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INVITED PAPER

Material model and revealing the truth

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> *You would increase knowledge not due to the ordinary benefit or vainglory but to spread out more and more truth from which become dependent the future and happiness of mankind.*
> The doctors' oath at Warsaw University of Technology

> *And what is truth? Pilate asked.*
> John 18, 38

Abstract. The paper refers to the approach used in science, specifically in building materials engineering, assuming the possibility of material modeling, including modeling of the technical characteristics of building materials of various compositions as well as modeling phenomena/processes that occur during the use of materials and structures made from them. The authors analyze the merits of the approach of modeling in the context of compliance computational models to reality, consider the significance of the selection of the proper model (type of mathematical function, number of input data) which should be based on the knowledge of modeled material or phenomenon and later adequate verification of the model. The authors also underline importance of proper interpretation of results obtained by calculation. Misrepresentation may result in a misstated model of the studied phenomenon and lead to incorrect conclusions, which puts the researcher far from the truth, that he or she should always seek for.

Key words: material model, analytical modelling, numerical modelling, modeling, computational tools, optimization, accuracy and precision of measurement.

1. Introduction

Science should be defined as the looking for the truth paradigm, a distinct concept of seeking and revealing the truth. We try to get closer to an essential reality. To convince one that something is true, it must be scientifically confirmed. E. Schrödinger [1] once said that "the scientist only imposes two things, namely truth and sincerity, imposes them upon himself and upon other scientists". But what if the scientific proof would be true only temporarily and in that case it is just a matter of time before the new facts are discovered thus the "new" truth is elaborated? "Desire to get things right" is the leitmotiv of the great book by T.S. Kuhn entitled "The Structure of Scientific Revolution" [2] which shows how the paradigm of science – the global and local one – is shifted when anomalies occur. However, Ian Hacking in his famous Introductory Essays to the 50th Edition of this book stressed that the old theory was not replaced by the new one because it was true but rather it is more away from less adequate conception. The progress in science is not a simple line leading to the truth. Situation is not simple and obvious even when is addressed to the local scientific workshop. It is not a problem if the new laws and rules are developing an existing solution or broadening the area of its application. For instance N. Bohr often emphasized that classical mechanics was not revoked by neither relativity mechanics nor by quantum mechanics but was an approximation of those both theories: "and the continuity of our science has not been affected by all these turbulent happenings, as the older theories have always been included as limited cases in the new ones" [3]. The problem starts when the new theory is questioning or paraphrasing the existing theory [4].

How far a theory or a model describing the reality is accurate and whether the numbers that are obtained as a result are true or true enough? R.A. Wilson [5] worked on the theory stating that every individual's beliefs and experiences cause that he or she interprets the same world differently, hence "truth is in the eye of the beholder". In the less literary language but more scientific or technical we can say that even the adoption of the reference system changes the picture of reality, perhaps even distort it. Even such a simple procedure as the adoption of a different scale (Fig. 1 and Fig. 2) can effectively distort the picture of reality and requires a different interpretation of the results. However, one must be aware that the apparent distortion is not a transformation and given information remains the same and true (e.g. the common definition of square is valid only in 2-linear system – Fig. 1). It was explained already in the 70s by T. Hofmokl [6] who performed a deformation of 2-D graphics of a pig by adopting different scales in both dimensions (Fig. 2). In the extreme case (quadratic and/or exponential scales) the object of trans-

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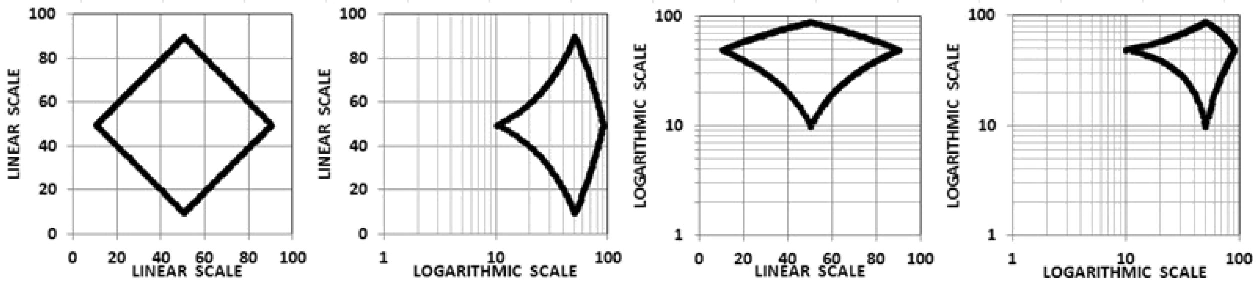

Fig. 1. Square deformation due to the damage of scale

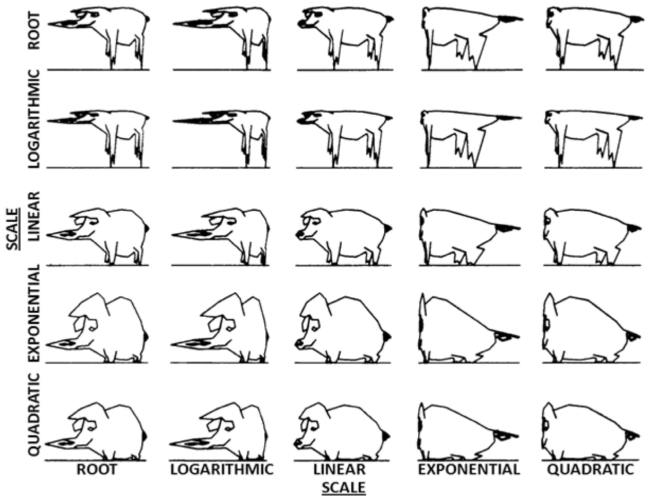

Fig. 2. Change of graphical presentation; deformations as a result of choice of scale [6]

formation resembles a bison rather than pig, though it is still the same set of data described by specific coordinates. Such image, although concerns the truth, is false. Interpretation of such deformed graphics is difficult since some details are expanded and the other are hidden and there is a risk that important information could be exaggerated, missed or incomplete. One must remember that “pictures and models finally have no other purpose than to serve as a framework for all the observations that are in principle possible” as E. Schrödinger [7] said during one of his lectures already in 1928.

When it comes to technology and engineering a lot of information need to be analyzed at the same time as many effects occurs simultaneously, the effects can overlap, which may create a synergy phenomenon [8]. Misleading or wrong interpretation of obtained information can lead to very serious consequences.

Since materials engineering is defined as a discipline that investigates the relationship between the structure and microstructure of materials and their macroscopic properties, material models are the mathematical descriptions of relations between the composition and properties. If they are well defined they can be valuable findings of this discipline. The models enable material optimization according to particular criterion or set of criteria and later – designing the material with demanded properties [9]. Modern computational and statistical tools allow finding the function of several variables which fit well to the analyzed data. The question is how the designated representation describes the actual state and how far we can trust designated solution. High values of correlation coefficient and determination coefficient indicate the level of fitting between observed values and the values expected under the model, however, the important issue is the selection of the type of model. The issue of modeling and optimization is raised in various engineering fields of research, including civil engineering [10] but also for instance in electromagnetics [11], electromechanics [12], robotics [13], etc., where the approaches to the modeling and their objects are very different, but all of the models or optimized solutions had been elaborated to become a useful tool for prediction the performance, optimization and general design [11]. However, regardless of the field of research, the selection of the model should be done not only on the basis of the knowledge of the statistical design principles but also on the knowledge of the investigated phenomenon.

2. Examples of material models

In the Civil Engineering domain, the new laws of nature are rather rarely discovered and developed. Existing equations rarely make any claims to new nature law formulations. Already existing laws are rather addressed to the given materials or composites under the given/expected conditions [14]. Table 1 contains several concepts of modeling various concretes (ordinary concrete OC, polymer-cement concretes PCC, polymer concretes PC) used for several past years as the useful tools of building material engineering. It lists both – material models (relations between material composition and properties) and models of phenomena/processes undergoing into the material (i.e. concrete carbonation, leaching). The particular models are described by different mathematical functions, including linear, nonlinear – polynomials, root, gamma. In most cases linear functions are not sufficient to accurately describe the modeled property or phenomenon – such description would be too big simplification (e.g. trial to determine the direct relation between pull-off adhesion strength of concrete and wave amplitude used in impact-echo nondestructive method failed [15]).

Table 1

Examples of material models used to describe the relations between properties of various concretes and their composition or the phenomena/processes undergoing in concrete

No	Type of material	Modeled property / phenomenon	Type of modeling function	Variables	General form of function equation	Coefficient R^2*	Potential application of the model	References
1	Ordinary concrete	compressive strength, f_c	Linear 1 variable (simplification of nonlinear function)	1. water-cement ratio, w/c *(combining 2 variables i.e. relative contents of water, w and cement, c)*	Bolomey equation: $f_{cm} = A_1\left(\frac{c}{w} - 0{,}5\right)$ or $f_{cm} = A_2\left(\frac{c}{w} + 0{,}5\right)$ f_{cm} – medium value; confidence interval stated at the 95% confidence level	0.80 ÷ 0.90 (in case of determining the real values of A_1 orA_2)	In design of concrete due to the strength class	PN-EN 206
2	Polymer concrete	compressive strength, f_c porosity, p	2-degree polynomial 1 variable	1. ultrasound wave velocity (going through the composite)	f_c $= a_0 + a_1.c_p + a_{11}.c_p^2$ p	0.90 0.90	To evaluate the properties of composite using NDT	A. Garbacz E.J. Garboczi [18] J.J. Sokołowska A. Lutomirski L. Courard [19]
3	Polymer-cement concrete and mortars	compressive strength, f_c adhesion, f_A	2-degree polynomial 2 variables	1. polymer-cement ratio, p/c 2. binder/aggregate ratio, b/a *(combination of 4 variables i.e. relative contents of: p, c, b, a)*	f_c $= a_0 + a_1.p/c + a_{11}.(p/c)^2 + a_2.b/a + a_{22}.(b/a)^2 + a_{12}.p/c{\cdot}b/a$ f_A	0.75 0.75	To predict values of properties on the basis of the composite composition	L. Czarnecki P. Łukowski [16]
4	Polymer-cement insulating coating	water penetration depth, p_w Flexibility index, I_{el}	2-degree polynomial 3 variables	1. polymer-cement ratio, p/c 2. polymer-fillers ratio, p/f 3. hydrophobic agent-cement ratio, h/c *(combination of 4 variables i.e. relative contents of: p, c,f, h)*	p_w $= a_0 + a_1.p/c + a_2.p/f + a_3.h/c + a_{11}.(p/c)^2 + a_{22}.(p/f)^2 + a_{33}.(h/c)^2 + a_{12}.p/c{\cdot}p/f + a_{13}.p/c{\cdot}h/c + a_{23}.p/f{\cdot}h/c$ I_{el}	0.85 0.85		L. Czarnecki J.J. Sokołowska [9]
5	Polymer concrete modified with fluidized fly ash	compressive strength, f_c flexural strength, f_b	2-degree polynomial 3 variables	1. aggregate-binder ratio, a/b 2. binder-microfiller ratio, b/m 3. fluidized calcium fly ash-microfiller ratio, cfa/m *(combination of 4 variables i.e. relative contents of: a, b, m, cfa)*	f_c $= a_0 + a_1.a/b + a_2.b/m + a_3.cfa/m + a_{11}{\cdot}(a/b)^2 + a_{22}.(b/m)^2 + a_{33}.(cfa/m)^2 + a_{12}.a/b{\cdot}b/m + a_{13}.a/b{\cdot}cfa/m + a_{23}.b/m{\cdot}cfa/m$ f_b	0.92 0.93	To assess the effect of modification on properties of modified composite on the basis of its composition	A. Garbacz J.J. Sokołowska [17]
6	Ordinary concrete	carbonation depth, h	root function 1 variable	1. time, t	$h = A\sqrt{t}$	0.55	To predict the concrete carbonation depth after particular time	G. Fagerlund [20]
7	Ordinary concrete	carbonation depth, h	root function 3 variables	1. water-cement ratio, w/c 2. early curing time, cp 3. time, t	$h = a(w/c) + b(cp) + (c{\cdot}t^{-0,5})$	0.94		L. Czarnecki P. Woyciechowski [21]
8	Ordinary concrete	Leaching, V	gamma 2 variables	1. point (range), x 2. time	$V(x,t) = 1 - \frac{E(\Gamma^x_{leach,max}(x,t))}{E_0}$	n.a.	To predict leaching effect in particular point / time	D. Gawin M. Koniorczyk F. Pasevant [22]
9	Ordinary concrete + repair material	Adhesion, f_h	1-degree polynomial 1 variables	1. surface tensile strength, f_{hs} 2.surface roughness index, SRI	$f_h = a_0 + a_1.f_{hs} + a_2.SRI$	0.67	To assess the bond strength between concrete and repair material	L. Courard T. Piotrowski

*) Values of determinationcoefficient calculated for the particular ranges of variables of the models – details given in the cited publication

When it comes to nonlinear functions used to formulate materials models the researchers point out that the use of a higher degree than second-degree polynomial would greatly complicate calculations, moreover, such approach would require performing greater number of tests, while the resulting model would not be much more accurate than model based on second degree polynomial [16]. Depending on the complexity of the model there are used second-degree polynomials of one, two or three variables. Higher number of variables would also greatly complicate calculations, moreover, the interpretation could be very difficult, especially, in the context of the synergistic effects that occur between the various components of the composite material. However, in many cases the number of actual material variables is higher than the number of variables included in the function equation. The variables are often expressed as the relative ratios between the contents of individual composite components. In this way, when modeling the property or phenomenon using function of two variables, the calculation is actually carried out on three or even four material variables (see Table 1, model No 3 [16]). This approach is often used in ordinary concrete technology – most often as variable is selected water-cement ratio w/c, combining relative contents of water and cement. Similar situation occurs in polymer composites technology: polymer-cement ratio, polymer-microfiller ratio or aggregate-binder ratio are often used as the variables in modeling [9, 16, 17].

One should be aware that calculating the mathematical function, when the type of function is selected unconsciously, just because of the statistical point of view it is well fit to the set of empiric data (e.g. obtained values of correlation and determination coefficients are high) is often a mistaken approach. The selection of the type of the model function should be based on the knowledge of the investigated phenomenon. Moreover, the researcher should be able to explain why the investigated processes occur according to the certain phenomenon, as an indication of general trends may be insufficient.

The following figures show the results obtained in several experiments in the field of building materials engineering. The first models (Fig. 3) concerned change of mass of epoxy mortars exposed to short- and long-term action of sodium hydroxide solution [24]. On the basis of the same empirical data two different regression functions were determined – in form of power and logarithmic functions. In both cases very high values of coefficients of correlation and determination were noted (R^2 higher than 0.95), suggesting a very good fit of the regression functions to the experimental data.

Both functions seemed to be a very good solution from the statistical point of view. However the functions describe a different course of physic-chemical phenomena. Although the both models assume that investigated phenomenon extends to infinity, i.e. the mass of the mortar will increase indefinitely, the first (power) model assumes, that the increase is faster than in a case of the second (logarithmic) model. Moreover, a logarithmic model is not limited by the horizontal asymptote, the shape of the curve suggests the mortars mass increase occurs much more slowly in time – the curve is getting flatter, and that phenomenon seems to be apparently a finite process. Taking into consideration physical mechanism of the phenomenon the second model seems to be correct as the mass of specimen does not increase indefinitely – the mass increase is the most probable result of the specimen solution absorption.

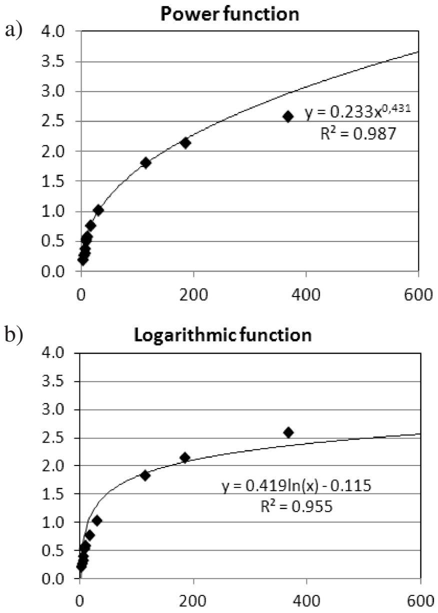

Fig. 3. Change of epoxy mortars mass (%) versus time (days) of exposure in sodium hydroxide: a) exponential function, b) logarithmic function (based on data from (after Ref. 24)

Another case concerns models of the concrete carbonation process (Fig. 4). The traditional model was remodeled and a new regression function describing the depth of concrete carbonation in time was elaborated. The new model assumes a new approach to the phenomenon of carbonation – it takes into account new variables: water-cement ratio, w/c and curing process, cp (expressed by early curing time) and the factor of time of carbonation occurring was reconsidered. As a result, a new regression function is limited by an asymptote, which corresponds with an approach that concrete carbonation is a limited process and the depth of a carbonated layer is also limited [21, 25]. The new model fits better to the laboratory data but the most important is that the new approach is describing the real situation more properly as authors have explained the investigated phenomenon [26].

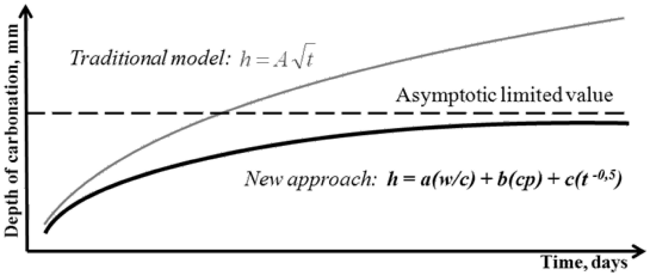

Fig. 4. Models of concrete carbonation process: traditional model and newly elaborated model (Refs. 21, 25)

The next case concerns the issue of fitting empiric data to the model. The subject of modeling is the effect of perlite powder, the by-product of expansion of perlite [27], on the polymer concrete properties. The statistical design of experiment assumed two variables (polyester bindermicrofiller ratio, S/M and perlite powder microfiller ratio, PP/M) and the modeling was performed in the 3-D space – the regression functions describe surfaces. The question is how well the regression function/surface should be fit. It is reasonable to seek for the surface that includes all the empiric points but is very developed with plenty local extremes? (Fig.5a) One of the aims of modeling is to simplify the form of the regression function and find the averaged function that still is characterized by high values of correlation and determination coefficients. This can be achieved by selecting in advance the appropriate form of the regression function. In the given case, it was decided that using second degree polynomial gives, from a technical point of view a sufficiently good representation (coefficient of correlation, $R = 0.84$) of the relation between the content of waste perlite powder in microfiller and the tested mechanical property (in the presented case – the flexural strength of the modified polymer composite – Fig. 5b).

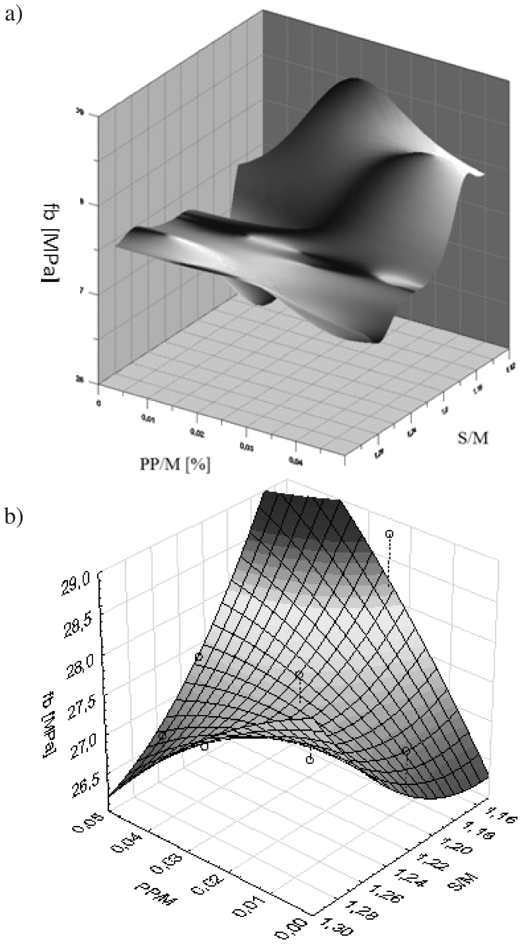

Fig. 5. Models of flexural strength in function of 2 variables (binder-microfiller ratio, B/M and perlite powder-microfiller ratio, PP/M – relative contents): a) trial of best fit of regression surface to empirical points, b) fit of second-degree polynomial (based on own research results)

3. Approach to model selection

The obligation of the researcher is to reject a solution that does not describe reality or contradicts the reality and to indicate the solution that is as close as possible to the investigated phenomenon. On the other hand there should be a balance between the accuracy and precision (Fig. 6) and the complexity of the calculations and a final form of the model.

The interpretation often requires a broader look at the issue and adoption of a different system or point of reference but it should be done in a conscious way. In technological area a complex model is often being simplified or completed by introducing elements obtained in an empirical way. Sometimes, such approach is the simplest way to make model accurate and precise. However it is necessary to be aware of difference between accuracy and precision (Fig. 6), as “it is better to be roughly right than precisely wrong” (J.M. Keynes). The terms “precision” and “accuracy” in everyday language are often interchangeable, but in the theory of experimentation they have strict and separate definitions. The “precision” characterizes internal consistency of a set of observations obtained under (hypothetically) identical conditions without defining the relation of the results to the real value of the characteristic under consideration, i.e. the less scattered are the results, the higher is the precision [28]. Meanwhile the “accuracy” characterizes the compatibility of the results with the real value of the characteristic which is being examined, i.e. the smaller are the errors the measurements towards the real value, the higher is the accuracy [28].

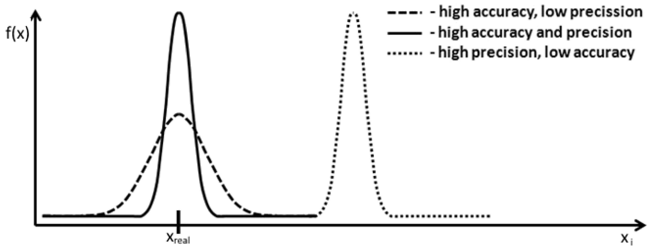

Fig. 6. Accuracy and precision of the measurement: x_i – result of measurement, x_{real} – real value, $f(x)$ – relation between the real value and random error of i-th measurement (based on [28])

The results of such a way of thinking are “rules of thumb” which are less popular in science but frequently used in engineering and presented in the technical literature. D. Fisher in his book “Rules of thumb for engineers and scientists” [29] gathered around six hundred rules which described many correlations that existed between different properties and different substances as well as between various factors in the given processes. There are several reasons why such rules appeared to be useful [29]:

- the universal use of computers and computer software has already created students who are rather out of touch with reality. We can act with imprecise concepts and/or values but we cannot act out of reality. In such case the Probably Approximately Correct Models, PACM [30] and values (number) involved with those models are of great value.

The PACM provides a quantitative framework in which designers can evaluate the expertise and the cost of achieving it,

- the rules of thumb prevent or even recreate the "engineering intuition",
- having a rough estimate of how material/construction and/or process should behave can quickly eliminate anomalous results,
- recalling a rule can help to avoid "re-inventing the wheel"; a process that is increasingly wasting space in scientific journals,
- rules of thumb can help to maintain links between science and technology and avoid just appearing crack between them which seems to extend in the current century. Contrary to that, the interpenetration of science and technology became in the current century gradually more obvious.

In the engineering activity the accuracy and precision of data frequently affect the reliability and in consequence the safety of construction [31]. It is easy to exemplify by a construction repair materials [32]. For the ideal homogenous material the variation and homogeneity coefficients should be equal: $v = 0$ and $k = 1$, accordingly. For engineering materials the evaluation criteria could be defined ($\alpha = 005$, $n = 35$) as follows:

$v \le 0.04 k \ge 0.92$ very good,

$0.04 < v \le 0.06$; $0.92 > k \ge 0.87$ good,

$0.06 < v \le 0.10$; $0.87 > k \ge 0.80$ sufficient,

$v > 0.10 k < 0.80$ insufficient.

Taking into consideration the technical responsibility involved with the repair performance the criteria mentioned above are relatively more than twice stringent than in case of the ordinary concrete. This gives an estimation of a suitable "material reliability" – the material safety factor on the given safety level and/or guarantee value. The relationship between the safety factor and the material variability factor (Fig. 7) depends on the values of accepted safety class. The safety class n is defined as follows: $-\log(1-P)$ or $P = 1 - 0.1^n$, where P is the desired (assumed) certainty of the non-failed work of the element; for $n = 1$, $P = 0.9$ and for $n = 6$, $P = 0.999999$. Acceptance of the safety class depends on the element as well as on the possibility and cost of its repair (Table 2).

We can say that the more material characteristic is closer to the true values and the more accurate is the process of understanding and description/modeling (compare [32]), the more diminished is the risk factor and the higher safety of the construction. The engineering benefit is a result of 'scholars seeking the truth'. In technical science the truth is valuated not only for its own sake.

Table 2
Contractual safety class n accepted for various cases of material reliability

Group	Subgroup		
	A	B	C
I	$n = 1$	$n = 2$	$n = 3$
II	$n = 4$	$n = 5$	$n = 6$

Explanation: I Possible failure does not cause the change of the usefulness of the element and only decreases the user comfort and aesthetics; II Possible failure causes the element not to comply with the usability state and is perilous for the user. A Repair is easy and non-expensive and can be done during routine maintenance; B Repair is possible but difficult and expensive; C Repair is complicated and after detailed analysis could be estimated as unreasonably

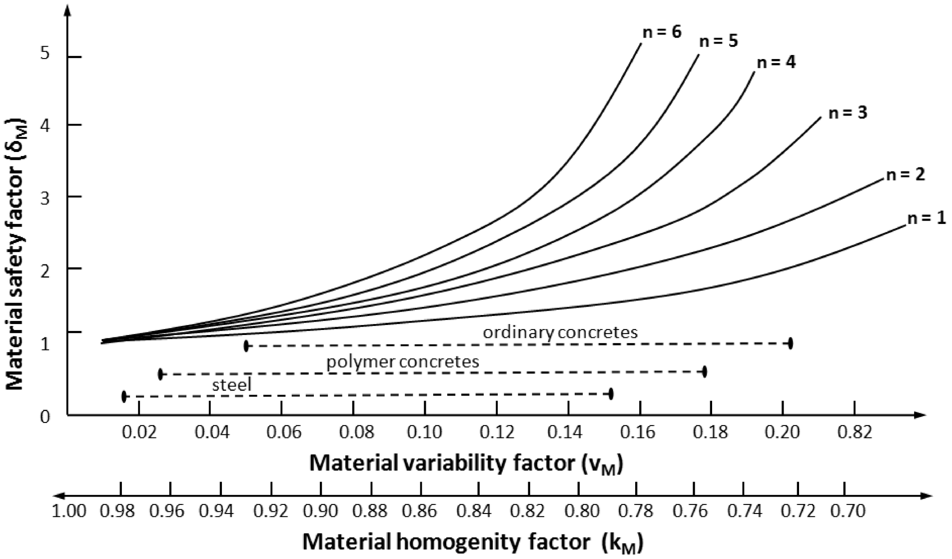

Fig. 7. Material safety factor (δ_M) vs material variability factor (v_M) and material homogeneity factor (k_M) for various safety classes (n) [32]

4. Summary

The model selection is the art of equilibrium obtaining between simplicity and accuracy. Proper selection of material model enables obtaining good and sufficient mathematical description of the investigated phenomenon, thus obtaining scientific or technical description of the truth. Wrong selection of the model (e.g. model function) can mislead the researcher by indicating different from the actual course of phenomena, and values estimated on the basis of the model may be incorrect. Underestimation or overestimation of the characteristics of the materials, including building or construction materials, can lead to serious construction disaster. That is why it is so important to lead modeling consciously, especially one must be able to assess the correctness of the results obtained through modeling.

The criteria of selection of the good model can be sum up as following:

- the number of input data (variables, constants, confounders, restrictions and limits) and output (modeled) data,
- simplicity of used mathematical description during modeling – including model designation and its statistical evaluation and verification,
- accuracy level of mapping of experimental points,
- precision level of mapping of experimental points,
- the compatibility of the designated model with the mechanism and nature of the modeled phenomenon supported by the discussion on physic-chemical determinants observed on the level of microstructure.

If above criteria are taken into account, there is a good chance that the designated target model will describe the investigated phenomenon properly and sufficiently close to an actual state, therefore will mathematically describe the foundation about this phenomenon.

Numbers, graphs and formulas are the means of communication in engineering [33, 34]. Even if in civil engineering only part of the numbers and quantitative relation express the laws of nature and there are lots of empirical or semi-empirical equations. They conveniently depicted very complicated process starting from natural resources via construction products to construction element and finally a structure itself. During this multistage process variability and uncertainty typical for raw materials gradually diminishes and become reliable and durable building structure. The authors realize that it has been more questions asked than answers formulated. Still remain subtle questions what should count as truth in material models, how much of the truth models include and what does it mean for the heart of the matter and practice of civil engineering.

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