Part 1. Unsaturated soils and the grading curve

1. Particle/pore size distribution & microstructure of saturation – key elements for rational description of mechanical behaviour of unsaturated soils

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Modelling the mechanical response of unsaturated soils is much more complex and challenging than that of dry or saturated soils. In the past few decades, many researchers have attempted to modify and extend existing models, in a rather ad-hoc manner, by incorporating additional state parameters such as Suction (S), its variation with degree of saturation (Sr) and volumetric strain (.v). These developments, however, ignore an important aspect of the behavior of unsaturated soils, viz. microstructure of saturation. This paper describes how the Particle Size Distribution (PSD) or Pore Size Distribution (POSD) and micro-structure of saturation play a crucial role in the determining deformation and failure of unsaturated soils. It is shown that mechanical response of two soils having the same initial conditions and Sr but different PSDs can be different. This difference, of course, disappears when soil is either dry or fully saturated.

Part 2. Constitutive laws, particle breakage.

2. A nonlinear continuum theory of finite deformations of elastoplastic media

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Contemporary flow plasticity theories in finite-strain elastoplasticity are either based on an additive decomposition of a strain rate tensor into an elastic part and a plastic part, or on a multiplicative decomposition of the deformation gradient tensor into an elastic part and a plastic part. While the former theories are considered to be ad hoc extensions of small-strain flow plasticity theories into the area of finite deformations to cover large displacements, but small strains in the material of the deforming body, the latter are now generally accepted as true finite-strain flow plasticity theories. Unfortunately none of the theories entirely satisfies the requirements of thermodynamic consistency, and as a result, the material models and their analysis results, when used in numerical analyses, are dependent on the description and the particularities of the material model formulation. Recently a nonlinear continuum mechanical theory of finite deformations of elastoplastic media has been developed, which allows for the development of objective and thermodynamically consistent material models. This means that the plastic flow, including 'normality rules' can be described in a thermodynamically consistent manner in terms of different stress measures and strain rates or their objective derivatives, which are conjugate with respect to the internal mechanical power, using various instances of the yield surface defined in the above stress spaces. A few results of the modified hypoelastoplastic and hyperelastoplastic material models based on the aforementioned nonlinear continuum mechanical theory will be presented and discussed.

3. Effect of crushing on critical states of soils: a DEM-based study

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Granular materials reach critical states upon shearing. The position and shape of a critical state line (CSL) in the compression plane are important for constitutive models, interpretation of in situ tests and liquefaction analyses. It is not fully clear how grain crushing may affect the identification and uniqueness of the CSL in granular soils.

Discrete-element simulations are used here to establish the relation between breakage-induced grading evolution and the CSL position in the compression plane. The study showcases an efficient discrete model of particle breakage simple to calibrate and able to track grading evolution.

4. Large strain plasticity for soils using the Particle Finite Element Method

Monforte, L. Arroyo, M. Carbonell, JM. Gens, A.:

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A computational framework for the numerical analysis of fluid-saturated porous media at large strains is presented. The proposal relies, on one hand, on the particle finite element method (PFEM), known for its capability to tackle large deformations and rapid changing boundaries, and, on the other hand, on constitutive descriptions well established in current geotechnical analyses (Darcy's law; Modified Cam Clay; Houlsby hyperelasticity). An important feature of this kind of problem is that incompressibility may arise either from undrained conditions or as a consequence of material behaviour; incompressibility may lead to volumetric locking of the low-order elements that are typically used in PFEM. In this work, two different three-field mixed formulations for the coupled hydromechanical problem are presented, in which either the effective pressure or the Jacobian are considered as nodal variables, in addition to the solid skeleton displacement and water pressure. Additionally, several mixed formulations are described for the simplified single-phase problem due to its formal similitude to the poromechanical case and its relevance in geotechnics, since it may approximate the saturated soil behaviour under undrained conditions. In order to use equal-order interpolants in displacements and scalar fields, stabilization techniques are used in the mass conservation equation of the biphasic medium and in the rest of scalar equations. Finally, all mixed formulations are assessed in some benchmark problems and their performances are compared. It is found that mixed formulations that have the Jacobian as a nodal variable perform better.

5. Linking true sphericity and particle rotation to calibrate DEM contact models

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Particle shapes affect the micromechanical interactions that underlie granular soil mechanics. Direct representation of particle shape in DEM is computationally costly. The alternative is to use a moment-rotation law. Such laws have parameters that are difficult to calibrate. We demonstrate how true sphericity may be used to bridge the gap between particle size information and soil mass behaviour.

Part 3. Grain shape, Grading Entropy and DEM, Entropy.

6. Volumetric consequences of mass loss in soils - A micro-mechanical perspective

Barreto, D[1]. McDougall, J[1]. Imre, E[2].

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Soil particles may be lost through dissolution, degradation or erosion. Regardless of the process of loss, there follows a change in soil structure both in terms of phase composition and grading. In this paper, the influence of size and amount of particle loss on phase composition at two stresses is investigated. The tests are performed on sand–salt mixtures, loaded in a modified permeation oedometer and subsequently dissolved. Changes in overall volume and void ratio are presented. Two significant observations about the volumetric consequences of particle loss can be made. First, overall volume changes are directly related to the amount of dissolved particles and to a lesser extent, the size of particle lost. Second, particle loss leads to an increase in void ratio; the magnitude of the increase is related to the amount of dissolved particles but appears not to be sensitive to either the size of particle lost or the pre-dissolution void ratio. Based on the observed response and a dissolution-induced void change parameter, the influence of different mechanisms of volume change is discussed. Tests were performed at two different vertical stresses with no discernible influence on void ratio change.

7. Preliminary study on the relationship between dry density and the grading entropy parameters.

Imre, E[1]. Singh, VP[2]. Baille, W[3]. Barreto, D[4].: Preliminary study on the relationship between dry density and the grading entropy parameters.

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The goal of the paper is to present and to further analyse the results of the pioneering research work on the dry density of sands made by Lőrincz (1990) and Kabai (1974) to elaborate a dry density model in terms of the grading curve. It is enough to consider the minimum dry density for sands only, according to Kabai [1974].

Lőrincz tested two kinds of grading curve series, continuous, fractal distributions and gap-graded soils with a fixed fraction numbers N (N=1…5) searching a relation between the maximum values of the minimum dry density e_{max} and the maximum value of the grading entropy. No direct relationship was found between the maximum density and the maximum entropy (the sum of the base entropy S_0 and the increment ΔS). The measured data of Lőrincz and some newly measured data concerning the minimum dry density e_{max} are split here into mean fraction density (on the basis of the measured fraction e_{max} values) and increment. These are related to the two entropy coordinates separately. It is shown that the first component (mean fraction density) is nearly linear in terms of the base entropy S_0, the increment is nearly linear in terms of the ΔS. The maximum density point is tentatively related to the maximum entropy S point for fractal mixtures. The DEM study enables to identify a relationship between the minimum dry density and the base entropy. The preparation of specimens is controlled and repeatable, and boundary effects can be avoided by using periodic boundary conditions.

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8. New aspects of the grading curve characterization. Mean or fractal gradings, natural (internally stable) soils. Strong force chains.

Imre, E[1]. Barreto D[2]. Goudarzy, M[3]. Rahemi, N[3]. Baille, W[3].:

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The grading curve is measured in discrete points, at the sieve hole diameters which are doubled. Applying the statistical entropy formula of the discrete probability distributions, two „grading entropy parameter pairs” were previously derived.

The space of grading curves with N fractions is represented by an N -1 dimensional, closed simplex. The two entropy coordinates are considered as a map of the simplex into the 2-dimensional Eucledian space. The inverse image creates a structure on the simplex.

Concerning the first grading entropy parameter, the *A* = constant condition means parallel hyper-plane sections of the simplex. Within this, the *B* = constant condition means subdivision centred to a point (the conditional maximum of *B*) which is a kind of centre point of the section, the related grading curve a mean grading curve with fractal distribution.

The physical meaning of the subdivision is as follows. The normalized form of the first grading entropy parameter *A* is a continuous internal stability measure, based on the simple physical fact that if enough large grains are present in a mixture then these will form a skeleton. The internal stability rule of the grading entropy theory - formulated in terms of this variable - separates the soils into natural (A>=2/3, stable) and artificial (A<2/3, unstable) ones. This statement is illustrated by micromechanical tools and some relations concerning liquefaction potential.

9. Preliminary study on the relationship between the small and intermediate strain properties of granular materials in terms of grading entropy parameters.

Barreto, D[1]. Imre, E[2].:

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It is well recognised that the small strains shear stiffness in granular materials is dependent on the particle size distributions. Earlier research relates descriptors of particle size distributions and shear stiffness. For example, Wichtmann & Triantafyllidis (2009) proposed relationships between the shear stiffness and the coefficient of uniformity (c_u) while Menq (2003) suggested using both c_u and the mean diameter (d_{50}) for the estimation of shear stiffness. More recently, Sun et al (2017) demonstrated that their newly proposed grading parameter (c_g) which considers the full range of particle sizes, correlates better to shear stiffness values than common grading parameters such as c_u and $d_{50.}$

However, grading entropy coordinates proposed by Lörincz (1986) are easier to calculate, they represent the entirety of any particle size distribution as a coordinate pair, and unlike c_g, they relate to c_u and $d_{50.}$ Earlier work has also shown that entropy coordinates are very well suited to describe and understand processes in which particle size distributions evolve such as particle breakage or mass loss due to mineral dissolution (e.g. Imre et al, 2012; McDougall et al, 2013).

Following the ideas by Sun et al (2018), in this study we use resonant column tests on sands with different gradings performed by Wichtmann & Triantafyllidis (2009) to establish relationships between grading entropy coordinates and shear stiffness. We demonstrate that grading entropy coordinates correlate as well as the parameter c_g to the corresponding material constants suggested by the popular shear stiffness formula by Hardin and Ricart (1963), while they are better related to physical phenomena and stress transmission in granular materials.

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10. Some comments on the internal stability rule of grading entropy (the probability of internally stable granular mixtures).

Talata, I[1]. Imre, E[2]. Singh, VP[3] Nagy L[4].:

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The overall soil stability – according to [1], in accordance with the experimental results [2] - is described by the criterion that A > 2/3. In soils which meet this criterion, the matrix of coarser soil particles is stable and able to form a resistant skeleton, even though suffusion may occur.

Some questions arise, for example, in regard to the stability of a single fraction which does not lie in a unique position on the entropy diagram. Since the change due to degradation is the appearance of smalls, which causes an increase in the A value, the one fraction case is likely on the safe side.

Another question is related to the probability that an arbitrary N-fraction soil is stable. This can be characterized by the relative size of the grading curve space separated with the A = 2/3 hyper-plane on condition that the probability is the same in the whole simplex. This number is decreasing with the fraction number (e.g. for N=2, the 1/3 part of the grading curve space is safe, for N=3, the 2/9 part of the grading curve space is safe).

Significant segregation is unlikely to occur, if the relative base entropy A is between the limits of 0.4 and 0.7. It is important to note that the same parameter - the relative base entropy A – is responsible for overall soil stability. In soils which meet this criterion, segregation may occur. Soils which meet both criterion may constitute very small part of the of the grading curve space and may need careful design in case of broadly graded soils.

The probability that an arbitrary N-fraction soil is stable and segregation free is characterized by the relative size of the grading curve space separated with the A = 2/3 and A = 0.7 hyper-planes (on condition that the probability is the same in the whole simplex) which is dependent on the space dimension of the simplex. The aim of the paper is to derive a recursive formula for the ratio of volumes of polyhedra obtained by cutting a simplex with a hyperplane into two parts.

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11. Approximate interpolation in terms of grading curves (density and SWCC functions),

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The interpolation over the space of the grain size distribution curves with N fractions is the same as the interpolation over a unit sided simplex with dimension N-1. The interpolation needs “too many” interpolation point for fraction number greater than about 4 (Table 1) since the number of sub-simplexes (sum of vertices, edges, faces etc.) increases exponentially with N. An approximate interpolation method is suggested which needs “less” interpolation points (2N).

The space of grading curves with N fractions is represented by an N -1 dimensional, closed simplex. The two entropy coordinates are considered as a map of the simplex into the 2-dimensional Eucledian space, the image of the map is the entropy diagram. The inverse image creates a structure on the simplex. Concerning the first grading entropy parameter, the A = constant condition means N-2 dimensional parallel hyper-plane cross-sections of the simplex. Within this, the *B* = constant condition means a submanifold centred to the point of the conditional maximum of *B* which is a mean point of the section, where the map is one-to-one.

The interpolation is made either on the grading entropy diagram (the image of the simplex) or on a properly selected, 2-dimensional topological section of the simplex (related to the fibration with the entropy map) which maps in a one-to-one manner into the entropy diagram by the entropy map.

The interpolation points are the (entropy) mean points and the extreme points of some *A* = constant cross-sections. The interpolated function is extended point-wise to the inverse image of the entropy diagram points by the constant function.

The suggested approximate interpolation method is started to be applied to interpolate some function of sands, the examples shown here are the related to the dry density and the parameters of some well-known SWCC functions (Imre et al, 2009 to 2014).

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Imre E , Lőrincz J , Hazay M , Juhász M , Rajkai K , Schanz T , Lins Y, Singh V P , Hortobagyi Zs Sand mixture density In: UNSAT2014. Sydney, Australia , 2014.07.02 -2014.07.04. pp. 691-697.

12. Tracking critical points on evolving curves and surface.

Sipos, A.: Tracking critical points on evolving curves and surfaces

*Hungarian Academy of Sciences -BME Morphodynamics Research Group.***s**

In recent years it became apparent that geophysical abrasion can be well characterized by the time evolution N(t) of the number N of static balance points of the abrading particle. Static balance points correspond to the critical points of the particle's surface represented as a scalar distance function r(u,v,t) measured from the center of mass of the particle. While N(t) is important for geophysicists, its computation poses challenges, because in the computational model r(u,v,t) is often replaced by its finely discretized approximation rΔ(u,v,t) and the number NΔ(t) of critical points corresponding to rΔ(u,v,t) is, in general, not identical to N(t). We describe the geometric theory relating NΔ(t) and N(t) and also provide an algorithm to compute N(t) based on rΔ(u,v,t).

13. A non-equilibrium foundation of thermodynamics

Martinás, K, Tremmel, B.: Basic Energy Concepts of Non-equilibrium Thermodynamics

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Thermodynamics as we know it today, including modern non-equilibrium thermodynamics, is based on the diligent study of equilibrium states.There is a hidden paradigm, a canonized assumption in thermodynamics that systems in non-equilibrium state can only be understood through equilibrium thermodynamics. By questioning the paradigm, we are going to present a new approach, which is built on non-equilibrium foundation.

Part 4. DEM, Grading Entropy, Entropy based Constitutive laws.

14. Multiple shear bands in granular materials.

Lévay, S. and Török, J.: Multiple shear bands in granular materials.

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from quasi-static to dynamic shear regime is studied by discrete element

method *(DEM)* and by means of a mesoscopic model. We show that at moderate shear rate multiple shear bands appear which eventually appear as a continuous shear profile for large shear rates. The model and the DEM simulations both show a minimum in the shear stress and a maximum for the number of simultaneous shear bands, however the position of the two do not coincide. The scaling analysis of the kinetic energy indicates that the peak in the latter is the relevant parameter. We also show how the long range order present in the quasi-static regime is gradually destroyed by the presence of multiple shear bands.

15. Frustrated packing in a granular system under geometrical confinement

Lévay, S. Fischer. D. Stannarius, R. Szabó, B. Börzsönyi, T. and Török, J.: Uniform sphere packing or frustrated packing in a granular system under geometrical confinement.

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Optimal packings of uniform spheres are solved problems in two and three dimensions. The main difference between them is that the two-dimensional ground state can be easily achieved by simple dynamical processes while in three dimensions, this is impossible due to the difference in the local and global optimal packings. In this paper we show experimentally and numerically that in 2 + □ dimensions, realized by a container which is in one dimension slightly wider than the spheres, the particles organize themselves in a triangular lattice, while touching either the front or rear side of the container. If these positions are denoted by up and down the packing problem can be mapped to a 1/2 spin system. At first it looks frustrated with spin-glass like configurations, but the system has a well defined ground state built up from isosceles triangles. When the system is agitated, it evolves very slowly towards the potential energy minimum through metastable states. We show that the dynamics is local and is driven by the optimization of the volumes of 7-particle configurations and by the vertical interaction between touching spheres.

16. Breakage properties and DEM modelling of Ballast material

Gálos, M. Orosz, Á.: Breakage properties and DEM modelling of Ballast material.

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In most cases, for technical and economic reasons, the foundation of the railway tracks is made up of crushed rocks. Besides, the size and material of the rocks, the shape plays a significant role in the load capacity of the ballast as well. The static and dynamic loads, that affect the railway ballast, lead to crack initiation and the crushing of the rocks, which causes fouling and changes in the shape and size of rocks. These failure mechanism results a decreased ballast strength.

The discrete element method (DEM) simulates materials with particles (elements) and interactions between them, which makes DEM ideal for modelling bulk materials. The oldest and simplest particle shape is the sphere, however other opportunities exist for modelling complex grains. Our focus is on the application of polyhedral elements, which are assumed to model the nature of crushed rocks more realistically than spheres. Different types of crushed rock aggregates are typical construction materials.

In our research, a crushable polyhedral material model was chosen, which defines the geometry of the particles and the constitutional law between them. The model is implemented in Yade software. The definition of the model was studied, then the program code was tested in different verification tests.

The model also performs random shape generation via Voronoi method. The resulting geometries were compared with natural rocks with the aid of 3D scanners and calibration studies were carried out with an application of uniaxial press test. Simulation and measurement results were compared, and conclusions were made about the application field of the current model and its development opportunities.

17. Analysis of particle movement conditions of open mixing screws.

Varga, A.: Analysis of particle movement conditions of open mixing screws.

Szent István University, Hungary.

In case of the drying process of agricultural grains in silos the main problem is that the distribution of the moisture content is not homogeneous within the granular assembly. These inhomogeneous zones could worsen the quality of the dried product. To reduce this effect mixing systems are used within the silos. The number of such screws, the geometry and kinematical parameters of their operation are determined by using experimental investigations, but little is known about what happens around the rotating mixing screw, and because of this, there are no clear guidelines for planning of them. In most of the cases the motion path and velocity of the screws are unchangeable. If the operational parameters are not set adequate then significantly additional costs could appears. The aim of my research was to determine the particle-flow about the mixing screws. To reach this goal I studied the literature in every detail. After to map the deficiency of the literature and choose the suitable modeling technique, an experimental apparatus was built. Next step was to define the measurement’s methods and determine the vertical displacement of the particles. The results of this measurement made it possible to verify the usability of my discrete element model. To describe the mixing phenomenon discrete element method was used which is a fairly new proceeding to model the mechanical properties of bulk materials. I had to decrease the simulation time, therefore the container’s size had to be reduced. In the case of size reduciton, attention must be paid that the original behavior of the bulk material does not change. After the modification of the experimental apparatus, it was proved that the vertical displacement has the largest influence over the mixing efficiency. Due to this statement, it was sufficient to examine the slice of the plexiglass cylinder.

Based on the test and the simuation results it can be supposed that the DEM model of the mixing apparatus can be used for the determination of the particle displacement field around open mixing screws. To compare the simulations with different parameters the effective radius has been determined. It can be found there is an optimal screw rotation angular velocity above which there is no reason to operate the mixing apparatus, as the mixing efficiency does not increase with the increase of screw angular velocity, as the change in the efficiency of mixing becomes smaller and smaller by increasing the angular velocity and the causeless increase of screw angular velocity results higher compressive forces acting on the mixed particles. I established that the mixed domain can be described with three functions and the shape of this volume does not depend on the particle's geometry. The mixed volume can be evaluated with the rotations of these functions about the vertical axis. The volume is affected by the following factors: leaf diameter and angular velocity of the screw. I proved that the pitch of the screw has no effect to mixed volume.

18. Calibration algorithm for discrete element models.

Safranyik, F.:

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Determination of micromechanical parameters (calibration of the discrete model) and computational demand of simulations are two main shortcomings of Discrete Element Method (DEM). Using this numerical technique, macro behaviour of granular assemblies is modeled with multiple, so-called micromechanical parameters of individual elements. Direct measurement most of these are impossible, because of this main aim of the calibration process is the finding of special combination of micromechanical parameters which are applicable to describe macro behaviour of the whole particulate assembly. Since nowadays there is no a robust, standardized procedure for calibrating micromechanical parameters in many cases the calibration itself consumes more time and resources, than modeling the mechanical process itself. To promote industrial application of DEM a shear test based discrete element calibration method, which is capable to model the behavior of the granular assembly through a wide domain of different precompression values is developed. It is demonstrated in our work, that a highly autonomous calibration algorithm can be constructed, which is capable to find desired macromechanical behavior by systematic odification of micromechanical parameters.

19. On the Topology of State-space, Linear vs. Nonlinear Theories and Dry Friction*

Verhás, J.: Morse lemma and entropy principle (Mohr Coulomb law and the properties of the friction)

Budapest University of Technology and Economics, Hungary

The work reported here aimed to eliminate the gap between static and sliding friction on the ground of non-equilibrium thermodynamics with dynamic (internal) degrees of freedom introduced into the state space of the system.

20. Mixture composition change due to breakage and grading entropy – A rock classification alternative?

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The grading entropy of a soil [*S*] - a kind of statistical entropy – is the sum of two terms (Lőrincz, 1998). The base entropy [S_o] is arisen from the fact that statistical cell width (fractions) in the conventional grading curve is not uniform. The entropy increment [ΔS] is arisen from the mixing of the fractions, expressing the entropy due to mixing the fractions. These “entropy coordinates” can be normalized resulting in the relative base entropy [*A*] and, the normalized entropy increment [*B*].
The entropy principle of the classical thermodynamics can be related to the directional properties of natural or spontaneous processes.The goal of the research is to study if any parts of the grading entropy may play the role of the “true” entropy in a thermodynamic sense (i.e. increases during an irreversible process). For this aim the crushing process was considered (eg., Coop et al, 2004, Lőrincz et al, 2005, Guida et al, 2016). The results of the experimental studies are as follows.

Similar behaviour is related to the compression and shear tests. During breakage the decrease of the mean diameter may occur under the following conditions. (i) the largest fraction remain due to cushion effect, (ii) the minimum grain size is limited by a crushing limit around some microns (Kendall 1978), (iii) the the minimum grain size may be assumed to appear at the start of the breakage

The entropy path is as follows. The base entropy S_o decrease (decrease of the mean diameter) occurs such that the entropy increment ΔS strictly monotonically increases. It follows that that the entropy increment ΔS can be related to the entropy principle of thermodynamics.

The normalised entropy path is as follows. The change of the normalized entropy parameters is the same for constant *N* but is discontinuous if the number of the fractions *N* is changing at the start of the tests when the new, smaller fractions appear. The ‘discontinuity’ causes a more stable grading in terms of the internal stability criterion of the grading entropy. The normalised entropy path seems to be independent of the material. Therefore, the rate of the entropy coordinate variation can be used for material qualification and rock classification.

It can be noted thet during lime modification the path opposite [Imre et al, 2012], (expressing the increase of the mean diameter and the decrease in the entropy increment ΔS).

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