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INTERACTION OF PARTICLES VIA SOLID INTERFACE: MODEL AND ANALYSIS − PARTICLES 2013

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Abstract. The paper addresses discrete element (DEM) models of the heterogeneous particulate solids where the normal interaction between two deformable spherical particles bonded via weaker solid interface is considered. The integral interaction model aimed for evaluation of the bond stiffness was developed, where analytical expressions of the stiffness parameters reflecting individual contribution of the two particles and of the interface properties are derived. Application of the developed DEM model to particulate solid with many particles is considered. The accuracy and the suitability of this approach are evaluated by considering refined 3D Finite Element analysis.

1 INTRODUCTION

Many of real engineering materials are heterogeneous solids. The focus of recent investigation is heterogeneous particulate solid consisting of solid particles of different size and shape embedded into the homogeneous matrix. The asphalt-type materials containing coarse particles and weak matrix may be considered as representative prototype of this model. Here, the stiff particles possess elastic behaviour, the matrix has, however, very complex mechanical properties including viscosity, load rate and temperature dependent behaviour. The above complexity makes it extremely difficult to obtain stress–strain state.

Among various numerical techniques recently used for analysis purposes using of them are basically shared between two alternatives – the conventional Finite Element Method (FEM) and the relatively new Discrete Element Method (DEM). Due to the heterogeneity of the particulate solids the routine application of the FEM using 3D continuum elements possesses

serious difficulties.

The DEM was originally aimed for the numerical modelling of discontinuous materials. Application of the DEM to solids requires serious theoretical analysis of the link between continuum and discrete parameters [1], [2]. Calculation of particles interaction forces is the most important issue of DEM technique. DEM interaction models were developed by different scientific communities using different approaches. Two technically different, particle-based and lattice-based, approached have been developed in the framework of DEM when applied to simulate solids. Particle-based approach presents a rather straightforward extension of the original DE method. The DE models aimed to solids assume bilateral or bonded interaction between particles and use the simplest contact laws such as linear contact of spherical shapes of particles, see Potyondy and Cundal [3], Hentz, Donzé and Daudeville [4], Rojek *et al*. [5].

An approach representing the continuum by material particles interacting via the network elements is called a lattice-type model. This type models dating back the earlier work of Herrmann *et al.* [6] is equivalent to structural network composed by various beam elements. Theoretical analysis and comprehensive review of the planar elastic lattice models which hold for micro-mechanical applications is given by Ostoja-Starzewski [7]. It was shown that the models require to use of the rotational degrees of freedom, therefore, they may be treated as a counterpart of non-classical continua. The Timoshenko type beams are analysed by Karihaloo *et al*. [8] and by Kozicki and Tejchman [9].

Most of applications are dealing with the homogeneous solids. the problem of inhomogeneity of solid is considered on the basis of disordered lattice or structural network by considering approach developed by Patyondy and Cundall [3].They have assumed normal bond stiffness implemented as stiffness of contacting particles cemented by a finite-size piece of interface material. Here, contribution of the interface was reflected by additional parallel bond.

Analysis of the heterogeneous structure of the material over different length scales is highly complicated. Several investigations demonstrate how lattice type elements were also able to reflect inhomogeneity of concrete. The three-phase element called generalized beam (GB) element composed of three sub-beams was presented by Liu *et al*.[10] To reduce computational expenses the meso-scale model seemed to be more attractive. The model simulates concrete meso-structure by means of a three-dimensional lattice was considered by Cusatis *et al*. [11]. Here, the lattice nodes are coincident with the centres of coarse aggregate pieces. Another type of applications concerns asphalt concrete presenting a two-phase composite of the asphalt mastic and the mineral aggregates size of which varies in millimetre scale. Extensive review of the DEM applications is given in [12].

It is clear that modelling of particulate solids is still under development while knowledge about the contribution of particular factors to their mechanical behaviour is not satisfactory.

Investigation addresses the Discrete Element model of the particulate solid, with emphasis on the normal interaction between two deformable spherical particles via weaker deformable interface. The integral interaction model aimed for evaluation of the bond stiffness was developed. This model is described by independently obtained analytical expressions of the

stiffness parameters reflecting individual contribution of the two particles and of the interface properties.

2 PROBLEM DESCRIPTION

The original heterogeneous particulate solid is composed by particles of various sizes and shapes (figure 1a). The particles are embedded into solid matrix. Macroscopically, geometry of the solid is characterised by fraction of matric volume and by fraction of the volume of particulate aggregates. The scale of particles is traditionally interpreted as micro scale, but in this case meso scale is more suitable. On the meso-scale geometry is defined basically by geometry and location of particles. Assuming spherical shapes, the geometry of each particle i is defined by radius R_i (figure 1b). If coarse distribution of particles prevails, no direct contact between them is allowed while the inter-particle distance, or the value of the gap L_g became an important parameter.

Mechanical properties of the particulate solid are introduced on meso-scale. The material of particles is assumed to be elastic and isotropic. Composition of particles is generally inhomogeneous, therefore, elasticity properties of each of the particle i may be different and characterized basically by the different elasticity moduli $E_{i.}$ The matrix is assumed to be homogeneous and isotropic. Elasticity properties of the matrix are characterised by the constant elasticity modulus E_{int}. The case of weaker matrix is of major practical interest, therewith $E_{int} < E_{i.}$ The Poisson's ratios are specified in the same manner. The matrix during deformation obeys viscosity properties typically defined by use of Prony series.

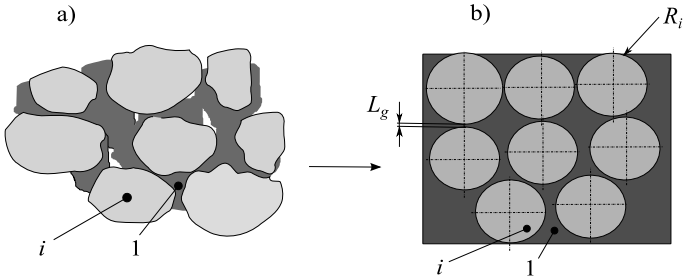

Figure 1. Heterogeneous particulate solid; a) general case, b) computational model composed by spheres; *i*-particle, 1- matrix

3 MULTI-LEVEL MODELLING CONCEPT

Formally, the above described heterogeneous particulate solid can be regarded as the 3D continuum and the stress-strain state of it can be computed directly by applying FE discretization approach and volume elements. This approach if it would be applied to real-scale volumes is restricted, however, by available computer resources, mostly by the CPU time. Consequently, it could be exploited exclusively for validation purposes. Elaboration and application of the multi-level modelling approach is expected to be more realistic.

On the macroscopic level, the particulate solid is regarded as a discrete system of the

bonded particles (figure 2c).

Therewith, the discrete model is implemented in the form of irregular triangular grid or lattice, structure with particles imbedded into the nodes of the grid, while grid lines are supposed to be deformable connection elements.

Description of the connection element has to be considered on the scale of particle by considering representative volume (figure 2a). This volume presents circular cylinder composed by hemispheres connected by weaker interface material of finite size termed usually a bond. Geometry of the model section (figure *2*a) is defined by its length *L* and diameter *2R*. Initial gap between particles is defined by L_g (figure *2*a).

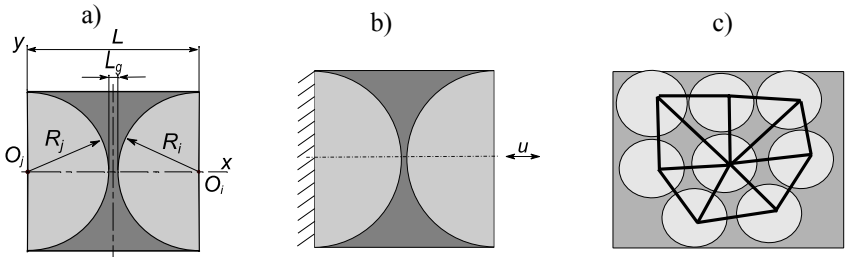

Figure 2. Multi-level modelling concept: a) representative volume; b) scheme of the normal interaction of particles; c) macroscopic model of the particles system

The connection element may be characterised by the constitutive relationship in terms of the force vector $\boldsymbol{F}$ and displacements $\boldsymbol{u}$. Finally, it is defined in conventional form:

$$\boldsymbol{F} = [\boldsymbol{K}]\boldsymbol{u} \ . \tag{1}$$

Here, $[\boldsymbol{K}]$ is the resultant normal stiffness matrix reflecting various properties of contacting particles and the interface. The relationship (1) and connection stiffness may calculated numerically by conducting various deformation tests or applying analytical methods. The effect of the initial particles gap size L_g could be studied numerically.

Once the connection element is characterised in a frame of the DE methodology, the macroscopic analysis will follow the conventional path of the DEM. On the other hand, such an element may be also regarded as synthetic 1D FE with user-defined properties.

4 THE INTEGRAL NORMAL INTERACTION MODEL

The connection element between two spherical particles *i* and *j* is defined through the axial deformation of representative volume (figure 2b). Deformation behaviour of element is characterised by the normal inter-particle displacement $u_n = u_i + u_j$. Consequently, the resultant constitutive relationship (1) of the connection element is transformed to simple relationship relating the normal force F_n and displacements u_n:

$$F_n = K_n \cdot u_n . \tag{2}$$

Here, K_n is the resultant normal stiffness reflecting various properties of contacting particles and the bond per unit length. The stiffness K_n of this connection element is resultant stiffness may calculated numerically by conducting various deformation tests or applying analytical methods Representative volume sample of the element model is a cylinder which may interpreted as composite rod. To define the stiffness, a generalised approach was proposed on the basis of the semi-analytical beam theory [13]. The 3D behaviour of connection element is simplified assuming cylinder to be assembly of deformable generatrix lines.

Each of the lines crosses regions of different homogeneity, i.e. regions occupied by particle and interface. It means that generetrix is always inhomogeneous line composed by sequentially connected sub lines. On the other hand, the cross-section of the cylinder may be divided into subsections. Regarding the above formulation, the cylinder volume may be imaginary presented as assembly of differently located inhomogeneous regions. Since stiffness nature is integral of material properties over the volume, evaluation of the stiffness is attributed to individual sub region. On this basis the resultant stiffness is obtained by composition of sequentially and parallel connected springs, while each of the springs is characterised using virtual displacement method.

This concept is demonstrated approach is demonstrated by showing two basic models – general model combining sequential and parallel elements (figure 3b, d) and the fully sequential (FSI) model (figure 3a, c). The FSI model comprises three sequentially connected springs. The stiffness of springs k_i and k_j reflect the contribution of particles i and j respectively. The stiffness of the middle spring k_{int} reflects contribution of region occupied by interface material. There values are calculated by integrating over respective volumes.

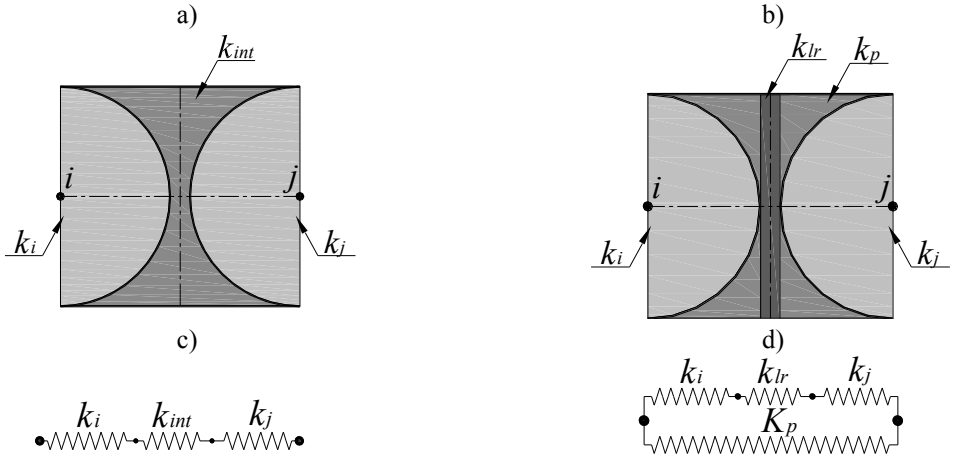

Figure 3. Normal interaction of spheres interacting via interface material: a, c) FSI model; b, d) general model.

The main differences of general model that an interface material is conditional divided into subregions. The middle stiffness of sequential part k_{lr} is predefined is by the constant layer

located between the particles, while the stiffness of parallel bond is attributed to parallel bond This model demonstrates that part of material, especially distanced from the central line may be attributed to the parallel spring.

Performance of the FSI model for wide range of relative interface elasticity modulus properties E_i/E_b for different interface thickness L_g is examined by the applying 3D FE discretisation of representative volume simulations, see Pilkavičius *et al*. [14], Rimša *et al*. [15].

Behaviour of the model obtained for interface thickness of L_g=0.5mm is illustrated in figure 4. Here variation of the stiffness K_n against relative elasticity modulus of interface is plotted in logarithmic scale. Each of the graphs presents variation of the separate bond stiffness parameters. The blue bold solid line stands for resultant stiffness K_n, thin solid cyan line for thickness interface stiffness k_{int}, while the horizontal dashed lines indicates the constant stiffness of particles k_i and k_j respectively. The red bold dots indicate the exact FE solution results obtained at selected points. The above results illustrate the excellent agreement of analytical model. It is also evident, that then drop of the relative interface modulus below $E_{i,j}/E_b$>12 the resultant stiffness is exclusively defined by interface stiffness and not depend on particles properties.

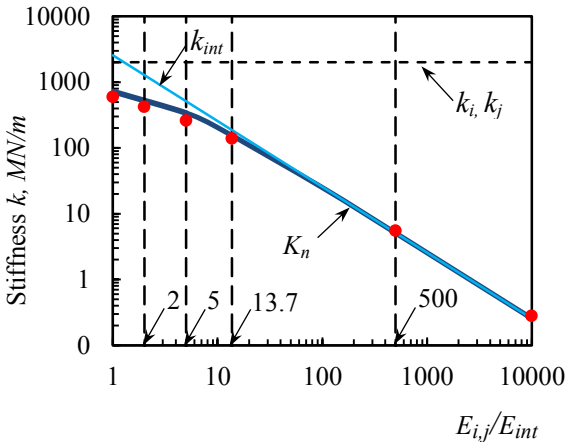

Figure 4 Evaluation of theoretical and FE models by variation of resultant bond stiffness against relative interface elasticity modulus properties $E_{i,j}/E_{int}$

5 NUMERICAL SAMPLE OF PARTICULTATE SOLID

Numerical sample of the particulate solid was considered to illustrate discretization technic. The system of eighteen identical spherical particles having radius R = 7.5 mm is considered as representative sample (figure 5). The relatively stiff elastic particles are embedded into rectangular box fulfilled by weaker viscoelastic matrix. The geometry of the box is defined by the length l = 112 mm, height h = 36 mm, and depth w = 18 mm. The locations of particles are defined by locations of the particles centres. All particles are located in the mid plane of the box.

Geometry of the particulate solid is defined by the distance between the particle's centres L = 15.5 mm and the gap between particles L_g = 0.5 mm.

The rigid boundary conditions are assumed on the bottom and implemented by fixing centres particles to the bottom wall. Interaction of particles with the vertical walls are softer, where flexibility is imposed by introducing the deformable layer between the particles and the box having minimal distance t in out-of-plane direction is equal to 1 mm.

The loading is defined by the motion of particles 1, 2 and 3 controlled by the prescribed displacement u = 0.5 mm.

Elasticity properties of granite are assigned for all of the particles, Therewith, the Young's modulus E is equal to $3 \cdot 10^{10}$ Pa, while the Poisson's ratio is defined as $\nu = 0.25$. Mechanical properties of the homogeneous matrix responding to the asphalt bitumen were taken from. Here, the time-independent elasticity properties are characterised by Young modulus E equal to $1.4 \cdot 10^{6}$ Pa and the Poisson's ratio equal to 0.46 and indicating relatively high incompressibility. The time varying properties are defined by the Maxwell element and expressed by coefficients of Prony series.

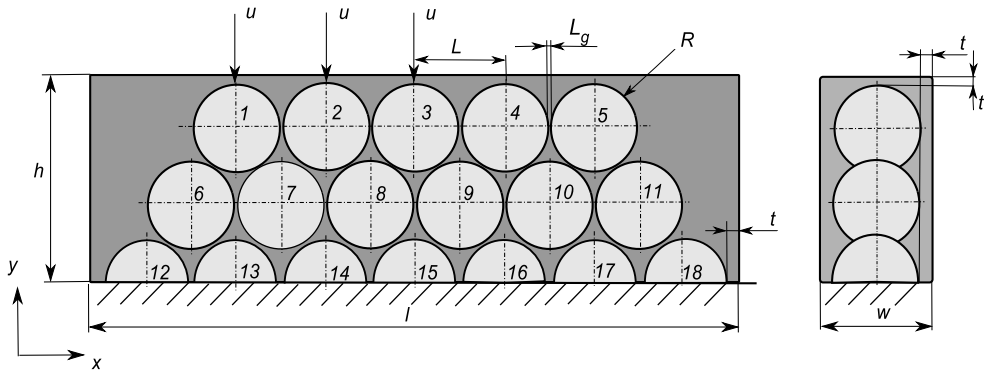

Figure 5. Geometry and boundary conditions of particulate solid in mid-sections of the specified box

6 DISCRETE ELEMENT MODEL

The DEM model of the above problem (figure 6) was developed to illustrate the discrete approach. Schematically, the model is presented as a regular triangular 2D structural network, geometry of which is predefined by location of the nodes. The model consists of eighteen nodes representing particles. The model lines are identified as connection elements.

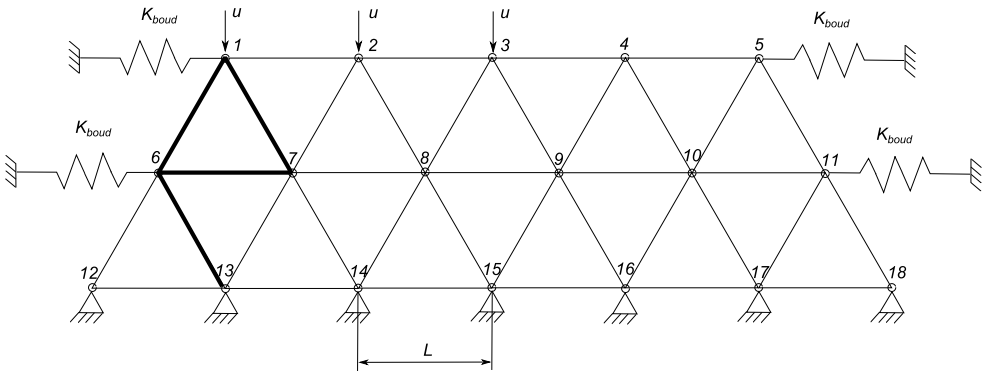

Figure 6. The discrete model of the sample

The discrete boundary conditions are specified to ensure the solid problem with the discretization accuracy. The rigid boundary on the bottom is implemented by suppressing motion of the corresponding nodes. Additional elements denoted by springs are added at nodes 1, 5, 6 and 11 to implement the transverse in-plane flexibility. The loading is specified by the prescribed displacement u of nodes 1, 2 and 3.

Elasticity properties of the solid are specified via connection elements Each of the element is able to undertake normal load and the above discussed normal interaction FSI model is applied for evaluation of stiffness K_n. Regarding inter particle distance L_g=0.5mm the stiffness $K_{0.5mm}=1.05\cdot10^5$ N/m. Boundary springs represent deformation of matrix which surrounds contacting particle area. Their stiffness is $K_{boud}=1.2\cdot10^2$ N/m.

7 THE SOLUTION ANALYSIS AND VERIFICATION OF THE DISCRETE MODEL

Verification of the model is performed by analysis of solutions of different models. Numerical sample of the particulate solid described above is considered for illustration purposes. It is assumed that the FE model of the heterogeneous 3D solid is more accurate when compared to the discrete element model composed by 1D elements.

To obtain the accurate solution the 3D FE model of the solid problem was generated by using the commercial FEM ANSYS code [16]. Tetrahedron type volume elements SOLID 187 with 10 nodes were used for generation of the model. As a result, the FE model consisting of 830098 nodes and 549098 elements was developed. In this context, the 2D Discrete Element model having 22 nodes with 22 degrees of freedom and 41 elements seems to be extraordinary simple. It should be noted that 3D FE model was solved in the linear and the finite strain formulations while difference between the models lies in the range of 3 %.

Direct comparison of the above DE and FE models is not a simple task. Various indirect approaches and various global and local criteria my by used for comparison purposes.

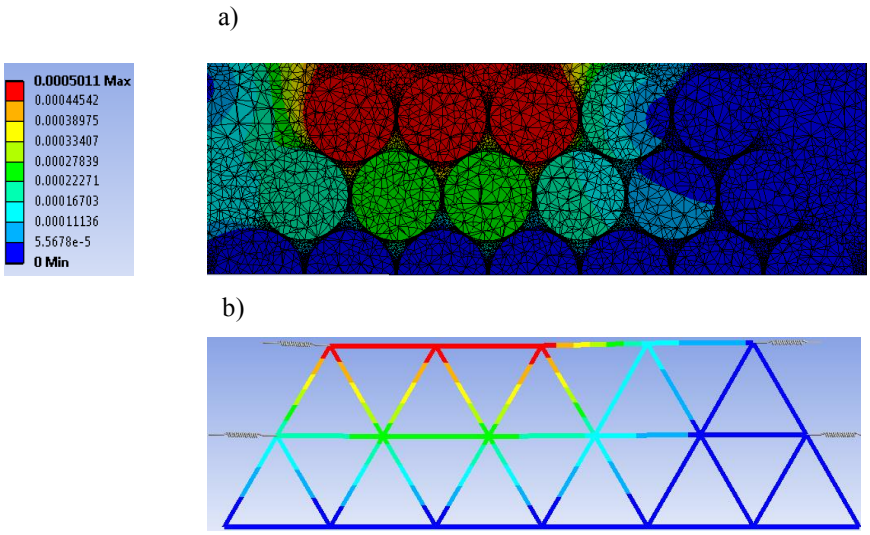

Figure 7. Contour plots of the displacement magnitudes in the mid-plane calculated: a) by the 3D FE; b) by the DE models

The simplest evaluation could be done by visual comparison of the calculated images. Contour plots of the displacement fields in the mid-plane of the box are shown in Figure 7, were colour scale indicate the displacement magnitudes. The colour pictures illustrate quite good similarity of the linear FE (Figure 7a) and DE (Figure 7b) models. It is obvious that the DE model properly reflects motion of the particles but the deformation behaviour of the weak matrix requires local analysis.

The rough evaluation of the model properties may be done, regarding composing of solid sample. The fraction value 35% of the particles volume is considerably smaller compared to the volume occupied by the matrix 65%; the volume of the interface material involved in the DE model is even smaller ~25%. Because of differences in the model structure, the only nodal displacements are directly comparable parameters

The deformation energy accumulated during loading evaluates deformation behaviour of the entire solution domain and yields information about the internal deformation behaviour. The 3D FE analysis yields the value of internal energy $U_{FE} = 0.0055$ *J*. The DE model yields the value $U_{DE} = 0.0052$ *J*.

The differences between the models are motivated by different response of them under action of the same prescribed displacement u. Thereby, the energy balance held for all of models indicates good conservation of energy. The higher deformation energy indicates the overestimated stiffness of the linear FE model. The difference between energies of the FE and DE models can be explained by different contribution of the local deformation modes between the particles. Energy obtained by the DE model is exceptionally attributed to the

axial deformation model. The value $U_{DE} = 0.0052\ J$ comprises 94.4 % of total deformation energy obtained by the FEM. It means that total contribution of shear and bending modes is smaller than 6.5 %.

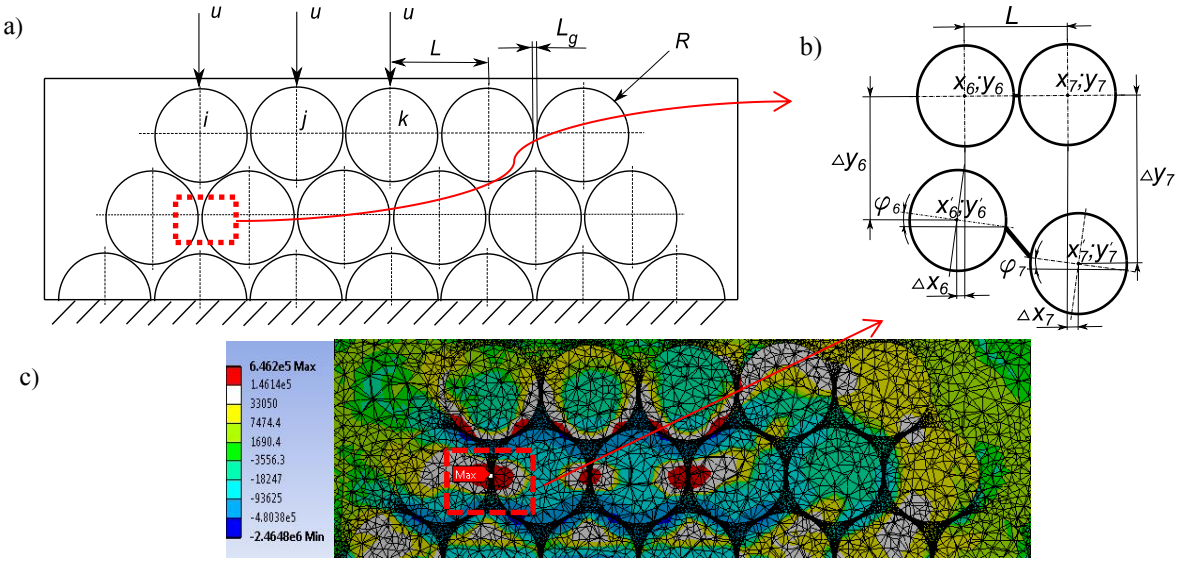

Figure 8. Local interaction analysis: a) geometry model in macro scale; b) initial and final positions of particles No. 6 and 7; c) contour plot of the principal stress

Comparison of models may be done using formal criteria. Euclidian norm of the nodal displacements u_i presents another global criterion. By comparing magnitudes of translational displacements, it was found that difference of displacements norms of the DE model $\|e\|_{DE} = 1.357 \cdot 10^{-3}$ m and of the FE $\|e\|_{FE} = 1.466 \cdot 10^{-3}$ m comprises 7.8% and indicates relativity good global similarity.

Identity or similarity of the global criteria not necessary matches the local behaviour, therefore, the detail local analysis required. For illustration of local effects, interaction of particles 6 and 7 is considered (figure 8). Local interaction analysis shows that particles rotations are relatively small. It is easy to persuade that angular deformation relative shift of particles could be explained by shearing deformation.

8 CONCLUSIONS

The heterogeneous particulate solid composed by particles bonded via weaker solid interface was considered and simplified discrete element (DEM) model was studied. Verification of the discrete model by comparing with the results of fully 3D finite element analysis illustrated the suitability of discrete model to capture macroscopic behaviour in terms of displacement of particles centres. It was also found that deformation behaviour of the solid

is predefined by the dominant axial interaction between the particles. This type of deformation comprises up to 95% deformation energy. It could be also stated that this accuracy is achieved by applying the newly developed interaction model regarding properties of interface. This approach applicable to confine state of particles is not sufficiently suitable for description of local inter-particle shear.

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