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# Nonlinear Inverse Dual Optimization for Hip Arthroplasty Ceramic Materials

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## ABSTRACT

Total hip arthroplasty constitutes an important group among the most frequent used implants in Biomedical Engineering and Medical Devices research field. In this contribution, dual modeling and non-linear optimization are performed with two commonly used ceramic materials for ceramic-on-ceramic hip arthroplasty – among the most surgically utilized currently. These are alumina and zirconium. Numerical results for dual optimization show acceptable figures with low residuals. Results with two-dimensional graphical optimization are demonstrated acceptable also. According to these findings and calculations, optimized model parameters are mathematically proven and verified. Mathematical consequences give raise for new non-linear optimization algorithms. Based on numerical optimization data results, applications lead to biomedical engineering and future bioengineering/biomaterials designs.

**Key words:** Artificial implants, biomechanical forces, ceramic-on-ceramic implant, dual non-linear optimization, hip implants, objective function, prosthesis materials, total hip arthroplasty, wear

## INTRODUCTION

THA in medical bioengineering has experienced an expansion of material specialization/variety, quality, and manufacturing design. The prevalence of longer lifetime of population has increased during recent decades. Among all types of THA, ceramic-on-ceramic (CoC) constitutes an important group.[2-5,11,21] Other group of patients derived for surgical implementation of THA come from traffic accidents injuries, accidents, or extreme/professional sport activities.

As a consequence for the elongation of lifetime and traumatological reasons, hip implants constitute the surgical routine at traumatology and/or orthopedic services at any general/specialized hospital. In elderly population, osteoporosis, associated diseases, degenerative pathologies, tumor invasion of zone or metastasis, and loss of biomechanical capability became some of the crucial THA factors.[5,17,18,21,23,25,27]

The biomechanical and physiological conditions at hip articulation are rather complicated/extent. For bipedal locomotion, hip constitutes the fundamental-mechanical meshing union between trunk and legs – essential for usual/normal movements. If hip articulation fails, the biomechanical consequence is rather difficult/very similar to be sorted compared, for example, to knee articulation failure or mechanical limitations. The economical outcome of this change in incidence/prevalence of hip diseases is a high demand of these types of THA implants. Therefore, actually there is a high industrial demand for mechanical/material improvements in medical technology production. One type is CoC, which is the objective of this study.

Thiscontributiondealswithmathematicaloptimization of usual CoC implant materials. These are alumina ($Al_3O_2$) and zirconium ($ZrO_2$).[5,21] Their tribological properties/functionality are computationally modeled using classical model equations. Reasons for this kind of choice are their extent use in medical engineering and histocompatibility of these materials. Numerical non-linear optimization and two-dimensional (2D) graphical optimization methods are applied with specific software. Results obtained are series of numerical data and imaging graphical surfaces

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to compare materials and get objective database for manufacturing and/or tentative tribotesting of implants at laboratory.

## BRIEF OF HIP CLINICAL BIOMECHANICS ARTHROPLASTY

The biomechanics of the hip articulation is shown in Figure 1. The force distribution is rather complicated. In the figure, force vectors are drawn in 2d. The trunk and abdomen loads are approximately perpendicular to the standing surface of the legs. This force, for biotribological purposes, is decomposed into a tangential component in-between interface of implant cup and implant head surface, and other perpendicular to the semi-spherical implant head toward the femur trochanter. Both force components of biomechanical load cause wear and debris at the implant surface while the rotation of the artificial articulation. The tangential component is one that originates abrasion between two surfaces, the implant acetabular cup surface and the implant head. The perpendicular force also causes wear and debris for pressure between both surfaces. Specifically for CoC implants, the debris caused by abrasion is not a trivial post-surgical problem. In hip articulation, the forces distribution is not symmetric, and the walk of any individual could differ compared to average people – at that anatomical zone, the range of forces is set around several hundred N. Trunk weight is supported also by hips. The gravity center of thorax-abdomen is located approximately at S2 level. Therefore, the biomaterial design of THA is laborious. This is an approximation, because usually the load is divided in X, Y, and Z components,[1,25] and average values and/or forces resultant values are taken. For non-linear optimization, the average values will be implemented in the program.[1,25] In this study, a load of around 200% of body weight (200%BW) is applied for optimization constraints, according to the most usual values of literature.[5,21,25,27]

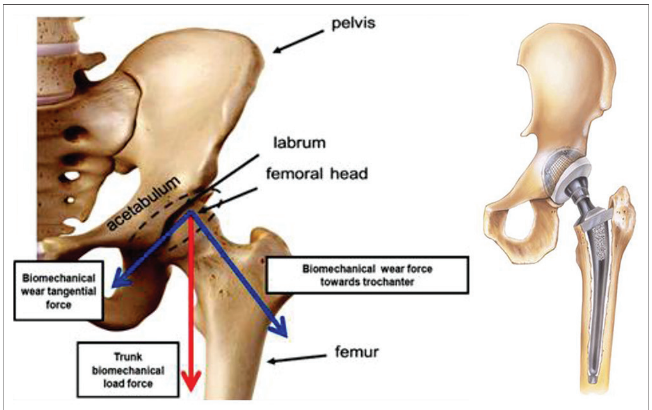


**Figure 1:** (Google free images with author's draws). On the left, from (ref…), basic forces distribution in normal hip. On the right, the elementary structure of the hip implant, cup, head, and leg. There are a wide number of implant apparatus kit variants in biomedical engineering. Before setting the implant, the bone has to be prepared according to implant geometry. In general, it is a complicated surgical intervention. Strong forces have to be exerted, and those have to be done precisely – the mechanical reason for modern robots usage. Ceramic-on-ceramic implants have a high hardness magnitude, in all their material variants

## NUMERICAL DATA IMPLEMENTATION

To perform mathematically correct optimization, definition of accurate magnitude data is a must.[1,21] The database comprises hardness of CoC material, implant head standard diameter, experimental interval of erosion widely published in literature, units, and other complementary data which are mentioned but not implemented on study models. In Table 1, numerical parameter database is detailed. Histocompatibility can be mechanical, surfactal, and chemical mainly. Further, histocompativility involves pharmacological biocompatibility and thrombus formation probability. Complementary data are cited without specifications.

## MATHEMATICAL INVERSE METHOD ALGORITHMS

The determination of hip implant wear in all the study is referred to cup and prosthesis head together (refs). The volume parameter is expressed in $mm^3$ always, the mass in kg, the force in N, time in seconds, and the constants of the models applied are function of these units always. The erosion or arthroplasty hip implants are specified in different ways along the literature,[5,21,25,27] namely, $mm^3$ of eroded material per million cycles (Mc) of the femoral head, mass of eroded material per year per Mc, very frequently $mm^3$ of eroded material per year, mass of eroded material per Mc or year, and others. Here, the $mm^3$ per Mc is selected for the entire study. It is considered a rough approximation $mm^3$ or mass of eroded material per year, because the number of cycles of the patient during a year is a non-precise measurement – unless large statistical data for age, kinetics, physical activity, etc., intervals are applied.

**Table 1:** Materials CoC data implemented in optimization models with complementary details

| Hip implants CoC numerical data | | | | |
|---|---|---|---|---|
| **Material** | **Hardness (GPa)** | **Density (g/cm³)** | **Histocompatibility** | **Standard head diameter (mm) and interval** |
| $Al_3O_2$ | 22.0 | 3.98 | Good | 28[22-28] |
| $ZrO_2$ | 12.2 | 5.56 | Good | 28[22-28] |
| Complementary Data for both | Elasticity modulus and fracture thougness are useful for other type of calculations. Density varies slightly in literature. The standard femoral head used diameter is 28 mm. Hardness also varies in literature | | | |

CoC: Ceramic-on ceramic, $Al_3O_2$: Alumina, $ZrO_2$: Zirconium

Other important parameter is to determine exactly/approximately what length has a cycle. According to kinesiology/anatomy of the natural hip, the rotation of femur head cannot reach 180°. This is valid for flexion, extension, abduction, adduction, and external/internal rotation. One cycle in this study is taken as the length corresponding to the maximum kinesiologic rotation angle. From literature, it varies, and post-operative movement range is different from normal movement and pre-operative.[24] The maximum value implemented here is 145° for flexion. Therefore, the erosion data resulted from the optimization always have to be considered as the maximum. In other words, it is considered that optimization parameters have to be calculated for the maximum erosion possible magnitude. This point is clarified at every optimization step. Using wear unit in mm³, the model constant K results dimensional, as it is proven. The load magnitude applied for optimization constraints is 200%BW.[5,21,25,27] This value was selected as usual in literature. Constraints for load are set for a 50 kg patient till an 80 kg patient. Fifty kilograms correspond, for example, to the body weight of elderly women, who present a high incidence/prevalence of femur head fractures.

The kinetics and dynamics of the patient are a multifunction of a number of varied parameters. They could be age, sport activity, physical work, walking habits, country, culture, individual circumstances, etc. Therefore, Mc within maximum rotation angle of 145° is considered a feasible approximation.

The algorithms that were implemented are based on classical Archard's model. However, from this model evolute algorithms were developed in previous contributions (Casesnoves, 2019–2020). The classical equation for optimization of hip implants reads,

$$W = K \frac{L \times X}{H} \; ; \tag{1}$$

Where, K is wear constant specific for each material, L biomechanical load (N, passed here to kg and mm), X sliding distance of the acetabular semi-sphere of the implant (mm), and H is the hardness of the implant material (MPa, here, it is used always kg and mm). X is measured as the number of rotations of the implant multiplied by half distance of its circular-spherical length. Number of rotations depends of the daily physical activity of the patient.

Hence, for setting OF,

$$W - K \frac{L \times X}{H} = 0 \; ; \tag{2}$$

Simple equation since model Equation (1) is used in integral form for finite elements techniques in hip implants,[1] K is parameter, although in previous contributions, this algorithm was implemented for more parameters,[12-15] such as optimal hardness or number of rotations. Number of rotations is calculated circumference implant head radius R by π for a factor of angle of 145°. Given this formulation, the OF with $L_2$ Norm that is used without fixed constraints reads,

minimize,

$$\left\| W - K \frac{L \times X}{H} \right\|_2^2 = 0 \; ; \tag{3}$$

subject to (generically),

$$\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} \le \begin{bmatrix} K \\ L \\ X \\ H \end{bmatrix} \le \begin{bmatrix} a_1 \\ b_1 \\ c_1 \\ d_1 \end{bmatrix};$$

Where, a, b, c, and d are constraint parameters to be selected. That is, any parameter(s) can be constrained for optimization. W values are experimental figures from the literature, in mm³. However, the most important one is H, since what is intended is to get practical optimal results for a dual group of arthroplasty materials. Load parameter is selected within a wide range 50 and 80 kg of patient weight. The reason is that this weight comprises from an older patient until a sporting young person, for instance.

The power 2 of the least squares algorithm converts the objective function into a non-linear function, although the model can be considered strictly as linear. Therefore, 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 (1). 2D graphical optimization several curves images were done with more complicated software that depends on subroutines in few parts.[2-5,23,26] This original software[2-5,26] was improved from previous contributions. Residuals and optimal values for K and the rest of parameters are also obtained in the programs. W is set in mm$^3$. The proof that for model Equation (1), using the selected unit kit, makes K dimensional follows straightforward selecting the given units.

## COMPUTATIONAL PROGRAMMING METHODS

The computational and mathematical methods of this study constitute an advanced evolution from previous publications[5] with MATLAB. Fortran was used to check/validate the numerical precision of the results. The variations/improvements are basically applications of 2D graphical optimization and interior optimization methods.[2-11,14,19,20] Complementary, implementations of results in 2D are presented. The algorithm (Casesnoves, 2021) implemented reads,

minimize,

$$\| F(W,K,H,L,X)\|_2^2 = ...... =$$

$$\sum_{i=1}^{i=N}\sum_{j=1}^{j=N}\sum_{k=1}^{k=N}\left(F_{ijk}\left(W_{ijk},K_{ijk},H_{ijk},L_{ijk},X_{ijk}\right)^2 + ..... + \right.$$

$$\left. F_N\left(W_{N,N,N},K_{N,N,N},H_{N,N,N},L_{N,N,N},X_{N,N,N}\right)^2\right);$$

subject generically to,

$$\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} \le \begin{bmatrix} K \\ L \\ X \\ H \end{bmatrix} \le \begin{bmatrix} a_1 \\ b_1 \\ c_1 \\ d_1 \end{bmatrix} \quad (4)$$

And K was selected as main variable for optimization. The 2D graphical optimization consists in the implementation of the objective function (OF) related to erosion interval and one selected parameter of the model. In this contribution, constraints are implemented in the objective function. N was chosen for 2 million functions. Therefore, the programs designed are varied and more complicated compared to a previous publication.[5] This fact implies the usage of several subroutines combined/complemented with new patterns. Software was designed to obtain minimum running time and clear visualization of results. In all calculations, always local minima are determined. The 3D volume matrix of the algorithm was converted to a 2D matrix with series of arrays for implementation in patterns (Casesnoves, 2020–2021).

The imaging 2D charts have surfaces, simple and combined parameter curves. The plotting of these curves and regions, when combined, is rather a difficult task. The reason is that to obtain sharp visualization of several or all model parameters together, it is necessary to set them in with scale factors. Those calculations involve a series of computational trials with approximations to get the best charts with clear local minima. Total running time for programs results be between 2 and 7 min because 2 million functions were chosen. A range of parameters chosen for 2D graphical optimization.[5,21,25] These are hardness, load, and model wear. Constraints for program software were selected as follows,

minimize,

$$\| F(W,K,H,L,X)\|_2^2 = ...... =$$

$$\sum_{i=1}^{i=N}\sum_{j=1}^{j=N}\sum_{k=1}^{k=N}\left(F_{ijk}\left(W_{ijk},K_{ijk},H_{ijk},L_{ijk},X_{ijk}\right)^2 + ..... + \right.$$

$$\left. F_N\left(W_{N,N,N},K_{N,N,N},H_{N,N,N},L_{N,N,N},X_{N,N,N}\right)^2\right)$$

subject to,

$N = 2 \times 10^6$,
$0.02 \le W \le 0.1$ mm$^3$,
$12 \times 10^6 \le H\ 23 \times 10^6$ kg, mm;
$7.5 \times 10^4 \times 9.8066 \le L \le 2.0 \times 10^5 \times 9.8066$;
$X = \pi \times 28 \times (145 \times 10^6)/180$ (1 Mc) (5)

## NONLINEAR DUAL OPTIMIZATION RESULTS

The results are presented both numerically and in graphics. Numerical results are detailed in Table 2.

Graphics software was designed to show local minimum in function of several parameters. In Table 2, the dual non-linear optimization for $Al_3O_2$ and $ZrO_2$ is shown. Figures 2-5 show the model graphical optimization. The curves and areas correspond to model objective function (Y-axis) related to parameter values (X-axis). Non-linear optimization matrix was set with 2 million functions. Running time was about 2–7 min to obtain local minima and graphics. The 2D surfaces obtained are filled with all the OF values for 2 million functions. Everyone has a different combination of parameters. Residuals are low considering the 2 million OFs of the optimization matrix.

Checking local minima values within model, it is obtained,

$$\left| K\left(optimal\right) \times \frac{Load\left(optimal\right) \times Mc}{Hardness\left(optimal\right)} \right| =$$

$$= 9.59 \times 10^{-9} \times \frac{1.10 \times 10^{6} \times Mc}{1.53 \times 10^{7}} =$$

$$= 0.0489 \in [0.02, 0.1];$$

Therefore, the optimal numerical values obtained with the software are within experimental interval. The figure 0.04 corresponds to about the center of the interval. That is a good numerical result, as it is not set around the boundaries of experimental interval. This implies that for both $Al_3O_2$ and zirconia materials, the optimal K value obtained is acceptable for the experimental wear magnitudes published in literature (ref). Just remark that units are always kg and mm for an erosion measured in $mm^3$. Table 2 shows all non-linear dual optimization results.

## BIOENGINEERING-BIOMEDICAL APPLICATIONS

Biomedical engineering applications of results are linked to optimal K coefficient. Furthermore, optimal parameters for hardness, load, and wear are

**Table 2:** Dual optimization numerical results. Acceptable figures

| Dual optimization numerical results | | | | | |
|---|---|---|---|---|---|
| **Material** | **Optimal K adimensional** | **Optimal hardness (Kg, mm)** | **Optimal Erosion ($mm^3$)** | **Optimal Load (kg, mm)** | **Residual** |
| $Al_3O_2$ | $9.587464 \times 10^{-9}$ | $1.526 \times 10^{7}$ | 0.0489 | $1.099 \times 10^{3}$ | $1.76697 \times 10^{3}$ |
| $ZrO_2$ | | | | | |
| Additional data | All units used in optimization are passed in Kg and mm. Number of nonlinear function for program is 2 million. The initial Volume-Matrix, that is, a 3D matrix with 3 variables, hardness, load, and experimental magnitudes was converted with programming arrays to a 2D matrix of 2 million functions. Absolute difference between (experimental wear interval)-(model wear interval) ϵ (0, 0.08). | | | | |

$Al_3O_2$: Alumina, $ZrO_2$: Zirconum, 2D: Two dimensional

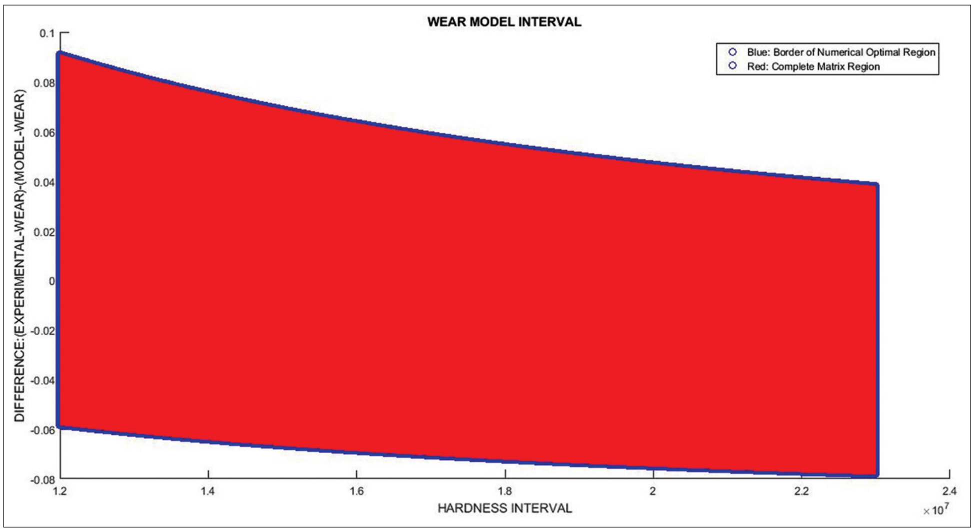


**Figure 2:** Twodimensional (2D) graphical optimization of model for K. All parameters are in Kg and mm (1 Mc). The matrix for all evaluated parameters in optimization program covers a 2D region. The numerical result of the difference between model and experimental wear axis Y. Matrix has all possible combinations of parameters, namely, load, hardness, and experimental wear. The initial volume matrix, that is, a 3D matrix with three variables, hardness, load, and experimental magnitudes was converted with programming arrays to a 2D matrix of 2 million functions. Optimal K is $9.587464 \times 10^{-9}$. Residual is $1.76697 \times 10^{3}$

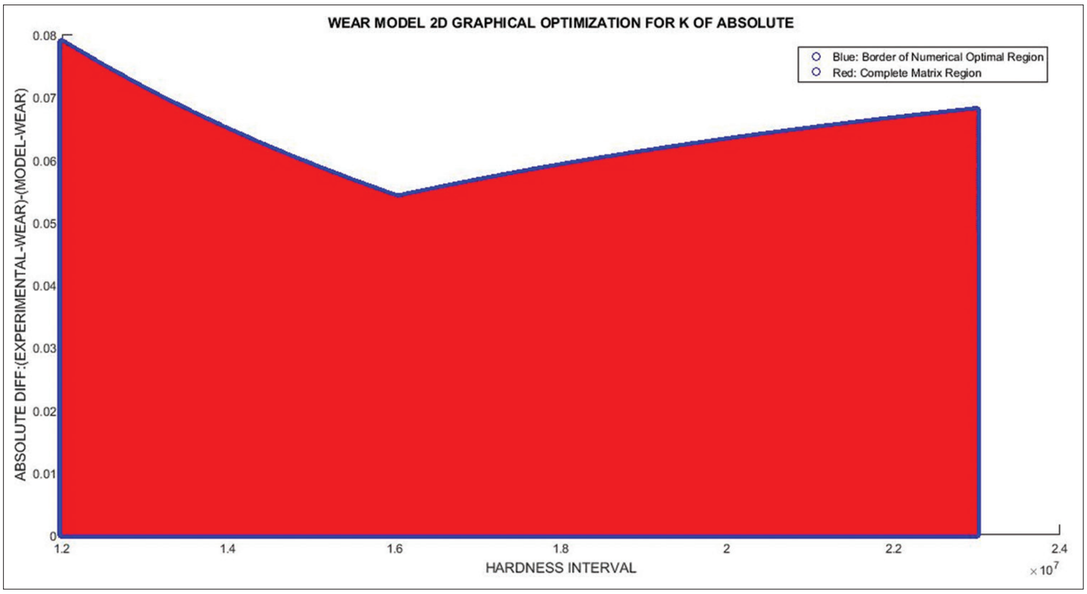


**Figure 3:** Twodimensional (2D) graphical optimization of model for K. Absolute value of OF. All parameters are in kg and mm (1 Mc). The matrix for all evaluated parameters in optimization program covers a 2D region. The numerical result of the difference between model and experimental wear axis Y. Matrix has all possible combinations of parameters, namely, load, hardness, and experimental wear. Optimal hardness can be observed at peak-concavity approximately at $1.5 \times 10^7$ (units at Table 2, Kg and $mm^3$). With graphical optimization is exactly $1.526 \times 10^7$. OF absolute value is within interval (0, 0.08), which is an acceptable result for the experimental data implemented (0.02, 0.1)

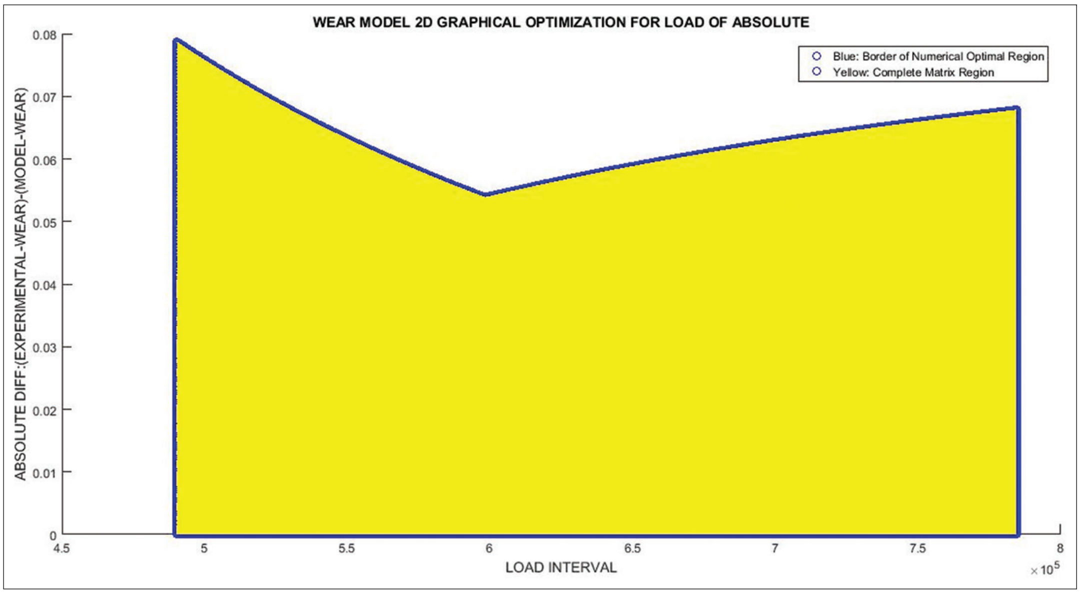


**Figure 4:** Twodimensional (2D) graphical optimization of model for load. Absolute value of OF. All parameters are in kg and mm (1 Mc). The matrix for all evaluated parameters in optimization program covers a 2D region. The numerical result of the difference between model and experimental wear axis Y. Matrix has all possible combinations of parameters, namely, load, hardness, and experimental wear. Optimal load can be observed at peak-concavity exactly at $1.099 \times 10^3$ Newton. For higher loads, the OF is approximately the same, but a global minimum cannot be reached for all model parameters

efficacious and useful. If it is applied the model of Equation (1), it is possible to use this K coefficient for similar materials with hardness values within the interval corresponding to $Al_3O_2$ and zirconia. That is, simulate/predict approximately the wear that will be caused in the implant for that load with higher number of rotations. The composed materials wear whose hardness fall within the computed interval can also be simulated with these optimal results.

Biomedical applications for THA are, therefore, extent if projected to higher number of Mc. Pre-operative simulations for THA to calculate approximately the durability time of the implant can be done with this model base. The advantage of dual optimization is that covers a hardness

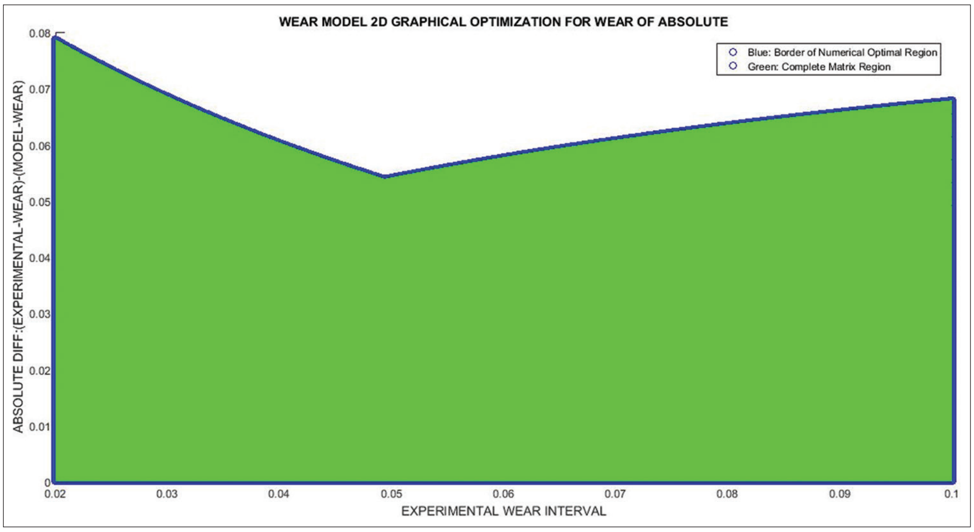


**Figure 5:** Twodimensional (2D) graphical optimization of model for experimental wear versus model OF absolute value. All parameters are in kg and mm (1 Mc). The matrix for all evaluated parameters in optimization program covers a 2D region. The numerical result of the difference between model and experimental wear axis Y. Matrix has all possible combinations of parameters, namely, load, hardness, and experimental wear. Optimal wear can be observed at peak concavity exactly at 0.0437 mm$^3$. It is a local minimum

interval of CoC. CoC arthroplasty has a high hardness magnitude and lifetime durability.[5]

## DISCUSSION AND CONCLUSIONS

A mathematical dual non-linear optimization study related to THA CoC implants was done. The inverse algorithm implemented was non-linear least squares. Optimal results show low residuals and acceptable model parameters. It is proven that global optimal values cannot be obtained for this model and experimental data. Local minimum values, however, show low residuals. The K optimal value implementation with the other optimal parameters gives good numerical results, matching the experimental data of the literature (ref). For load interval implemented at the model, average values of the patients were implemented with basic approximations (ref). The Mc total length was corrected/approximated for biomechanical kinetics of hip.

The number of functions optimized to obtain the local minima is 2 million with a complete combination of parameters. The running time of software is about 2–7 min. 2D graphical optimization charts of the programming patters give a good visualization of OF, differences between OF and experimental data, and model parameters. The K value is functional/useful both for $Al_3O_2$ and zirconia THA implants. All dual optimization processes can be objectively considered acceptable, numerically efficacious, and effective.

In summary, a group of optimal parameters applicable for this THA erosion model was obtained to be applied in THA $Al_3O_2$ and zirconia CoC implants.

## SCIENTIFIC ETHICS STANDARDS

This contribution is based on graphical visualization-optimization methods for cadaveric specimens of lumbar spine with software improved from previous articles. Graphical-optimization methods were created by Dr. Francisco Casesnoves on December 2016. The software was originally developed by author. This advanced article has a few previous paper information, whose inclusion is essential to make the contribution understandable. The non-linear optimization software[2-5,19,20,26] was improved from previous contributions in subroutines modifications, patters, loops, graphics, and optimal visualization. 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.[16,29] This research was completely done by the author, the software, calculations, images, mathematical propositions and statements, reference citations, and text is original for the author. When anything is taken from a source, it is adequately recognized. Ideas from previous publications were emphasized due to a clarification aim.[16,29]

## AUTHOR'S BIOGRAPHY

Francisco Casesnoves is Engineering and Natural Sciences PhD by Tallinn University of Technology (started thesis in 2016, thesis defense/PhD earned defense in December 2018, official graduate diploma 2019), 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 C Navamuel and I Vela, in Renaissance-Humanism ideas – later on with the motivation manuscripts of Nobel and Von Helmholtz prizes Santiago Ramon y Cajal. Casesnoves resigned definitely to his original nationality in 2020 for ideological and ethical-professional reasons. 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 100 recognized publications with 50 papers. His main branch is computational-mathematical non-linear/inverse methods optimization. Casesnoves best achievement is the Numerical Reuleaux Method in dynamics and non-linear optimization (books 2019–2020). Casesnoves scientific service since 2016 to the Free and Independent Republic of Estonia for technological development (and also at Riga technical University, Power Electrical and Electronics Department) is about 28 physics engineering articles, two books, and 1 industrial radiotherapy project associated to Europe Union EIT Health Program (Tartu University, 2017).

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