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DISCRETE ELEMENT MODELLING OF PARTICLE DEGARDATION OF RAILWAY BALLAST MATERIAL WITH PFC^{3D} SOFTWARE

Purpose. It is a very important issue to be able to determine the accurate particle degradation of railway ballast material. There are three different – but connecting – methodology for that: 1) full scale field tests, 2) full scale or reduced scale laboratory tests, 3) computer modelling, mainly with discrete element method (DEM). Options no. 1 and no. 2 need a lot of time and money, but for option no. 3 sophisticated software is needed that can consider the accurate micromechanical characteristics of ballast bed material. **Methodology.** In this paper the authors summarize their results related to modelling, having applied a software that uses DEM for calculation, as well as laboratory tests, namely uniaxial compression tests with reduced scale and computer tomography. **Findings.** The authors obtained the results that the uniaxial compression test in laboratory was able to be modelled by DEM software with an initial precision but in the future should be specified. The results are certified by measurements performed by computer tomography method. **Originality.** It is a very complicated issue to model the particle breakage of railway ballast not only particle movements in DEM software. There are many available software packages at the 'market', e.g. PFC, EDEM, YADE. Some of them are quite expensive, the others can be controlled by significantly difficult manner (special programming technique is needed, command line, etc.) The authors applied not only laboratory loading tests, but sophisticated computer tomography for their research. **Practical value** The results can be useful for railway engineering area. This article is a part of a PhD research at Szechenyi Istvan University, the PhD student is Erika Juhász. Her aim is to develop a method to be able to determine the more accurate ballast breakage, as well as develop assessment methodology related to special measurement techniques (e.g. GOM techniques, computer tomography, etc.). The publishing of this paper was supported by ÚNKP–19-3–I–SZE–13 project.

Keywords: discrete element modelling; particle degradation; breakage; laboratory test; static pressing test; CT-equipment

Purpose

Construction of the conventional railway tracks have the highest proportion of crushed stones. The crushed stone is responsible for the solid but flexible support of the track. Besides they include important load bearing, drainage and stability functions [6].

The authors' research has focused on laboratory tests, whereas other scientific research like computer modelling in the field of technical sciences are the focus of the 21st century.

In this article, the authors present computer modelling and its capabilities, and attempt to compare its results with laboratory results. From several computer modelling the discrete element modelling is suitable for analysing the effects of railway crushed stone bed degradation according to the state of the art. In the aggregation, the deformation of the structure of the grains can be used to qualify the changes, so it is possible to examine the whole aggregate and the behaviour of the individual grain. In any case, the physical parameters of the models can be determined. The latter aspect is – if not the only one – one of the most important parts of discrete element modelling, that is more precisely the adjustment and refinement of the micromechanical parameters of the model. So the model can be validated using the results of the modelled test in the laboratory.

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Methodology

About Discrete Element Modelling. The discrete element method is used to simulate particulate or granular modelled material and processes. Granular material is for example sand, soil or in this paper: railway crushed stone. In addition, it is a numerical method in which the set to be simulated is made up of discrete elements with independent displacements and degrees of freedom of motion. Relationships between elements can be established and terminated. In addition, it is possible to specify relationships between predefined grains, which can be characterized by the addition of strength properties to the «small» grains that form «large» grains; and even models of larger structures can be constructed in this way, e.g. geogrids, engineering structures, etc.

Computer simulations can significantly reduce the number of laboratory tests that need to be performed if the parameters of the computer model and the laboratory test and also the results can be prepared (this is the ‘model validation’ mentioned earlier). In this way in DEM simulation (discrete element method) by modifying individual parameters, more extensive research can be done, avoiding and minimizing costly and time-consuming laboratory tests.

Discrete element simulations do not work as usual with finite element methods (FEM simulation): due to the random location of discrete particles, the same result cannot be obtained for all samples with the same parameters. However, in finite element simulations the same mesh resolution will always have the same result.

Introduction of the used computer software. For the purpose of this article, the authors applied PFC^{3D} (Particle Flow Code in 3 Dimensions), a software developed and marketed by Itasca Consulting Group Inc. (the authors’ software version is 4.0, released around 2009 – currently the latest version is 6.0). The software is used for three-dimensional micromechanical analysis of particulate material systems: mainly to determine particle motions and particle shape changes (fractures, fragmentation, etc.) and the occurring forces-stresses during these processes. It offers analytical and investigative capabilities to characterize the interaction between individual (granular) components by friction, modelling of cohesion relationships, and considering material continuity when examining engineering structures. In this way, e.g. three-dimensional load simulation of a reinforced concrete beam (naturally with steel reinforcement) can also be solved with the software by replacing both concrete and reinforcing bars with discrete elements, and working together can be defined.

The software is also capable of modelling the dynamic behaviour of the particulate set, which may be important in the future due to the vibration effect of the passing railway units. The shape of the granules may be different from the ideal sphere shape (so-called ‘ball’). So formed of contact and/or intersecting spheres, modelling of complex particles (so-called ‘clumps’) is also solved. Depending on the particle size distribution of the required particulate material, the particle set to be modelled can be generated either as a single particle set or as a Gaussian distribution, or it can be used to generate a predetermined specific particle size distribution.

PFC is a general-purpose framework for modelling discrete elements, available in two- and three-dimensional programs [16, 17]. It is applied for modelling synthetic materials of variable size, stiff particles that form particulate and solid materials. PFC models simulate the independent motion (translation and rotation) and interaction of many stiff particles that can interact with each other based on internal force and torque. Particle shapes can include 2D plates or 3D spheres, nodes of stiffly connected plates in 2D, convex polygons in 2D, or 3D polyhedra. The PFC includes twelve built-in contact models with the ability to even create a custom C++ user-defined contact model (UDM).

Since its first release in 1994, PFC has been successfully used by a number of scientific institutions and private companies in a variety of high-level research, ranging from basic micro-size to specific applications including hydraulic fracture, soil mechanical interactions, slope stability, bulk material flow / mixing and cavern mining, but was also used to simulate a number of other activities.

Thermal Analysis: The PFC thermal module allows simulations of transient heat conduction and storage in PFC particle materials and the development of heat-induced deformations and forces. The PFC supports both thermal and coupled thermomechanical analysis.

C++ Contact Models: Enables users to add new contact models (particle force-displacement

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relationship) to the PFC using C++ scripts. This option provides a high degree of freedom of application and the ability to individually program in the software the physical properties and operating mechanisms relevant to each problem.

Among the PFC software – in the authors' research – the authors worked with PFC^{3D} 4.0. version (as it has been already mentioned), which besides the previously mentioned granular elements, it also works with wall elements ('walls'), which can be finite and infinite flat plates, and other walls of other geometry (cylinder, cone, etc.).

In general, the program should specify the mechanical properties of the particles and the parameters of the grain-grain or grain-wall relationship. The PFC program considers the particles as infinitely stiff and compresses all the mechanical properties of the material into a relationship between the particles, which can also be deformed. Since the crushed stone bedding has no internal bond, it is not necessary to define tensile strength in contact bonds in this case.

In addition, the authors have a wide range of applications, e.g. the software can also be used to build geogrids (providing tensile strength and bending stiffness properties).

The calculations are based on the combined cyclical application of Newton's laws of motion and the force-displacement law.

Generic Adhesive Contact Model. The Adhesive Rolling Resistance Linear Model is a new contact model now available in PFC 6 to represent a simple cohesive granular material. The cohesion arises from a short-range attraction, which is a linear approximation of the van der Waals force law. For these materials, the attraction force is always present when the contact surfaces fall within a specific range of attraction force. Assemblies of cohesive grains exhibit much larger variations in their equilibrium densities than do corresponding assemblies of non-cohesive grains, because the cohesive grains may form loose, solid-like cohesive granulates. Such granular systems can stay in mechanical equilibrium at lower solid fractions (down to 25-30%) than cohesionless granular systems (with typical solid fractions of 58-64%). Cohesive granular materials have much less frequently been investigated by numerical simulation than cohesionless ones. The new contact model in PFC encompasses both types of materials and could be used to study macroscopic behaviour of a variety of cohesive granular materials including cohesive powders such as xerographic toners (in which cohesion stems from van der Waals interaction) and wet bead packs (in which cohesion stems from liquid bridges joining neighbouring particles) [17].

Soft-Bond Contact Model. The soft-bond model can be used to simulate both unbonded and bonded systems.

In an unbonded state, it behaves essentially similar to the contact model, providing the ability to transmit both a force and a moment at the contact point, with frictional strength parameters limiting the shear force, bending moment, and twisting moment.

In its bonded formulation, the behaviour is similar to that of a linear parallel bond model, with a frictional strength parameter limiting the shear force, and the possibility for the bond to fail if the bond strength is exceeded either in shear or in tension. However, contrary to the linear parallel bond model, the bond is not removed upon failure. Instead, it may enter into a softening regime until the bond stress reaches a threshold value at which the bond is removed and considered broken. The slope and tensile breakage strength during softening can be specified by the user (via the softening factor and the softening tensile strength factor, respectively). Another difference with the linear parallel bond model is that only one set of stiffnesses is used for both the unbonded and bonded formulations. This behaviour is essentially similar to that proposed, with the difference that the bond elongation used to update the normal stress in the softening regime accounts for both the normal displacement and bending increments [17].

Behaviour Summary. A soft bond can be envisioned as a set of elastic springs with constant normal and shear stiffnesses, uniformly distributed over a {rectangular in 2D; circular in 3D} cross-section lying on the contact plane and centred at the contact point. Relative motion at the contact causes a linear force and moment to develop, that act on the two contacting pieces. If the bond is inactive, frictional strength parameters cap the shear force, bending and twisting moments. If the bond is active, the force and moment can be related to maximum normal and shear stresses acting within the bond material at the bond periphery. If either of these maximum stresses exceeds its corresponding

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bond strength, the bond may enter a softening regime to a specified failure criterion. After failure, the behaviour reverts to the unbonded formulation [17].

As balls, clumps, rigid blocks, and walls (i.e., pieces) are rigid in PFC, all deformation between surfaces of adjacent pieces occurs at contacts. Specific contact models (i.e., particle-interaction laws) can be inserted to represent different physical situations using a soft contact representation where the pieces do not deform but and piece overlaps are allowed. Forces and moments are computed based on the degree of overlap. Contact models can use the piece properties to determine the resulting interactions. Contacts are created and deleted automatically during model cycling. PFC uses the null model contact model by default and therefore the user is required to explicitly specify which contact model(s) should be used in each PFC model. Each contact is assigned a single contact model manually or via the Contact Model Assignment Table (CMAT). [16]

Built-in Contact Models. [16]

Null. The null contact model is the default contact model with no mechanical interaction. No force or moment is generated.

Linear. The linear model reproduces the mechanical behaviour of an infinitesimal, linear elastic and frictional interface that carries a point force. The interface does not resist relative rotation and optional viscous dashpots may be activated.

Linear Contact Bond. The linear contact bond model provides the behaviour of an infinitesimal, linear elastic, and either frictional or bonded interface that carries a point force and does not resist relative rotation.

Linear Parallel Bond. The linear parallel bond model provides the force-displacement behaviour of a finite-sized piece of cementitious material deposited between two pieces in the vicinity of the contact location, acting in parallel with a linear model.

Soft-Bond. Similar to the linear parallel bond with the addition that a softening parameter can be specified to modify the stiffness in the post tensile failure regime, allowing for a degradation of the tensile stiffness as a function of increasing bond elongation.

Rolling Resistance Linear. Based on the linear model but incorporates a torque acting on the contacting pieces to resisting rolling motion for granular applications.

Adhesive Rolling Resistance Linear. Based on the rolling resistance linear model to which an adhesive component is added. The cohesion arises from a short-range attraction, which is a linear approximation of the van der Waals force law.

Flat joint. A flat joint contact simulates the behaviour of an interface between two notional surfaces, each of which is connected rigidly to a ball or pebble. The notional surfaces are called faces, which are lines (PFC^{2D}) or disks (PFC^{3D}).

Smooth Joint. The smooth joint model simulates the behaviour of an interface regardless of the local particle contact orientations along the interface. The behaviour of a frictional or bonded joint can be modelled by assigning smooth-joint models to all contacts between particles that lie on opposite sides of the joint.

Hertz. The Hertz contact model in PFC consists in a non-linear formulation based on an approximation.

Hysteretic. The Hysteretic contact model in PFC consists in a combination of the elastic portion of the Hertz model, combined an alternate dashpot group consisting in a nonlinear viscoelastic element in the normal direction.

Burger's. Simulates creep mechanisms by using a Kelvin model and a Maxwell model connected in series in both the normal and shear directions.

Walking around the topic, computer programming (and discrete element modelling within it) already allows assembled elements to be built on not just from a sphere or multiple spheres ('clumps'), but polyhedra [4]. This method is already used by many Hungarian researchers. This also gives us a more accurate picture of the movement and relationship of the particle shapes with each other, but the authors were not able to model the authors' laboratory analysis with the mesh shapes built into this system (due to the fact that only PFC^{3D} 4.0 software is available at Széchenyi István University). For example, the YADE software, which is an open source, programmable software, with its problems and difficulties, is also suitable for simulation with polyhedra. The authors' model is made up of several larger spheres (balls) made up of smaller spheres (balls). The test principles are very similar, so in the first approach the authors found PFC^{3D} 4.0 perfectly suitable for

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‘testing’ discrete element modelling and getting to know the method. Since the modelling of crushed stone granules as spherical granules can lead to incorrect behaviour (singularities in the calculations), it was necessary to use composite granules for realistic results of the simulations [2].

About the simulation and the built model, the basics of the model. The authors would like to illustrate the basics of the simulation: let's take a particle that produces displacements under the influence of a contact (even it can be considered as a set of grains). The displacements cause the disappearance of existing contacts and the formation of new contacts, but at these points of contact, forces awaken. This is called ‘cycling,’ which is performed by the software up to the specified limit, and finally this process is called ‘cycling’ leading to equilibrium.

Fragmentation of railway crushed stone bed granules was observed in laboratory tests in a 160 mm external diameter HDPE (hard polyethylene tube). The tube was lined with 1200 g/m^2 geotextile. The tube was filled to a standard height of about 15 cm with a standard 31.5/50 mm rail crushed stone (with two types of andesite from mines). This is how the authors achieved the approximately equal height-to-width ratio determined by the CT device used in the study. A set of rock material consisted of approximately 16 to 20 individually measured and photographed rock particles [6].

The authors could create a slightly different model with using DEM. While in reality (measurement in laboratory) the authors crushed it in the form of a cylinder with an inside diameter of approximately 14 cm – filled at a height of 15 cm with two dozen rocks which have sharp corners and oblong-cubic shape; in the DEM simulation the authors loaded three dozen spherical macrospheres into a rectangular container. The size of the container is 2-2.5 cm.

The PFC^{3D} 4.0 version is capable of working with significantly fewer elements in the fracture calculations and exponentially increases the time required for running number of items (compared to either 5.0 or 6.0).

The authors also experimented with small granular (crushed) laboratory tests. Components suitable for garden watering systems (HDPE 25 tube – outer diameter 25 mm, wall thickness 2.3 mm – and HDPE 25 end cap) were assembled into several test tube pieces, in which NZ 4/8 andesite material filled – approx. 25-25 pieces – the specimens are shown in Fig 1. Rock physical parameters of the fraction 10/14: LA – 13.2%, m_{DE} – 23.4%. Small granular DEM simulations were made with these laboratory tests in mind.

Fig. 1. Test specimens for NZ 4/8

Fig. 2 shows the load design, the loading of the samples carried out with a ZD-40 type crusher.

Fig. 2. The laboratory test assembly

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A total of 6 samples were tested with unidirectional (vertical) pressure: 3 samples with max. 300 kPa (samples no. 1, no. 2 and no. 4), 3 more samples max. 900 kPa (samples no. 3, no. 5 and no. 6) with a single-stage load (see [6]).

The authors performed a CT x-ray on each of the crushed samples as described in the authors' previous article [6] with the help of Imre Fekete department engineer on the pre- and post-workout states, as shown in Figures 3-4 (mainly the displacements could be observed). For this measurement, we did not separate numbering, weighing, and one-by-one photography of the particles, as the authors did with the 31.5/50 crushed stone bed.

The loading graphs of the laboratory samples are presented together with the DEM modelling in the 'Originality and practical value' Paragraph.

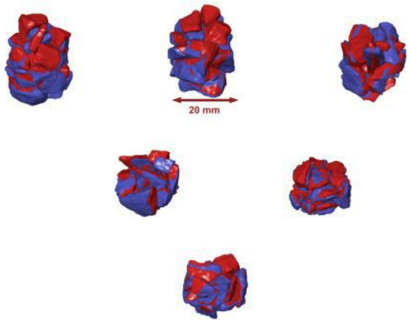

Fig. 4. X-ray CT scans of uniaxial compression tests with NZ 4/8 material by axonometric representation (red for pre-load and blue for post-load; sample numbering: sample no. 1 in the bottom row; from left to right no. 2, no. 3 in the middle row; from left to right no. 4, no. 5, and no. 6 in the top row)

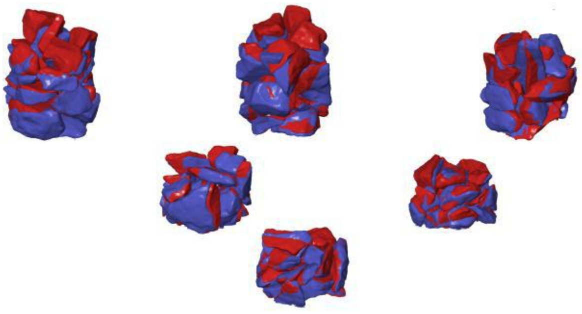

Fig. 4. X-ray CT scans of our uniaxial compression tests with NZ 4/8 material from top view (red for pre-load and blue for post-load; sample numbering: sample no. 1 in the bottom row; from left to right no. 2, no. 3 in the middle row; from left to right no. 4, no. 5, and no. 6 in the top row)

Presentation of the macroparticle fragmented aggregation. The authors' aim with the DEM test was to get to know the simulation first and to identify possible directions of the research.

During the creation of the DEM model, the authors generated a set of macroparticles, which consisted of the following steps:

- the microparticles were produced by random distribution which fills the range defined by the diameter of the macroparticles,
- the properties of certain inhomogeneous microstructures of the macroparticles (the individual macroparticles, which consisted of the same number of microspheres, were not completely similar in microstructure) were also important aspects in the random distribution of the microparticles.

The geometric properties of the macroparticles for the numerical study performed are summarized in Table 1.

Table 1

The geometric properties of the macroparticles

Diameter of the macro-grains [mm]	Number of the macrograins in the aggregation [piece]	Number of micro-particles within a macroparticle [piece]
4.0	17	51
6.0	12	148
8.0	7	322

There are two types of contacts that can be identified in the macroparticle aggregation model for fragmentation. The first type of contact is non-bonded, described by the Hertz-Mindlin contact model. This is also relevant along the macro particulate aggregate and microparticulate cracks. The second type of contact is based on a contact model defined by the microparticles inside the same macroparticle, which are linked by the normal and shear properties of parallel bonds. The diameter of the microparticles were selected to the resulting macroparticles contain sufficient microparticles to perform a proper simulation of the fragmentation process. As can be seen in Table 1, one of these macroparticles (so-called 'clumps') contains 51-322 microparticles, which significantly increased the run time.

The mechanical properties of the ‘clumps’ used in the simulations were the same as those of the spheres.

The assumed contact properties in this article are summarized in Table 2.

Table 2

Micromechanical properties

Contact bond (parallel contact bond)	
Normal and shear stiffness [N/cm]	4.7×10^5
Normal and shear strength [N/cm^2]	7.9×10^3
The ratio of the ‘bond radius’ to the microparticle radius	0.5
Friction factor in particle-particle Contact	0.55
Friction factor in the particle-wall contact	0.55

Container (crucible) size: 19.0 (width) × 19.0 (long) × 26.5 (height) [mm].

Odometer examination of the aggregate. All of the macroparticles (build from the micrograins) were randomly placed at one point and then allowed to gravitationally enter into the receiving container.

When the sample was completed (the first balanced status was formed) and the top sheet was in place, the ‘pressing process’ began, consisting of small steps. The pressure plate (on the top of the set) moved downward in 0.16 mm increments at a constant speed of 8 mm/s (10 to 6 seconds). In all cases, this was sufficient to allow the set to reach a state in which the initial macroparticles (as the encapsulating ‘spherical particles’) almost completely disintegrate into microparticles.

Here it is important to mention the fact that the simulation ran until the authors crushed all the macroparticles into microparticles. Of course, this is not possible and realistic conditions, as any loaded material will eventually become incompressible. However, the simulation has been able to compress each particle over and over again. So some of the authors’ resulting values were ignored as they would not give a realistic picture of the load. This ‘over-compression’ is illustrated in Fig. 5.

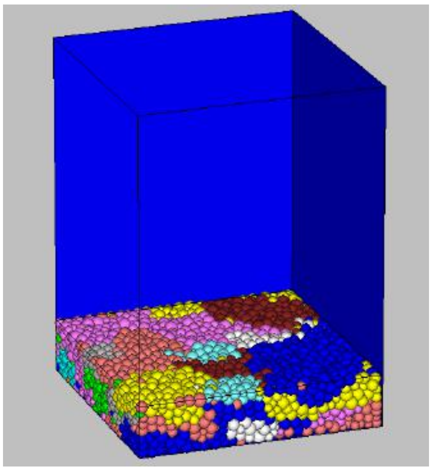

Fig. 5. Excessive compression in simulation (state of cycle 3280)

Pictures of the simulations are shown in Figures 6-8. Fig. 6 shows the state for 45th, 1115th, 1520th and 1960th cycle with modelled walls and microparticulate macroparticles. In Figures 7-8 the authors could see the direction of the forces in the contact and the parallel bond between the microparticles. In Fig. 6 the authors could also see the awaken forces in the contact bonds for the used cycles.

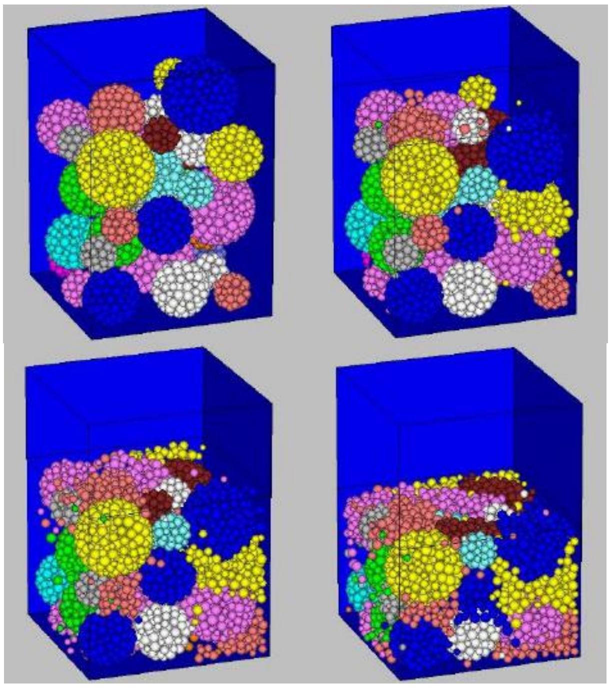

Fig. 6. The gradual compression, in which the macroparticles are reduced to microparticles (from left to right and from top to down: after a given 45th, 1115th, 1520th and 1960th cycle)

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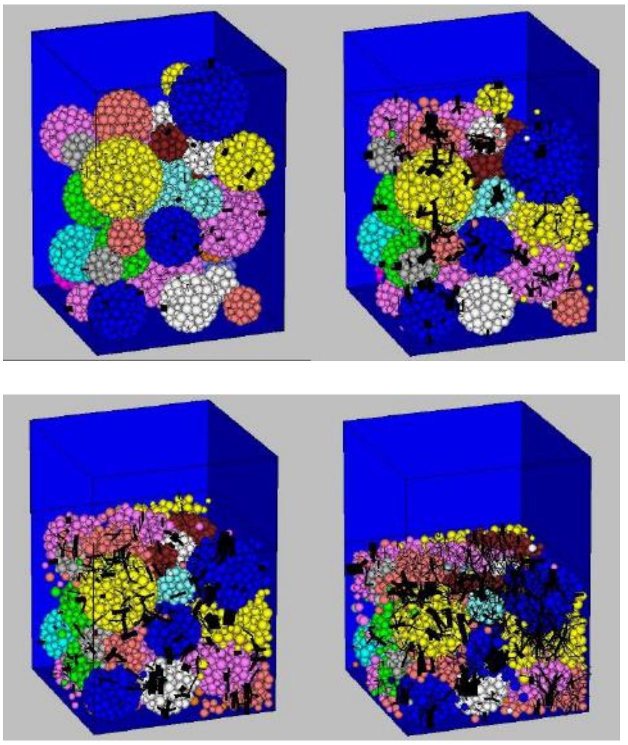

Fig. 7. Contact forces in particle-particle and particle-wall contact bonds (line thickness is consistent with force, line direction is same as force vector) (from left to right and from top to down: after a given 45th, 1115th, 1520th and 1960th cycle)

Findings

In Fig. 8, the 'parallel bonds' (indicated by red lines in the pictures) gradually disappear as the number of cycles increases, that is, the macroparticles disintegrate into microparticles; so the macrograins become degraded.

As a first approximation (without taking into account the results of laboratory tests), the condition that may be the limit of real behaviour can be put into about 1960th cycle of the authors' simulation. So up to this point, the authors could actually compress the aggregate. Until this data (as a limit), the authors have created load diagrams for the following parameters as a function of the number of cycles (Figures 9-10):

- position of the horizontal load plate of the Odometer load (initial value 26.5 mm),
- vertical normal voltage (voltage applied to the load plate),
- void ratio (calculated in the usual way in geotechnics, i.e. the volume ratio of air to particles in relation to the reference volume).

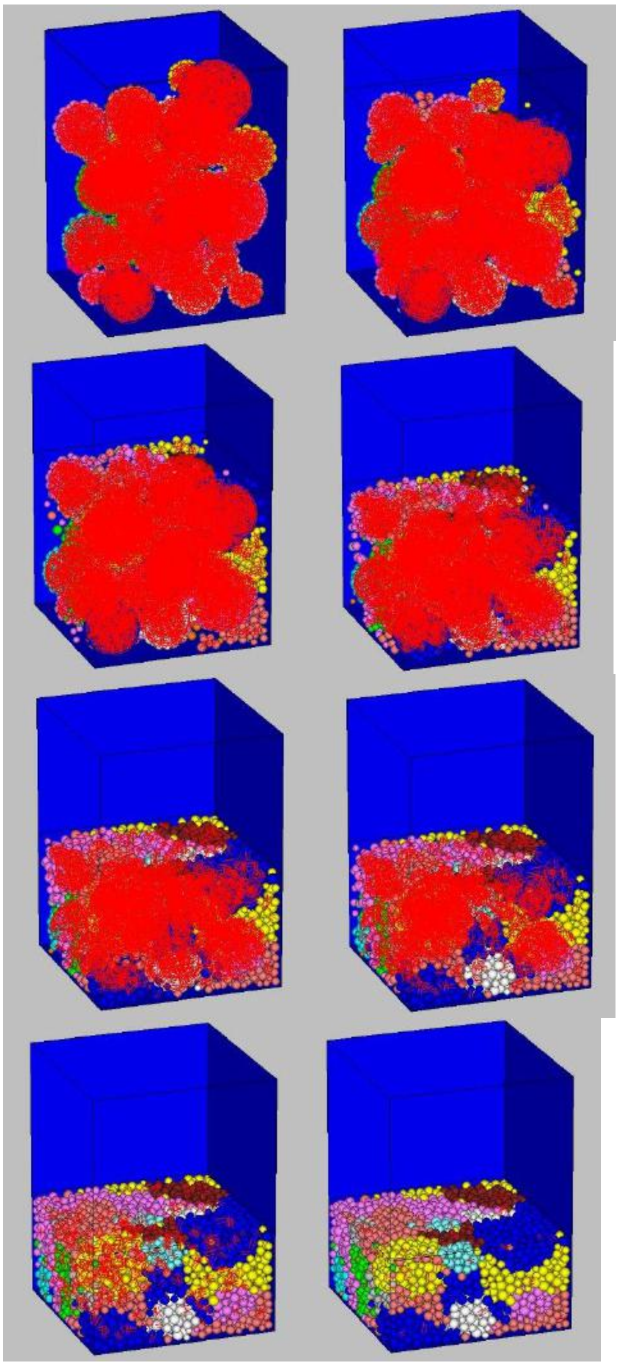

Fig. 8. Contact forces in parallel bonds between microparticles (from left to right and from top to down: after a given 45th, 1115th, 1520th, 1960th, 2180th, 2290th, 2400th and 2510th cycle)

Fig. 11 shows the magnitude of the vertical loading of sample compression (this type of representation was required for consistency with laboratory measurements).

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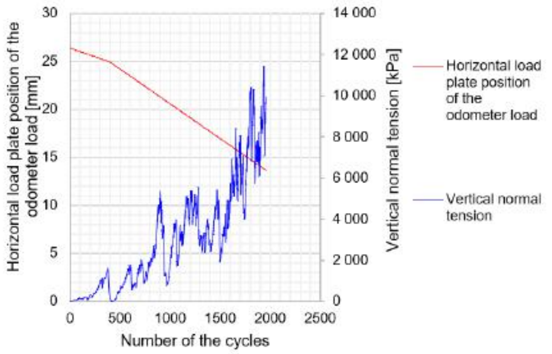

Fig. 9. Loading diagram 1

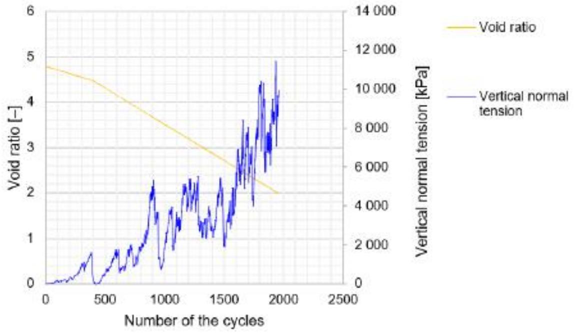

Fig. 10. Loading diagram 2

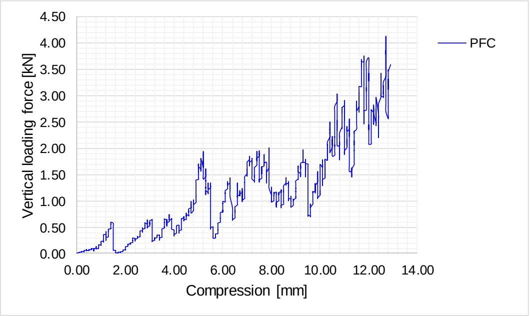

Fig. 11. Loading diagram 3

In Figures 9-11 it is interesting to observe that the void ratio decreases from an initial value of 4.8 to a value of 2.0 in the 1960th cycle. Both the 4.8 and 2.0 void ratio are unrealistic in a real circumstance. Nevertheless, it should be noted that the software also includes the volume of air between the microparticles, which of course is not true.

Figures 9 and 11 show that, according to the simulation, about the 1960th cycle the compression is 12.9 mm, which is still an unrealistic data for a 25.6 mm initial tall jar filled with macrograins. Because of this reason, the results of the laboratory samples, which are plotted in Fig. 12, are also required.

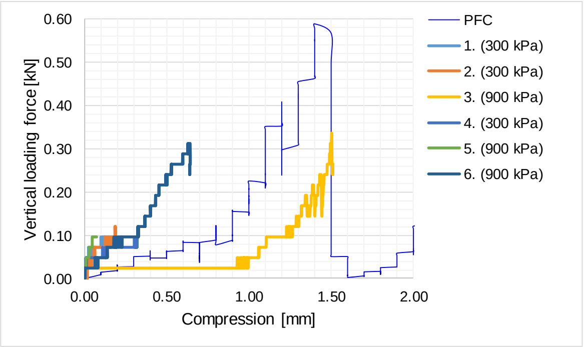

Fig. 12. Loading diagram 4

Analyzing some of the result lines in Fig. 12, it can be concluded that the simulation was a good approximation, despite that the authors' laboratory samples were in 20.4 mm diameter cylinder and in the DEM simulation the authors used a 19.0 x 19.0 mm cuboid. According to the Fig. 8 the consideration of the 1960th cycle is an excessive approximation. For the 2.0 mm compression (see Fig. 12) belongs to the 459th cycle (see Fig. 13) in the DEM model. The authors need to mention that the 6-series samples measurement data (see Fig. 12) is too stairy to the applied force measuring cell: that because in the Structure Testing Laboratory of Széchenyi István University the authors are mainly equipped to measure multi-ton loads. For example, in the range of forces below 1 kN, the applied measuring cells can produce similar phenomenon – regardless of the movement and fracture of the particles. This must be taken into account in the future, meaning that smaller measuring cells may be required with higher precision design.

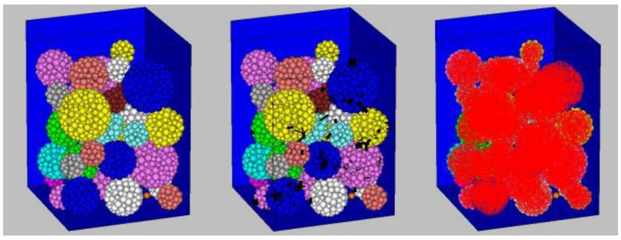

Fig. 13. Condition according to load cycle 459
(from left to right: linkage forces between
macroparticles of microparticles, particle-particle
and particle-wall; parallel bonds)

When comparing the graphs in Fig. 12 with the Figures 3-4 and the Fig. 13., it can be stated that the minimal degradation observed is realistic according to the results – the actual degradation was

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negligible in the laboratory measurements based on the CT X-ray images.

In DEM simulation, – although spherical macroparticles were used, in real circumstances the authors utilized amorphous, sharp and fractured particles – the fragmentation occurs in around the 1000**th** cycle, which comes with 6 mm compression. This deformation is probably including 2 kN load (see Fig 11) which means that the HDPE tube with its ending cap would not bear this load without failure. So the authors would need to use different measurement setup to investigate.

Originality and practical value

With the discrete element modelling presented above, the authors proved that the method is capable of numerically calculating of the degradation of the ballast particles in up to even 3 dimensions, but in the future the authors need to fill in the gaps described below and refine the used parameters. During the authors' modelling, the authors were aware of the limitations of the authors' calculations and results:

1. The particles should be taken into account in the real grain size corresponding to the crushed stone bed of the railway, so the 31.5/50 mm or 31.5/63 mm fraction instead of the currently used 4/8 mm fraction.
2. In accordance with the 1st point, it is also necessary to refine the particle shapes to the real one [4, 15, 18], which will require the application of a DEM program more advanced than PFC^{3D} version 4.0.
3. The approximately 20-30 grains will be too small for a more accurate simulation, but with higher item number, the authors will also encounter obstacles to more than 10 years of PFC^{3D} version 4.0 (unmanageable runtime – the authors' presented results required about 2 months of computer runtime, which is unacceptably in 2019).
4. The authors need to specify micromechanical parameters for validation of the DEM model by laboratory measurements, which requires easy-to-use, relatively fast-running software (free, open source, programmable DEM software available on the Internet, such as costly professional advances software: PFC^{3D} version 6.0, EDEM, etc.).
5. Among the refinements that can still be made in PFC^{3D} version 4.0 are:
   a. validation of the DEM model according to laboratory measurements,
   b. quantify and record the number of terminated/broken parallel bonds,
   c. by changing the micromechanical and geometric parameters of the validated model the authors can obtain further important results from the runs.
6. In the future, instead of static loads (with properly managed DEM software), dynamic loads should be considered which are closer to real circumstances.
7. Sophisticated software (like EDEM) can be used to model manual/machine bedding and bed screening as well as the bed's degradation effect.
8. Complemented with CT X-ray records [13], although limited in geometry and with a jar of material limited in translucency, the method can be improved and the cracks and deformations measured under laboratory load can be more accurately controlled.
9. Ignoring fragmentation, it is also possible to calculate the deformation of the granular assemblies, in which case it is possible to calculate the 'only' particle displacement (3D shifts and 3D rotations) and the resulting voltage trajectories [1, 14] – static and/or dynamic loads – which may be sufficient under certain modelling frameworks.
10. The authors would mention that other interesting research methods like measurement and evaluation capabilities based on digital image and video processing, which have already been successfully used in another university research (GOM Atos, Tritop and Aramis [5]) as a research of fiberglass-reinforced plastic composite rail joint. (The Széchenyi István University's Faculty of Audi Hungária Vehicle Engineering has these tools.) This would require loading the particles in a transparent plexiglass tube or plexiglass column while taking digital pictures/videos of the aggregate (and the particles). The tools and their evaluation software are capable of accurately locating displacements fields up to a hundredth of a millimetre – in this case, the rotation of the particles can cause problems in the application of the method, which affects accuracy and actual behaviour.

All in all, discrete element modelling can be a very useful method to reduce the cost of expensive laboratory and/or field tests, but you should also be aware of the limitations of DEM simulations.

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These include the fact that simulations can give unrealistic results if configuration is not properly, like for example the used structure in the simulation can be ‘overloaded’ unlike in real circumstances. To do this, the authors need to have proper engineering thinking and to be able to judge the correctness of the results and to adjust the parameters of the model.

This paper is the continuation of the authors previous papers [2, 3, 6, 7, 8, 9, 10, 11, 12].

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ДИСКРЕТНО-ЕЛЕМЕНТНЕ МОДЕЛЮВАННЯ РУЙНУВАННЯ ЧАСТОК ЗАЛІЗНИЧНОГО БАЛАСТНОГО МАТЕРІАЛУ ЗА ДОПОМОГОЮ ПРОГРАМНОГО ЗАБЕЗПЕЧЕННЯ PFC^{3D}

Мета. Визначення точного руйнування часток залізничного баластного матеріалу є досить важливою проблемою. Для цього існують три різні, але пов’язані між собою методики: 1) повномасштабні польові випробування; 2) повномасштабні або скорочені лабораторні випробування; 3) комп’ютерне моделювання, в основному з використанням методу дискретних елементів (МДЕ). Перший і другий варіанти вимагають багато часу і грошей, а для третього варіанта потрібне складне програмне забезпечення, яке може враховувати точні мікромеханічні характеристики матеріалу баластного шару. Метою цієї роботи є розробка методу, який дозволяє визначати більш точне руйнування баласту, а також розробка методології оцінки, пов’язаної зі спеціальними методами вимірювання (наприклад, методами GOM, комп’ютерною томографією тощо). **Методика.** У цій роботі автори підводять підсумки проведеного моделювання з використанням програмного забезпечення, що застосовує для розрахунку МДЕ, а також лабораторних випробувань, а саме скорочених випробувань на одновісне стискання, і комп’ютерної томографії. **Результати.** Автори отримали результати, згідно з якими лабораторні випробування на одновісне стискання можна було змоделювати за допомогою програмного забезпечення МДЕ з початковою точністю, що в подальшому потребує вдосконалення. Результати підтверджені вимірюваннями, виконаними методом комп’ютерної томографії. **Наукова новизна**. Моделювання руйнування часток залізничного баласту, а не тільки їх руху, у програмному забезпеченні МДЕ є складним завданням. Сьогодні на ринку є багато доступного програмного забезпечення, наприклад, PFC, EDEM, YADE. Одні програми досить дорогі, іншими складно управляти (необхідна спеціальна методика програмування, командна лінія тощо). Для своїх досліджень автори застосували не тільки лабораторні навантажувальні випробування, але й складну комп’ютерну томографію. **Практична значимість.** Результати цього дослідження можна застосовувати в галузі залізничного будівництва. Дана робота є частиною дослідження в аспірантурі Університету Іштвана Сечені, виконана аспіранткою Ерікою Юхас. Її метою є розробка методу, що дозволяє визначити більш точне руйнування баластного шару, а також розробка методології оцінки, пов'язаної зі спеціальними методами вимірювання (наприклад, методами GOM, комп'ютерною томографією і т. д.). Публікація цієї статті підтримана проектом ÚNKP–19–3–I–SZE–13.

Ключові слова: дискретно-елементне моделювання; руйнування часток; розлом; лабораторні випробування; випробування на статичне пресування; КТ-обладнання

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ДИСКРЕТНО-ЭЛЕМЕНТНОЕ МОДЕЛИРОВАНИЕ РАЗРУШЕНИЯ ЧАСТИЦ ЖЕЛЕЗНОДОРОЖНОГО БАЛЛАСТНОГО МАТЕРИАЛА С ПОМОЩЬЮ ПРОГРАММНОГО ОБЕСПЕЧЕНИЯ PFC^{3D}

Цель. Определение точного разрушения частиц железнодорожного балластного материала является крайне важной проблемой. Для этого существует три разные, но связанные между собой методики: 1) полномасштабные полевые испытания; 2) полномасштабные или сокращенные лабораторные испытания; 3) компьютерное моделирование, в основном с использованием метода дискретных элементов (МДЭ). Первый и второй варианты требуют много времени и денег, а для третьего варианта требуется сложное программное обеспечение, которое может учитывать точные микромеханические характеристики материала балластного слоя. Целью этой работы является разработка метода, позволяющего определять более точное разрушение балласта, а также разработка методологии оценки, связанной со специальными методами измерения (например, методами GOM, компьютерной томографией и т. д.). **Методика.** В данной работе авторы подводят итоги проведенного моделирования с использованием программного обеспечения, использующего для расчета МДЭ, а также лабораторных испытаний, а именно сокращенных испытаний на одноосное сжатие, и компьютерной томографии. **Результаты.** Авторы получили результаты, согласно которым лабораторные испытания на одноосное сжатие можно было смоделировать с помощью программного обеспечения МДЭ с первоначальной точностью, что в дальнейшем требует усовершенствования. Результаты подтверждены измерениями, выполненными методом компьютерной томографии. **Научная новизна.** Моделирование разрушения частиц железнодорожного балласта, а не только их движения, в программном обеспечении МДЭ является очень сложной задачей. Сегодня на рынке есть много доступного программного обеспечения, например, PFC, EDEM, YADE. Одни программы довольно дорогие, другими сложно управлять (необходима специальная методика программирования, командная линия и т. д.). Для своих исследований авторы применили не только лабораторные нагрузочные испытания, но и сложную компьютерную томографию. **Практическая значимость.** Результаты данного исследования можно быть применять в области железнодорожного строительства. Данная работа является частью исследования в аспирантуре Университета Иштвана Сечени, выполненная аспиранткой Эрикой Юхас. Ее целью является разработка метода, позволяющего определить более точное разрушение балластного слоя, а также разработка методологии оценки, связанной со специальными методами измерения (например, методами GOM, компьютерной томографией и т. д.). Публикация данной статьи поддержана проектом ÚNKP–19–3–I–SZE–13.

Ключевые слова: дискретно-элементное моделирование; разрушение частиц; разлом; лабораторные испытания; испытание на статическое прессование; КТ-оборудование

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