International Journal of Scientific Research in Computer Science, Engineering and Information Technology
 | Volume 2 | Issue 3 | ISSN : 2456-3307

Mathematical Models in Biotribology with 2D-3D Erosion Integral-Differential Model and Computational-Optimization/Simulation Programming

—a mathematical model construction based on experimental research

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ABSTRACT

Following from previous computational-research of biotribology models, the study of wear, abrasive wear, corrosion, and erosion-corrosion in bioengineering artificial implants, interior, exterior, partlially-interior/exterior biomedical devices, or artificial-bone implants, is directly linked to the operationa-solution of their bioengineering/biomechanical difficulties. Additionally, this kind of deterioration could also involve external medical devices, prostheses, temporary prostheses or orthopaedic supplies, surgical permanent devices, and even surgery theatre devices or tools, causing a series of important associated functional difficulties. This usually happens during surgery and the post-operation stage, or rehabilitation time. The consequences of this industrial-biomedical design complexity are extent, from re-operation, failure of medical devices, or post-surgical discomfort/pain to complete malfunction of the device or prostheses. In addition to all these hurdles, there are economic loss and waste of operation-surgical time, re-operations and manoeuvres carried out in modifications or repair. The wear is caused mainly by solid surfaces in contact, abrasive or sliding wear with frictional resistance. Corrosion/Tribocorrosion of protective coatings also constitute a number of significant mechanical and bioengineering difficulties. Mathematical modelling through optimization methods, initially mostly developed for industrial mechanical systems, overcome these engineering/bioengineering complications/difficulties, and reduce the experimental/tribotesting period in the rather expensive manufacturing process. In this contribution we provide a brief review of the current classified wear, erosion and/or corrosion mathematical models developed for general biotribology—based on recent modelling international publications in tribology, as an introduction to research. Subsequently the aim focus on specific tribology for biomedical applications and references to optimization methods and previously published new graphical optimization for precise modelling with computational formuli, programming presentation, and numerical-software practical recipes. Results comprise an initial review of tribological models with further simulations, computational optimization programming, new graphical optimization, and visual data/examples both in mechanical and biomechanical engineering. The corollary of this research is a mathematical integral-differential model for abrasive erosion is developed based on experimental laboratory data and previous mathematical modelling contributions. All in all, this study constitutes a contribution to modelling optimization in bioengineering with a model development and imaging optimization/simulation recent advances.

Keywords : Tribology, Erosion, Corrosion, Wear, Biomedical Devices, Erosion-Corrosion, Mathematical Modelling, Nonlinear Optimization, Advanced Programming And Software

I. INTRODUCTION

Human life-biology constitutes a type of matter natural organization at earth with an special evoluted cognitive brain, together with animal, vegetal, atmosphere and mineral ones. This fact implies that any environmental physical-chemical phenomena that cause changes in the structure of all these kinds of material-structurated varieties involve common physical/chemical mathematical laws and parameters.

The engineering and science advances in modern research focused on tribology, biotribology and wear, erosion and corrosion are not an exclusive study of these phenomena. Natural earth surface has been modified by geophysics laws/parameters by wear, and erosion during periods of millions of years. Human/animal physical biomechanics and tissue-biology is linked to these physical-chemical changes along the lifetime of the natural beings. What is more, recent climate change has became an additional factor to modify previous natural conditions/stages of erosion and corrosion of earth, in such a way that today, for easy example, it is well-known that antartic surface-glaciars are performing a significan objective modification in their structure and melting-volume. Secondarily, the production results of the human industry is modified along their usability-time by tribological conditions, and even the increasing industrial residuals, specially non-biodegradable matter, and all kind of waste are subject of tribological constraints not only in the elimination/transformation phase but also during the storage of industrial-human and/or solid-residuals and waste.

As a logical consequence of all these phenomena, we can classify tribology and biomedical tribology among the groups natural, artificial, and natural-artificial. The interaction between/among these strands are evident, for instance, the modification of farming over the soil during the harvest grow or the links between the wood industry modification of natural spaces that yield the erosion of free land-surface alteration. An external biomedical implant directly causes influence over the surrounding muscles and tissues, since the biomechanics of that part of the human body is different as a result of the insertion of the medical device.

To summarize these emvironmental-human-tribocorrosion concepts, and prove the natural-artificial extensive interrelation, a logical example is the probably modification along the large-decades of the physiological temperature-control, due to the sudden climate changes and overlapping of the natural climate terms—in other words, in the same way that diet habits transformation during recent times have resulted in different body-shape of new generations, the external conditions get similar influence. To guess akin phenomena, the skin physiological cycle of melanocites could be become dissimilar for the long-term increase of the solar radiation, and the alike high-augment to electromagnetic radiation overall dose, e.g., cell-phones or comparable devices around radio-sensitive zones of head and neck, could result in decades in neural-axon transmission conversion to a new environmental circumstances.

Biomedical Tribology and Tribocorrosion constitutes a mixed up branch whose specialization shares parts of every group defined previously [8,9,13]. In other words, Biomedical Tribology involves artificial wear of medical implants and devices but also natural biochemical corrosion or wear of any medical device which is set into the human biomechanical system [8]. This fact implies that there are special and difficult mathematical, computational, numerical, physical, and chemical/biochemical conditions when the mechanical device of interest is biomedical and is surrounded by human/animal tissues. Another important evolution-factor is the biomedical technology advances linked to the progress towards a longer lifetime in human population. This incidence/prevalence fact implies that a significant percent of population will experience during their lifetime substitution(s) of body parts for a large number of pathological reasons, or traumatological-accidental causes [35,37,36,39]. It is not risky to pre-hypothesize that in the future decades the human body will experience changes along the life with increasing substitution of damaged/degenerated tissues/body-parts because the expectation of lifetime will be significantly longer [72].

Therefore, according to all these conditions/constraints, 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, biomedical tribology essentials and environmental-geophysical factors. For built-up mechanized purposes, pure mechanical or biomedical, given the economic loss caused by erosion and corrosion in an extensive range of engineering/technology areas, the selection of materials became a must. 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.

The advances during the XXth Century in mathematical methods towards their applicability in a large field of sciences that were not initially subject of strict-numerical objective determinations has supposed a quality jump in investigation, and not limited for this field but also extended, e.g., to social sciences, industry design/planification, classical agricultural/food-production techniques, physical-sport science, etc. Just the same occurred with materials engineering, whose classical trial-and-error testing involved a large series of defects and discarded intends in the field of machinery, metal coatings or power-energy stations, among many other areas.

The computational era of XXIst Century supposed a further upstep in research-applicable mathematical methods for engineering, and the selection/optimization of materials began to be subject of mathematical modelling and computational calculations—mainly accompanied with the electronics advances in microprocessors speed and memory quality standards. Complementary, the creation of simulators to avoid large laboratory investigation-terms supposed in these recent years a small revolution in scientific work methods [14,23,35,37,39,56].

The third leap-stage for mechanical materials engineering was the extension of the industry from first to next towards the manufacturing of medical devices. This fact was caused by the parallel advances of technology applied on medicine, surgery, and rehabilitation physical-therapy [23,35,37,39,56].

These objective real-world facts implied that investigation of biomaterials was born as a new specialization/branch within biomedical engineering. In other words, simulators, optimization methods, mathematical modelling and computational software constitute daily tools of advance in biomaterials investigation.

“Trial and error” methods, that is, the Forward Empirical Problem Technique, was found expensive, imprecise and time consuming [5,55]. In consequence, applications of the Inverse Problem methods were used to determine, *a posteriori*, the validation/refinement of theoretical mathematical models previously approximated [6,7,8,6,9]. 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 [5,10]. Since the optimization task has become a routinary/compulsory task at daily research routine, [35,36], and not necessarily all the investigators got used to work with optimization programming and tools, graphical optimization, among several optional-practical methods arose in recent years—for instance, see section with images focused on graphical optimization with Freemat and Matlab.

In terms of general mechanics/machinery/devices, material coatings erosion,corrosion,deformation and stress cracks are considered an industrial hurdle that creates loss of budget, energy, reparation-time, and operating time. Material substrate, although important also and chemically/physically linked to these processes, does not constitute the primary problem. Statistically, a rate higher than 90%, of mechanical-machine failures are linked to fatigue, friction,and wear. Succintly, according to [11], the aggressive environments that cause degradation in general are, wear, corrosion, oxidation, temperature, gas-particle size/velocity [12,16,17,22,27], and any combination of these factors. In biomedical tribology the degradation is more specific, chemical factors take a fundamental role, and biomechanical forces that cause wear are also essential for durability of artificial implants, phisiologycal acid-dase ions are fundamental in this phenomenon. Hence, the practical objective to find out engineering/bioengineering solutions is to use new/improved optimal materials for the technical design, in such a way according to precision of durability and functional operation of the mechanical system/device or group of any kind of apparatus/prostheses. Actually there is a number of mathematical models for tribilogy, biotribology, wear, erosion, corrosion, and combined erosion-corrosion or tribocorrosion. 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 device, could be improved in durability, tribology/biotribology capabilities, and erosion-corrosion resistance.

Engineering solutions, as said, for these problems that cause economic loss, together with a waste of, e.g., functioning time and expensive reparations, re-operations in biomechanical and mechanical structures, power plants, bioengineering and mechanical apparatus/equipment are based on precision-design of both coating materials resistant to abrasion-erosion, and/or friction [1,3,4,6], and mechanical optimization of the operational structure of the device/mechanical system/mechanical-chain-group–in fact, temperature of components, e.g. hardmetal or cermets, constitutes also an important factor-and stress of materials also. 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 [14,16]. 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 [16] –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 [1,3]. Tribotests for biomedical wear and corrosion involve different and more uncommon/sophisticated conditions since the human physiology and biomechanics comprise different and rather more complicated parameters in several circumstances compared to classical mechanical systems [ref]. In other words, biomedical tribotests both *in vivo* and *in vitro*, involve a more complicated/constrained experimental conditions and even medical-ethical legal norms.

This contribution deals with an up-to-date modelling-presentation of tribology/biotribology wear,erosion, corrosion, and erosion-corrosion mathematical models, both from an objective and critical point of view. 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 materials/machinery/device 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. In general is a continuation of previous modeling contributions but complemented and developed towards a biomedical and biotribology scope [35,36,37,39,72].

The simulations that are presented comprise both mechanical systems modeling for tribology and biomedical modeling also. Graphical optimization, [Casesnoves, 2017], is detailed with series of images and sharp conclusions that are evidenced by visual information. Optimization algorithms and computational examples are also shown with detailed and sharp-learning explanations. A group of highlights and important key points following all the article development from theory to computational practice are gathered at final sections to summarize the results of this research. The mathematical model developed constitutes a realistic presentation of a theoretical-experimental development of equation for hip implants wear [Casesnoves,2017].

II. SIMPLIFIED CLASSIFICATION OF GENERAL MODELS FOR EROSION AND CORROSION

Erosion and corrosion concepts imply the interaction between/among physical structures that could be in any physical state, namely, solid, liquid-solid,deformable-solid, or metastates. There have been several classifications, developed for erosion and corrosion mathematical models, tribology and biotribology in general.

The interaction complexity is rather high, (Table 1). In the literature [17,10,55], it is 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 biotribology and specifically E/C causes the necessity to design particular models almost for every type of interaction.

Type1 and Type2 interactive classification constitutes a simple and fast practical use/selection of models in each

particular materials choice –proposal of authors previously published [55], Table 2. The predominant criterion of this 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, biotribology, erosion, and corrosion. Therefore, it is defined as follows,

Type 1 (T1) Mathematical Tribology, Biotribology and specifically 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.

TABLE I

BIOMATERIALS INTERACTION CONDITIONS FOR MECHANICAL TRIBOLOGY AND BIOMEDICAL TRIBOLOGY	
Conditional Factor	**Variables/Parameters/Comments**
State	solid (cristallographyc variety),liquid,gas,metaestates
Physical Magnitude	particles velocity,kinetic energy,materials particle temperature
Geometry	rather difficult in most cases,particle impact angle(s),interaction angle(s), interaction surface(s)
Material Composition	chemical,molecular,nano-quantum composition
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
Stress Residual and Strain in hip implants	Stress and strain of prosthesis conditions for hip implant (modelled in equations)
Biomechanical Conditions	For Biotribology and biomedical devices very important rather essential in engineering design

BIOMATERIALS INTERACTION CONDITIONS FOR MECHANICAL TRIBOLOGY AND BIOMEDICAL TRIBOLOGY	
Conditional Factor	**Variables/Parameters/Comments**

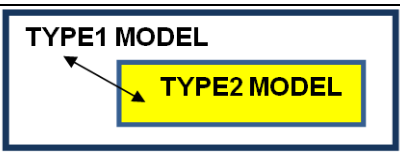
INTERACTIONS FLOW CHART

Physiological-chemical-composition of plasme, blood flow, and surrounding tissue composition	Very important for the tribocorrosion conditions and durability of the implant. Acid and base ions of plasma and surrounding chemical pH parameter constitutes a corrosion factor for metal/composites/plastic surfaces
Associated diseases in the patient subject of biomechanical implant	Any concomitant disease of the patient that is subject of biomedical device implant surgery is a factor interacting with the implant materials and biomechanics, e.g., ostheoporosis, diabetes, clots, metasthasis, tumoral physical growth/pressure, etc
Biomechanical Specific Body-types	Not all the patient anatomy and therefore biomechanical constitution are equal, and what is more, the particular physical activity of every person also is an important factor
Histocompatibility Contrast Internal External	Internal devices are subject of biocompatibility Mandatory conditions, not the case for external implants, mixed requirements for internal-external [8]
Medical Device Biomaterials personalization	In not few cases, personalization of a medical device for special/complicated patients yields to the particular design of biomaterials

In Table 1 a general overview of Triblogy and Biotribology definition of this classification is detailed—improved from previous publications [55].

TABLE II

TRIBOLOGY AND BIOTRIBOLOGY MATHEMATICAL MODELS CLASSIFICATION WITH DETAILS		
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
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)
Flexible Classification	T1 and T2	It is meant that an initial model in tribotesting stage/improvement could pass from T1 to T2, or vice-versa, derive in other models with new lab findings or be modified in optimization process
DIAGRAM OF FLEXIBLE CLASSIFICATION OF MODELS		



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III. BIOMEDICAL TRIBOLOGY/TRIBOCORROSION MATHEMATICAL MODELS, AN INTRODUCTION

This section is mainly focused on hip prostheses models for femur acetabular joint replacement, and brief reference to other biomedical models. The predominat phenomenon in biotribology is not pure wear or corrosion. Since the environment in internal implants is human tissue, tribocorrosion is what mostly occurs. Tribocorrosion is defined as the degradation of material surfaces both physical and chemical—wear,cracking,corrosion, abrasion etc.

In Diagram 1, the process of model construction is briefly detailed. Tribocorrosion involves sliding among 2 or three bodies, which could be unidirectional or reciprocating, that is, corrosive wear or chemo-mechanical polishing. Fretting phenomenon happens in dentistry implants and body joints, just the same that occurs in rolling. Microabrasion is linked to rolling, grooving and slurry in general [9].

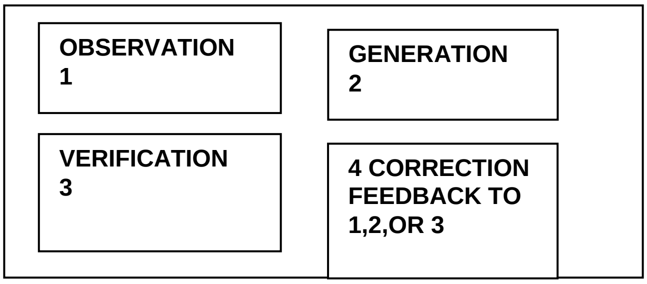

Diagram 1.-Basic construction and verification of a mathematical model

The reasons for more significant incidence/prevalence of biotribology linked to hip prostheses are multiple, from the high prevalence /incidence of hip articulation degradation/fracture or similar surgical/medical pathologies to traumatological or genetic malformations that involve severe biomechanical problems in hip articulation system. In fact, hip gait constitutes a fundamental part for walk, run and general mobility of the whole human anatomy. In other words, hip is the biomechanical mesh between the trunk and the legs walking muscular-articular system. No matter whether legs are functional or not, a mobility default in the hip causes such a complicated biomechanical consequences that all the inferior member of the body could claudicate completely. In addition, load magnitudes on knee, taking into account tendons and ligaments forces during walk, are around 2000 N, and similar values can be expected in hip, both natural articulation or implant. This number gives an idea of the severe constraints/difficulties, both biomechanical and material characteristics (stress, strain, hardness, etc) when designing the prostheses [53,66]. Hip and knee are crucial biomechanical articulations for mobility, and the industrial focus of bioengineering medical devices sets an important part of activity/investigation in this field. A classical model for wear in hip arthroplasty is,

W = K • (L X)/H

Equation [1]

where K is a wear parameter/constant, L is biomechanical load, X is sliding distance, and H is hardness of implant. This equation is optimized in computational section. Originally, this model was conceived with Flow-Pressure instead Hardness, although hardness can be approximated to flow-pressure. Besides, it is used as a basic formula to develop a mathematical model with a continuous hardness function of matrix in WC-Co reinforced composites to demonstrate an integral equation wear model [Casesnoves,2017]—provided the fact that Titanium-Titanium-Boride are the [1] histocompatible election composite choice [8]. This model reads as follows,with hardness defined as a continuous function H(s),

$$\frac{dw}{ds}=\frac{dw}{dH}\times\frac{dH}{ds}=$$
$$=(KLX)\times\left(\frac{-1}{H^2(s)}\right)\times\left(\frac{dH(s)}{ds}\right);$$
$$\text{integrating along all matrix average length,}$$
$$\int_{w_0}^{w} dw=\int_{s_0}^{s}(KLX)\times\left(\frac{-1}{H^2(s)}\right)\times\left(\frac{dH(s)}{ds}\right)ds;$$
$$\text{or,}$$
$$\int_{w_0}^{w} dw=\int_{s_0}^{s}(KLX)\times\left(\frac{-p_1(s)}{p_2(s)}\right)ds;$$
$$\text{with } p_{1,2}(s) \text{ as integrand polynomials;}$$

Eq [2]

In the following it is developed two generic models that are basis for new derived types. One of the initial classifications of wear is the Barwell types, a follows,

$$(1)\quad \Omega=\frac{\beta}{\alpha}\left[1-e^{-\alpha T}\right];$$
$$(2)\quad \Omega=\alpha T;$$
$$(3)\quad \Omega=\beta e^{\alpha T};$$

Eq [2.1]

where Ω is volume removed, alpha is a constant and T is the time. It is an initial overview useful for further research and development of models, applicable in biomaterials also. For friction in polymer-matrix composites or similar compounded materials, the Rhee model reads,

$$\Omega=K\times F^{(K_1)}\times V^{(K_2)}\times T^{(K_3)}\quad;$$

Eq [2.2]

where Ω is volume removed, F load, V velocity, and T time, Ks are constants of laboratory experimental determination. Lubrication modeling in hip prostheses, [53], constitute also a base for development of mathematical formulation, and as an example we refer to Rabinowitsch model that reads,

$$\eta=\eta_\infty+\frac{\eta_0-\eta_\infty}{1+\left(\frac{\tau}{G}\right)^2};$$

Eq [3]

where mu is viscosity, and tau is shear-stress, the other parameters are constants determined by regression, [53]. And also the Carreau's and Cross model,

$$\eta=\eta_\infty+\frac{\eta_0-\eta_\infty}{\left(1+\left(1+\left[\frac{\dot{\gamma}}{\dot{\gamma}_c}\right]^2\right)\right)^{m/2}};$$

Eq [4]

where gamma is the notation for the shear rate. Actually hip arthroplasty constitutes an important branch of medical devices industry with several super-specialization branches for the extensive area of investigation. Lubrication is essential for several reasons, among them, the minimization of the surfaces

[1] **Integral-Differential Model was created by Francisco Casesnoves in December 2016 at Tallinn University of Technology based on Computational results from experimental lab data.**

in contact wear, and other motive is the better mechanical performance of the implant.

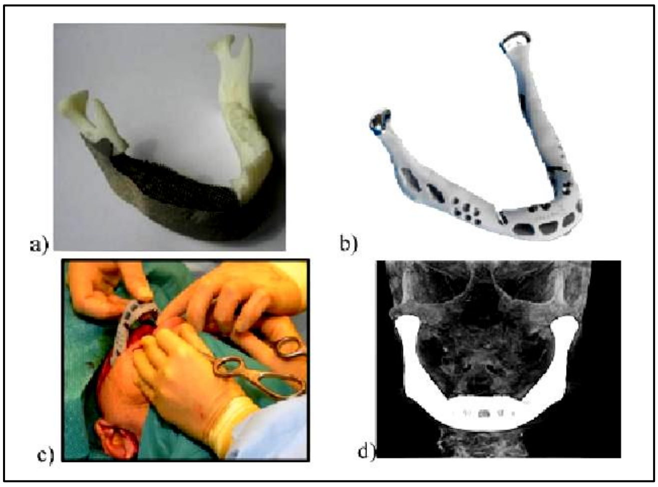

Figure 1.-From reference [8], excellent biomechanical sketch of Bartolo and Colls, [8], showing the recent progress in biomedical design-implants and surgery-implementation of an artificial mandibule at surgical theatre. Projection of this kind of advances could involve/result in future towards a significant increase of lifetime with additional acceptable level of quality of life and personal-independence-capability standards. Note the well-overcome difficulty of that anatomical region, and the resolutive solution with bioengineering design of muscles and tendons slits/holes to Insert them properly in the artificial implant [37]. That is, the mandibule and neck-cranial group of muscles is a risky-complicated zone for surgery with important vascular parts, essential nerves and glandules.

Creep, [67], constitutes an additional parameter in rolling surfaces, for instance, for external implants. It is very usual the use of FE method which is essential in contact mechanics, specially in hip implants. One of the most important problems to be sorted to implement and obtain acceptable results is the biomechanical angle between the system acetabular-cup—femoral-head. If that angle would be 0°, modelling and biomechanical functioning would be easier. What is more, since this group of forces project its biomechanical consequences along the femur, which is the longest bone of the body, the results for the normal walk are significant. For basic contact mechanics and FE methods/models, contact radius and maximum stress have been modeled from Hertz theory, [66], namely, ….

$$A = \left[\frac{3F_y\, R \left(1 - \nu^2\right)}{2E} \right]^{1/3} ;$$

$$\sigma_c = \frac{3F_y}{2\pi A^2} ;$$

Eq [5]

where R is the effective radius, v is Poisson ratio, and E is elasticity Modulus.

Mathematical models based on fundamental partial differential equations, [63], have been also used for hip replacement. For instance, by using heat transfer equation, Navier Stokes one, fluid dynamics flow, and stress-equilibrium PDEs [63]. Here it is detailed a primary formula of model for stress-equilibrium formula, which is used for implementation of FE models. Succintly,

$$\rho \frac{\partial^2 u}{\partial t} - \left(\frac{\partial \sigma_x}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} \right) = F_x \,;\, \sigma(\text{stress})\,;$$

$$\rho \frac{\partial^2 v}{\partial t} - \left(\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} \right) = F_y \,;$$

and,

$$\varepsilon_x\,(\text{strain}) = \frac{\partial u}{\partial x} ; \varepsilon_y\,(\text{strain}) = \frac{\partial v}{\partial y} ; \qquad \text{Eq [6]}$$

$$\text{then, } 2\varepsilon_{xy}\,(\text{strain}) = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} ;$$

with the fundamental equivalence,

$$\begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} d_{11} & d_{12} & \\ d_{21} & d_{22} & \\ & & d_{33} \end{pmatrix} \times \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_{xy} \end{pmatrix} ;$$

where u and v are displacements in x and y directions respectively, F loads in x and y, and sigma and epsilon stress and strain classical tensors. These formulas are developed to obtain a larger equation for final implementation [63]. These mathematical formuli seem to be complicated but in modern FE software can be used fastly and obtain good imaging sketches of the complete result [13,15,19,22].

The wear of a hip prosthesis is a complicated phenomenon, which generally depends on the contact status between the ball and the cup (i.e., friction regime), characteristics of the tribocouple, physiological conditions [60], production quality of the prostheses [61], lubricants [62], etc. For example, despite a low friction torque, the polymer-on-metal configurations exhibit higher wear, than metal-on-metal or ceramic-on-ceramic ones [63] due to the boundary lubrication regime between the wearing surfaces [64,65]. For the same reason, small-size metal-on-metal hip joints perform worse, than large-size ones [64]. Properly designed and manufactured metal-on-metal hip joint prosthesis work, *vice-versa*, under mixed lubrication regime [65], and ceramic-on-ceramic hip joints function even under hydrodynamic lubrication conditions [64], what provides extremely low friction—linked to the articular movement of acetabular hip, that is, number of rotations in a day is extremely high, arms and legs are basic in human daily movements.

The three principal wear mechanisms in hip joints were found to be adhesive wear, abrasive wear and fatigue wear [55], accompanied by tribocorrosion in the case of metal-on-metal configurations [60]. With time, one mechanism may change to another. For polymer-on-ceramic hip joints, adhesive wear of polymer with the subsequent formation of the tribolayer on the ceramic surface is characteristic. For polymer-on-metal configurations, both adhesive and abrasive wear mechanisms were reported, whereas the last was found to be more probable [61,62,63]. Surface fatigue in combination with three-body abrasion and tribochemical reactions was found to cause wear in the case of metal-on-metal tribocouples [60]. Despite the absence of clear literature data, for ceramic-on-ceramic configurations, surface fatigue and abrasion may be named as the most probable wear mechanisms.
For simulation of wear of a hip prostheses the Archard's wear law is usually applied [61,62]. Its is more convenient to present the integral equation from this model once obtained from the finite elements method mathematical development. According to it, the wear volume V (mm^3), vanished from the contact surface, may be determined as

$$W = \int_{\Gamma_{t0}}^{\Gamma_t} \int_{S_{t0}}^{S_t} K_w \, \sigma \, dS \, dA \quad ;$$

Eq [7]

where Γ is the contact surface, mm^2;S_t is the sliding distance, m; k_w is the wear coefficient; $k_w = (0.18–0.80)\times10^{-6}$ mm^3/Nm for the ultra-high-molecular-weight polyethylene (UHMWPE) in tribocouple with the stainless steel [61,63], and $k_w = 0.10–0.31 \times 10^{-6}$ mm^3/Nm for UHMWPE in tribocouple with alumina (Al_2O_3) [1];σ is the normal contact stresses (Hertz contact stresses), N/mm^2, which may be calculated by the corresponding formulas.The maximum normal force (F_N) may be taken as $F_N = 3500$ N [61] and the swing angle of foot is 23 degrees in the forward and backward directions.For the real simulations, the volumetric wear rate (mm^3/year) is usually calculated. By the literature data, it is in the range of 5–50 mm^3/year. The difference between the modeling of hip and knee is given mainly by the methods used. In knee implants, because of the extreme loads that are acting over a rather small bone surface, the usual method is Finite Elements modeling, with precise distribution of stress and strain magnitudes [47,51]. However, substitution of tibial parts are also made with metallic implants, e. g., titanium plasma spray coatings [47,51]. Archard's wear law has several formuli developments depending of the type of implementation an dis extensively applied in Tribology and Biotribology.

Spinal biomechanics modeling is also usually focused on Finite Elements Modeling, [Casesnoves, ref 12]. In spinal reconstruction, a large number of prostheses types are used given the complicated and risky system of the vertebral biomechanics. Finite elements are combined with other biomechanical constraints in order to obtain precision and functionality.All in all, in Tables IV, a succinct brief of biotriboly are presented with advantages and inconvenients. The extension of the optimization/simulations of Appendix 1 will give in following publications additional algorithmic data for this important field of the Biotribiology.

IV. NOTES OF NONLINEAR OPTIMIZATION METHODS AND ALGORITHMS

In previous publications, a modern review of main optimization methods was developed with numerical examples. In [55], these methods are described for complementary information and graphical optimization is set in its proper section. We refer the reader to that publication to find more data and complementary optimization simulation methods and erosion and corrosion models in Appendix 2.

TABLE III

SELECTED MEDICAL-BIOTRIBOLOGICAL MODELS						
BIOTRIBOLOGICAL MODELS/ALGORITHMS FOR HIP ARTHROPLASTY						
NAME AUTHOR AND/OR REF	**TYPE**	**SETTING VARIABLES**	**ADVANTAGES**	**WEAKNESSES**	**USAGE GRAD E**	**COMMENTS**
Classical General Model Jin and others [51]	T1	Hardness, Load, Rotation Velocity	Simplicity	Accuracy to be improved and specified	2	classic model for further developments
Rabinowitsch Model for lubrication [53]	T2	Viscosity constants and shear-stress	Specific for lubrication and minimize wear	Required precision in constants	2	useful
Carreau's Model [53]	T2	Viscosity constants and shear, shear rate	Evolution of previous model with shear rate	Not useful totally for synovial fluid	2	Derived models are more improved
Archard's wear model	T1	Finite Elements Integral equation	Integral/Differential model precision	More computational time	2	Step forward towards a infinitesimal model
Integral-Differential model for basic Hip-Implant Wear Determination [Casesnoves, 2017]	T2	Direct empirical computational-determination of Hardness continuous function	Integral-differential calculus applicable	Lab samples required, statistical requirements	2	This model is in mathematical development and validation actually
Contact Mechanics Hertz parameters modelling	T1	Radius, Elasticity Modulus, and Poisson ration	Implementation on FE methods	Large computational-geometrical work	1	For FE methods but also applicable in contact biomechanics
Stress-Strain Equational Model for Hip implants	T1-T2	Stress and strain matrices mostly	Applicable also in TE methods	Partial differential equation, not simple	1	Useful in several development, there are more similar modelss
Barnwell Classification	T1-T2	All range of variables	General to be improved	Initial approach	1	First modelling
Polymer-Matrix Model	T2	Load, velocity, timey	applicability	Only polymers	1	useful
BIOTRIBOLOGICAL MODELS/ALGORITHMS FOR KNEE ARTHROPLASTY (THOSE MODELS ARE USUALLY DEVELOPED WITH SPECIFIC FINITE ELEMENTS GENERIC METHOD)						
NAME	**TYPE**	**SETTING VARIABLES**	**ADVANTAGES**	**WEAKNESSES**	**USAGE GRAD E**	**COMMENTS**
Finite Elements Modelling	T1	Physical variables	Extensive and multifunctional applications	Errors at implementation	2	Simulation processes feasible
Corrosion Models applied on solid metallic implants for knee [52]	T2	Chemical parameters	Specific accuracy	For durability of metal-coated knee implants	1	useful
BIOTRIBOLOGICAL MODELS/ALGORITHMS FOR SPINAL ARTIFICIAL IMPLANTS						
Dynamics of deformable Compliant Artificial Intervertebral-Lumbar Disks [Casesnoves 2017]	T1-2	THE NUMERICAL REULEAUX METHOD APPLIED ON ARTIFICIAL DISKS [Casesnoves, 2007] Synergic model for deformation-biomechanical-stress of artificial disks	Applicability on deformable solids dynamics/kinematics	Computational algorithms And framework necessary	2	Connected with Deformable solid theory and General Numerical Reuleaux Method (Casesnoves, 2007) Modelling
Finite Elements Modeling	T1	Corrosive activity,time, and force acting on the oxide layer	Both corrosion and erosion determination Extensive applicability	Specific for tubes and boilers	2	Largely developed by Ots with series of equations

V. MATHEMATICAL METHODS FOR NUMERICAL-GRAPHICAL NONLINEAR OPTIMIZATION WITH ALGORITHMS

This section is intended to explain several new/improved methods for direct approximated graphical optimization. Advantages of this method are the nimble/fast search of the global/local minima/maxima and the sharp imaging visualization of the objective function shape and spatial geometry-distribution along the selected interval. Inconvenients are the limitation to 2 variables in plane x/y, and the strict necessity of simulation-graphical accurate software instead simple numerical-programming software, e.g., a FORTRAN compilator. Then it is defined,

Definition 1 [Casesnoves, 2017].-Graphical nonlinear optimization[2] is a constructive approximated method to set the global/local minima/maxima of an Objective Function provided two strict conditions,

-computational graphical simulation of the objective function is precise and imaging software is sufficiently proved as accurate in its imaging algorithms.

-Objective Function mathematical development and constraints, are strictly mathematically linked to the graphical implementation.

Proposition 1.-Approximated Optimization by Separation of Variables [Casesnoves, 2017].-Any OF can be developed/expanded by variables separation method, to obtain several approximations kinds of equations to fastly calculate minima/maxima and set the surfactal imaging-representation of that OF.

Proof: beginning with a classical L_2 OF,and for simplicity taking one-term,

$$F(\vec{x}_i) = \|\vec{a} - f(\vec{x}_i)\|^2 = \|\vec{a}\|^2 + \|f(\vec{x}_i)\|^2 - \\ - 2\|\vec{a}\|\,\|f(\vec{x}_i)\| \cong [\text{separation of variables expansion}]; \qquad \text{Eq [8]}$$

And the expansion divide the minima calculation in a series of independent terms which are multiplied or summed, giving several options to get further minimization/maximization approximations [23,35,36,37,39,56,72].

VI. COMPUTATIONAL SIMULATIONS OF BIOTRIBOLOGY AND MECHANICAL MODELS WITH PROGRAMMING RECIPES

The beguine of this section is with 3d graphical optimization examples and Region of Interest selection methods. We continue with previous research models both for simplicity and clarification in learning.This example of 2 variables simulation is done with the Menguturk and Sverdrup (1979) model, developed as an empirical erosion model for carbon steel material eroded by coal dust. The model shows that erosion is largely a function of particle impact velocity and angle. It is important to remark that what is shown with is model is totally applicable on any bioengineering mathematical mdel. The selection of this algorithm is justified for primary new 3D simulations with surfaces in an attempt to demonstrate the practical materials engineering/bioengineering usage of this kind of 3D representation—in other words, the cursor of the software can give the numerical desired values for lab or experimental of any type.The model for small and large particle impact angles is given as a easy tool to carry out a graphical optimization, as follows,

$$E = v^{2.5} \times \left[\left(1.63e-6\bullet(\cos\alpha)^{2.5}\right) + \left(4.68e-7\bullet(\sin\alpha)^{2.5}\right)\right];$$

This is the simplest equation valid for particle impact angles ≥ 22.7°. For angles < 22.7°, the model formulation reads],

$$E = v^{2.5} \times \left[\left(1.63e-6\bullet(\cos\alpha)^{2.5}\bullet\sin\left(\frac{180}{45.4}\,\alpha\right)\right) + \left(4.68e-7\bullet(\sin\alpha)^{2.5}\right)\right];$$

Eqs [9]

where E is the erosion rate in mm3 g−1 , and impact velocity and angle α, measured in m s−1 and radians,respectively. The volumetric erosion rate (mm^3 g−1). That is, 2 variables. This simple equation illustrates the following series of computational simulations, because the implementation of programming matrices algebra-operations is fast, although the application of the matrix-algebra concepts in programming requires special calculations to obtain

[2] **Graphical-3D Nonlinear Optimization Method was created by Francisco Casesnoves at Tallinn University of Technology in December 2016. The method was a result of the numerical-mathematical study with Fortran and F# Software of lab experimental data.**

accurate/realistic/precise results.

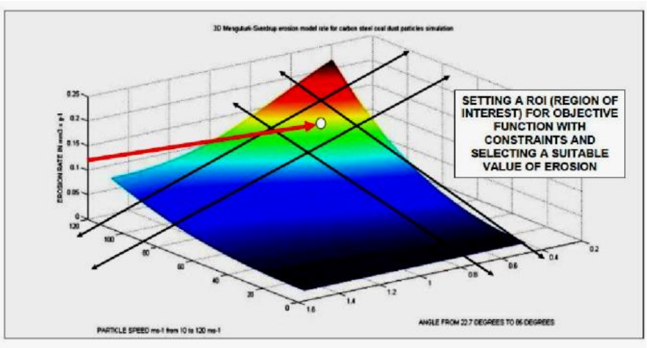

Fig 2.- [Enhanced in Appendix 1] Mathematical-geometrical Method of selection of graphical optimization values for a ROI, (region of interest), within the objective function with constraints [Casesnoves,2017]. The picture is a matrix-simulation for a velocity range from 10-120 ms^{-1} of the model and matrices 1000x1000, quite large numerical imaging programming—running time around 4 seconds, perspective-imaging change time about 10 seconds, taking into account the large matrices. The projection of this kind of graphical optimization onto large series of different models is realistic and mathematically acceptable—for instance, the subsequent simulations of the hip implant wear equation. The setting of constraints in this type of optimizations yields to a new concept in ROIs selection to save time and lab tribotesting.

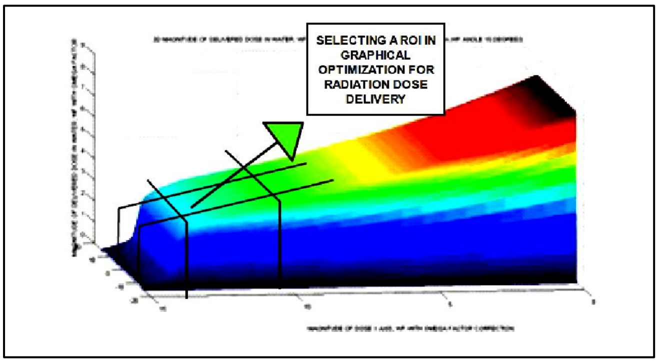

Fig 3.-Graphical 3D optimization example, [Casesnoves,2017], of a radiotherapy dose delivery selection of a Region of Interest with constraints in Matlab—enhanced in Appendix 1. Any numerical data within the ROI can be determined with the design of the software, and selection of the optimal values are straightforward.

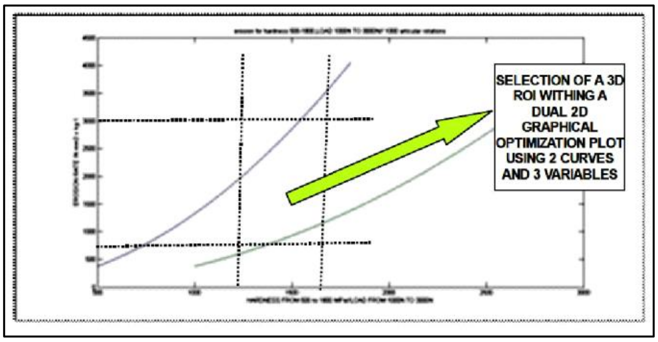

Fig 4.-Graphical 2D-3D optimization example, [Casesnoves,2017], of a hip implant simulation with a selection of a Region of Interest with constraints in Matlab—enhanced in Appendix 1. This software is more complicated for the subroutine to conform the optimal graph to select further the ROI. Any numerical data within the ROI can be determined with the design of the software, and selection of the optimal values are straightforward. Note that the choice of the ROI is essential to get comparison sharing all variables.

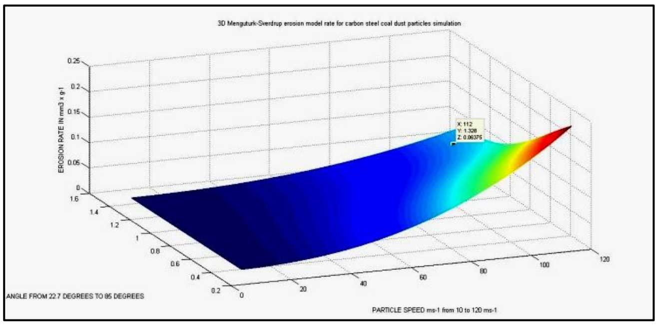

Fig 5.- Pictured with cursor-magnitude-inset, the narrowly-same numerical Matlab-2009-10, jpg format, surface-matrix-simulation for a velocity range from 10-120 ms^{-1} of Menguturk and Sverdrup (1979) model and matrices 1000x1000, quite large numerical imaging programming. Cursor indicates speed 112 ms^{-1} , angle of particle 1.326 radians, and erosion rate about 0.084 mm^{3} g^{-1} . The choice of the imaging perspective is intended to show the smooth surface growth towards the maximum speed and angle optimal value that gives the maximum erosion magnitudes for the model. Note the the practical utility of the cursor to search optimal experimental-theoretical values for modeling research both for simulation and nonlinear optimization.

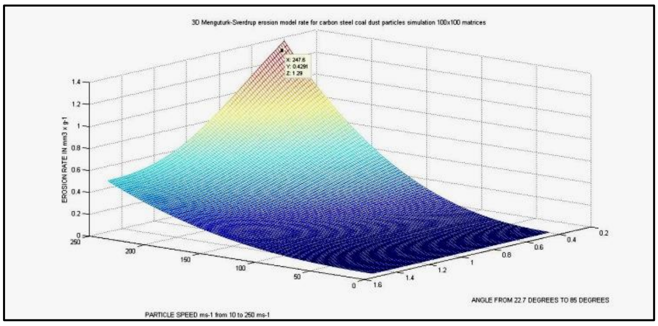

Fig 6.- This simulation shows maximum-model cursor-values of speed about 247 ms^{-1} , angle of particle 0.4291 radians, and erosion rate about 1.29 $mm^3\ g^{-1}$ .So pictured with inset-cursor it is a different simulation of the previous figure in also different angles, to show the surface extension, jpg format, a matrix-simulation for a velocity range from 10-250 ms^{-1} of the model and matrices 100x100, rather simple numerical imaging programming—running time around 2 seconds, perspective-imaging change time about 1-3 seconds, taking into account in this case the small matrices. Cursor in at peak of The choice of the imaging perspective is intended to show better the smooth surface growth towards the maximum-peak speed and angle optimal value, with the surface-sheet totally pictured, that gives the maximum-medium-minimum erosion magnitudes for the model, and also the surface part for minimum values.

Following with 2D type of simulations., this example of 2 variables simulation is developed with the the classical wear of hip implants prosthesis mainly. It is simpler programming and can be easily executed both in Freemat or Matlab as it is here presented.

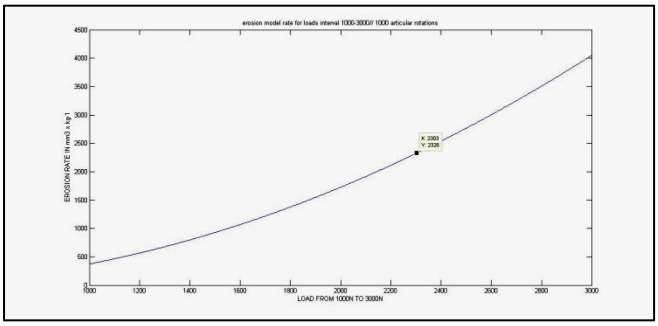

Fig 7.-In this 2D-simulation-program for hip implant in Equation [1], the load range was [1000,3000] in MPa. This program was designed for erosion rate versus load with Matlab subroutines for 1000 rotations. The simulation with inset cursor is showing selected data in the plotted curve. It was selected a cursor-point with higher than average load value. The matrices of imaging programming are 1000x1000.

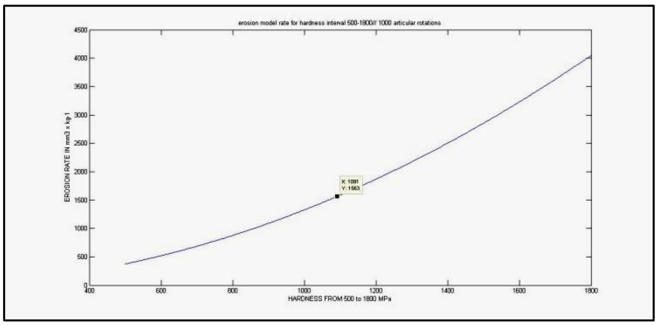

Fig 8.-In this 2D-simulation-program for hip implant in Equation [1], the hardness range was [500,1800] in MPa. This program was designed for erosion rate versus hardness for 1000 rotations. The simulation with inset cursor is showing selected data in the plotted curve. It was selected a cursor-point with middle-hardness value. The matrices of imaging programming are 1000x1000.

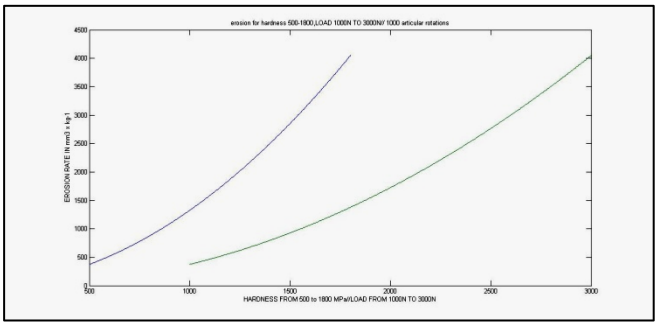

Fig 9 [enhanced in Appendix 1]**.-**In this 2D-simulation-program the software was specially designed to show both previous images in the same graph for comparison—ranges are just the same.Hardness range was [500,1800] in MPa. This program was designed for erosion rate versus hardness and load for 1000 acetabular-cup rotations. The simulation with inset cursor could show selected data in the plotted curves. The matrices of imaging programming are 1000x1000. In Matlab, as it also happens in Freemat, this is not the unique subroutine that can be used for 2D graphs.

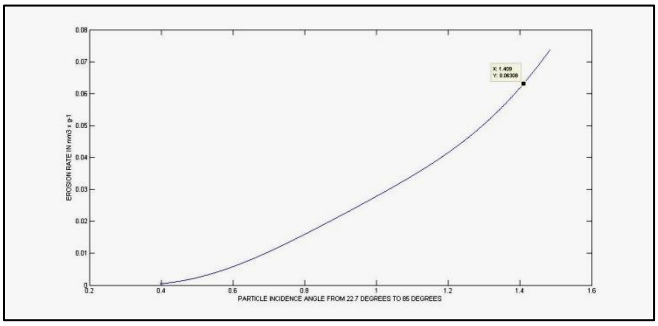

Fig 10.-In this 2D-simulation-program the speed range was from 10-120 ms^{-1}—Menguturk and Sverdrup (1979) model. This program was designed for erosion rate versus angle range of particle incident. The simulation with inset cursor is showing angle of 1.409 radians and erosion rate about 0.063 $mm^3\ g^{-1}$. It was selected a cursor-point with rather extreme incident-angle value. The matrices of imaging programming are 1000x1000.Note the cosine and sine variations and exponentials low values in the model according to changes within the velocity/angles range.

To summarize this section,in Appendix 1, pictured table, a series of optimization trials in non-linear least squares for wear in biotribological hip prostheses and mechanical systems—usually done with lsqnonlin subroutine or similars. This group of data is an improvement of computational work presented in previous publications. The laboratory measurements were set randomly, and the most important is the well-performance of the subroutines of Matlab for nonlinear optimization. The hip implants materials are selected as significantly different, with hardness interval from metal to the highest values of ceramic-ceramic implants [51, 61,62]. In Freemat there are also a number of subroutines with nearly similar applications, or the reader can find a Freemat program example for Newton-Rapson method with Hutchings model from previous contributions [55].

VII. IMAGING AND GRAPHICAL NONLINEAR OPTIMIZATION METHODS WITH SPECIFIC HIP IMPLANTS 3D SETTINGS

In this section global-local minima with a random simulated laboratory measurements are computed in order to obtain a 2D plot series of global minimum visual location. In the same way, a number of imaging optimization pictures are shown with additional comments.

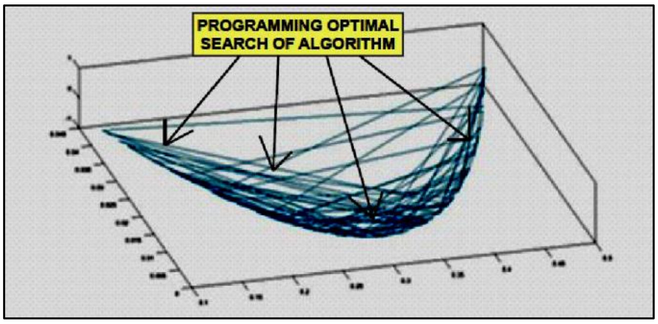

Fig 11.-In this Freemat 3D-simulation-program the classical Hutchings model search for the minimum with random simulations is shown. The programming search for global minimum is seen sewing points of the curve. Since values of simulations are stochastic, the program is joining these curve model points in the neighbourhood of the minimum. This picture is intended to show both the several alternatives in nonlinear optimization software, e. g., Matlab and Freemat, and the easy use of all this number of subroutines with sharp intuitive-visual interpretation—in other words, for non-specialized researchers in optimization, only with basic learning of concepts the practical caption of the results is caught up.

The new practical concepts in approximated/constructive optimization have derived from the current available software facilities and applications. A model of hip implants is developed and simulated in 3D with graphical sharp images. It is not unfrequent that lab experimental requires fast calculations, roughly speaking approximated, to try tentative trials or get a quick view of maximum and minimum, usually local, optimal values of a model with/without constraints. From Proposition 1 and Lemma 1, it can be guessed the availability to represent any 3D Objective Function with/without constraints in a graphical way.

The significant improvements of the 3D/2D graphical software and the extensive choice of tools available in the graphics prompts, obtain the maximum of a function in a previously selected range with the simple program and parameters range takes a few seconds. Complementary, errors, residuals and even with a few improvements in the program determinations coefficients can be calculated.

For example, in previous figures the approximated local maximum of the function is easily determined by the use of the cursor. Just the same approach for the approximated local minimum determination can be done, and further ROIs of constraints can be calculated.

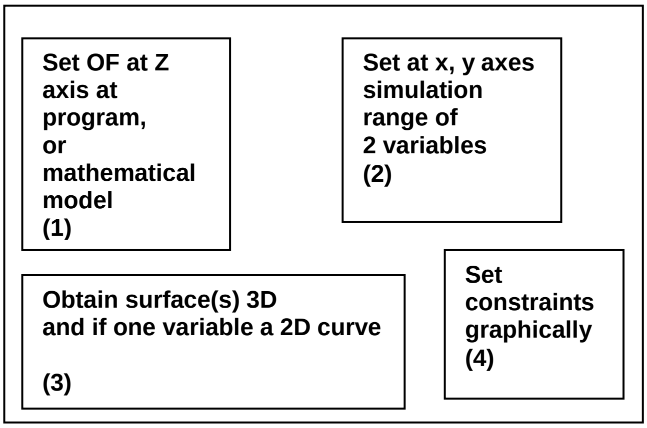

Diagram 2.-Basic application of graphical optimization and setting of objective function.

Furthermore, it is possible to try a constructive approximation with straight lines and even curves, so settings constraints or constraints groups in 3D. That is, fixed a value for one variable, we drag the cursor in that direction to find the maximum or minimum of the z axis objective function obtaining at the same time the optimal local value of the other axis variable. That is, we have set an upper graphical constraint for one parameter and found the search for both optimal values in the other parameter and the z-axis objective function. In Figs 16,17 an even more evident instance is shown with a radiotherapy dose distribution of radiation dose distribution—from the author's previous publication, with new software in Freemat, that has very explicit imaging simulations examples [36,54]. The global maxima line of the radiation dose distribution is sharply found and just the same occurs for the global minima—minima and maxima are in a line since the distribution in 3D is symmetric. Therefore, to use this method when, for example, we are designing further programs of simulations/optimization and the need is to get a caption of approximate values is suitable and practical—and this happens usually in engineering fast experimental works/trials.

Advantages of this method are a quite series ones, provided that the program for simulation is precise and accurate—and this is a mandatory condition. The fastest method to check whether a simulation is accurate is to carry out random calculations and verify all the interval ranges precisely.

Not all the laboratory staff are experts in programming and optimization, and instead they can get sharp learning from this graphical method. In addition, it is not necessary to design more optimization codes, e. g., a multiobjective optimization program, to obtain a local minimum for any selected interval. Other significant advantage is the fact, provided the accuracy of the simulation, that to use a searching-optimization program could yield wrong results from an inconsistent choice of the initial search. However, using the graph, if there are several concavities in the objective function surface, to locate the local minimum is visually fast/precise instead.

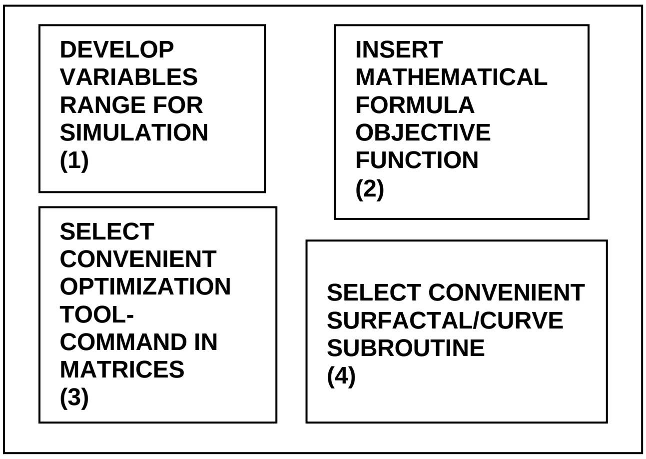

Diagram 3.-Flow chart of a graphical optimization program (basic).

Definitely, the constant progress/improvements in software for simulations or optimization graphs justify this usage for practical engineering trials and experimental. Disadvantages of this method exist obviously, since it is an approximated method, are the simplification/approximation of data obtained, and the limitation of the function to 3D and a closed interval range of parameters. In conclusion, it is suggested this method for fast and visual optimization with simple computational programming and convenient tolls at prompt.

While using Matlab software, for instance, the cursor can determine the optimal point of intervals, but with Freemat it is not possible, only to get a general overview of the surface objective function and guess the regions of maxima and minima. However, imaging both in Matlab and Freemat is overall acceptable and good for their respective subroutines.

In the following, a series of figures with 3D plots are shown and commented—both for hip implant equation and a Triple Gaussian Model in radiation therapy.

According to previous simulations, we pass on proper biomedical models such as hip implants wear basic formula. This deals with direct imaging software results of objective function representation of hip implant equation [1] subject to realistic experimental data from references. Each image has specific software developed to prove the utility of the presented mathematical-graphical method(s). The formula developed in the following serias of simulations, Eq [1], reads,

$$W = K \bullet (L\ X)/H \ ;$$

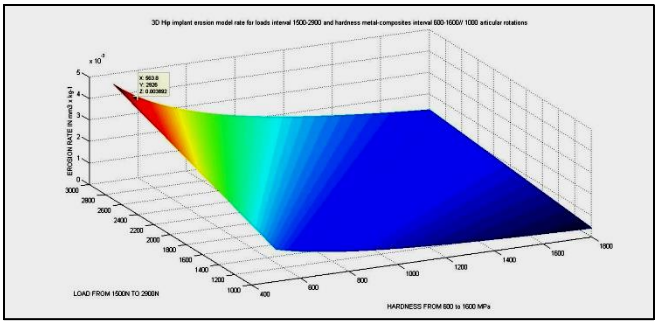

Fig 12.- [Enhanced in Appendix 1] Maximum of Equation (1) model for hip implants with cursor inset showing numerical values. Matrices are 1000x1000, and Matlab sharpness of this image is very good, and running time is acceptable.

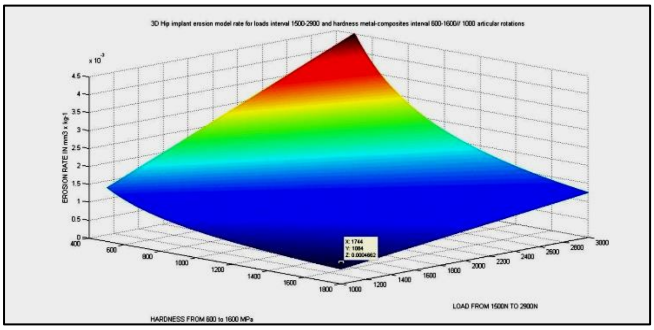

Fig 13.- [Enhanced in Appendix 1] Minimum of Equation [1] model for hip implants with cursor inset showing minimum numerical values. Matrices are 1000x1000, and sharpeness of this image is very good, and running time is acceptable.

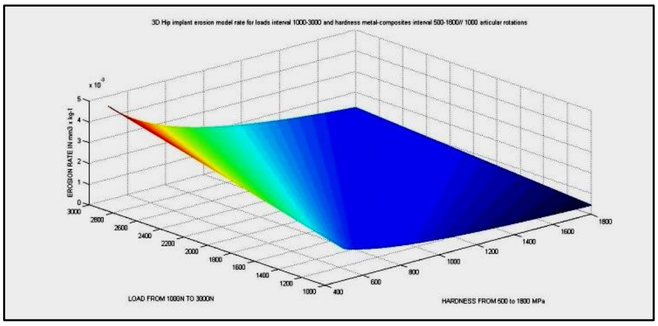

Fig 14.-Maximum of Equation (1) model for hip implants without cursor but convenient angle showing numerical values for erosion rate. Matrices are 1000x1000, and Matlab sharpness of this image is very good, and running time is acceptable.

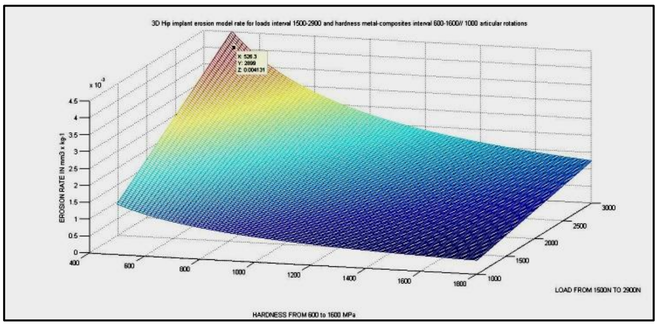

Fig 15.- Simulation of Equation [1] maximum of Equation [1] model for hip implants with cursor inset showing numerical values. Matrices are 100x100, and sharpness of this image is very good, with running time is acceptable.

To support all these arguments with additional-variated mathematical development, a graphical radiotherapy simulation is shown in next picture. It corresponds to a Triple-Gaussian radiotherapy model, so-called AAA, analytic anisothropical algorithm, algorithm. In particular, a corrected model representation for a wedge filter at depth of 15cm and 18Mev beam physical parameters. This image was done with Freemat instead of Matlab, as used in previous radiotherapy contributions, [36,54], to prove the adaptation of the designed simulation-optimization software on several types of programs.

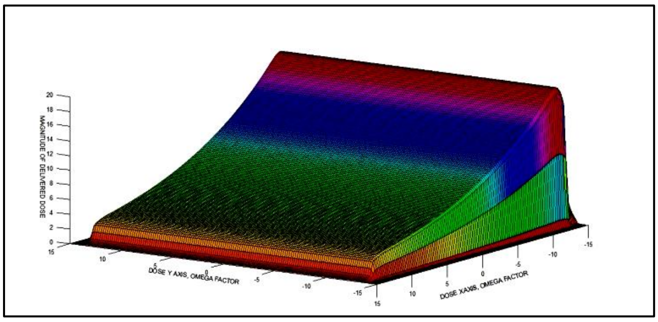

Fig 16.-A Freemat 4.1 (Samit Basu General Public License), 3D objective symmetric-function of radiotherapy photon-dose surface with clear determination of the straight marginal lines of global minima/maxima in radiation delivery dose distribution. Matrices are 150 x 150, and with Freemat 4.1 the running time is longer than Matlab—at the same time the matrices size for normal running-time is lower in standard microprocessors. This simulation is Freemat original based on previous computational contributions [refs].For 150 x 150 matrices imaging view setting takes about 5 seconds, and spatial-changes of imaging-set about 7 seconds. If 50x50 matrices are used, the time is reduced around 2 seconds.

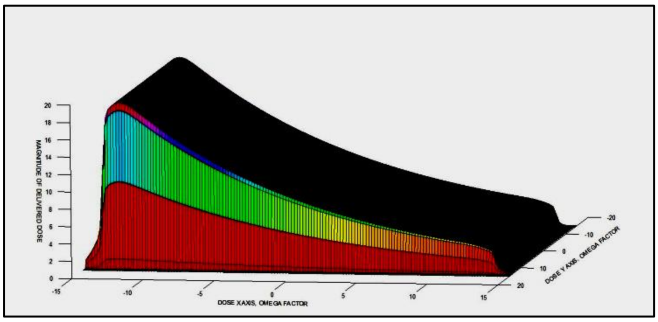

Fig 17.-A Freemat 4.1 (Samit Basu General Public License), 3D objective symmetric-function of radiotherapy photon-dose surface with clear determination of the straight marginal lines of global minima/maxima in radiation delivery dose distribution. Matrices are 150 x 150, and with Freemat 4.1 the running time is longer than Matlab—at the same time the matrices size for normal running-time is lower in standard microprocessors. This simulation is Freemat original based on previous computational contributions [refs].For 150 x 150 matrices imaging view setting takes about 5 seconds, and spatial-changes of imaging-set about 7 seconds. If 50x50 matrices are used, the time is reduced around 2 seconds.

VIII. BRIEF MARKS OF F# FUNCTIONAL PROGRAMMING APPLICATIONS IN COMPUTATIONAL SIMULATIONS

F# programming, [73], a non-classic programming language, shows advantages and inconvenients to simulate some kind of formulation. This language, for instance, in a Visual Studio compiler, can download a number of packages to carry out several options to be included in the codes—and also interact with web information and html programming. Inconvenients, again, of F#, apart from cyber-security questionable use when programming design, are its limitation in numerical methods compared to other specific software, whether as it is a different construction sometimes simpler, whether in other cases results more complicated, related to other languages—namely the powerful-precise FORTRAN in numerical methods [37,56].

In the following, a hip implant extremely simple code is shown, [Casesnoves,2017], for a tentative program to be developed in double precision and more extensive features in F#. In addition, it is presented the F# interactive output at prompt, that gives the random simulation values of the program.

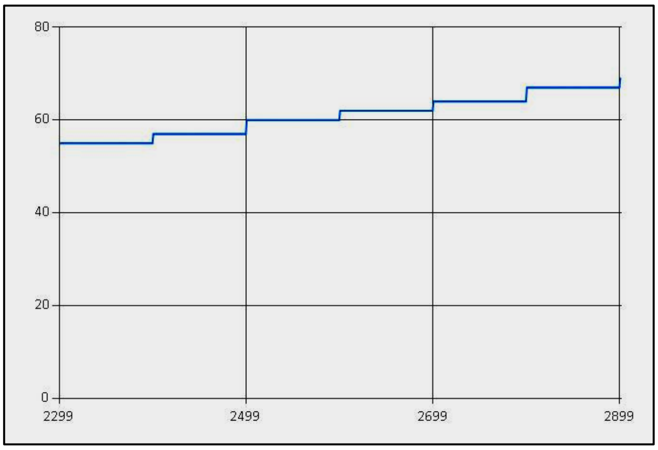

Fig 18.-A F# chart developed with functional programming software in visual studio for a hip implants erosion model simulation.It is seen sharply the good image given by the compiler, although other types of programming software facilities could make better and faster plots without downloading chart-F# specific packages. This program was developed in F# by the authors originally [Casesnoves,2016].

```
open FSharp.Charting
open FSharp.Charting.ChartTypes
//approximate value of grup of constants.We simulate a chart of
implant wear with loads from 2300 to 2900
//taking K value approximated as 37e-2. X axis is load and y axis is
wear mm3 after 10e6 cycles of
//biomechanical movement and we remark that this is a simulated
approximation according to references values studied.
Chart.Line([for x in 2300 .. 2900 -> x,(x/100)*12*2/10]).ShowChart()

//
let randomPoints = [for i in 0 .. 1000 -> rand(),  rand()]

Chart.Point randomPoints

let randomTrend1 = [for i in 10.0 .. 0.1 .. 200.0 -> i, 5.1*sin i *
rand()]//velocity
let randomTrend2 = [for i in 10.0 .. 0.1 .. 10.0 -> i, sin i *
rand()]//density
```

Fig 19.-A F# simple code to generate random hip implant simulation, for further improvements in formuli and double-precision. It was developed with functional programming software in visual studio for model simulation.It is seen sharply in previous picture the good image given by the prompt interactive, although other types of programming software facilities could make better windows and faster debugs. This program was developed in F# by the authors originally [Casesnoves,2016].

```
val randomTrend1 : (float * float) list =
  [(10.0, -0.1404662546); (10.1, -2.293313682); (10.2, -0.4796590218);
   (10.3, -2.565416081); (10.4, -3.606794148); (10.5, -2.266275941);
   (10.6, -3.395426854); (10.7, -3.575901385); (10.8, -4.231986696);
   (10.9, -2.471837757); (11.0, -4.917058251); (11.1, -1.521487212);
   (11.2, -3.408112815); (11.3, -4.747778067); (11.4, -3.276653312);
   (11.5, -3.014259536); (11.6, -2.358532016); (11.7, -3.050279046);
   (11.8, -1.725775824); (11.9, -1.913584685); (12.0, -1.997005739);
   (12.1, -2.074145695); (12.2, -1.627197805); (12.3, -0.7537396074);
   (12.4, -0.2311059042); (12.5, -0.2110616309); (12.6, 0.1217366107);
   (12.7, 0.5014503174); (12.8, 0.1745334274); (12.9, 1.074303317);
   (13.0, 1.451865401); (13.1, 2.394991471); (13.2, 1.429399931);
   (13.3, 3.175968384); (13.4, 0.78170315); (13.5, 3.459722022);
   (13.6, 1.188891998); (13.7, 3.893001325); (13.8, 2.549692091);
   (13.9, 0.2632960671); (14.0, 0.3871546167); (14.1, 2.572510299);
   (14.2, 1.413911938); (14.3, 4.931114415); (14.4, 1.78025936);
   (14.5, 4.518372979); (14.6, 3.205197617); (14.7, 3.445987855);
   (14.8, 3.587155339); (14.9, 0.7329472398); (15.0, 0.9765795428);
   (15.1, 1.060163802); (15.2, 2.307318118); (15.3, 1.762342793);
   (15.4, 0.6408115451); (15.5, 0.1538954116); (15.6, 0.4554263128);
   (15.7, 0.02326797247); (15.8, -0.1788710209); (15.9, -0.2241753176);
   (16.0, -1.167613296); (16.1, -1.916410736); (16.2, -1.409758032);
   (16.3, -0.576836707); (16.4, -2.633927112); (16.5, -0.1485404028);
   (16.6, -3.28121609); (16.7, -3.212355205); (16.8, -3.479961159);
   (16.9, -4.050878599); (17.0, -1.979813082); (17.1, -3.610775974);
   (17.2, -1.297227257); (17.3, -2.217032697); (17.4, -2.68504735);
   (17.5, -1.119521787); (17.6, -3.032619744); (17.7, -4.239053458);
   (17.8, -0.884402902); (17.9, -1.351877714); (18.0, -3.52988045);
   (18.1, -3.165478399); (18.2, -2.608622658); (18.3, -2.527956556);
   (18.4, -0.7730081439); (18.5, -0.5477665466); (18.6, -1.250858038);
   (18.7, -0.4577508974); (18.8, -0.1302407619); (18.9, 0.01565350602);
   (19.0, 0.01165143649); (19.1, 0.8827452538); (19.2, 0.8071007276);
   (19.3, 0.664913319); (19.4, 0.6879906614); (19.5, 0.2876200617);
   (19.6, 3.198532505); (19.7, 0.2878878552); (19.8, 0.7074857359);
   (19.9, 1.418498008); ...]
val randomTrend2 : (float * float) list = [(10.0, -0.1776498577)]

>
```

Fig 20.-A F# simple output in interactive from the previous program [Casesnoves,2017]. Data in prompt is well-presented and storage of files and execution usually does not show too many complications compared to other software programming in numerical methods, such as Freemat.

IX. INTEGRAL-DIFFERENTIAL MATHEMATICAL MODEL CONSTRUCTION FOR WC-Co REINFORCED METAL COATINGS, EXPERIMENTAL-THEORETICAL METHOD

This section is focused on general fundamental steps to develop a mathematical model starting from experimental and heading towards the theory.

Biomedical implants are manufactured with a large type of materials. Among them, metal coatings constitute an important variety used in manufacturing both in medical devices and internal/external biomedical implants, subjected to histocompatibility always—provided that this condition is applicable on contact tissue-material surfaces, particularly well-accomplished by titanium. There are two essential requirements for biomaterials, specially when implants are internal, namely, biocompatibility or histocompatibility, and biodegradability [8].Additional desirable/compulsory properties are appropriate porosity, bioactivity, mechanical strength, adequate surface finish, and easily manufactured and sterilization conditions. Among this kind of biomaterials, the promising shape memory/development, and geometrical-conformally-adapted materials are creating a new specific branch of applications in biomedical engineering.

Recently, [8], reinforcements are used to increase titanium hardness, such as titanium boride in a titanium matrix—explicitly Ti-TiB_W . Published results show that this kind of composite is not cytotoxic and has an acceptable hemolysis level.

The material of this model-example, composite Fe-based hardfacings with coarse WC-Co reinforcement types are used in industry but closely similar materials are manufactured also for medical devices with the constraint of histocompatibility when they are internal ones.

In this example the model construction in its principal outlines is detailed for Fe-based self-fluxing alloy (FeCrBSi) with spherical WC-Co hardmetal reinforcement. In biomedical implants this kind of composites are used but with histocompatible metal titanium, when the implant is internal [8].

Conceptual mathematical an danalytic geometry problem in this kind of coatings is the non-constant hardness distribution, phenomena that occurs in the matrix, hardface, and at interface—absolutely necessary to remark in this point that interface constitutes an essential part linked to the binding between matrix and reinforced hardface. This implies that if hardness is not constant, wear is not also. Therefore, the material modelling is more complicated. What is meant here is a method to construct a model that can be generalized with different equations/algorithms.

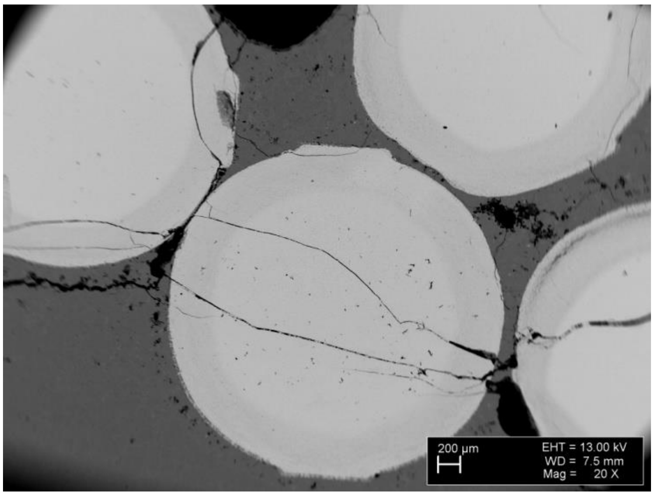

Fig 19.-Image of matrix, hardface and transition zone in composite Fe-based hardfacings with coarse WC-Co reinforcement [Andrei Surzhenkov, Taavi Simson and Colls, Tallinn University of Technology Lab]. Images of composite obtained with scanning electron microscope (SEM) EVO MA-15 at Tallinn University of Technology Lab.

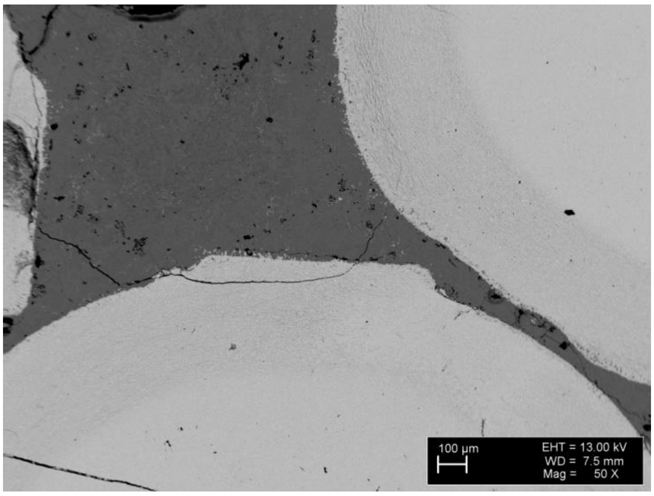

Fig 20.- Enhanced image of matrix, hardface and transition zone in composite Fe-based hardfacings with coarse WC-Co reinforcement [Andrei Surzhenkov, Taavi Simson and Colls, Tallinn University of Technology Lab]. The matrix average distances from the minimum hardness points to the borders of hardface are measured randomly using images and, for instance, Monte-Carlo Method [Casesnoves, 2017, refs]. Images of composite obtained with scanning electron microscope (SEM) EVO MA-15 at Tallinn University of Tecnnology Lab. Interface crown is sharply seen at the right-upper corner inset. Although minimum is coating-surface extension, interface is essential in the binding and cohesion of the composite.

TABLE IV

Type of component	**Type of material**	**Chemical composition [wt.%]**
Matrix	Fe-based self-fluxing alloy (FeCrBSi)	13.72 Cr, 2.67 Si, 0.32 Mn, 2.07 C, 0.02 S, 3.40 B, 6.04 Ni, bal. Fe
Reinforcement	Spherical WC-Co hardmetal	85 WC, 15 Co

Table 4 .-Detailed composition of the laboratory sample for modeling construction. The geometry of the reinforcement in this case is spherical, not angular. The spherical hardmetal size in this manufactured composite can be considered rather high, which is a geometrical advantage for the model construction.

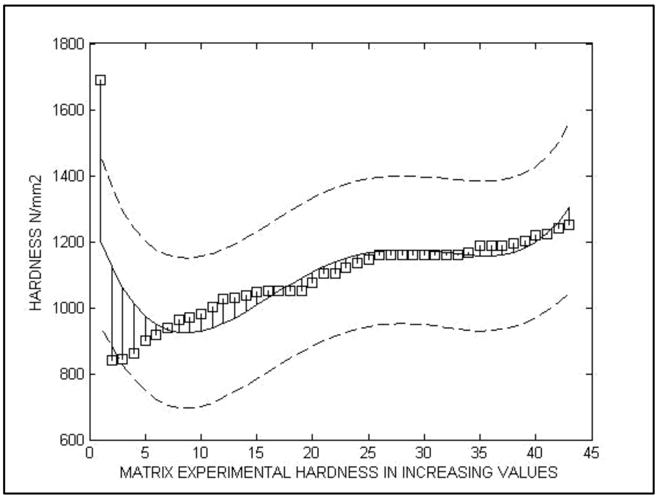

Fig 21.-Pictured, Matlab 4-degree-polynomial numerical fitting with error plotting intervals of matrix experimental hardness in intervals of average distance from center of matrix to the next hardface spherical spot. This is calculated with random measurements

over the ultramicroscopic images instead the classical Weibull distribution [1,9,23,37].It is seen sharply the acceptable goodness of the approximation, with the exception of the beginning of the curve—these extremal-dispersed values are usually discarded for model construction. In the x axis 43 increasing measurements that correspond each one to an statistically distance calculation from matrix center geodesic to interfaces around hardfaces.

TABLE V

EXAMPLES OF EXPERIMENTAL DATA FOR MODEL DEVELOPMENT [TALLINN UNIVERSITY OF TECHNOLOGY LABORATORY,ESTONIA]	
NUMBER OF MEASURE	**HARDNESS [MPa]**
1	689
2	841
4	861
30	1161
35	1189

Table 5 .-Experimental data examples of matrix hardness carried out at Tallinn University of Technology Mechanics Lab. These 43 values where implemented to construct the mathematical model for matrix.

The mathematical development begins with the assumption that hardness is not constant as a results of the polynomial fitting of data of **Fig** , and it s equation related to distance reads,

$$H(s) = 10^3 \bullet \left[(-0.0003)x^3 + (0.0094)x^2 + (-0.1050)x + 12984\right];$$
$$\text{Residual of numerical fitting} = 657.6564;$$

Therefore, for the model in matrix, it is straight to guess that hardness in classical hip implants, with similar materials, has a nonlinear distribution according to distance from WC-Co reinforcement spherical spots. The formulation gets modified,

$W = K \bullet (L X)/H(s)$;

As a first approximation, considering K, L, and X constants, it is reasonable to take derivatives of wear respect to distance, [Casesnoves, Integral-Differential model,2017], reads,

$$\frac{dw}{ds} = \frac{dw}{dH} \times \frac{dH}{ds} =$$
$$= (KLX) \times \left(\frac{-1}{H^2(s)}\right) \times \left(\frac{dH(s)}{ds}\right);$$
$$\text{integrating along all matrix average length,}$$
$$\int_{w_0}^{w} dw = \int_{s_0}^{s} (KLX) \times \left(\frac{-1}{H^2(s)}\right) \times \left(\frac{dH(s)}{ds}\right) ds;$$

Eqs [10]

Which is the total wear for all the matrix length, and a part of the total wear of the composite metal. This type of numerical-differential modelling, is applicable on Composite Fe-based Hardfacings with coarse WC-Co reinforcement, and also in titanium-varieties histocompatible coatings, usually Titanium-Boride composites, of this material type for hip implants. What is clear, as guessed,is the development fom the experimental to the theoretical modelling of this rather difficult metals given their complex chemical composition, increased for the geometrical-spation distribution of every constituent.

The construction of the model follows straightforward from this equation since the hardness at matrix is a continuous and differentiable function, instead a series of discrete values. Given the Hardness Function, the insertion of the function into any other suitable model of wear, subject to constraints, constitutes a new method for erosion rate determination.

The evolution of this model in its differentiable equation will be continued in next contributions since the development to obtain useful calculations could be extent and its applications at least substantial.

X. DISCUSSION AND CONCLUSIONS

An objective analysis of mathematical models for erosion, corrosion, and tribocorrosion in bioengineering was presented with introductory ideas and appendices of general mechanical engineering tribology models. The evolution of the concept of investigation method in Biotribology was enlightened and justified.

The mathematical development of a model for the matrix of a composite metal Fe-based coating was determined and sharply explained with mathematical formulation, lab images, and explicit equations—Intergral-Differential Model. Graphical Optimization Methods, with/without constraints in region of interest, was explained and linked to clear imaging-computational pictures and software details.

In summary, according to the volume of new research and innovative optimization methods presented, the advances of this study could be considered acceptable and well-backgrounded with special nonlinear optimization procedures.

XI. ACKNOWLEDGEMENTS AND SCIENTIFIC ETHICS STANDARDS

TUT is gratefully acknowledged for all the facilities for research. 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. 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. The research publication in United States is exclusive.This article contains also unique numerical data and special new-improved images. The principal sketches were made originally, and the figures, tables, or data that corresponds/developed-from previous papers is properly clarified. When anything is taken from a source, it is adequately recognized [58]. Ideas from previous publications were emphasized due to a clarification aim.

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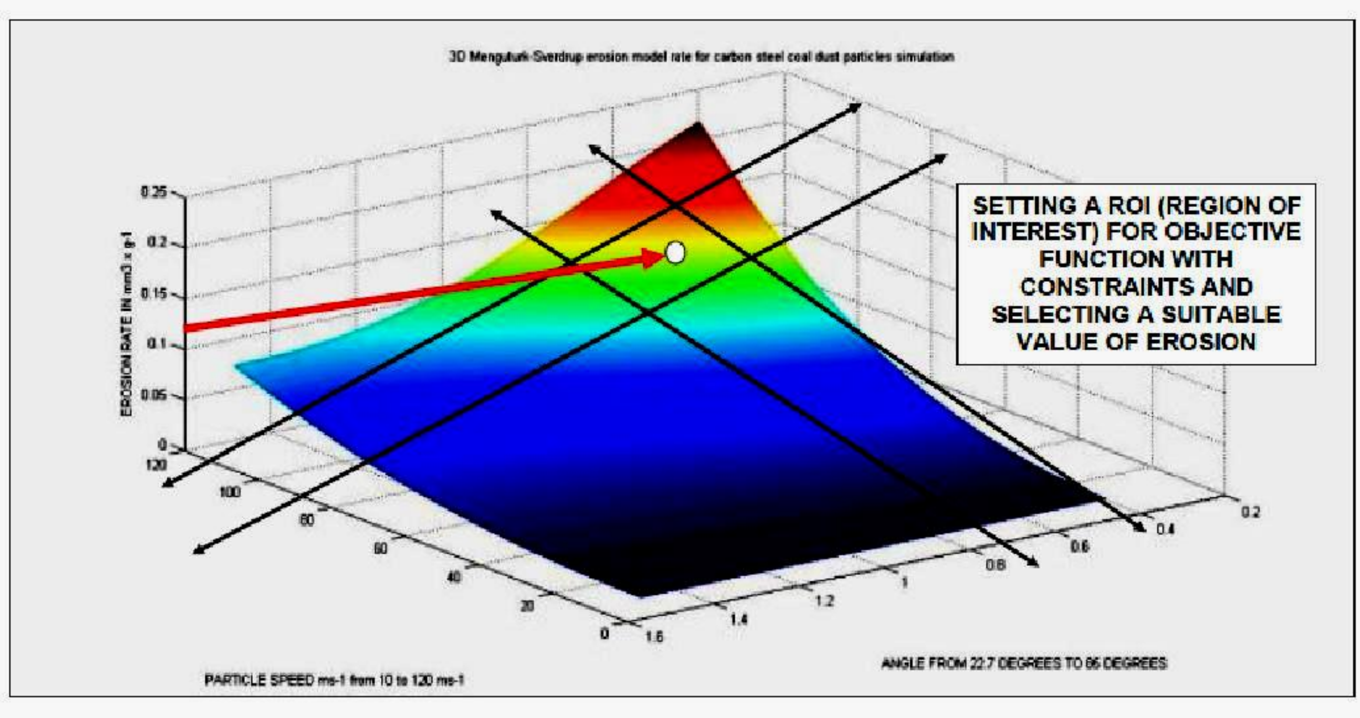
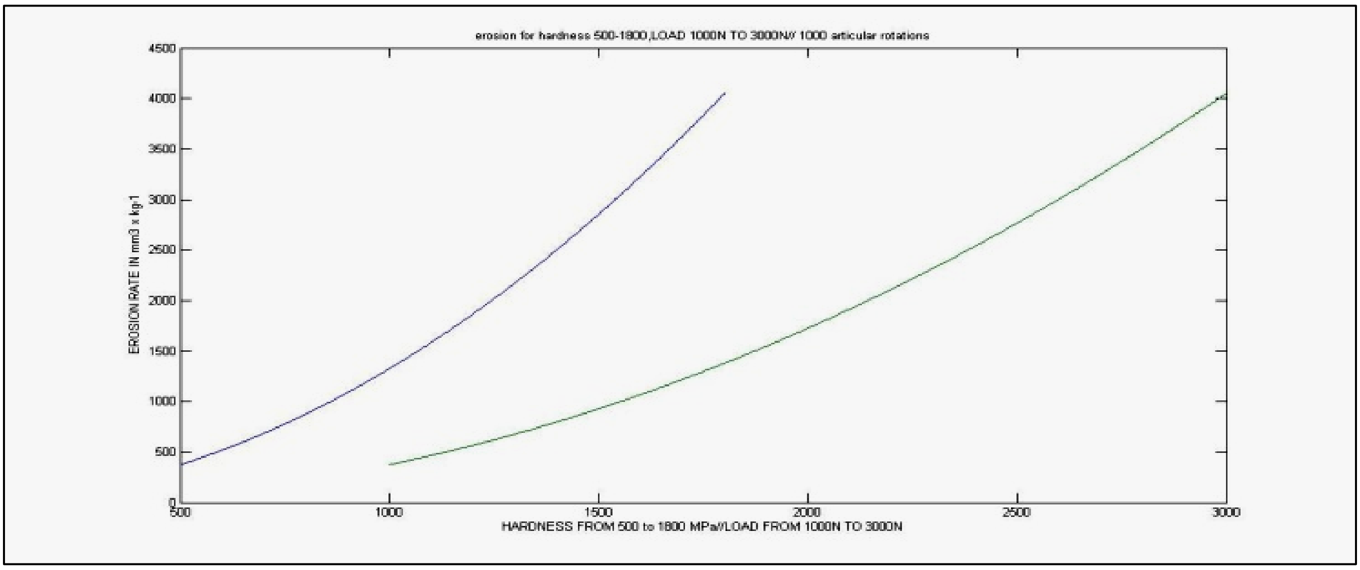
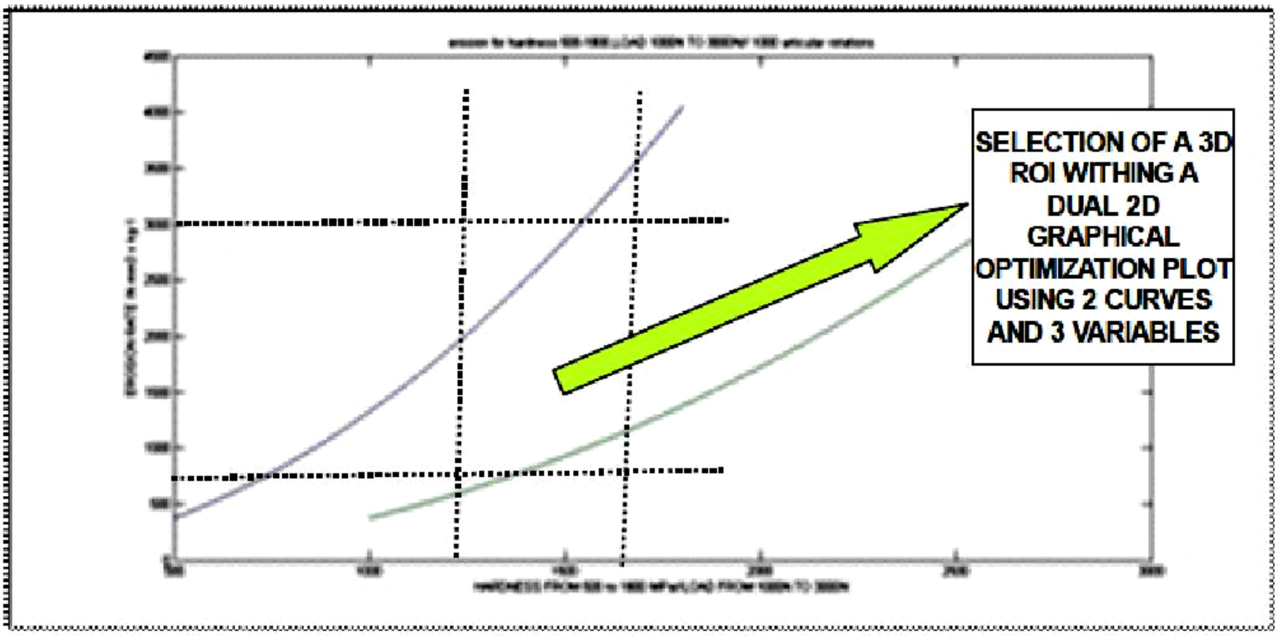
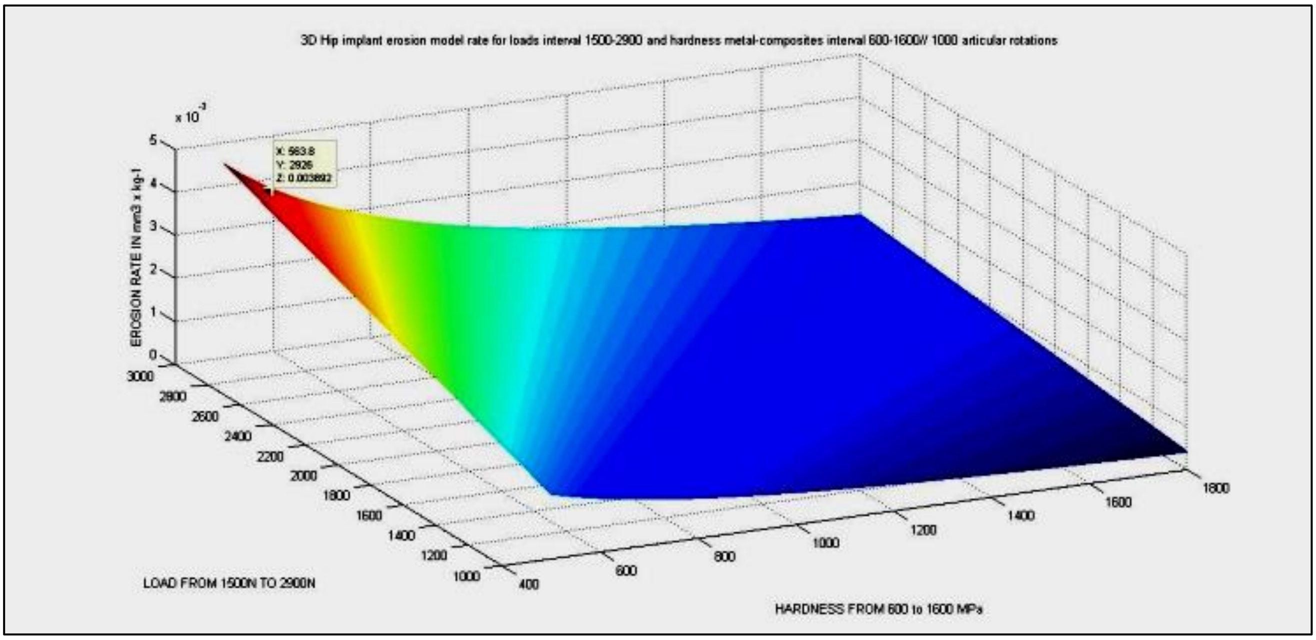
APPENDIX 1

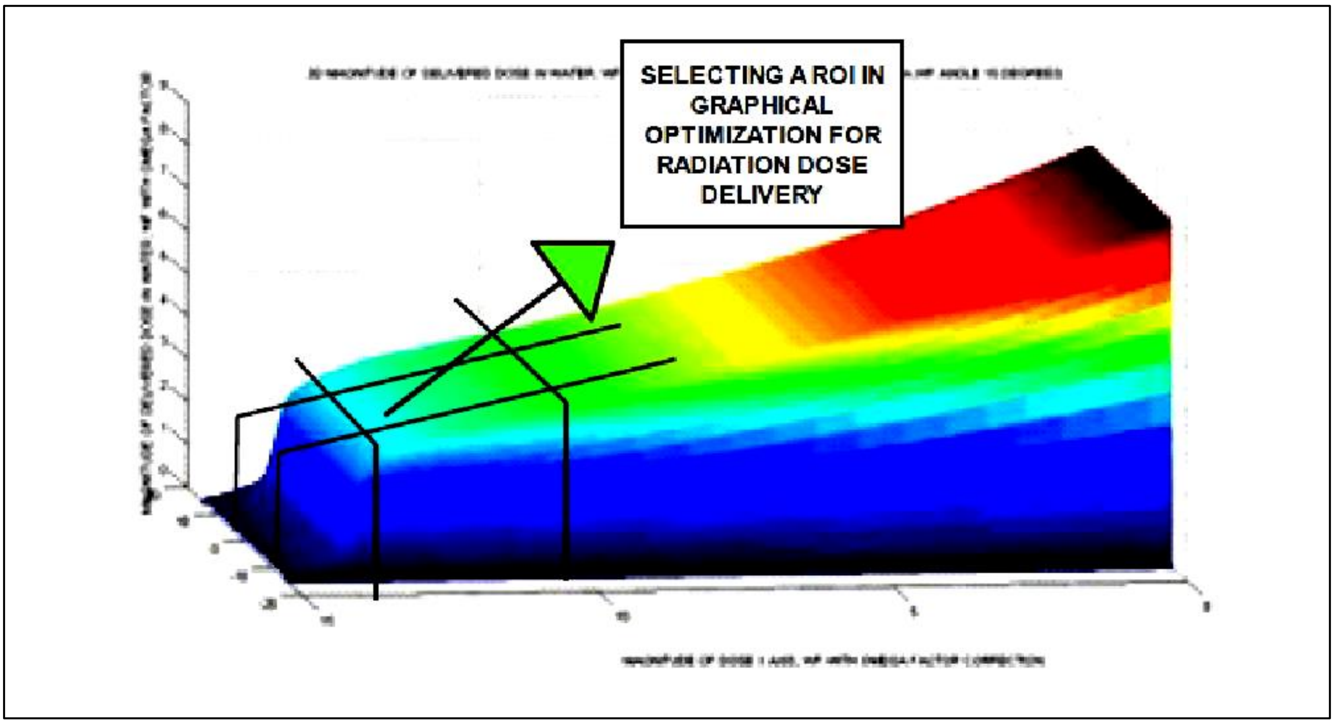
NON-LINEAR OPTIMIZATION SIMULATUION SFOR BIOTRIBOLOGICAL AND MECHANICAL SYSTEMS AND INAGING ENHANCED PICTURES

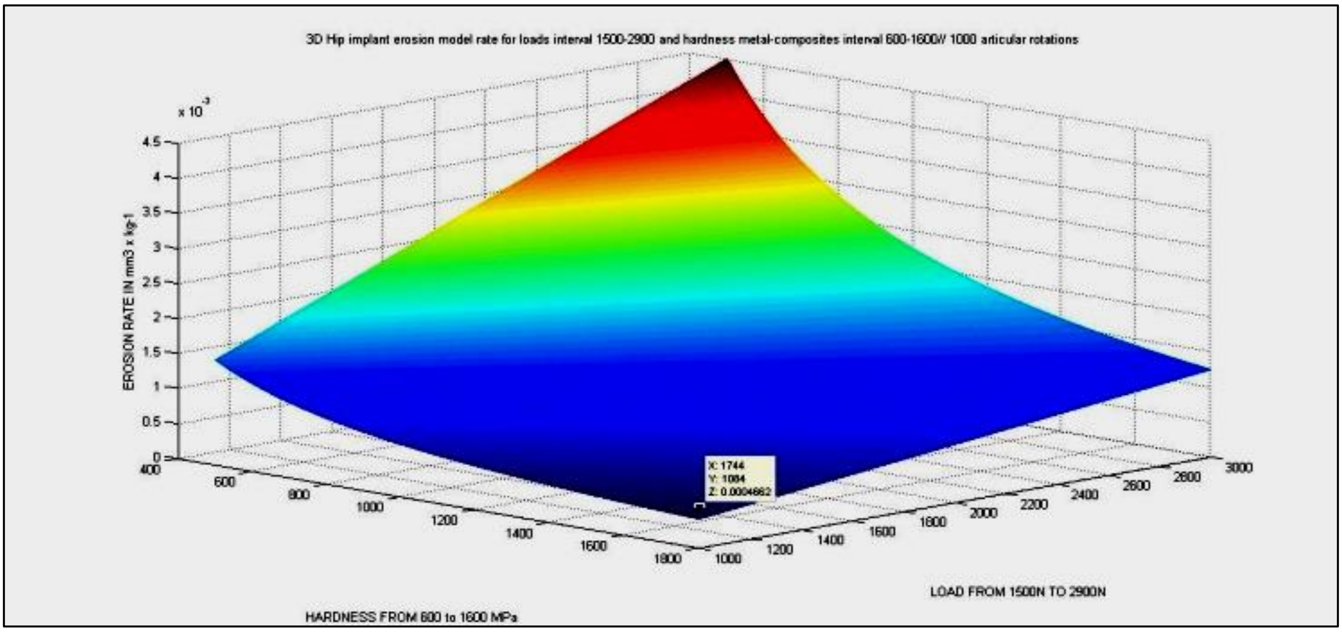





SELECTION OF A 3D ROI WITHING A DUAL 2D GRAPHICAL OPTIMIZATION PLOT USING 2 CURVES AND 3 VARIABLES


3D Hip implant erosion model rate for loads interval 1500-2900 and hardness metal-composites interval 600-1600// 1000 articular rotations
EROSION RATE IN mm3 x kg-1
LOAD FROM 1500N TO 2900N
HARDNESS FROM 600 to 1600 MPa


SELECTING A ROI IN GRAPHICAL OPTIMIZATION FOR RADIATION DOSE DELIVERY


3D Hip implant erosion model rate for loads interval 1500-2900 and hardness metal-composites interval 600-1600// 1000 articular rotations
x 10^-3
EROSION RATE IN mm3 x kg-1
X: 1744
Y: 1084
Z: 0.0004662
HARDNESS FROM 600 to 1600 MPa
LOAD FROM 1500N TO 2900N

APPENDIX 2 PROGRAMMING SOFTWARE WITH NUMERICAL NONLINEAR OPTIMIZATION RESULTS COMPLEMENTED

NON-LINEAR OPTIMIZATION NUMERICAL DATA FOR BIOMEDICAL/MECHANICAL TRIBOLOGY WEAR/EROSION MATHEMATICAL MODELS					
MATLAB SUBROUTINES USED LSQNONLIN, FMINCON INTERIOR POINT AND ACTIVE SET ALGORITHMS, MATLAB OPTIMIZATION TOOLBOX					
MODEL TYPE AND SIMULATION #	**NUMBER OF OPTIMIZATION VARIABLES**	**NUMBER OF RANDOM SIMULATED LAB MEASUREMENTS**	**SEARCH POINT**	**OPTIMAL SOLUTION**	**APPLIED DOUBLE PRECISION AND COMMENTS**
Hutchings	2, k v	50	(0.2,10)	0.0003, 12.0	N
Hutchings	2, k v	100	x=(0.2 ,10)	0.0005 9.9919	N
Hutchings	2, k v	10000	x= (1, 14)	0.0003 13.8600	N,running fast
Hutchings	2 k v	1000	x=(0.2, 10)	0.2821 0.4159	N
Hutchings	2 k v	1000	x=(0.3, 10)	0.2834 0.4159	N
Menguturk and Sverdrup	2, v, angle 25 degrees	10000	X=5	138.4362	N
Menguturk and Sverdrup	2, v, angle 25 degrees	1000	X=5	139.0728	Y
Menguturk and Sverdrup	2, v, angle 25 degrees	10000	X=1	138.3685	N, precision
Menguturk and Sverdrup	2, v, angle 25 degrees	10000	X=4	138.2630	N
hip metal implant	1, k, Hardness 350 MPa	10000	X=5	5.5802e-04	Y, search point not too much influence
hip metal implant	1, k, Hardness 350 MPa	10000	X=2	5.6087e-04	Y
hip metal implant	1, k, Hardness 350 MPa	10000	X=2.5	5.6087e-04	N
hip metal-coated implant $C_OC_RM_O$	1, k, Hardness 884 MPa	10000	X=5	0.0014	N
ceramic implant 2300	1, k, Hardness 2300 MPa	10000	X=4	0.0037	N
ceramic implant 2300	1, k, Hardness 2300 MPa	10000	X=7	0.0037	N aceptable results
ceramic implant 2300	1, k, Hardness 2300 MPa	10000 at interval [1,5]	X=7	0.0368	N
ceramic implant 2300	1, k, Hardness 2300 MPa	10000	X=6	0.0368	N
CONCLUSIONS: Initially acceptable optimization results conditioned to further improvements, however further improvements will be done in next contributions.					