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Mathematical Models for Tribology/Biomedical Engineering with Graphical Optimization Software-Simulations

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ABSTRACT

Surface damage and wear in materials engineering and medical implants, both external and internal, in manufactured materials, or power plants causes economic loss, unnecessary plant stops, medical-surgical difficulties, and post-operation severe functional troubles. In the case of power plants, of operational time in modifications or repair. The wear in power plants is caused mainly by solid particles and water droplets. In medical technology, erosion and corrosion of implants, together with histocompatibility of the materials, creates serious surgical and post-surgical inconvenients. Erosion and corrosion of protective coatings constitute a number of significant engineering difficulties. "Trial and error" type methodology to improve the materials design is rather expensive, inaccurate and time consuming. Inverse methods [4, Casesnoves, 2017] and mathematical optimization and modelling are the current tools for overcome these difficulties. Mathematical modelling through optimization methods can solve partially/totally these engineering complications/difficulties, and reduce the experimental/tribotesting period. In medical technology/devices biotribotesting is more complicated because the clinical trials, in-vitro, and in-vivo tests require animal or human specimens and in the last stages of these clinical trials the medical ethics implies a carefully and cautiously upper-level phase to obtain the final device/implant ready for surgery or orthopedics. In this paper we provide a brief review of the current classified erosion and/or corrosion models and, additionally, detailed modern optimization methods for precise modelling of given applications. The Integral-Differential Model/Method is presented (Casesnoves, 2017), followed by the Stratrified Model (Casesnoves, Kulu, Surzhenkov, 2018). Bioengineering models for medical devices in hip implants, in erosion, are computationally-graphically optimized with specific algorithms. Ever the precision, from optimization algorithm to laboratory data implementation, computational optimization trials for an erosion models are presented with brief software details/approximations. Graphical Optimization (Casesnoves, 2017) for models is presented in materials tribology and biotribology with sharp images.

Keywords : Erosion, Corrosion, Erosion-Corrosion, Mathematical Modelling, Nonlinear Optimization, Bioengineering, Graphical Constrained Optimization, Tribotest

I. INTRODUCTION

Although the common technical concept of wear, erosion, and corrosion is usually related to materials in mechanical engineering/physics, these physical-chemical phenomena are widely extended both in nature and artificial world. In the nature, the earth planet surface and several of its fundamental structures have been configured by erosion and corrosion, that is, interaction among natural components/phenomena with subsequent erosion and corrosion, during millions of years. In the artificial world, erosion and corrosion are not only linked to specific machinery materials engineering. They are found also, for example, related to textile-design manufacturing industry, mixed natural-artificial human implants, wear of human physical body interacting with machines or age increase in Health Sciences, special aerospace engineering design, or extensive branches of mechanical tools, footwear, jewelry, or defence industry -in other words, artificial material-material interaction(s).

Pure natural erosion and corrosion belongs to any kind of compounds of earth materials that change in structure or superficial constitution along the decades/centuries, i. e., wind particles with rocks, humid air with stones, or plants whose roots create chemical corrosion in rocks before the subsequent erosion of them commences. Between both groups, (Tables 1,2), we find a mixed type of natural-artificial erosion-corrosion phenomena, such as wear of buildings structures caused by natural compounds, automotive erosion-corrosion with natural wind impact, or changes of air chemical composition in the environment, etc. Recently [33], earth climate changes have set influence and varied the natural and artificial conditions for erosion and corrosion. The increase of temperature has impact in oxidation phenomena, and also so the air humidity. Furthermore, the changes in temperature and natural phenomena out of usual time, such a storms, rain, snow, hurricanes, tsunamis, tornados, floods, increase of sea leveland water temperature, etc, suppose a new factor to vary the natural erosion at earth surface. Therefore, it is straightforward to guess and estimate the importance of the study/research of wear, erosion, and corrosion in technology and science as industrial-material essentials and environmental-geophysical factors. For built-up mechanized purposes, given the economic loss caused by erosion and corrosion in an extensive range of engineering/technology areas, the selection of materials became a must. In medical technology, specially internal implants, corrosion has influence in durability of the implant and immunological factors constitute an important condition. External implants or orthopedic mechanical devices are linked to erosion of materials since the dynamics and biomechanics conditions are essential. As a result, a large number of technical approaches to deal this question have been put in practice, mainly since the beginning of the industrial era.

"Trial and error" methods, that is, the Forward Problem technique, was found expensive, imprecise and time consuming [1-4]. In consequence, applications of the Inverse Problem methods were used to determine, *a posteriori*, the validation/refinement of theoretical mathematical models previously approximated [1-4]. In doing so, the modelling optimization time arose, in order to carry out an initial mathematical approximation for a subsequent experimental choice of the most convenient materials [10].

TABLE I

CLASSIFICATION OF EROSION AND CORROSION FOR ORIGIN/CAUSE	
TYPE	**EXAMPLES**
Natural	Geophysical earth changes, rocks corrosion-erosion, human body wear for ageing and biomechanical movement
Artificial	Coatings damage with particles in gas/vapor or gas/vapor, wear in machinery parts, corrosion of coatings after erosion
Natural-Artificial	Degradation of concrete caused by natural impact, metal corrosion for natural air humidity,
Biomedica l	It is both natural, inmunological and artificial when the implant is interior, if exterior natural and artificial

Power-Stations or other Energy Thermal-Production Systems constitute a classic-standard source of energy obtained through combustion of materials such as shale, biomass, coal, or several others, constantly in industrial improvement during the recent centuries. This combustion creates a heat focus that can be used to evaporate water and carry out the physical steam-force to move electrical generators-engines which ultimately produce electrical-AC current/power. Material coatings erosion,corrosion,deformation and stress cracks are considered an industrial hurdle that creates loss of budget, energy, reparation-time, and operating time. Statistically, a rate higher than 90%, of mechanical-machine failures are linked to fatigue,friction,and wear. Succintly, the aggressive environments that cause degradation in general are, wear, corrosion, oxidation, temperature, gas-particle size/velocity [10], and any combination of these factors. In medical technology, and as a cautious pre-hypothesis, we consider unpredictable, in near future, the amount of body parts that can be substituted by artificial devices, natural-artificial devices, or genetically-engineered tissues. A strong factor for the support of former assertion, is the increase of the population life expectation and the enlargement of work-time-life. Hence, the practical objective to find out engineering solutions is to use new/improved optimal materials for the plants design and medical technology, in such a way according to precision of durability and functional operation of the energy power source and devices. Actually there is a number of mathematical models for erosion, corrosion, and combined erosion-corrosion. The objective of these modelling algorithms is to design accurate theoretical optimization models for initial search of optimal material characteristics, before passing on to the type of material testing/tribotesting with (approximated) those previous parameters- given as a solution of the theoretical model. In such a way, that mainly the coatings of the plant, could be improved in durability and erosion-corrosion resistance. The coatings of the medical devices require more complicated design.

In general, wear constitutes a common/frequent cause of deterioration in the generic group of energy production systems, based on gas-turbine engines, for electrical power production. A significant number of several parts of the energy plant can be eroded, corroded or eroded-corroded by micro/macro drops/particles of different types of gas –also downstream components, such as turbine valves, nozzles, drains, exhaust, vanes, or blades. The mechanical properties of abrasive particles, that is, hardness, density, or fracture toughness, form the external aggressive factors for coatings, boilers, pipes, or any other system component in contact with erodents. Engineering solutions, as said, for these problems that cause economic loss, together with a waste of functioning time and expensive reparations, are based on precision-design of both coating materials resistant to abrasion-erosion, and/or friction, and mechanical optimization of the operational structure of the plant –in fact, temperature of components, e.g. hardmetal or cermets, constitutes also an important factor. Since materials testing apparatus have became more sophisticated and at the same time more accurate, the testing-process economical cost, therefore, has increased in recent times –we refer to them as the so-called tribotest in general [1-4,10]. Tribotests could be based on almost realistic simulations for all the components of the mechanical system, some of them, or a reduced number of them –simplified-tests or single-component tests. As a result of the optimal variable-magnitude determinations with the mathematical model, it is imperative to link this objective data to perform, subsequently, experimental testing at lab. Then figure out a definite evaluation, in order to choose the optimal material usually for coatings or other structures. Medical testing [12,32], can be divided into two main strands, the biomechanical for external medical devices, and the biochemical-chemical for internal devices. In-between these groups, there are mixed medical devices that comprise external and internal parts. This contribution deals with an up-to-date bibliography of erosion, corrosion, and erosion-corrosion mathematical models, from an objective presentation point of view, with an intended minimum biased analysis. Complementary, in this article, we explained basic/functional nonlinear/linear optimization techniques to make an optimal choice of erosion and corrosion models, in order to minimize surface damage. The results and conclusions comprise a group of modern series of data, applicable in materials selection optimization, both for further research, and engineering design in the energy field.

Recently two new models/methods were developed and published [1-4],. Namely, Integral-Differential Model (Casesnoves, 2017), and the Stratified Model Model (Casesnoves, Kulu, Surzhenkov, 2018, Appendix I) are presented and further extensive data can be found at [1,2,3,4,5]. An example of applicability of a simple model for a series of simulations based on simulated experimental data was developed in Sections VI-VII. It was intended to show nonlinear optimization with least-squares L_2 Norm in to prove the explained methods mathematical possibilities [15,20].

II. T1, T2, CLASSIFICATION OF MODELS

2.1 General Classification

Erosion and corrosion concepts imply the interaction between/among physical structures that could be in any physical state, namely, solid, have been developed several classifications for erosion and corrosion mathematical models.

However, at present and for future research, we do not try to emulate the already published classifications [16]. Instead, it is liquid, gas, metastates, or varieties of them. The interaction complexity is rather high, (Table 2). In the literature [16,10], there possible to simplify the classification(s) on the basis that, given the rather large number of models, it is guessed that the extensive complexity of E/C causes the necessity to design particular models almost for every type of interaction. In other words, the lack of existence of widely-applicable general models for E/C, constitutes the main reason for such kind of mathematical models variety. A brief of conditional factors is included in Table 2.

It was intended to set a common classification frame both for erosion and corrosion, in terms of simplification and fast practical use/selection of models in each particular materials choice –proposal of authors to be improved in further research. The predominant criterion of the classification is the practical engineering selection, that is, *for what is used every model*, and its advantages and limitations.The frame of classification is just the same for erosion and corrosion. Erosion-corrosion models can be included at anyone.

TABLE II

E/C MATERIALS INTERACTION CONDITIONS	
Conditional Factor	**Variables/Parameters**
State	solid (cristallographyc variety),liquid,gas,metaestates
Physical Magnitude	particles velocity,kinetic energy,materials particle temperature
Inmunological Factors	In Medical Devices caused by histocompatibility
Phisiological Factors	In Medical Devices caused by human fluids components (Oxigen, free radicals, etc)
Biomechanical Factors	In Medical Devices external or internal caused by body dynamics
Geometry	rather difficult in most cases,particle impact angle(s),interaction angle(s), interaction surface(s)
Material Composition	chemical,molecular,nano-quantum composition

E/C MATERIALS INTERACTION CONDITIONS	
Conditional Factor	**Variables/Parameters**
Material Structure	physical-chemical and nanomaterial complexity
Material Origin	natural (unpredictable), artificial
Environment	temperature, humidity, thermical insulation, adiabatic and/or isothermical conditions
Residual Stress and Fatigue	influence in erosion and corrosion rates and surface cracks
Mutual Interaction	any possible interaction among/between all the former factors

In this line, according to the variety of physical states of the materials performing E/C at any kind of interaction, whether wear, corrosion or erosion, and their applications, it is defined,

Type 1 (T1) Mathematical E/C Models.-Those ones that can be implemented for several applications/material-interactions. Degree of usage is from 1 (lowest application range) -4 (highest application range).

Type 2 (T2) Mathematical E/C Models.-Those ones that can be implemented, and are designed/optimized for a specific or super-specific physical application. Degree of usage 1.

2.2 Mathematical Methods/Modelling Techniques for E/C

It is up to the researcher to include them in classification, or take the methods as a reference to characterize any Type 1 or Type 2 model.The criterion actually is the inclusion within the classification to clarify any model analysis precisely. In Table 4 a brief of the models presented in this paper is gathered with advantages, degree of usage, classification, and specific parameters for each one.

TABLE III

E/C MATHEMATICAL MODELS CLASSIFICATION WITH DETAILS (PROPOSAL OF AUTHORS)		
Group/Brand	**Model Type**	**Definition/Examples**
TYPE 1 (T1)	Models with several applications	Models for several E/C interactions in different conditions
TYPE 2 (T2)	Specific, and superspecific models with one application	Precise or extremely-accurate design for a unique materials physical interaction
BIOIMEDICAL TYPE 2 (T2)	The usual models in Biomedical Engineering. Human biomechanics and physiology is complicated for general modelling.	Approximately accurate design for a unique materials physical interaction conditioned by histocompatibility, inmunocompatibility and biomechanics.
Mathematical Methods	Mathematical And Optimization Techniques applicable to characterize Type 1 and Type 2, linked to any model	Heuristic (H) Empirical (E) Random (Monte Carlo) (R) Deterministic (D) Mixed (M) Finite Element (FE) Dynamic Model (DM) Others (O) Degree of Usage (1-4)

It is convenient/obliged to discuss a few concepts about the extensively used methods for E/C, usually characterized as heuristic and/or empirical. Additionally, to remark the essentials/significance of Finite Elements Method, which is a formal mathematical theory instead a simple method. Given the complexity of E/C, all models can be considered heuristic. Heuristic means, *grosso modo*, an approximate solution for a problem, non-perfect but functional in practice. The engineering heuristic method comprises a pre-evaluation, an evaluation, the discussion of the evaluation, and finally the usability discussion. E/C models are considered heuristic in our criteria. Empirical, [20], means knowledge based on whether experience, evidences, facts, experimental, or whether combinations of these factors. Formally, empirism asserts that the knowledge comes from perceptual representation systems and perceptual states.

In E/C modeling, the empirical ones are not necessarily bad/limited, and can be considered in some cases as the initial stage for a more theoretical model, e. g., the classical Finnie model. Besides, it is extensively denominated in the literature FEM as a modelling/exclusive modelling method, and we respectfully differ from this interpretation. FEM is a mathematical theory, that can be widely applied from numerical methods, differential/partial-differential equations, physical applications of differential equations, (e. g., Boltzmann diffusion equation in radiotherapy), to mechanical systems, E/C modeling, and many others. Therefore, in Classification of Table 3, FEM is used as a reference to develop/characterize/improve an equational model, but not as a model itself.

III. BRIEF OF EROSION MODELS

This section deals with a bibliographic description of E/C models, setting advantages, inconvenients, and prospective considerations. However, the citations/mentions are brief, and more extensive mathematical development is oncoming in next contributions. In the following, some classical and practical models are detailed, and afterwards a brief of several models currently in use are explained with longer details, and all of them with T1, T2 classification. A large number of references for these models can be found in [1-4].

3.1 Finnie Model (T1) This simple model, [16], was one of the first model invented for quantification of eroded material magnitude. This formulation (T1, ductile materials) is a cutting model and sets a rigid-plane surface. Finnie algorithm is the base for further developments of other models, and remains today as a formal reference. Its basic formulation reads,

$$\begin{aligned} &W = c \times \frac{M\,V^2}{\psi\, p\, K} \times \quad f(\alpha); \quad \text{with}, \\ &f(\alpha) = \sin(2\alpha) - \frac{6}{K}\sin^2(\alpha), \quad \alpha \le \arctan(\frac{K}{6}); \\ &f(\alpha) = \frac{K\cos^2(\alpha)}{6}, \quad \alpha \rangle \arctan(\frac{K}{6}); \end{aligned} \tag{1}$$

where,

K= geometrical ratio between vertical to horizontal forces,V, particle speed, p, material flow stress, W, material volume remove, c is a correction factor for impact failure/mutual-particle-impact. Ψ is the ratio of depths, contact to cut. Note the factor MV^2 that corresponds to a kinetic energy magnitude inserted implicitly within the formula.

3.2 Bitter Model (T1) This model sums erosion for plastic deformation (W_d) and cutting erosion (W_c). Its formulation derives from Finnie T1. Main equations for both removals are,

$$
\begin{aligned}
&\text{Deformation Wear Erosion},\\
&W_D = \frac{M\left[V\sin(\alpha) - V_{el}\right]^2}{2\varepsilon_b} \text{ for } V\sin(\alpha)\rangle V_{el} \text{ and}\\
&\text{null if } \langle\, V_{el};\\
&\text{and subsequent, cutting wear erosion},\\
&W_C = \frac{2M\,C'\left[V\sin(\alpha) - V_{el}\right]^2}{2\varepsilon_b} \times\\
&2MC'\left[V\cos(\alpha) - \frac{C'\times\left[V\sin(\alpha) - V_{el}\right]^2}{\sqrt{V\sin(\alpha)}}\,\phi_C\right]\\
&\text{if } \alpha \le \alpha_0 \quad \text{or}\\
&M\left[V\cos(\alpha) - \frac{M\left[V^2\cos^2(\alpha) - K_1\left[V\sin(\alpha) - V_{el}\right]^{3/2}\right]}{2\phi_C}\right] \qquad (2)\\
&\text{for } \alpha\rangle\alpha_0 \quad ;
\end{aligned}
$$

This Bitter Model has many parameters, detailed in literature extensively, and the most important ones that are in (1), namely,

Alpha is the attack angle, ε_b is the deformation wear factor (obtained experimentally), and V_{el} is the threshold velocity (velocity at collision at which the elastic limit of the workpiece material is just reached). V_{el} can be calculated from the Hertzian contact theory. V_{el} depends on several factors, and some approximations were carried out. Parameter Φc is a material dependant wear factor obtained experimentally and C', K1 are constants.

3.3 Bitter Model Simplified (Neilson and Gilchrist's Model, T1) Neilson and Gilchrist's, simplified the Bitter model combined to express a ductile erosion model and using this Bitter model for brittle erosion, as follows,

$$
\begin{aligned}
&W = \frac{MV^2\cos^2(\alpha)^2}{2\phi_C} + \frac{M\left[V\sin(\alpha) - V_{el}\right]^2}{2\varepsilon_b};\\
&\alpha \ge \alpha_0 \quad ;\text{and}, \qquad (3)\\
&W = \frac{MV^2\cos^2(\alpha)^2\sin(n\alpha)}{2\phi_C} +\\
&+\frac{M\left[V\sin(\alpha) - V_{el}\right]^2}{2\varepsilon_b};\ \alpha \le \alpha_0\,;
\end{aligned}
$$

The details of parameters are rather extensive and correspond to the previous equations. However, this simplification does not save the experimental work required to determine the erosion constants.

3.4 Hutchings Model (T1) This model and its derivations were a primary ones. It was designed for erosive wear by plastic deformation, without deformation factors. The angle of impact is 90 degrees, that is, normal incidence. The result is a summatory of impacts, with an erosion rate, E, as follows,

$$
E = \frac{K\rho U^2}{2H} \quad ; \qquad (4)
$$

where ρ is the density of the material being eroded, U is the initial particle velocity and H is the target surface hardness. K represents the fraction of material removed from the indentation as wear debris and is also known as the wear coefficient. The value of K can be thought of as a measure of the efficiency of the material removal process. Derivations of this model inserting the impact angle have been developed and constitute an specific variety [1-4]. This model was used to make an optimization example with software-subroutine in Section VI.

3.5 Hashish modified model for erosion (T2) This model is based on Finnie one and includes the velocity term and the conditions of the particle shape. Basic formulation is as follows,

$$
\begin{aligned}
&W = \frac{7}{\pi}\times\frac{M}{\rho_p}\times\left(\frac{V}{C_K}\right)^{5/2}\sin(2\alpha)\times\left(\sin(\alpha)\right)^{1/2} \ ; \qquad (5)\\
&\text{and},\\
&C_K = \sqrt{\frac{3\,\sigma_f\,R_f^{3/5}}{\rho_p}} \ ;
\end{aligned}
$$

where R_f is the particle roundness factor. This model does not require any experimental constants. It is uniquely based on the ductile properties of the eroded material, and therefore useful/focused for shallow impact angles for ductile materials, T2.

3.6 Computational Fluid Dynamics Models (T1) This method is used for solid particle erosion inside pipe geometries, rather T2 but since it could be applied on several kinds of materials, T1. Its weakness is that this technique is complicated and time consuming and as such is most appropriate for complex, non-standard geometries.

Additional difficulties are the determination of percentage of particle on a fixed surface, their impacting angle, and specific/individual velocity. An example of formulation for this type of modelling is,

$$E = A\,F_S\,V_0^n\,f(\theta)\ ; \tag{6}$$

where, E is the erosion rate, V_0 is the particle impingement velocity, A is a material dependent coefficient, F_s is a particle shape coefficient, n is an empirical constant, 1.73, and f(θ) is a particle impact angle dependent function.

3.7 Micro Scale Dynamic Model (MEDM,T1) This model, is designed to be implemented with FE method and is useful for erosion-corrosion. It is based on fundamental physical forces equations, such as,

$$\vec{F} = m \times \frac{d^2\vec{r}}{dt^2}\ ; \tag{7}$$

The MEDM approach is applied to modelling an abrasion process compared to plastic-elastic mechanical elements, such as wheels or similar mechanical components. This tribotesting method is widely used to rank wear-resistant materials under low stress condition. Abrasive particles pass through the opened-gap between the mechanical sample and the specimen. As a result the specimen surface is eroded/abraded. The mass loss of a tested material is dependent on the mechanical properties of the tested material and the abrasive particles as well as the wear conditions. All this is carried out with 2D modeling and the resulting equations have a physical mechanical frame and do not present important complications.

3.8 A series of models with corresponding approximations Nepomnyashchy, asserted that erosive wear of metals is caused by low-cycle fatigue or microcutting, and depends on the impact angle. Abramov applied Hooke's law for metal erosive deformation, and supposed breakings are linked to maximum shear stress magnitude.

Beckmann and Gotzmann derived an analytical expression for the erosion of metals from the hypothesis that, in abrasive and erosive wear, the volume removed is proportional to the work of shear forces in the surface layer. The basic model was formulated from the study of deformation caused by a single spherical particle.

Peter [16] in his model used Beckmann and Gotzmann`s erosion theory after the replacement of the equations for computing the indentation depth of the particle and the specific shear energy density.

3.9 Finite Element (FEM) and Monte-Carlo/Quasi Monte-Carlo Models Broadly, FEM is a mathematical method, and not an specific model. Therefore, what is included here is the FEM that has been applied on specific model equations to obtain practical results for erosion determination.The same consideration holds for Monte-Carlo, that is, Monte Carlo is a mathematical method that was used for erosion modeling, e.g.,thermal barrier coatings or physical vapor deposition. Monte Carlo simulation techniques uses continuous software random loops to reach an optimal value for particle size, properties, the material surface condition and the local dynamic impact condition.

Miller model (**T2, 1957**). This model is for ductile-cutting and its equations are formulated for abrasive particles with cubic shape. However, it can be considered simple in structure as follows:

$$E_M = K \times \frac{A\, d_m\, f\, F\, P_{atm}}{b_w\, G_w\, q_w\, R\, V_{wg}\, \rho_a} \times \frac{C}{C+1} \tag{8}$$

depth of cut per unit time is,

$$DE_M = K \times \frac{A\, d_m\, f\, p\, P_{atm}}{b_w\, G_w\, q_w\, R\, V_{wg}\, \rho_a} \times \frac{C}{C+1} \ ,$$

where E_M is material removal rate (mm³/s), DE_M - depth of cut per time unit (mm/s), K - constant of proportionality, A - cross-sectional area (mm²) , b_w - Burger vector work surface (mm), d_m - mean diameter of abrasive (mm), P_{atm} - atmospheric pressure (MPa), F - mean static force over a period (N), f - cyclic frequency of vibrations (cycles/s), G_w - shear modulus (MPa), q_w - work hardening capacity (MPa), R - surface roughness (µm), V_{wg} - volume of tool-work gap (mm³), C - volumetric concentration of abrasives (adimensional). The first equation is to determine the erosion rate, the second is to calculate the depth of cut per unit time caused by erosion. This model is applicable for ductile materials, and has similar applications than Finnie model. In general, the units can be adapted on specific laboratory requirements [1-4, 10].

Lee and Chan model for brittle fracture (**T1-T2, 1997**). This nonlinear model is very specific for a hemispherical indentation fracture. Abrasives are assumed as spherical particles and rigid. The formulation is:

$$E_L = \frac{2\pi K_1^2 f}{3N} \times (aF + bA)^2 ; \tag{9}$$

where,

$$a = \frac{T}{\Delta t} ; b = \frac{A_t\, E_t}{L_t} \quad 1 + \frac{T}{\pi\, \Delta t} \cos(wt_a - \varphi) \ ;$$

$$and,\ A(t) = A \sin(wt - \varphi),$$

where E_L is material removal rate (mm³/s), and φ - the phase of the amplitude equation (radians), A and $A(t)$ - wave amplitudes (mm), K_1 - constant of proportionality, F - mean static force over a period (N), f - cyclic frequency of vibrations (cycles/s) , N - number of active abrasive grains in the working gap, a quotient between T and Δt adimensional, b Burger vector (mm), T - time period of vibrations (s), A_t - cross sectional area of cutting tool (mm²), E_t - Young modulus of tool (MPa), L_t - contact length of tool (mm), w - angular frequency (cycles/s), t_a - time corresponding to abrasive contact (s). This model specific fro brittle can be considered less general than Parbhakar model.

Finnie model (T1, 1958, 1960). This model was one of the first models invented [16] for quantification of eroded material magnitude. It is a cutting considering model, which sets a rigid-plane surface. Today Finnie algorithm is used as a formal reference for improved models. The formulation reads:

$$E_F = c \times \frac{M V^2}{\psi\, p\, K} \times \ f(\alpha) ; \quad with, \tag{10}$$

$$f(\alpha) = \sin(2\alpha) - \frac{6}{K}\sin^2(\alpha), \quad \alpha \le ar\tan(\frac{K}{6}) ;$$

$$f(\alpha) = \frac{K\cos^2(\alpha)}{6}, \quad \alpha \ \ge \ ar\tan(\frac{K}{6}),$$

where E_F is the material removal (mm³ /mass of abrasives in kg) , K - the geometrical ratio between vertical to horizontal forces adimensional, V - the particle speed (mm/s), p - material flow stress , M mass of abrasives (kg), c - a correction factor for impact failure/mutual-particle-impact, Ψ - the ratio of depths, contact to cut, adimensional, α is the attack angle (radians or degrees). Note the factor MV^2 that corresponds to a kinetic energy magnitude inserted implicitly within the formula. This model is classical, and erosion is characterized by high flow stress compared to others for both ductile materials and brittle materials.

Bitter model (T1, 1963). This model sums erosion for plastic deformation (E_{Bd}) and cutting erosion (E_{Bc}). Principal equations are as follows:

$$\begin{aligned}
&\text{Deformation wear erosion,}\\
&E_{Bd} = \frac{M\left[V\sin(\alpha) - V_{el}\right]^2}{2\varepsilon_b} \text{ for } V\sin(\alpha) \geq V_{el} \text{ and}\\
&\text{null if} \leq V_{el};\\
&\text{and subsequent, cutting wear erosion,}\\
&E_{Bc} = \frac{2MC'\left[V\sin(\alpha) - V_{el}\right]^2}{2\varepsilon_b} \times\\
&2MC' \; V\cos(\alpha) \; \frac{C' \times \left[V\sin(\alpha) - V_{el}\right]^2}{\sqrt{V\sin(\alpha)}} \varphi_C\\
&\text{if } \alpha \leq \alpha_0 \text{ or}\\
&M \; V\cos(\alpha) \; \frac{M\left[V^2 \cos^2(\alpha) - K_1\left[V\sin(\alpha) - V_{el}\right]^{3/2}\right]}{2\varphi_C}\\
&\text{for } \alpha \geq \alpha_0 \; ,
\end{aligned} \tag{11}$$

where α is the impact angle (degrees or radians), ε_b - the deformation wear factor obtained experimentally (J/mm³), and V_{el} - the threshold velocity (velocity at collision at which the elastic limit of the workpiece material is just reached), (m/s). V_{el} can be calculated from the Hertzian contact theory. V_{el} depends on several factors, and some approximations were carried out. Parameter ϕ_c is a material dependent wear factor obtained experimentally (J/mm³) and C' and K_1 are constants of a specific material. This model has similar advantages compared to (10).

Parbhakar model (T2, 1993). This model was designed for brittle fracture with spherical particles and Hertz fracture theory was applied. The equation of this model is:

$$\begin{aligned}
&E_P = N f V_a C_s \; ;\\
&\text{where}, V_a = \frac{1}{3}\pi c^2 \delta \; ,
\end{aligned} \tag{12}$$

E_P - is volume removal rate , (mm³/s) V_a - volumetric removal rate (mm³/s), N - number of active abrasive grains in the working gap, f - cyclic frequency of vibrations (cycles/s), C_s -ratio of effective contact length to the mean diameter of abrasives, adimensional, V_a - conical volume removed by a single particle (mm³/s) , c - radial extension of crack (mm), δ - depth at which crack originates (mm). This model is simple and specific for brittle compared to similar ones is more simple to apply and for indentation fracture.

Bitter simplified model (Neilson and Gilchrist's Model, T1, 1968). Neilson and Gilchrist simplified the Bitter model [1], combined to express a ductile erosion model and using this Bitter model for brittle erosion as follows:

$$\begin{aligned}
&E_N = \frac{MV^2\cos^2(\alpha)^2}{2\varphi_C} + \frac{M\left[V\sin(\alpha) - V_{el}\right]^2}{2\varepsilon_b};\\
&\alpha \geq \alpha_0 \; ; \text{and},\\
&E_N = \frac{MV^2\cos^2(\alpha)^2\sin(n\alpha)}{2\varphi_C} +\\
&+\frac{M\left[V\sin(\alpha) - V_{el}\right]^2}{2\varepsilon_b}; \alpha \leq \alpha_0 \; ,
\end{aligned} \tag{13}$$

where α - is the impact angle (degrees or radians), ε_b - the deformation wear factor obtained experimentally (J/mm³), V_{el} - the threshold velocity (velocity at collision at which the elastic limit of the workpiece material is just reached), (m/s). V_{el} can be calculated from the Hertzian contact theory. V_{el} depends on several factors, and some approximations were carried out. Parameter ϕ_c - is a material dependent wear factor obtained experimentally (J/mm³) and C' - and K_1 - are constants of a specific material. Experimental work is required to determine the erosion constants ε_b and ϕ_c. This model is a simplified evolution of (11), and applicable in brittle and ductile erosion. Compared to others, it results in formulation very similar and efficacious.

Hutchings models (T1, 1981) [1, 2, 16]. There are several types of this model and this is a primary one. In Paper III, the classical equation was calculated for discrete models. It was designed for erosive wear by plastic deformation, without deformation factors. The specific formula for normal impact is:

$$E_H = \frac{K\rho v^2}{2H} \; , \tag{14}$$

where E_H is erosion rate (mm³/kg s in this study), ρ - the density of the material being eroded (kg/mm³), v - the initial particle velocity (mm/s) and H - the target surface hardness (MPa to mm and kg). K represents the fraction of material removed from the indentation as wear debris and is also known as the wear coefficient. The value of K can be thought of as a measure of the efficiency of the material removal process. Derivations of this model inserting the impact angle have been developed and constitute a specific variety. This model was used to make an optimization example with software-subroutine in Section 3.3. It cannot be considered a good model compared to (10) and (11), because it is a generalization.

Sheldon model (T2, 1996). This model is for brittle materials, particles are set as rigid, spherical and angular. Constraints of the impact angle are always normal.

$$E_S = K_4 \left(\frac{r_m^6}{r'}\right)^{\frac{0.6n}{n-2}} \times (v_a)^{\frac{2.4n}{n-2}} \;, \tag{18}$$

where K_4 forms a series of consecutive equations with products and exponentials,

where E_S is volume of material removed by particle, v_a - article impact velocity, r parameters - geometrical distances, K_4 - proportionality constant, n - flaw parameters.

Hashish modified model for erosion (T2, 1987). This model [1] is based on the Finnie model and includes the velocity term and the conditions of the particle shape. Basic formulation is as follows:

$$E_{HM} = \frac{7}{\pi} \times \frac{M}{\rho_a} \times \left(\frac{V}{C_K}\right)^{5/2} \left(\sin(2\alpha) \times (\sin(\alpha))^{1/2}\right) ; \tag{16}$$

and,

$$C_K = \sqrt{\frac{3\sigma_f R_f^{3/5}}{\rho_a}} \;,$$

where R_f is the particle roundness factor (mm), alpha - the impact angle (radians or degrees), C_k - the characteristic velocity factor defined by the second equation (mm/s), M - particle mass (kg), ρ_a - particle density (kg/mm³), σ_f - flow strength of the work piece (MPa). This model requires no experimental constants. It is uniquely based on the ductile properties of the eroded material, and therefore useful/focused for shallow impact angles for ductile materials, T2. It is an improved Finnie model specific for deformation wear.

Computational fluid dynamics models (T1, 2000, 2009). This method [2,16] is used for solid particle erosion inside pipe geometries, rather for T2 but since it could be applied on several kinds of materials, for T1 as well. Its weakness is that this technique is complicated and time consuming and as such is most appropriate for complex, non-standard geometries.

Additional difficulties are the determination of particle percentage on a fixed surface, their impacting angle, and specific/individual velocity. An example of formulation for this type of modelling is:

$$E_{CD} = A F_S V_0^n f(\vartheta) \;, \tag{17}$$

where, E_{CD} is the erosion rate (mm³/kg s), V_0 - the particle impingement velocity (mm/s), A - a material adimensional dependent coefficient, F_s - a particle shape coefficient (mm), n - an empirical constant, and $f(\theta)$ - a function dependent on the impact angle. Computational fluid dynamics models are used, for example, for pipe erosion.

Neema model (T2, 1993). This model is suitable exclusively for brittle materials at normal impact angle.

$$E_N\,(Kg/s) = 0.1156 \times \frac{\rho_a M_a v_n^2}{10^3 \sigma_{fw}} \;; \tag{18}$$

brittle and normal impact constraints, where E_N is the volume of material rate (kg/s), v_n - normal component of particle speed (mm/s), M_a - mass of abrasive particle (kg), σ_{fw} - flow stress of target of workpiece material (MPa or N/mm^2), ρ_a - density of abrasive particles (kg/mm^3). Neema model is very specific compared to similar others.

Microscale dynamic model (MSDM, T1). This model [2] is designed to be implemented with the FE method and is useful for erosion-corrosion. It is based on the equations of fundamental physical forces, such as:

$$\vec{F} = m \times \frac{d^2 \vec{r}}{dt^2} \ , \tag{19}$$

where m is mass defined in Newton's law (any convenient unit of mass), r - position of particle (any convenient unit of longitude) , t – time (any convenient unit of time), F – force (any convenient unit of force related o equation). The MSDM approach is applied to modelling of an abrasion process compared to plastic-elastic mechanical elements, such as wheels or similar mechanical components. This tribotesting method is widely used to rank wear-resistant materials under low stress condition. Abrasive particles pass through the opened-gap between the mechanical sample and the specimen. As a result, the specimen surface is eroded/abraded. The mass loss of a tested material is dependent on the mechanical properties of the tested material and the abrasive particles as well as the wear conditions. All this is carried out with 2D modelling and the resulting equations have a physical mechanical frame and present no important complications.

Beckmann and Gotzmann (T1-T2, 1985), [19]. These are discrete models in Equations of text [10, Appendix I], and their formulation is rather long. They were derived as an analytical expression for the erosion of metals from the hypothesis that in abrasive and erosive wear, the volume removed is proportional to the work of shear forces in the surface layer. The basic model was formulated from the study of deformation caused by a single spherical particle. A discrete extended model of this type was implemented completely in [6].

Finite Element (FEM) and Monte Carlo/Quasi Monte Carlo models. Broadly, FEM is a mathematical method [1, 2] and not a specific model. Therefore, what is included here is the FEM that has been applied on specific model equations to obtain practical results for erosion determination. The same consideration holds for Monte Carlo, i.e., Monte Carlo is a mathematical method that was used for erosion modelling, e.g., thermal barrier coatings or physical vapor deposition.

Monte Carlo simulation techniques [20,22] use continuous software random loops to reach an optimal value for particle size, properties, the material surface condition and the local dynamic impact condition. Monte Carlo methods were applied in the dynamics of deformable solids and radiotherapy delivery dosimetry optimization [22]. Monte Carlo methods are also applied in turbulence analysis for aerospace dynamics [22].

In this section, corrosion models are explained with their main formulation. One difference between erosion modelling compared to corrosion is the relative complexity of the chemical process of corrosion equations. In the following, a series of corrosion models are presented. In corrosion, depending on the imperative condition of every chemical compound of the materials, T2 models are found very frequently in the literature. We recommend [20,22] to develop these concepts with formulation. Usually, the most frequent opinion is that erosion can accelerate corrosion, and less common that corrosion can accelerate erosion; oxidative-corrosion is an important engineering question in seawater technology and marine engineering. Corrosion in power plants [6] is caused principally by oxidation whose general chemical equation reads:

$$\begin{aligned}&aM+\frac{b}{2}O_2\leftrightarrow M_aO_b\ ;\\&feasible\ corrosion, if,\\&\Delta G\le 0\ ,\\&G: Gibbs\ Free\ Energy\ ,\end{aligned}\qquad(20)$$

where a, b are chemical reaction proportionality constants, O_2 - oxygen molecule, M - the metal oxidized, G - Gibbs energy. Apart from that, recently, corrosion combined with wear/erosion, i.e., wear plus abrasion, has become a promising and applicable new investigation line – so called tribocorrosion. Tribocorrosion joins in applicable algorithms, both chemical and physical concepts and equations, and constitutes a simplification to share two simultaneous phenomena in one modelling-formulation. In the following, a series of erosion-corrosion models are presented whose references are detailed in classical FEM literature.

Chemo-hygro-thermo-mechanical model for concrete (T2, 1990). This model is developed in FEM and is used for reinforcement of concrete at any kind of special construction. It comprises chemical and mechanical characteristics. It can be considered a specific model of T2, and with features of corrosion-erosion duality.

Pipe corrosion models based on neural-network theory (T2, 1996). This model [16] works in pipes, based on neural-networks mathematical methods. It is applicable in power plants since pipes constitute an important structure in energy systems and corrosion in oil-gas pipelines. The internal corrosion of a pipeline is a multivariable nonlinear system, and Genetic Algorithms (GA), in combination with artificial neural network, are used in its optimization. The computational development of this model follows usual steps of the GA programming; it can be considered a specific T2 model.

Stress corrosion model (T1, 1981). Stress corrosion, in combination with environmental agents, causes cracks in a number of mechanical structures. The environment component diffuses within the cracks and causes a positive feedback for the cracking-mechanical process.

The modelling is rather complex, and some approaches were used. The role of the geometry of the cracks added to fracture mechanics principles constitutes additional factors to increase the difficulties. Some equations for this kind of stress are published in the literature, as follows, for a hyperbolic notch:

$$\begin{aligned}&\sigma_X=\frac{K}{(2\pi r)^{1/2}}\times\\&\times[\ \cos(\ \frac{\vartheta}{2}\ )\times(\ (1-\sin(\ \frac{\vartheta}{2}\ )\sin(\ \frac{3\vartheta}{2}))\ -\ \frac{\rho}{2r}\times\cos(\ \frac{3\vartheta}{2}\ )\ ]\ ;\\&\sigma_Y=\frac{K}{(2\pi r)^{1/2}}\times\\&\times[\ \cos(\ \frac{\vartheta}{2}\ )\times\ (1-\sin(\ \frac{\vartheta}{2}\ )\sin\ (\frac{3\vartheta}{2}))-\ \frac{\rho}{2r}\times\cos(\ \frac{3\vartheta}{2}\ )]\ ,\end{aligned}\qquad(21)$$

where θ is the polar angle of r, K - a geometrical constant, and ρ - the curvature parameter. The study and modelling of the interrelation among cracks (mechanical) and corrosion (chemical) is a complex mathematical-geometrical challenge.

Three-dimensional geometric models of corroded steel bars (T2, 1996). This geometrical model, [5], T2, is based on the experimental fact that a corrosion pit can be given with a hyperbola. The effects/physical consequences of geometric parameters for a hyperbola on the mechanical properties of corroded steel bars are applied. Therefore, there is a link with any kind of energy plant applications. It is a rather empirical model based on simple hyperbolic geometry of pits and steel bars. Stress and strain parameters are fundamental in the implementation of this model.

Wagner model and derived equations for oxidative corrosion (T2, 1996). This equation is basic for the mathematical analysis of the kinetic process of oxidation-corrosion rates. Oxidative corrosion rate usually has two stages: the initial stage (formation of superficial layer) and the main stage (the growth of the thickness of oxidative layer and formation of the multilayer of oxide), with an intermediate stage between both. The Wagner primary equation is used to derive practical formulas for high-temperature corrosion and low-temperature corrosion, and a series of intermediate approximations. Wagner's differential equation reads

$$J = CB\ \frac{d}{dx} + ze\frac{dE}{dx}\ , \tag{22}$$

were J is the rate of number of particles through oxide layer, C - particle concentration, B - the particle velocity for unit of force applied, φ - the chemical potential (we refer to Nerst fundamental equation), z - the valence of the particle, e - the electron charge, and x - the thickness of the oxide layer. From this Wagner equation, a series of models for different oxidative stages have been developed in the literature, mainly in an exponential differential equation frame or integral equation. This model is a milestone for power plant functionality Survival Time Function $R(t)$ in the reliability determination of the plant.

In classic contributions, Ots in refs of [10] developed corrosion models both in metal in general at low, high, discrete or continuous temperature, and in metal pipes with the same variations, but under the effect of oil shale combustion.

The series of equations/approximations is rather large; nevertheless, it is possible to refer to some fundamental formulas that could be modified according to specific metal material or geometry of basic plant components. For general metal corrosion at high temperature, the following equation holds:

$$\text{Amount of oxidized metal, } W, \qquad W = K_{02}\, e^{\frac{Ez}{RT}} \times t^{n}\ , \tag{23}$$

where t is time (s), T - absolute temperature (Celsius degrees), K_{02} - derived from a temperature-dependent coefficient, R - chemical constant of gas, n - a corrosion rate factor. Variations of these formulas are detailed in [5] for, i.e., specific for diffusion-controlled region of the oxide layer, particular for the kinetic region of the layer, etc.

Models of corrosive-erosive wear of heat-transfer tubes (T1, 1996). In the literature [5], a series of equations/approximations for Erosion-Corrosion Models preferably/more-specific for oil shale combustion have been developed. In order to refer/show a basic equation with differential-frame of a function of several variables, which is W, the specific mass of corroded material, in the function of, namely, P, force acting on the layer, K, corrosive activity of the deposit (e.g., a boiler), and t, the time.

That formulation reads:

$$W(P,K,t)\ \text{differential}, \qquad dW(P,K,t) = \left[\frac{\partial W(P,K,t)}{\partial t}\right]_{P,K} + \left[\frac{\partial W(P,K,t)}{\partial P}\right]_{t,K} + \left[\frac{\partial W(P,K,t)}{\partial K}\right]_{P,t}, \tag{24}$$

where W is mass of corroded metal (kg), P – pressure (MPa), K - gas constant, t - temperature. A similar mathematical observation is applicable, this and these formulas in general, could be modified according to a specific metal material or geometry of basic plant components.

Todinov synergic model of erosion and corrosion (T2). This is a model for erosion and corrosion for powdered material coatings developed by Todinov [5]. The synergism between erosion and corrosion reads:

$$E_T = E + C + S\ , \tag{25}$$

where E_T is the total mass loss rate from [72], i.e., the erosion–corrosion rate, E - the pure erosion rate, C - the pure corrosion rate, and S - the loss due to the synergistic effect between erosion and corrosion – the object of interest of this equation. This synergistic term may be separated into two terms:

$$S = S_{EC} + S_{CE} \,, \qquad (26)$$

where S_{EC} represents the erosion-induced corrosion rate (i.e., increase in corrosion rate due to erosion) and S_{CE} represents corrosion-induced erosion rate (increase in erosion rate due to corrosion). This is the synergism modelling base, and further developments and approximations can be found in the literature. By way of explanation, it sharply differs from a corrosion process over a previously eroded powdered material surface, S_{EC} from an erosion with loss of material in a previous corroded area S_{CE}.

IV. INTEGRAL-DIFFERENTIAL MODEL AND STRATIFIED MODEL

In this section the Integral-Differential Model (Casesnoves, 2017), and the Stratified Model Model (Casesnoves, Kulu, Surzhenkov, 2018, Appendix I) are presented and further extensive data can be found at [1,2,3,4,5].

1.-Integral-Differential Model/Method (T1).- This model can be considered both a model and a mathematical method, and is based on the conversion of the classical models of erosion with fixed parameters to functions. Its advantage is that this method can provide with instant erosion, instant erosion rate, and cumulative erosion. Calculations-software is rather more complicated than discrete models, but precision, by theory, is more promising for future accuracy/prediction. The mathematical framework is not complicated but the demonstrations and formulas are long. It is referred to [1,2,3,4].

2.- Stratified Model (T1).- (Casesnoves, Kulu, Surzhenkov, 2018, Appendix I) .This model is a discrete one, and is based on several stages with application of Hutchings, Beckmann and Gotzmann formulas. It requires experimental data to calculate the final erosion and software programming to perform the long but simple numerical task [5]. The model is on improvements stage at this time.

V. BRIEF OF CORROSION MODELS

In this section corrosion models are explained with their main formulation. One difference between erosion modeling compared to corrosion is the rather complexity of the chemical process of corrosion equations. In the following a series of corrosion models are presented. In corrosion, depending of the imperative condition of every chemical compounds of the materials, T2 models are found very frequently in the literature [5]. Usually the most frequent physical phenomena is that erosion causes corrosion, and less common that corrosion causes erosion –oxidative-corrosion is an important engineering question in seawater technology and marine engineering [5]. Corrosion in power plants is caused principally by oxidation, [5], whose general chemical equation reads,

$$\begin{aligned} & aM + \frac{b}{2} O_2 \leftrightarrow M_a O_b \;\; ; \\ & \text{feasible corrosion, if,} \\ & \Delta G \langle \, 0 \;\; , \\ & G : \text{Gibbs Free Energy} \;\; ; \end{aligned} \qquad (27)$$

Apart from that, recently, [5,10], corrosion combined with wear/erosion, i. e., wear plus abrasion, has become a promising and applicable new investigation line –so called tribocorrosion. Tribocorrosion joints in applicable algorithms both chemical and physical concepts and equations, and constitutes a simplification to share two simultaneous phenomena in one modeling-formulation.

Energy Plants, such as nuclear or other kinds of steam-turbines type got significant improvements from these recent advances. In the following we pass on the corrosion models direct description.

4.1 Chemo-hygro-thermo-mechanical model for concrete (T2) This model, [5], is developed in FEM and is used for reinforcement concrete at any kind of special construction. It comprises chemical and mechanical characteristics. It can be considered an specific model of T2, and with features of corrosion-erosion duality.

4.2 Pipe Corrosion Models based on Neural-Network Theory (T2) This model works in pipes, based on Neural-networks mathematical methods. It si applicable in Power Plants since pipes constitute an important structure in energy systems -corrosion in oil-gas pipelines. The internal corrosion of pipeline is a multivariable nonlinear system, and Genetic Algorithms (GA), such as Neural Network analysis, are used in its optimization. The computational development of this model follows the usual steps of the GA programming –it can be considered specific T2 model.

4.3 Stress Corrosion Model (T1) Stress corrosion, in combination with environmental agents, causes cracks in a number of mechanical structures [5]. the environment component diffuses within the cracks and causes a positive feedback for the cracking-mechanical process.

The modeling is rather complex, and some approaches were done. The role of the geometry of the cracks, added to fracture mechanics principles constitute additional factors to increase the difficulties. Some equations for this kind of stress are published in the literature, as follows, for an hyperbolic notch,

$$\sigma_X = \frac{K}{(2\pi r)^{1/2}} \times$$
$$\times\left[\cos\left(\frac{\theta}{2}\right)\times\left(1-\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{3\theta}{2}\right)\right)-\frac{\rho}{2r}\times\cos\left(\frac{3\theta}{2}\right)\right]; \qquad (28)$$
$$\sigma_Y = \frac{K}{(2\pi r)^{1/2}} \times$$
$$\times\left[\cos\left(\frac{\theta}{2}\right)\times\left(1-\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{3\theta}{2}\right)\right)-\frac{\rho}{2r}\times\cos\left(\frac{3\theta}{2}\right)\right];$$

where θ is the polar angle of r, K a geometrical constant, and ρ the curvature parameter. The study and modeling of the interrelation among cracks (mechanical) and corrosion (chemical) is a complex mathematical-geometrical challenge.

4.4 Three-Dimensional geometric models of corroded steel bars (T2) This geometrical model, (T2), is based on the experimental fact that corrosion pit can be given with a hyperbola. The effects/physical-consequences of geometric parameters for a hyperbola on mechanical properties of corroded steel bars are applied –there is a link, therefore, with any kind of energy plant. It is a rather empirical model based on simple hyperbolic geometry of pits and steel bars. Stress and strain parameters are fundamental in the implementation of this model.

4.5 Wagner Model and derived equations for oxidative corrosion This equation, explained here longer, is basic for the mathematical analysis of the kinetic process of oxidation-corrosion rates. Oxidative corrosion rate usually has two stages, the initial stage (formation of superficial layer) and the main stage (the growth of the thickness of oxidative layer and formation of the multilayer of oxide), with an intermediate stage between both [5]. The Wagner primary equation is useful to derive practical formulas for high-temperature corrosion and low-temperature corrosion, and a series of intermediate approximations. Wagner's Differential Equation reads,

$$J = -CB\left[\frac{d\varphi}{dx} + ze\frac{dE}{dx}\right];$$

J is, (29)
Rate of Number of particles through oxide layer;

were C is particle concentration, B is the particle velocity for unit of force applied, φ is the chemical potential (we refer to Nerst fundamental equation), z is the valence of the particle, e is the electron charge and x is the thickness of the oxide layer. From this Wagner equation a series of models for different oxidative stages have been developed in the literature

[4, 5, 10], mainly in a exponential differential equation frame or integral equation. This model is a milestone for power plant functionality Survival Time Function R(t) in Reliability determination of the plant. In classic contributions, Ots, [5], developed corrosion models both in metal in general at low,high, discrete or continuous temperature, and metal pipes with the same variations, but under the effect of oil shale combustion. The series of equations/approximations is rather large, nevertheless it is possible to refer some fundamental formulas that could be modified according to specific metal material or geometry of basic plant components. For general metals corrosion, at high temperature, the following equation holds,

$$W = K_{02}\, e^{\left(\frac{-Ez}{RT}\right)} \times t^{n} \;; \quad \text{W is, Amount of oxidized metal;} \qquad (30)$$

where t is time, T absolute temperature, K_{02} is derived from a temperature-dependent coefficient, and n is a corrosion rate factor. Variations of these formulas are extensive and detailed [5], i.e., specific for diffusion-controlled region of the oxide layer, particular for the kinetic region of the layer, etc.

4.6 Models of Corrosive-Erosive Wear of Heat-Transfer Tubes (T1) In the literature, Ots, [5], developed also in his contributions a series of equations/approximations for Erosion-Corrosion Models prefereably/more-specific for oil shale combustion. In order to refer/show a basic equation with differential-frame of a function of several variables which is W, the specific mass of corroded material, in function of, namely, P, force acting on the layer, K, corrosive activity of the deposit (e.g., a boiler), and t, the time. That formulation reads,

$$dW(P,K,t) = \left(\frac{\partial W(P,K,t)}{\partial t}\right)_{P,K} + \left(\frac{\partial W(P,K,t)}{\partial P}\right)_{t,K} + \left(\frac{\partial W(P,K,t)}{\partial K}\right)_{P,t} \;; \quad \text{W(P,K,t) is, Specific mass of corroded metal;} \qquad (31)$$

The similar mathematical observation is applicable, this and those formulas in general, could be modified according to specific metal material or geometry of basic plant components [7, 30].

4.7 Todinov Synergic Model of Erosion and Corrosion A model for Erosion and Corrosion for powdered materials coatings was developed by Todinov [5]. Synergism between erosion and corrosion reads,

$$T=E+C+S; \qquad (32)$$

where T is the total mass loss rate from, (i.e., the erosion–corrosion rate), E is the pure erosion rate, C is the pure corrosion rate, and S is the mass loss rate due to the synergistic effect between erosion and corrosion –the object of interest of this equation. This synergistic term may be separated into two terms:

$$S=S_{EC}+S_{CE}; \qquad (33)$$

where, S_{EC} represents the erosion-induced corrosion rate (i.e., increase in corrosion rate due to erosion) and S_{CE} represents corrosion-induced erosion rate (increase in erosion rate due to corrosion). This is the synergism modelling base, and further developments and approximations can be found in the literature, [5]. By way of explanation, it is sharply different a corrosion process over a previously eroded powdered material surface, S_{EC}, from an erosion with loss of material in a previous corroded area, S_{CE}.

VI. BRIEF OF BIOMEDICAL MODELS

In this section, it is introduced an example and algorithm of a model for biomedical hip implants. Other biomedical models can be found at [1]. The objective function of nonlinear optimization is also explained. Complete numerical data can be found at [1].

Computational Method and Optimization Objective Function for Hip Implants in medical devices. Matlab nonlinear optimization subroutines with handle function were used to obtain numerical results. The optimization program was complemented with a graph of the value of the objective function (axis y), and the value of the hardmess (axis x, hardness in Kg and mm, so for that reason the exponential). The development of the Objective Function (OF), is the method that was implemented in [1-5] and in other dynamics publications such as [18,19,20].

From Archard's model [39],

$$W = K \frac{L \bullet X}{H};$$

It is known L, X, H values from [25], and W simulated values are set in Table 2. Thus,

$$W - K(\text{opt parameter}) \frac{L \bullet X}{H} = 0; \qquad (34)$$

Simple equation since model (34) is used in integral form for finite elements techniques in hip implants, [5]. K is parameter, although in previous contributions this algorithm was implemented for more parameters, such as optimal hardness or number of rotations. Number of rotations is calculated multiplying the semi/circumference width value of the implant, πr, from Table 3, 50mm, by number of rotations, Table 3, 10^7. Given this formulation [39], the OF with L_2 Norm that was used without fixed constraints reads,

minimize,

$$\left\| W - K \frac{L \bullet X}{H} \right\|_2^2 = 0; \qquad (35)$$

Although constraints are not fixed, the program was runned setting tentative constraints to search both for optimal initial search vector and verify that the minimum was global. The values can be found in Table 1, Appendix I. The OF is a nonlinear least squares one, that has provided acceptable results in materials engineering, [1-5]. The data set was hardness of implants types, and loads, the parameter without constraints to be determined, as said, is the K coefficient of (34). 3D Graphical Optimization surfactal images were done with more complicated software that depends on subroutines in few parts [1,4,39].

This original software, [1,4,39], was developed in previous contributions. Residuals and optimal values for K are were also set in the program, all in Kg and millimeters as it is the standard at Tallinn University of Technology usually. In Table 1, Appendix I and Figures 1-2 optimization results are shown. The K coefficient of Eq. 1 is the optimization parameter. Loads were selected for mature persons rather slim to average persons with standard weight. Angular velocity was chose 1 radian per second.

In Table 1, Appendix I and [39], there are two types of optimization. The first one is for all material together to obtain a common optimal K coefficient. This creates higher residual. The second and third are the optimization of K for Titanium and Co-Cr alloy. Fig. 2 is determination for Co-Cr implants and Figs. 3-4 for specific implant materials, namely Titanium and Co-Cr and an example of surfactal graphical optimization [1-4]. In **Table 1** (at Appendix 1), the residual for the optimization of K value for all materials together is shown. At X axis, it is set the variation of the OF residual for the range of hardness of the simulated materials. The hardness of every material was implemented in the program as a vector, and the graph shows the optimal value of hardness of that vector that gives the global minimum for OF, while the optimal value of K, 0.1932, is released at prompt.

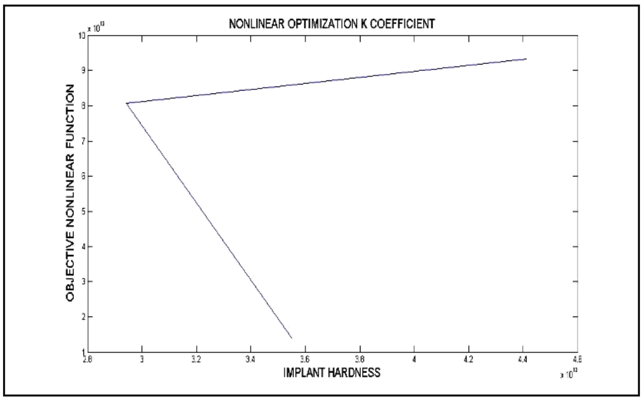

Figure 1.-Graphical result of optimization. Materials are Titanium, Co-Cr, and Cast Co-Cr alloy.

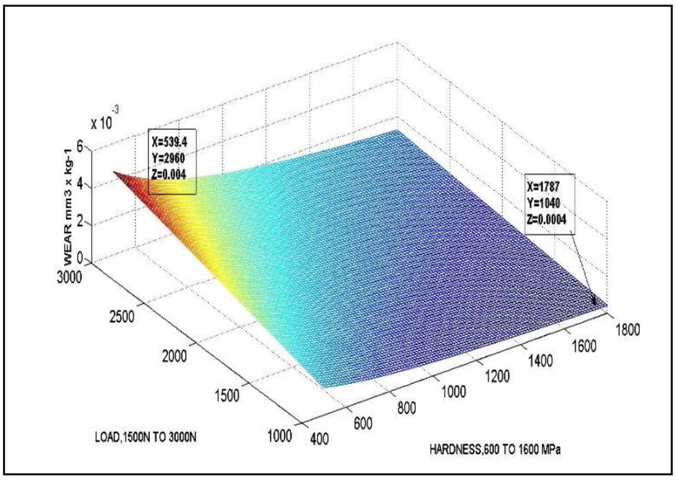

Figure 2.-Graphical 3D Optimization-Simulation. Global minimum and Global Maximum determined by cursor in Graphical Optimization Method, [1-4]

In Figure 2, the simulation presented comprises a range of loads between 500 and 300 N, and a range of implant-material hardness between 600 and 1600 MPa—not specific material a range that can cover several ones, such as metal-metal or ceramic-ceramic.

The number of articular rotations was selected as 1000 ones. The constant K was chosen for metal-composites type implant. The programming of this algorithm for graphical simulations was done with subdivision method and 3D surfactal imaging subroutines both in FREEMAT and Matlab.

Biomedical engineering applications of results are linked to optimal K coefficient. If it is applied the model of (34), it is possible to use this K coefficient for similar materials with similar values of hardness. That is, predict approximately the wear that will be caused in the implant for that load with higher number of rotations.

VII. GRAPHICAL SOFTWARE-OPTIMIZATION AND SIMULATIONS

This section comprises basic definitions in tribology for graphical matrix-algebra optimization and a graph with a ROI selection for learning. Convexity concept of a 2D or 3D objective function was applied in optimization development.

In all the Publications and in, a large series of plots with model implementations of graphical optimization were included.

Definition 1: *Graphical nonlinear optimization is a constructive approximated method to set the global/local minima/maxima of an objective function provided when two strict conditions are met:*

(1) Computational graphical simulation of the objective function is precise and imaging software is sufficiently proved as accurate in its imaging algorithms.

(2) Objective function of mathematical development and constraints is strictly mathematically linked to the graphical implementation.

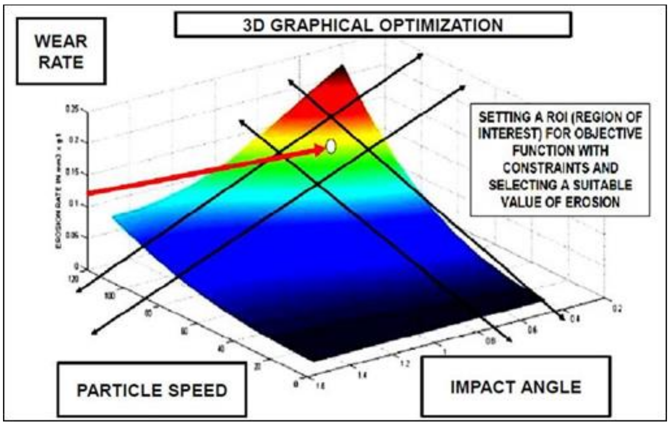

Figure 3.-Basic concept of Graphical Optimization. Numerical data is not relevant, the important is the caption concepts.

A graph of ROI selection in graphical optimization is included in Figure 4. The algorithms of graphical optimization were developed in a series of programs, both in FREEMAT and MATLAB. The subroutines for 3D implementation of the graph are given by those software options. The formulation of a model for graphical optimization is a rather complicated task and depends specifically on each type of the model. This means that to obtain appropriate size and congruent operations of the matrices, such as multiplications, powers, summatories, and division, it is mandatory to perform a model operations division in a number of parts. This original technique was developed along all series of papers published [1-4]. In Figure 4, a ROI selection of Menguturk model with constraints is presented. Matrices are 1000x1000, and MATLAB sharpness of this image is very good, and running time is ≤0.5 s with a Linux Station 16.2 and AMD processor. Region of interest is velocity [61.6, 104.3] ms^{-1}, angle in degrees [42.9, 57.3], and erosion rate [0.1, 0.2] mm^3/g.

3D and 2D Graphical optimization of ROI selections are detailed in all contributions, and multiple graphical optimization methods are included in the conclusions specifically.

To select a ROI, a specific tool is provided in MATLAB. When a ROI is selected graphically, the complete numerical matrices data is set at prompt. Therefore, the selection of the desirable values for the model can be easily chosen from the numerical data. FREEMAT does not offer this option, and the matrices-values for a ROI have to be extracted with commands at prompt.

In plain language, suppose that the laboratory apparatus has some functional constraints (or the material that we would manufacture will only be exclusively exposed to a range of erodent velocities and impact angles). That is, the velocity of particles can be in the interval [61.6, 104.3] ms^{-1}, the impact angle in radians at [1.0, 0.7]. Then, within that ROI it is possible to click the optimal minimum erosion approximately at 0.1 mm^3/g for a particular velocity and angle. This is possible if the model surface representation is sharply concave-concavity / convexity concept that is fundamental in the optimization. If it is necessary to see all the matrix values within the region of interest, set the vectors of the axes x,y,z at prompt, or more easily, use the MATLAB tool that automatically gives the ROI magnitudes at screen. With many variants and different algorithms, this method was previously used in the selection of optimal ROIs for the implementation of surgical prostheses at the selected surface parts of the vertebras [12,32].

The biotribological optimization and simulations were developed in Paper IV. Numerical computing was focused mainly on hip wear prostheses models. The wear of a hip prosthesis is highly complicated. Generally, it depends on the contact status between the ball and the cup (i.e., friction regime), characteristics of the tribocouple, anatomical and physiological conditions, age, type of physical activity, production quality of the prostheses, lubricants, diseases history, concomitant diseases, etc. There are prostheses made of metal, composites, metal with ceramics, metal with

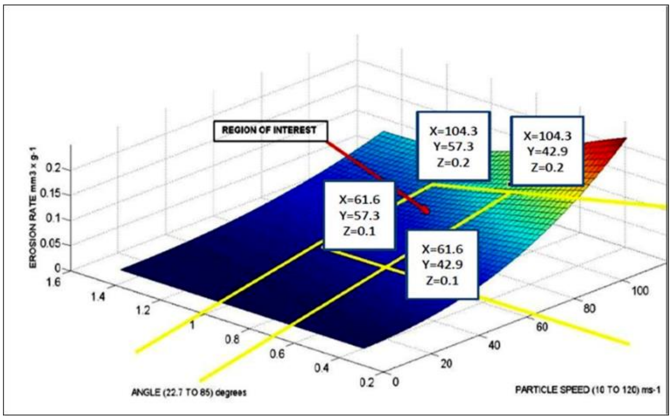

Figure 4. ROI selection of the Menguturk model with constraints.

composites etc. [1-5,10]. For example, in spite of a low friction torque, the polymer-on-metal configurations exhibit higher wear than those of metal-on-metal or ceramic-on-ceramic due to the boundary lubrication regime between the wearing surfaces. For the same reason, small-size metal-on-metal hip joints perform worse than large-sized ones. If properly designed and manufactured, metal-on-metal hip joint prostheses work, *vice-versa*, under mixed lubrication regime, and ceramic-on-ceramic hip joints function even under hydrodynamic lubrication conditions, which provide extremely low friction. It is related to the articular movement of acetabular hip that is estimated as the number of rotations in a day and it is high since arms and legs are basic in human daily movements. If sports or high physical effort/activity is added, the result in the modelling involves a large number of factors. Figure 5 presents a 3D Graphical optimization for a hip implant basic Archard's law model for abrasion. Matrices are 1000x1000, and MATLAB sharpness of this image is good, and running time is ≤ 0.5 s with a Linux station 16.2 and AMD processor. Maximum load is 2960 N, wear rate 0.0040 mm^3/kg, hardness 539.4 MPa. Minimum load is 1040 N, wear rate 0.0004 mm^3/kg, hardness 1787 MPa.

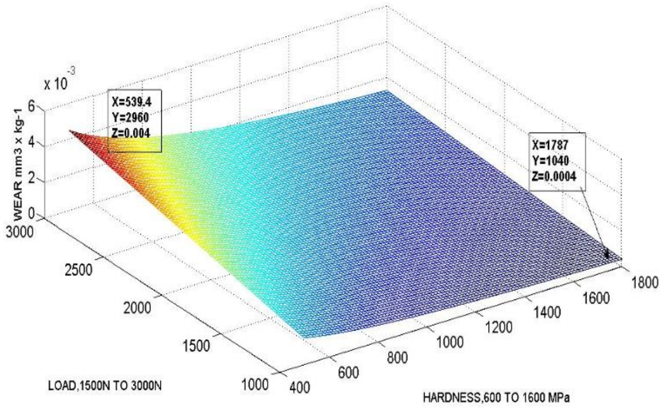

Figure 5.- Model for hip implants with cursor inset showing numerical values of maximum and minimum.

For graphical optimization of hip implants, the following equation was applied:

$$W = K\frac{L \bullet X}{H}, \qquad (36)$$

where K is the wear constant specific for each material, L - biomechanical load (N), X - sliding distance of the acetabular semi-sphere of the implant (mm), and H - the hardness of the implant material (MPa). X is measured as the number of rotations of the implant multiplied by half distance of its circular-spherical length. The number of rotations depends on the daily physical activity of the patient.

In Figure 5, the simulation presented comprises a range of loads between 1500 and 3000 N, and a range of implant-material hardness between 600 and 1600 MPa. The number of articular rotations selected was 1000. The constant K was chosen for a metal-composites type implant. The programming of this algorithm for graphical simulations was done with the subdivision method and 3D surfactal imaging subroutines both in FREEMAT and MATLAB.

This equation was implemented computationally for graphical optimization with varied constants depending on the material of the hip implant. In Paper IV, a series of nonlinear constrained and non-constrained optimization results are shown. Among these hip implant materials selected were: ceramic implants, metal implants, metal-coated and mixed-implants such as metal-composites [1-5]. Additionally, in [1,39], important biotribological models are described in detail.

To date, in hip implants, tribological design constitutes an increasing bioengineering demand in the market and Health Services, both public and private. The increase of the population age in the European Union creates an increment of incidence/prevalence of surgical interventions for femoral-hip articulations replacement with artificial implants. In [39], the objective functions for geometrical modelling of cloud data to a surface are set and developed with MATLAB and FreeMat subroutines. Specifically, in [12,32], a 3D hyperboloid geometry was fitted to ¼ million cloud data from a medical scanner with results of high values, (> 75 %), in statistical error determination coefficients.

VIII. DICCUSSION AND CONCLUSIONS

This study presents a series of Erosion, Corrosion, and Biomedical models in the field of tribology wear and Tribocorrosion. The models can be an initial point for further investigation and tribotesting at laboratory, subject to specific parameters. Therefore, the engineering practical use of the contents was the primary main objective of the article. The paper continues the research in these fields that was started in previous publications [1,-8, 12, 21 ,22, 24, 39]. The second part refers to Graphical Optimization Methods that can be applied to any selected model, with software and 3D images examples for sharp learning. This second section requires the design of computational software and optimization algorithms with the tribotesting data, much better using Inverse Methods. The Integral-Differential Model/Method (Casesnoves, 2017) and the Stratified Model (Casesnoves, Kulu, Surzhenkov, 2018) are included. One simple hip-wear algorithm for objective function optimization was presented.

In summary, the focus of the study is to provide with engineering methods to choose a model, carry out tribostesting of theoretical study, and obtain realistic and practical industrial applications. Specific data is referred to Medical Devices materials design, that involve more complicated experimental validation *in-vivo* and *in-vitro*. Materials Engineering, Biomedical/Biotribology, manufacturing-industry and theory are included in the focus of this contribution for practical applications and model/algorithms improvements.

IX. ACKNOWLEGMEMENTS AND SCIENTIFIC ETHICS STANDARDS

This study was carried out, and their contents are done according to the European Union Technology and Science Ethics. Reference, 'European Textbook on Ethics in Research'. European Commission, Directorate-General for Research. Unit L3. Governance and Ethics. European Research Area. Science and Society. EUR 24452 EN [50, 67]. This research was completely done by the authors, the software, calculations, images, mathematical propositions and statements, reference citations, and text is original for the authors. This article contains also unique numerical data and special new-improved images together with algorithms original from author. The paper can be considered both a research article and a technical review one. Therefore, some data and author's previous work has been introduced into the text. In addition, the basics of some paragraphs/algorithms of the some previous papers are set to understand mathematics and optimization of the present contribution. When anything is taken from a source, it is adequately recognized. Ideas from previous publications were emphasized due to a clarification aim, [30,38].

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XI. AUTHOR'S BIOGRAPHY

Francisco Casesnoves is Engineering PhD by Talllinn University of Technology (started thesis in 2016, thesis defence/PhD-graduated in 2018), Estonia, and computational-engineering/physics independent researcher at COE, MSc-BSc, Physics/Applied-Mathematics (Public Eastern-Finland-University), Graduate-with-MPhil, in Medicine and Surgery (Public Madrid University Medicine School). Casesnoves studied always in public-educational institutions. His education/scientific vocation was motivated very young, by Profs Candida Navamuel and Isabel Vela, in Renaissance-Humanism ideas—later on with the motivation manuscripts of Nobel and Von Helmholtz prizes Santiago Ramon y Cajal. His constant service to International Scientific Community and Estonian technological progress (2016-present) commenced in 1985 with publications in Medical Physics, with further specialization in optimization methods in 1997 at Finland—at the moment approximately 90 recognized publications. His main branch is Computational-mathematical Nonlinear/Inverse Optimization. His service to International Scientific community also comprises the publication of two recent books with Estonian affiliation, the first is the computational dynamics book, 'The Numerical Reuleaux Method' (200 pages, 2019), the second is a sociological and medical philosophy book (300 pages, 2019). Casesnoves best-achievement is the Numerical Reuleaux Method in dynamics and nonlinear-optimization. This Numerical Reuleaux Method constitutes, among others, an advance in Space Aerodynamics Computational Methods and Bioengineering. Casesnoves speaks, reads, amd writes Estonian language at B1-2 levels, with corresponding official diplomas in A2 and B1. Also participates/registers in sporting Estonian activities such as Tallinn Marathon. Casesnoves played as defender and middle-fielder at Junior Madrid Football League, and as physician is supporting agnostic healthy life and all sporting activities. Casesnoves publications are always according to International Scientific Standards. He sets his medical technology papers, specially in cancer radiotherapy methods, always in open access for benefit and use of any public health system according to the Fundamental Right for health care. Recently has written new mathematical modelling radiotherapy articles affiliated to Estonia, Tallinn (2019). Casesnoves has contributed to technological development in Estonia (and also at Riga technical University, Power Electrical and Electronics Department) with 18 articles, two books, and 1 industrial project associated to Europa Union EIT Health Program (Tartu University, 2017).

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XII. APPENDIX I

OPTIMIZATION NUMERICAL RESULTS					
Material	**Hardness [MPa]**	**Hardness for optimization [mm, Kg]**	**Prostheses Radius [mm]**	**Biomechanical Loads [Kg x mm/s²]**	**Angular Speed /Number of rotations**
Cast Co-Cr alloy	2942	2942×10^9	For all 50	For all 500×10^3 750×10^3 1000×10^3	1 rad/s 10^7
Titanium	3550	3550×10^9			
Co-Cr alloy	4413	4413×10^9			

OPTIMIZATION NUMERICAL K COEFFICIENT RESULTS			
Material	**Optimal k**	**Residual**	**Comments**
Cast Co-Cr alloy Titanium Co-Cr optimization	0.1392	1.2415e13	Optimization was performed for these materials together setting vector of respective hardness
Titanium	0.1420	3.6e-4	Low residual
Co-Cr alloy	0.1765	5.5e-4	Low residual

Table 1.-Nonlinear optimization parameters for biomedical hip model [39].

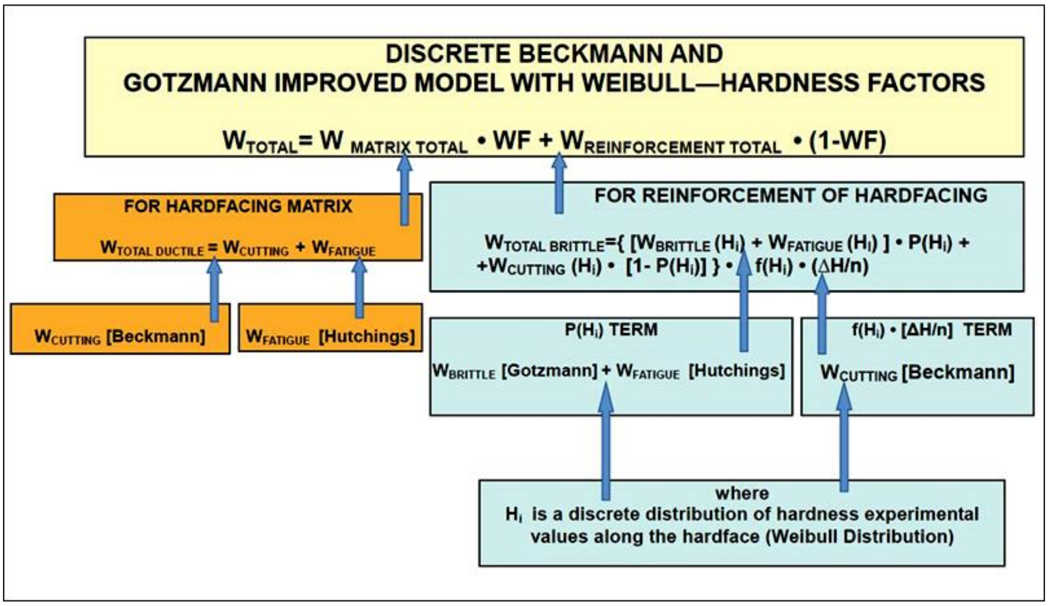

Figure 1.-Basic procedure to obtain erosion magnitude with Stratified Model (Casesnoves, Kulu, Surzhenkov, 2018)