Soil parameters in terms of entropy coordinates

Emőke Imre[1*], *Tibor* Firgi[2], *Wiebke* Baille[3], *Maria* Datcheva[4], *Daniel* Barreto[5], *Shuyin* Feng[6], and *Vijay* Singh[7]

[1]EKIK HBM Research Centers and Bánki Donát Faculty of Mechanical and Safety Engineering, Óbuda University, H-1081 Budapest, Hungary
[2]Ybl Miklós Faculty of Architecture and Civil Engineering, Óbuda University, H-1174 Budapest, Hungary
[3]Ruhr-Universität Bochum, 44801 Bochum, Germany
[4]Institute of Mechanics and Institute of Information and Communication Technologies, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria
[5]School of Computing, Engineering and the Built Environment, Edinburgh Napier University, EH10 5DT Edinburgh, United Kingdom
[6]Birmingham City University, B42 2SU Birmingham and University of Bristol, BS8 1QU Bristol, United Kingdom
[7]Texas A&M University, College Station, TX 77843, United States of America

Abstract. In the ongoing research, an approximate, grading entropy based, advanced interpolation method is applied to establish empirical functions between the grading curves and the model parameters of sands. The space of the grain size distribution curves with N fractions is isomorphic to the space of the unit-sided simplex with dimension N-1. The traditional interpolation over the simplex with dimension N-1 is problematic since the number of the sub-simplexes (and the interpolation points) may increase exponentially with N. To overcome this difficulty, the function is approximately interpolated, which means that the interpolation is made on some 2-dimensional sections of the simplex and is extended to the whole simplex, using the grading entropy map. Two kinds of 2-dimensional sections can be used based on either fractal distributions or partly fractal partly on some maximal gap-graded distributions. In this paper the experiments were made on the artificial mixtures of natural sand grains earlier. Two kinds of functions were approximately interpolated for the minimum dry density using the measured data. One kind of function was determined for the parameters of an SWCC model directly from the level lines previously graphically interpolated from fractal distribution data.

1 Introduction

1.1 Space of grading curves

To characterise a grading curve, an abstract fraction system is defined. The diameter limits are doubled with the serial number j (j =1, 2. , Table 1):

$$2^{j} d_0 \geq d > 2^{j-1} d_0, \tag{1}$$

where d_0 is the smallest diameter which may be equal to the height of the SiO_4 tetrahedron ($d_0=2^{-22}$ mm).

The relative frequency of x_j of grading curves fulfil:

$$\sum_{i=1}^{N} x_i = 1, \quad x_i \geq 0, \; N \geq 1. \tag{2}$$

where the integer variable N is the number of the fractions between the finest and coarsest non-zero ones.

The relative frequencies x_i can be identified with the barycentre coordinates of the points of an N-1 dimensional, closed simplex. The space of the grading curves with N fractions can be identified with the N-1 dimensional, closed simplex.

1.2 Grading entropy and diagrams

The grading entropy S is the sum of two parts [1, 2]):

$$S = S_0 + \Delta S \tag{3}$$

where S_0 is base entropy, ΔS is entropy increment. The base entropy and its normalized form are the weighed (normalised) means of the fraction entropies:

$$S_0 = \sum x_i S_{0i}, \; A = \frac{(S_o - S_{o\min})}{S_{o\max} - S_{o\min}} \tag{4}$$

where S_{0k} is the k-th fraction entropy (Table 1), S_{0max} and S_{0min} are the entropies of the largest and the smallest fractions, respectively. The entropy increment ΔS and its normalized form B:

$$\Delta S = -\frac{1}{\ln 2} \sum_{x_i \neq 0} x_i \ln x_i, \; B = \frac{\Delta S}{\ln N} \tag{5}$$

Any grading curve can be represented as a point in the entropy diagram using the normalised or non-normalised grading entropy coordinates (Fig. 1(b)) using the smooth entropy map. The inverse image (Fig. 2) of a regular value is an N-3 - dimensional sphere, the

* Corresponding author: imre.emoke@uni-obuda.hu

critical values of the map (maximum line of the diagram) is the optimal line. A point of it, the optimal point or optimal grading curve which has fractal distribution, with the following relative frequencies:

$$x_1 = \frac{1}{\sum_{j=1}^{N} a^{j-1}} = \frac{1-a}{1-a^N},\; x_j = x_1\, a^{j-1} \qquad (6)$$

where parameter a is the root of the equation:

$$y = \sum_{j=1}^{N} a^{j-1}[\,j-1-A(N-1)] = 0. \qquad (7)$$

The optimal grading curve is a kind of mean grading curve for all the grading curves for given A value.

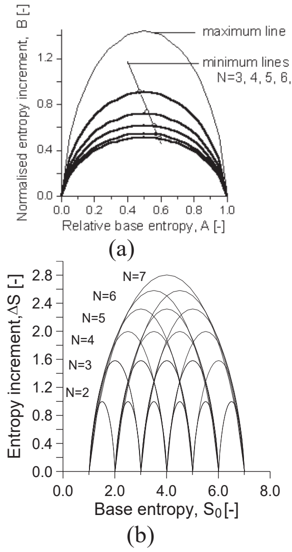
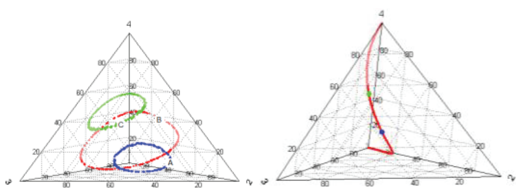


Fig. 1. The entropy diagrams. (a). The normalized entropy diagrams for simplexes with N varying from 2 to 7. Note the fixed maximum (optimal) line and the N-dependent edge 1-N. (b) The optimal lines separate in the non-normalised diagram.



(a) (b)

Fig. 2. Inverse images for an N=4 simplex [2]. (a) The inverse image of three regular entropy diagram points (N-3=1 dimensional spheres). (b) The optimal line.

Table 1. Fractions in terms of a fixed d_0, serial numbers and fraction eigen-entropies

j	1	...	23	24
Limits	d_0 to 2 d_0	...	2^{22} d_0 to 2^{23} d_0	2^{23} d_0 to 2^{24} d_0
S_{0j} [-]	1	...	23	24

1.3 Interpolation, goal of paper

The direct interpolation of a function over the space of the grading curves (Fig. 3(a)) needs $c(2^N$-1) interpolation points, this number is exponentially increasing in terms of the number of the fractions N (see Table 2). To overcome this difficulty, an approximate interpolation method is suggested, based on the grading entropy concept, needing ~c N to ~c N^2 data. The paper briefly presents the method and its application to the minimum dry density and, to the parameters of the Fredlund-Xing soil water characteristic curve equations [3] for sands.

2 Approximate interpolation

2.1 Some definitions

In topology the fibration is defined for topological spaces as follows:

$$F \rightarrow E \rightarrow B \qquad (8)$$

where the first map is the inclusion of fiber F into the total space E and the second map π: E → B is a projection of the total space onto the base space B.

The fibration is locally trivial if in small regions of the base space B the total space E behaves just like a projection from corresponding regions of $B \times F$ to B.

A subspace I in E is a section of the fibration if there is a continuous map g: B→ I and the map g(π) is the identity of B. A locally trivial fibration is trivial if the base space is contractible. In this case E is diffeomorphic to B x F or I x F, E can be decomposed such that one fiber is attached to each section point.

2.2 Interpolation using the entropy map

The simplex (total space) maps to into entropy diagram (base space B). The fiber F is the inverse image (Fig. 2).

We can interpolate on the entropy diagram (or equivalently on a section I of the fibration in the total space E). The function is extended onto the fibers by the constant map point-wise. The extended function – according to the continuity of the composite functions – is continuous, but approximate over the total space.

The entropy map is twofold for the triangle diagram (n=2), having two sections as shown in Fig. 3. The optimal line maps into the upper boundary of the entropy diagram and the related grading curves reflect a kind of mean behaviour. It is the part of the boundary of both sections. The other part of the boundary is either the edges 1-2, 2-3..(N-1)- N or the edge 1-N, resp.

The s_{min} iso-lines on the entropy diagram are different if section 1 or section 2 is mapped (upper/lower part of the triangle diagram, resulting in near linear/curved lines, respectively, Fig. 3).

Table 2. Number of sub-simplexes

N	2^N-1 (# of sub-simplexes)	(N+1)N/2 (# of continuous sub-simplexes
2	3	3
3	7	6
4	15	10
7	127	28
10	1023	55
14	16383	105

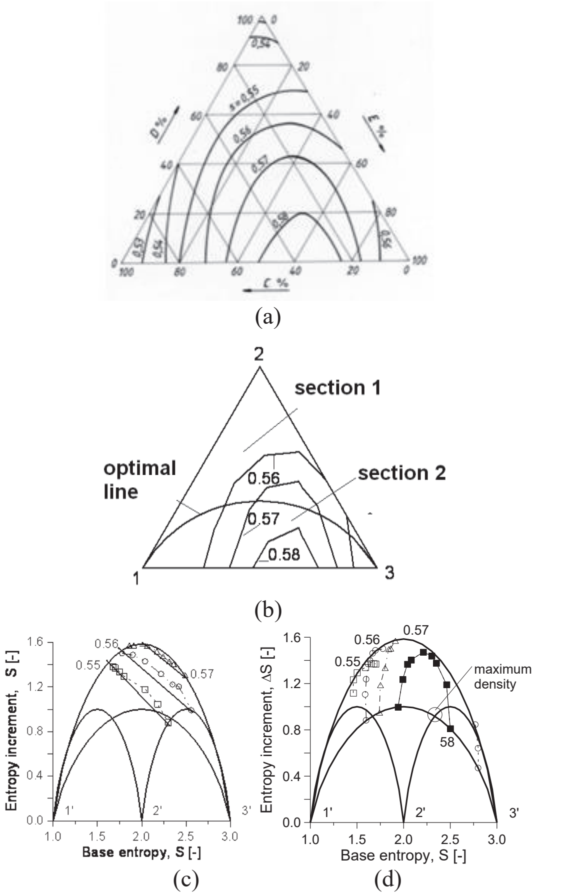


Fig. 3. The image of the s_{min} iso-lines of the 2-dimensional simplex by the entropy map. (a) The triangle diagram and the direct interpolation of the s_{min} iso-lines using data sampled at the intersection points of the coordinate lines [1]. (b) The optimal line, the section1 and section 2 definition. (c, d) The image of the s_{min} iso-lines from Section 1 and 2.

3 Materials and methods

3.1 SWCC data measurements and processing

The Fredlund – Xing (1994) equation reads [5]:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\left\{ \ln \left[e + \left(\frac{u_a - u_w}{a} \right)^n \right] \right\}^m} \tag{9}$$

where u_a – air pressure, u_w – pore water pressure, θ – volumetric water content, a [kPa], n, m – non-linear model parameters, θ_r, θ_s are linear model parameters.

The measurements were performed on seven sand fractions and their artificial, optimal mixtures with A=2/3 (see Tables 3, 4, [7 - 10]). In the suction range of u_a-u_w $\leq$ 50 kPa sand boxes were used, in the higher suction range axis translation technique was used. For the model fitting, a nonlinear method was applied [6].

Using the identified parameters, section 1 interpolation was made where not only the fractal gradings related to N=7, but also the fractal gradings N<7 were also used (ie., optimal points of the continuous sub-simplexes were also used, Table 3, [3]). In this work the so determined isolines were approximated by simple parametric functions in terms of the non-normalised grading entropy coordinates.

3.2 Dry density measurements

The measurements were performed on five sand fractions and their artificial, optimal mixtures by Lőrincz earlier (see Table 5, [11 - 15]).

The minimum dry density level lines were interpolated in two cases, either from the of 50 fractal distributions with various N, or from 9 / 5 maximal gap-graded / maximal fractal distributions ([11 - 15]).

In this work the so determined isolines were approximated by simple parametric functions in terms of the non-normalised grading entropy coordinates.

.

Table 3. SWCC measuring – A=2/3 optimal (fractal) mixtures [7].

N		Maximal fraction j	Notation	Fractions in mixture
2		2	22	1-2
		3	23	3-3
		4	24	3-4
		5	25	4-5
		6	26	5-6
		7	27	6-7
3		3	33	1-3-3
		4	34	3-3-4
		5	35	3-4-5
		6	36	4-5-6
		7	37	5-6-7
4		4	44	1-3-3-4
		5	45	3-3-4-5
		6	46	3-4-5-6
		7	47	4-5-6-7
5		5	55	1-3-3-4-5
		6	56	3-3-4-5-6
		7	57	3-4-5-6-7
6		6	66	1-3-3-4-5-6
		7	67	3-3-4-5-6-7
7		7	77	1-3-3-4-5-6-7

Table 4. Fractions [7].

Fraction	d [mm]	S_0 [-]
1	0.03 – 0.06	12
2	0.06 – 0.125	13
3	0.125 – 0.25	14
4	0.25 – 0.50	15
5	0.50 – 1.0	16
6	1.0 – 2.0	17
7	2.0 – 4.0	18

Table 5. Fractions of Lőrincz [1]

Fraction	d [mm]	S_0 [-]
A:	0.06 – 0.125	13
B:	0.125 – 0.25	14
C:	0.25 – 0.50	15
D:	0.50 – 1.0	16
E:	1.0 – 2.0	17

 https://doi.org/10.1051/e3sconf/202338225003

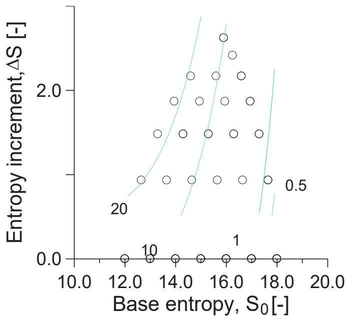


Fig. 4. Parameter *a*, fractal interpolation points, Eq. 10

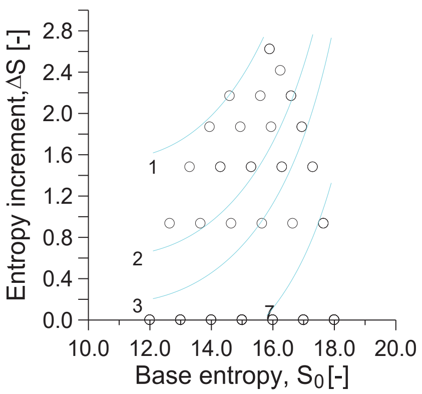


Fig. 5. Parameter *n*, fractal interpolation points. Fredlund-Xing model. Eq. 11

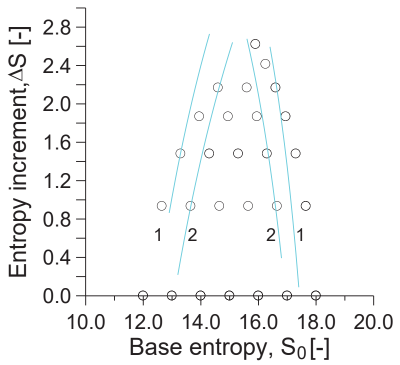


Fig. 6. Parameter *m*, fractal interpolation points and approximate isolines. Fredlund-Xing model. (Eq. 12)

Table 6. Fredlund-Xing model. Parameter values for the *m* equation.

	C_1	C_2	C_3	C_4
$S_0 > 15$	-2.04454	-2.23865	0.265252	14.13297
$S_0 < 15$	1.563788	-0.5288	-0.16316	-1.24706

4 Results

4.1 SWCC

The entropy coordinates were computed here by assuming that the fraction d = 0.03 to 0.06 mm has a base entropy of S_0 = 12. The iso-lines of the parameters *a, n, m* of the SWCC model of Fredlund-Xing were possible to be graphically interpolated on the entropy diagram, see e.g., in [7 to 10].

In this work the so determined isolines were approximated by simple parametric functions in terms of the non-normalised grading entropy coordinates (Figs 4 to 6). The *m*-equation was approximated in two parts, with the same parametric function:

$$m = C_1\, S_0 + C_1 \Delta S + C_1 \Delta S S_0 + C_4 \tag{10}$$

Different parameter values were valid in the range of $S_0 > 15$ or $S_0 < 15$, respectively, as shown in Table 6. The equations suggested for parameters *a* and *n*:

$$a = -4.995\, S_0 - 9.376\, \Delta S + 0.212\, S_0 \Delta S \Delta S + 89.033 \tag{11}$$

$$n = \exp(17.27)(100 - S_0 S_0)^{-2.76}(\Delta S + 3)^{-2.99} \tag{12}$$

4.2 Minimum dry density

The entropy coordinates of the data base of Lőrincz ([1, 11 to 15]) were computed here by assuming that fraction d = 0.06 to 0.125 mm has a base entropy of S_0 = 13.

Two sections were used. In the first case, fractal gradings of the continuous sub-simplexes of the 4-dimensional simplex were used for the measurement. The isolines shown in Fig.7 were determined directly from the following regression equation:

$$s_{\min} = 0.0195 S_0 + 0.0318 \Delta S + 0.2482 \tag{13}$$

In the second case, the 4-dimensional version of section 2 (see Fig. 3) was used, the interpolation points were selected on the optimal line and on the gap-graded edge 1-*N*. The iso-lines shown in Fig. 7(b) were computed from the following regression equation:

$$s_{\min} = 0.7126 A - 0.5668 A^2 + 0.5232 B - 0.3067 B^2 \tag{14}$$

Eq. 14 can be applied in the "lower half" of the simplex where the largest fraction is dominant (see Fig. 3 and Table 4).

4.3 Preciseness by the inverse image

To test the variability of the SWCC or the minimum dry density related to a fixed entropy diagram point, a set of grading curves were generated as the inverse image of the entropy diagram point.

Concerning the variability of the SWCC-s related to a fixed entropy diagram point, results can be seen in Fig. 8. The drying and wetting curves are similar, when the fine content is larger, the SWCC is keeping more water, the difference is about 0.2 of total saturation volumetric water content at 10 kPa.

The variability of the dry density related to two fixed entropy diagram points is presented in [13]. According to the results, the preciseness is determined by the size of the inverse image of the entropy diagram point.

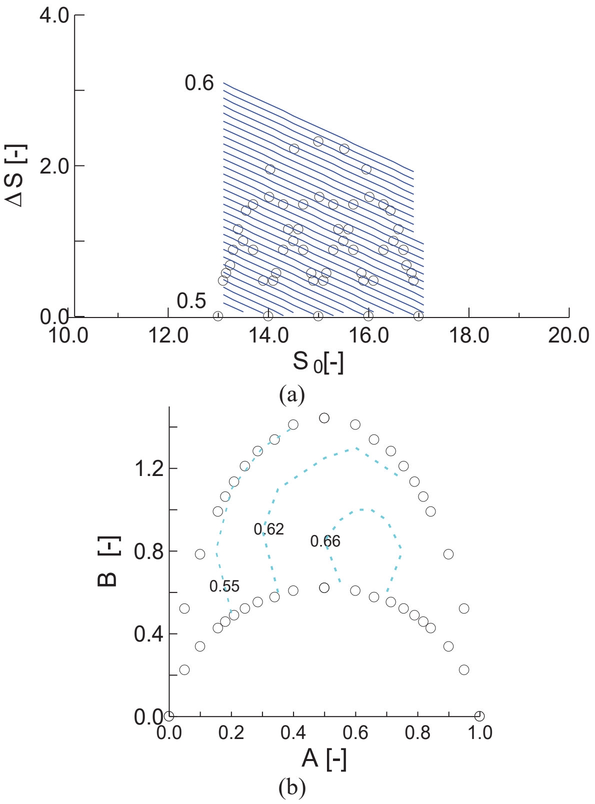


Fig. 7. N=5, s_{min} iso-lines (a) constructed from optimal (fractal, mean) mixture data (Eq. (13), (b) constructed from maximal gap-graded and maximal optimal mixture data (Eq. 14).

5 Discussion

5.1 Dry density

Comparing the linear level lines for section 1 interpolation in case of N=3 and 5 (see Fig. 3. and Fig. 7(a)), the similarity is apparent. Comparing the curved level lines for section 2 interpolation in case of N=3 and 5 (see Fig. 3. and Fig. 7(b)), the similarity is also apparent. The relationship seems to be similar for any N, to be practically independent of the value of N.

Concerning section 1 interpolation, linear relation is found for not only the tested fractal mixtures with (R^2 > 0.9) but also for two additional data bases for continuous mixtures (see [17], where it was mentioned that the linear relation supports the idea raised in Edwards statistical mechanics approach [16] that the dry density and the entropy are closely related).

The linear relation is not valid for gap-graded mixtures. However, it is known from earlier study [15] that gap-graded mixtures are slightly denser in the loosest state than the optimal ones at a given A.

5.2 Minimum number of interpolation points

If the interpolation is based on mean (fractal) gradings of the whole simplex, and on some 2-fraction mixtures, then the minimum number of data used for the interpolation is equal to ~5+5N and ~ 5+5 for section 1 and 2 interpolation, respectively ([15]).

The similarity of the level lines for section 1 or section 2 interpolation may explain that the minimum number of the interpolation points is hardly changing with N which has some significance since for a unit-sided simplex, representing the space of the grading curves, the ratio of surface/volume increases with N and, the number of sub-simplexes increases exponentially with N (see Tables 8, 2, [15]). In case of section 1 interpolation, according to the experiences, optimal points of the continuous sub-simplexes can also be used as ~c N^2 interpolation point.

Table 7. Definition of lower half of the simplex (see e.g., [9, 15]) where Eq. 14 can be applied.

A [-]	Relative frequency of largest fraction	
	Minimum [%] Optimal grading	Maximum [%] Edge 1-N
0.06	2.5	6
0.14	3	14
0.26	7.5	26
0.38	10	38
0.5	20	50
0.63	30	63
0.74	50	74
0.86	70	86
0.94	90	94

Table 8. Surface/volume ratio for the n-dimensional simplex

Dimension, *n*	**1**	**2**	**3**
Volume, V	1	0.43	0.12
Surface, K	0	3	1.73
K/V	0	6.93	14.69

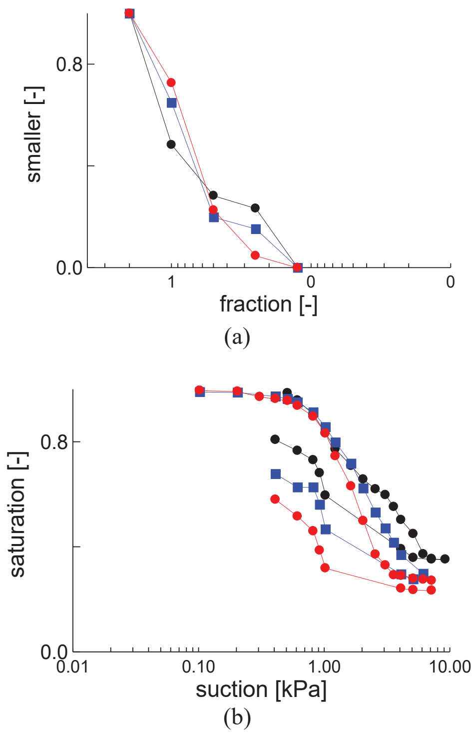


Fig. 8. Inverse image at entropy coordinates A=2/3, B=1,2, N=4. (a) Grading curves. (b) SWCC-s of the grading curves.

5.3 Type of the entropy diagram

The normalised grading entropy coordinates are not unique, zero fractions may change their value, but this is not the case for the non-normalised grading entropy coordinates, which are unique. The normalised and non-normalised diagram representations are equivalent in case of applying zero fractions up to fixed maximum and minimum diameters [4, 17, 18]. The representation is simpler and theoretically more precise in the non-normalized diagram since no zero fractions are needed.

6 Conclusions

In this paper some analytical functions were elaborated to describe the non-linear parameters of the Fredlund-Xing model [4] in terms of non-normalised grading entropy coordinates, based on the previously interpolated level lines. In further research, the preciseness will be analysed and some regression equations will be elaborated directly from measured data.

In this paper it was found that the dry density level lines are similar in dimensions 2 and 4, indicating that level lines interpolated in the triangle above and below the optimal line may qualitatively characterize the level lines of the larger dimensional simplexes determined by section 1 (continuous mixtures) and section 2 (near maximal gap-graded) interpolations.

Especially, linear level lines were found for fractal and continuous mixtures with R2>0.9. This linear relationship supported the idea that dry density and entropy are closely related, as indicated by Edwards' statistical mechanics, the link will be further investigated for fractal gradings.

A quadratic function was elaborated to describe the minimum dry density from near maximal gap-graded and fractal mixtures, the preciseness will be investigated.

The suggested interpolation method can be used for the approximation of any parameter of the complicated critical state models of sands, this and the use for silts and plastic soils will be investigated.

The work by M. Datcheva is supported by Grant No BG05M2OP001-1.001-0003, financed by the Science and Education for Smart Growth Operational Program (2014–2020) and co-financed by the European Union through the European Structural and Investment Funds.

References

1. J. Lőrincz; E. Imre; V. P. Singh. Chapter in Granular Materials. Rijeka: InTech doi: 10.5772/intechopen.69167, (2017)
2. E. Imre (2023) *The approximate interpolation in terms of the grading curve*. ESB 2021 Conference (submitted).
3. E. Imre; J. Lőrincz, Q. Trang, S. Fityus, J. Pusztai, G. Telekes, T. Schanz, KSCE Journal of Civil Engineering **134,** 257-272 (2009)
4. E. Imre, Á. Bálint, Á. L. Nagy, J. Lőrincz, J., Zs. Illés, D. Barreto, F. Casini, G. Guida, S. Feng, *Examination of saturated hydraulic conductivity using grading curve functions*, in Proc. of ISC6, Budapest, Hungary, 26-29 September 2021, https://doi.org/10.53243/ISC2020-373 (2021)
5. D.G. Fredlund, A. Xing, Can. Geot. J. **31**, 521-532 (1994)
6. E. Imre, C. Hegedűs, S. Kovacs, L. Kovacs, *Reducing numerical work in non-linear parameter identification,* arXiv:2102.08210 *(*2021)
7. E. Imre, K. Rajkai, R. Genovese, C. Jommi, J. Lőrincz, L. Aradi, G. Telekes, *Soil water-retention curve for fractions and mixtures*, in Proc. UNSAT-ASIA, Osaka, 451-45 (2003)
8. E. Imre, K. Rajkai, T. Firgi, Q. Trang, G. Telekes, *Closed-form functions for the soil water-retention curve of sand fractions and sand mixtures*, in Proc. of 4th Unsat 2006, Carefree, 2408-2419 (2006)
9. E. Imre, K. Rajkai, E. Genovese, S. Fityus, *The SWCC transfer functions of sands*, in Proc. of 4th Asia Pacific Conf on Unsaturated Soils. Newcastle, Australia, 23.-25.11.2009, 791-797 (2009)
10. E. Imre, K. Rajkai, T. Firgi, I. Laufer, R. Genovese, C. Jommi, *Modified grading curve – SWCC relations*, in Proc. E-UNSAT, Naple, 39-46 (2012)
11. E. Imre, J. Lőrincz, J P. Rózsa. *Characterization of some sand mixtures*, in Proc. 12th IACMAG Goa, India, 2064-2075 (2008)
12. E. Imre, J. Lőrincz, E. Gerendai, R. Szalkai, Y. Lins, T. Schanz, *Some notes concerning the dry density testing standards*. 18th ICSMGE. Paris, 349-352 (2013)
13. E. Imre, J. Lőrincz, M. Hazay, M. Juhász, K. Rajkai, T. Schanz, Y. Lins, V. Singh, Z. Hortobágyi, *Sand mixture density*, in. UNSAT2014, Sydney Australia, 2-4.07.2014, 691-697.
14. E. Imre, G. Kecskés, K. Rajkai, T. Schanz, Z. Hortobágyi, V.P. Singh, S. Fityus*, Sand behaviour in terms of the grading curve*, in Proc. 16th ECSMGE 2015, 3753-3758.
15. E. Imre (2015) *Soil physical characteristics to solve water flow problems*. Thesis submitted at Budapest University of Technology and Economics Habilitation Committee and Doctoral Shoool of the Faculty of Civil Engineering (in Hungarian).
16. A. Baule, F. Morone, H.J. Herrman, H.A. Makse, Rev. M. od. Phys. **90**(1):015006 (2018)
17. E. Imre, D. Barreto, M. Datcheva, V. P. Singh, W. Baille, S. Feng, S. Firgi, *Minimum dry density in terms of grading entropy coordinates*, (accepted 17ARC 2023)
18. S. Feng, P. J. Vardanega, E. Ibraim, I. Widyatmoko, C. Ojum, *Géotechnique* **69**, 646–654 (2019)