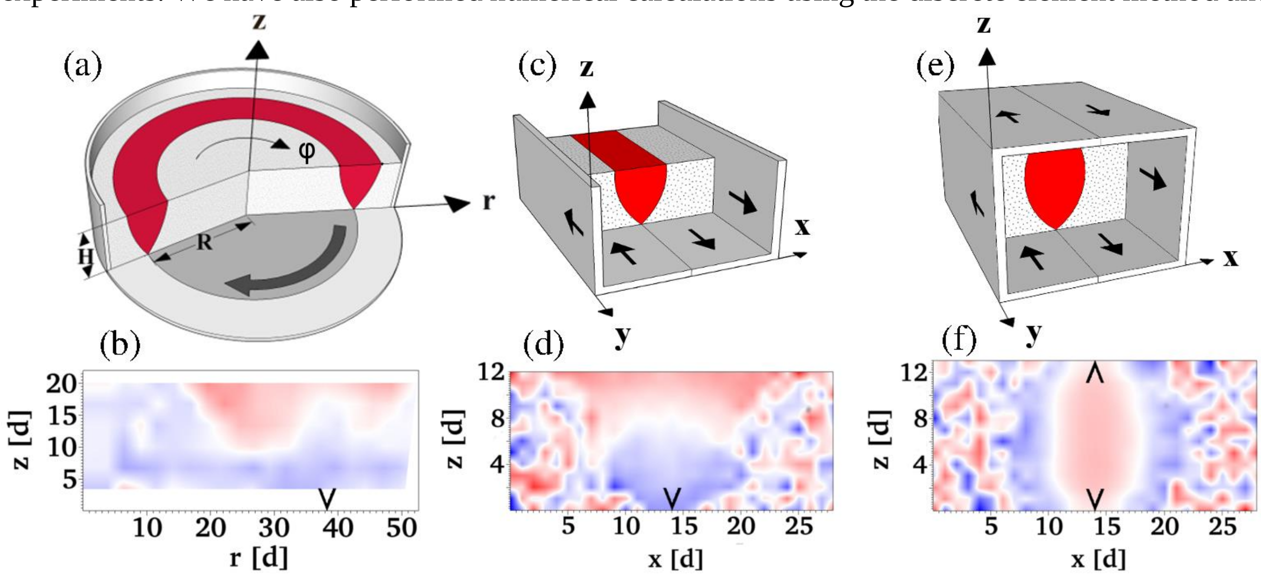

Fig. 7. Shear induced segregation in a binary mixture, where the two types of grains only differ in their surface friction. In the presence of gravity [(a-b) – experiments], [(c-d) – simulation] the smooth grains (blue) migrate to the bottom of the cell, while in the absence of gravity [(e-f) – simulation] the smooth particles migrate out of the shear zone.

observed the same phenomenon. The phenomenon is similar to kinetic sieving in particle mixtures with size heterogeneity. In the present case the smooth particles have a higher probability to penetrate into voids created by the shearing than the rough ones. These results were published in a paper [Soft Matter **13**, 415 (2017)]

We have also performed experiments to study flow induced segregation in a rotating drum. We have shown, that the initial composition of the mixture has a similarly strong influence on the segregation dynamics as the filling height of the bed [Phys. Rev. E **93**, 032903 (2016)].

Publications supported by this project:

Peer-reviewed journal articles:

[1] R. Moosavi, M. R. Shaebani, M. Maleki, J. Török, D. E. Wolf, and W. Losert*: 'Coexistence and Transition between Shear Zones in Slow Granular Flows'*. Phys. Rev. Lett. 111, 148301 (2013)

[2] S. Wegner, R. Stannarius, A. Böse, G. Rose, B. Szabó, E. Somfai and T. Börzsönyi: *'Effects of grain shape on packing and dilatancy of sheared granular materials'*. Soft Matter 10, 5157 (2014)

[3] B. Szabó, J. Török, E. Somfai, S. Wegner, R. Stannarius, A. Böse, G. Rose, F. Angenstein and T. Börzsönyi: *'Evolution of shear zones in granular materials'*. Phys. Rev. E 90, 032205 (2014)

[4] I. Fejér, L. Halmai, and J. Török: Erhöhung der Verwerfungssicherheit von lückenlosen Gleisen, Der Eisenbahningenieur, pp.6-11, 2014/03., (2014)

[5] J. Török, L. Halmai, I. Fejér: A recézés növeli a betonalj keresztirányú ellenállását, Innorail magazin, pp. 38-41, 2014/1., (2014)

[6] G. Wortel, T. Börzsönyi, E. Somfai, S. Wegner, B. Szabó, R. Stannarius, and M. van Hecke: *'Heaping, secondary flows and broken symmetry of elongated granular particles'*. Soft Matter 11, 2570 (2015)

[7] T. Finger, F. von Rüling, S. Lévay, B. Szabó, T. Börzsönyi, and R. Stannarius: *'Segregation of granular mixtures in a spherical tumbler'*. Phys. Rev. E 93, 032903 (2016)

[8] T. Börzsönyi, E. Somfai, B. Szabó, S. Wegner, P. Mier, G. Rose and R. Stannarius: *'Packing, alignment and flow of shape-anisotropic grains in a 3D silo experiment'*. New J. Phys. 18, 093017 (2016)

[9] D. Fischer, T. Börzsönyi, D.S. Nasato, T. Pöschel and R. Stannarius: *'Heaping, and secondary flows in sheared granular materials'*. New J. Phys. 18, 113006 (2016)

[10] A. Ashour, S. Wegner, T. Trittel, T. Börzsönyi, and R. Stannarius: *'Outflow and clogging of shape-anisotropic grains in hoppers with small apertures'*. Soft Matter 13, 402 (2017)

[11] K.A. Gillemot, E. Somfai, and T. Börzsönyi: *'Shear-driven segregation of dry granular materials with different friction coefficients'*. Soft Matter 13, 415 (2017)

Papers in peer-reviewed conference proceedings:

[12] T. Börzsönyi, E. Somfai, B. Szabó, S. Wegner, A. Ashour, and R. Stannarius: *'Elongated grains in a hopper'*. Powders and Grains, AIP Conf. Proc. accepted (2017)

[13] J. Török, S. Lévay, B. Szabó, E. Somfai, S. Wegner, R. Stannarius and T. Börzsönyi: *'Arching in three-dimensional clogging'*. Powders and Grains, AIP Conf. Proc. accepted (2017)

[14] R. Stannarius, D. Fischer, and T. Börzsönyi: *'Heaping and secondary flows in sheared granular materials'*. Powders and Grains, AIP Conf. Proc. accepted (2017)

[15] L. Brendel, J. Török, A. Ries, and D. E. Wolf: *'Relaxation Times in Simple Shear and the Role of Walls'*. Powders and Grains, AIP Conf. Proc. accepted (2017)

Diploma/TDK works:

Béla Csengeri: Investigation of granular flows (2014, BSc, Eötvös University, Budapest)
Sára Lévay: Modeling and simulation of granular materials (2014, BSc, Budapest University of Technology and Economics)
Bence Szabó: Flow detection by digital image analysis (2017, BSc, Eötvös University, Budapest)
Sára Lévay: Szemcsés anyagok nyírásának modellezése és szimulálása, OTDK 1st prize

PhD dissertations:

Balázs Szabó: Shear zones in dry granular materials (2015, Eötvös University, Budapest)

In addition to the above publications the results of this project were presented at international conferences in *16 talks* and *6 poster presentations*.