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Mathematical Optimization for Molecular Effect Model in High Temperature Superconductors Lattice TET Pb Class compared to Tl Group [$T_C > 0°$]

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ABSTRACT

The objective of this research article was to apply/compare Inverse Least Squares (ILS), 2D Numerical/Graphical Optimization in Molecular Effect model for two High Temperature Superconductors (HTSC) groups. These are Pb Tetragonal (TET) Lattice Class [mostly $T_C > 0°$] and [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] one constrained to those with $T_C > 0°$ C exclusively. Both groups show have got innovative electronics physics applications. Results are obtained with 2D optimization/simulations, classical ILS, 2D Interior Optimization, and 2D Graphical Optimization. Numerical and imaging solutions are obtained as in previous contributions with Tikhonov Regularization algorithms, at this stage depending on Molecular Mass uniquely. For Thallium HTSC Class results demonstrate/corroborate proven 2D sinusoidal analytic geometry model curve in former publications. Findings for Pb Tetragonal (TET) Lattice Class in Molecular Effect ILS optimization display acceptable theoretical Numerical, and 2D Graphical Optimization parabolic-like curves with low residuals. Complete results comprise two parts for these two HTSCs classes, the numerical modelling for T_C Molecular Effect, and the ILS software/imaging methods. HTCS Electronics Physics are guessed from numerical and graphical results.

Key Words: Interior Optimization (IO) Methods, Graphical Optimization, Systems of Nonlinear Equations, Tikhonov Regularization (TR), Critical temperature [Tc], Isotope Effect (IE), Inverse Least Squares (ILS), Electronics Superconductors, High-Temperature Superconductors (HTSC), BCS Theory, Pb Tetragonal HTSC Class, TET Lattice, Thallium HTSC Class [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] Molecular HTSC Group, Molecular Mass (MO).

Introduction

Superconductors Modelling Optimization research field [1,4-6], both for standard superconductors and HTSC was studied and presented in previous contribution series [1,4-6]. In this article a new HTSCs Pb class, [3-5, 12-15, 32-34, 37], is compared to Thallium HTSC group. Namely, the HTSCs group [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] whose $T_C > 0°$ centigrades exclusively. These HTSCs classes forma recent materials innovation in HTSCs with $T_C \in$ [230 °K , 80 °C] . The number of HTSC new material compounds developed is extensive [3-5, 12-15, 32-34, 37]. The HTSC materials-class whose $T_C > 0°$ marks a significant physical-chemical and thermodynamical-materials difference related to other HTSCs classes.

The superconductors study commenced with the milestone of BCS theory, constructed on interactive-materials with electrical and magnetics fields physical-chemical phenomena. BCS theory framework is based on a series of theoretical parts of physical-chemical equations. The mathematical structure is rather extensive. *Grosso modo*, the superconducting effect begins with [thermodynamical effect of material-cooling summed to electrical J implementation], and this causes [→ electrons-subsequent lattice structural deformation]. Because of which, subsequently, the [electrical-resistance magnitude decrease →], this phenomenon causes phonons (special particles) production. The last stage produced by phonons effect is [→ high acceleration of current of electrons].

The superconducting background shows a series of material physics, theoretical physics, and chemistry matter-structure mathematical models. Therefore, the variety of algorithms is rather long, some of them simple and most complicated, with modifications related to molecular/atomic specific properties [3-5, 12-15, 32-34, 37]. Type 2 Superconductors (HTSCs), constitute the most recent/innovative class subject to improvements/evolution. Their most likely further industrial applications have got going be learnt.

HTSC, that is, Type 2 superconductors, have a different superconducting state background in their transition to superconducting effect phenomena compared to classical Type 1 ones [3-5, 12-15, 32-34, 37]. The properties of this HTSCs transition are subject of study/improvements continuously.

Isotope Effect forms a primary BCS theory stage when superconducting effect got going to find experimental evidences. IE algorithms uphold that ‘differences in atomic mass of a chemical element determines the variable critical transition temperature of a superconductor’ [3-5, 12-15, 32-34, 37] . In consequence, the published Molecular Effect hypothesis is supported by a similar criterion [Casesnoves, 2020, 1-5]. In other words, in case a HTSCs class has a very similar nano-molecular-atomic composition, its changes in T_C magnitude within the HTSC class could be mathematically-modelling linked to valences,

and type of isotopes and isotope proportions in the material conformation. That is, an isotopes mixture of the same molecular structure compound with several isotopes forming just the same molecules.

Molecular Effect model is at initial hypothesis stage [Casesnoves, 2020, 3-5]. The reasons are that smatter-structure equations, flux-lattice vortices concepts, and quantum mechanics and inter-related physical-chemical algorithms, are not implemented yet if in case they would be necessary to improve MEM model.

Previous study, [1], showed primary optimization for Sn class of HTSCs with $T_C > 0°$ centigrade [1]. Roughly speaking, [1-6, 14-16, 26-29], the classical HTSCs are those ones whose Tc is approximately higher than 80 K—precisely 77 K [3-5, 12-15].

In BCS theory, the Isotope Effect model [1-6, 14-16, 26-29] for uni-element superconductors equation reads,

$$[M_i]^{\alpha} T_{Ci} - K \cong 0; \quad \text{for } i = 1,\ldots..n; \tag{1}$$

where, [1], K and α are numerical-experimental constants, M Atomic Element Mass (AMU) of an element with (n) isotopes, T_{Ci} is critical temperature (usually Kelvin) for every isotope; (i) is the corresponding isotope for the element. The optimization search is to find an optimal K, α, and an optimal T_C for all the isotopes of the selected chemical element. T_{Ci} is critical temperature (usually Kelvin) for every isotope and in some specific elements it varies in one or decimal units [26,27,29]. This paper study deals with the comparative Molecular Effect Model 2D Graphical/Numerical-Algorithms model for HTSCs [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] and Pb HTSCs classes. Most of the selected compounds properties for optimization are constrained to $T_C > 0°$.

Equation (1), is a simplified algorithm for every element-isotope-atomic mass of a Type 1 superconductor with its corresponding Critical Temperature Tc. From [1], two main parameters [M , T_C] , and two constants [K , α] got to be optimized/determined both experimental and numerically. IE model Equation (1), both in exponential structure and logarithmic forms, has proven be approximated with some impreciseness [3-5, 12-15] .

In this contribution, the TET Lattice Pb class and Thallium one HTSCs chemical groups whose molecular composition/formulation diverge in proportion of valences/elements [1-9,12-15] are compared and 2D numerically/graphically optimized with ILS polynomial-algorithm model used in [1].

Succintly, the article proves a 2D Numerical-Graphical optimization study for the primary hypothesis of Molecular Effect model set on Pb and Thallium groups. Software and programming-formulas are set with Matlab Optimization Toolbox and imaging-processing software. 2D Graphical models plots are presented. The improved software related to [1, 4-6] is based on previous this research [1, 4-6]. 2D numerical/graphical solutions show low numerical errors/residuals. The model Pb shape is parabolic-like and the Thallium one results confirms/fits approximately sinusoid curves.

Mathematical Algorithms and Computational Methods

The numerical experimental data for setting the Molecular Effect model for [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSC group is shown in Table 1. The differences among the 13 group compounds are given by a number of elements. Tl , Ba, Cu and O, always form molecule part, instead, Sn, Mn, Ti, Si, Pb, and Mg, are complementary in specific compounds within this HTSCs class.

Valences are not always discrete figures, and are set without subscript format for better reading/differentiation. In this HTSCs class, exclusively those compounds whose $T_C > 0°$ are selected for the model optimization . For Pb TET Lattice class, Table 2, T_C is given in Kelvin, and five compounds are selected.

The programming method is similar to [1, 4-6], but in this study the software loops, 2D patterns, and imaging processing tools for 2D Graphical and statistical programming were improved according to this HTSCs class characteristics. Errors are indicated in graphs, Figures 1-4. Algorithm is based on Tikhonov Regularization Theory [7,13,31] as in previous contributions.

Numerical Experimental Data

Table 1.- The development of optimization of parameters for [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] Thallium class implemented in this study [1,4-6, 14-16]. Note the differences among the group compounds. Tl , Ba, Cu and O, always form molecule part, but for instance Pb, Mn, Mg, and Si are present exclusively in specific compounds within this HTSC class.

NUMERICAL OPTIMIZATION DATA [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] CLASS [HT-SUPERCONDUCTORS, [Tc > 0°] MOLECULAR EFFECT HYPOTHESIS]	
FORMULATION	MOLECULAR WEIGHT (UAM) / APPROXIMATE T_C (CENTIGRADES)
Tl7Sn2Ba2MnCu10O20	2.9531e+03 / 77
Tl7Sn2Ba2TiCu10O20	2.9461e+03 / 65
Tl6Sn2Ba2TiCu9O18	2.6462e+03 / 56
Tl7Sn2Ba2SiCu10O20	2.9263e+03 / 53
Tl6Ba4SiCu9O18	2.6636e+03 / 48
Tl5Ba4SiCu8O16	2.4479e+03 / 44
(Tl5Sn2)Ba2SiCu8O16	2.3264e+03 / 42
(Tl5Pb2)Ba2SiCu8O16	2.5034e+03 / 38
(Tl5Pb2)Ba2Si2.5Cu8.5O17	2.5933e+03 / 35
(Tl5Pb2)Ba2Mg2.5Cu8.5O17	2.5839e+03 / 30
(Tl5Pb2)Ba2Mg2Cu9O18	2.6195e+03 / 28
(Tl5Pb2)Ba2MgCu10O20	2.6907e+03 / 18
(Tl4Pb)Ba2MgCu8O13	2.0401e+03 / 3

Tables 1-2 present Numerical Experimental Data for modelling . [3-5, 12-15, 32-34, 37]. In Thallium class, Table 1, there are differences among the respective compounds T_C and element-compositions. However, the differences among those molecular masses are not significative. In Table 2, all the molecular masses are similar with the exception of [Pb_3MgO_5].

NUMERICAL OPTIMIZATION MEM DATA FOR HTSC TET LATTICE Pb CLASS	
FORMULATION	MOLECULAR MASS (UAM) APPROXIMATE T_C (Kelvin)
Pb2Sr2(Ca, Y)Cu3O8	1.04e+003 / 70
(Pb1.5Sn1.5)Sr4Ca2Cu5O15+	1.48e+003 / 95
Pb3Sr4Ca2Cu5O15+	1.61e+003 / 101
Pb3Sr4Ca3Cu6Ox	1.63e+003 / 106
Pb3MgO5	725.90e+000/307
COMMENTS	
725.90e+000 MOLECULAR MASS IS NOT FOLLOWING THE MOSTLY CURVE FITNESS	

Table 2.- Numerical optimization data for HTSC TET Lattice Pb class. All the molecular masses are similar/coherent with Molecular Effect with the exception of [Pb_3MgO_5]. This one causes an error at 2D Optimization fitness in Figures 1-2.

Computational-Software Algorithms

For this Molecular Model optimization, the algorithm with constraints for parameters is shown in Equation (2). Tikhonov functional method is applied as [1]. Therefore, algorithms set for ILS Molecular Effect, with a polynomial p(MO) read,

$$
\begin{aligned}
&\text{minimize Tikhonov functional } J(\alpha),\\
&\text{with } \alpha 1=0 \text{ and } L_2 \text{ Norm},\\
&J_{\alpha}(u)_{u\in X} = \left\| A\,u - p(MO) \right\|_2^2 + [\alpha 1]\, J(u);\\
&\text{Hence minimize},\\
&\left\| T_{Ci} - p(MO_i) \right\|_2^2 \quad ,\\
&\text{for } i = 1,\ldots..n\\
&\text{subject to} \quad ,\\
&a \le MO_i \le a_1 \; ;\\
&b \le T_{Ci} \le b_1 \; ;
\end{aligned}
$$

(2)

where MO_i is the molecular weight of the HTSC selected (i) within a HTSC group with (i) elements, and [a-b] are constraints intervals. T_{Ci} is critical temperature (Centigrades for Thallium class, Kelvin for Pb group) for every (i) member of HTSCs group. The figure α1 is a constant specific Tikhonov Regularization Parameter, to be appropriately selected. The constraints [a-b] are applied for 2D modelling optimization. This OF was selected with ILS programming in Matlab.

The selected group of HTSCs constitutes a modern HTSCs materials whose $T_C > 0°$ centigrades, with prospective applications [1-6, 14-16, 26-29]. Table 1 shows a narrow T_C differences interval, namely, approximately T_C-group ϵ [3 , 77] centigrades. For Pb class, Table 2 shows the Pb, such as $T_C \epsilon$ [70 , 307] Kelvin.

Numerical and Graphical Results

Molecular Effect modelling results for Pb class are 2D Graphical, Figures 1-2, and Numerical, Table 5, with model equations parameters. Molecular Effect modelling results for Thallium class are 2D Graphical, Figures 3-5, and Numerical, Tables 3-4, with explicit model equations. Matlab Graphical results for 2-degree and 4-degree ILS polynomial model Pb group are shown in Figures 1-2, with parabolic-like analytical geometry shape. Matlab Graphical results for 3-5 degree ILS polynomial model Thallium group are shown in Figures 3-5. All 3, 4 and 5-degree show a sinusoid curve-shape for model. Graphical errors can be considered acceptable/low, with the exception of [Pb_3MgO_5] in Figures 1-2, and Table 1. Results for ILS Thallium and Pb class equations are detailed in Tables 3-5, with approximations and errors.

ILS 2,3,4,5-Degree Graphical Optimization Model Results Pb Class compared to Tl Group

Figures 1-2 show parabolic-like shape model curves for ILS [2,4-degree] Molecular Effect model in Pb class. Figures 3-4 show sinusoid-shaped model curve for ILS [3,5-degree]

Molecular effect model in [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. Geometrical analytic differences in shape compared to parabolic model-curves obtained in previous studies with different HTSCs class [1, 4-6] are clear. The study at this stage shows that every Superconductor and HTSC class has an specific Molecular Effect analytic geometry equations type.

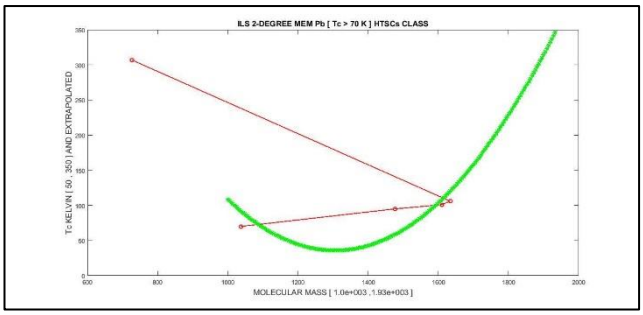

Fig. 1.- 2-degree ILS polynomial optimization of Molecular Effect Model for Pb HTSCs group. Matlab Extrapolated modelled curve (green) and experimental data (red). The model results to resemble a parabolic equation, approximately. The exception of [Pb_3MgO_5], with very different molecular mass, Table 1, creates an error-break in the fitness (long red line).

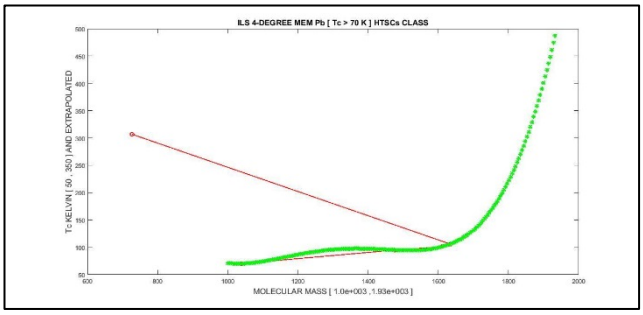

Fig. 2.- 4-degree ILS polynomial optimization of Molecular Effect Model for Pb HTSCs group, at y-axis T_C in Kelvin. Matlab Extrapolated modelled curve (green) and experimental data (red). The model results confirms to resemble a parabolic equation. As in 2-degree model, the exception of [Pb_3MgO_5], with very different molecular mass, Table 1, creates an error-break in the fitness (long red line).

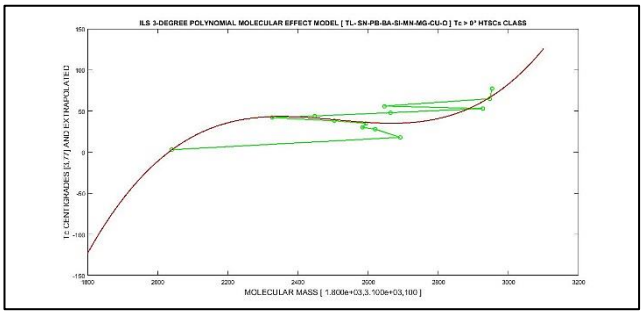

Fig. 3.- First attempt with 3-degree ILS polynomial optimization of Molecular Effect Model for [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. Matlab Extrapolated modelled curve (red) and experimental data (green). The model results to resemble a sinusoid equation, approximately. Since this HTSCs class has a number of compounds with $T_C < 0°$, the model confirms that trend.

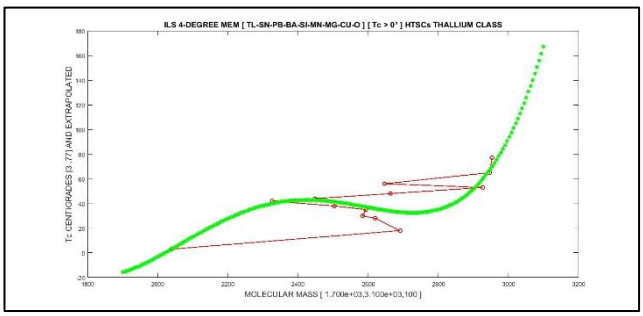

Fig. 4.- The 4-degree ILS polynomial optimization of Thallium Molecular Effect Model for this HTSCs group. It confirms the 3-degree ILS polynomial model analytic geometry shape. Extrapolated modelled curve (green) and experimental data (red). The model results be almost linear at intermediate values and becomes sinusoid for significant absolute-values increments in $T_C < 0°$ and $T_C > 0°$ [1,12-15, 32-34, 37].

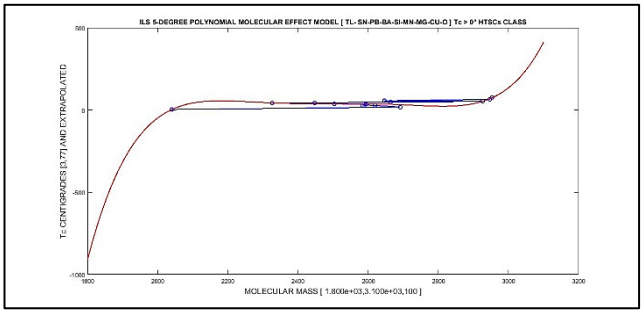

Fig. 5.- The 5-degree ILS polynomial optimization of Thallium Molecular Effect Model for this HTSCs group. It confirms the 3-degree ILS polynomial model analytic geometry shape. Extrapolated modelled curve (red) and experimental data (blue). The model results be almost linear at intermediate values and becomes sinusoid for significant absolute-values increments in $T_C < 0°$ and $T_C > 0°$ [1,12-15, 32-34, 37].

ILS Model Equations Pb Class and Tl Group

Tables 3-4 show 3 and 5 Thallium ILS model equations without/with approximations, discarding very low polynomial coefficients if numerically necessary. Table 5 presents 4-degree ILS MEM model equations results for Pb class.

MATLAB MEM [3-DEGREE] WITHOUT APPROXIMATIONS	
COEFFICIENT	VARIABLE X SELECTED
-8.2906e+003	CONSTANT
10.0383e+000	X
-4.0163e-003	X^2
533.5328e-009	X^3
RESIDUAL = 5.8316e+000	
MODEL EQUATION	
Tc = [-8.2906e+003] +... ... + [10.0383e+000] MO + ... +[-4.0163e-003] MO^2 +... ...+ [533.5328e-009] MO^3	

Table 3.- Without approximations, 3-degree ILS polynomial optimization of Molecular Effect Model Equation. Approximations were not numerically possible since there are not coefficients very high with negative powers.

ILS MOLECULAR EFFECT MODEL (5-DEGREE) WITH APPROXIMATIONS	
COEFFICIENT	VARIABLE X SELECTED
-829.6301e+003	CONSTANT
1.6793e+003	X
-1.3557e+000	X^2
545.7033e-006	X^3
-109.5228e-009	X^4
≈ 0	X^5 [not significant]
RESIDUAL = 5.6351	
MODEL EQUATION	
Tc = [-829.6301e+003] +... ... + [1.6793e+003] MO + ... +[-1.3557e+000] MO^2 +... ...+ [545.7033e-006] MO^3 +... ...+ [-109.5228e-009] MO^4	

Table 4.- 5-degree ILS polynomial optimization of Molecular Effect Model Equation. In this case, approximations were numerically possible since there are coefficients with very high negative powers [$\approx 10^{-12}$].

MATLAB MEM Pb HTSC CLASS [4-DEGREE] WITHOUT APPROXIMATIONS	
COEFFICIENT	**VARIABLE X SELECTED**
9.1379e+003	CONSTANT
-28.9614e+000	X
34.1860e-003	X^2
-17.6773e-006	X^3
3.3859e-009	X^4
RESIDUAL = 5.3789e-006	
MODEL EQUATION	
Tc = [9.1379e+003] +... ... + [-28.9614e+000] MO + ... +[34.1860e-003] MO^2 +... ...+ [-17.6773e-006] MO^3 +... ...+ [3.3859e-009] MO^4	

Table 5.- 4-degree ILS polynomial optimization of Molecular Effect Model Equation for Pb class, T_C in Kelvin. In this case, approximations are not applicable/necessary.

Discussion and Conclusions:

The objective of this study was to get and compare 2D graphical/numerical models for Molecular Effect Model in [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs class subject to $T_C > 0°$ C, to Pb HTSC TET Lattice class. Thallium class 2D Graphical optimization shows a clear sinusoid-shape curve, and Pb HTSC TET Lattice class shape is parabolic-like one.

Actually, both groups of these HTSCs materials are in prospective research and development for a number of electronics applications. They own new/useful electronical-thermodynamical properties. In this HTSCs group, MEM model was 2D graphically and numerically determined.

Results are 2D Graphical and Numerical for both HTSC classes. 2D graphical results confirm the steady analytic geometry shapes, for Thallium group, sinusoid, and for Pb one, parabolic-like. Algorithms in these groups can be considered acceptable with low residuals. In contrast with previous research for other groups of HTSCs materials [1, 4-6], the Thallium model shows a sinusoid clear analytic geometry shape. Thallium class analytic geometry does not depend on ILS polynomial-model degree selected. Pb class has low number of compounds, but shows a distinct parabolic-like form. Pb group has an exception with [Pb_3MgO_5], whose molecular mass differ signiflicantly from other class compounds ones. Equations/Approximations for 2, 3, 4 and 5 degree ILS polynomial methods have been obtained and approached with software developed in patterns, loops, imaging processing tools, and arrays. Programming modifications were made specially for each HTSC class.

In summary, 2D ILS Molecular Effect polynomial-modelling and 2D Graphical Optimization methods for HTSCs Thallium and Pb groups materials were determined. Applications in Electronics Physics emerge from all research Numerical/Graphical results.

Scientific Ethics Standards:

The study comprises a totally new class of HTSCs materials. Molecular Effect model was created by author in 2020-1. Equations set are algorithms previously used for different materials class models. 2D/3D Graphical Optimization Methods were created by Dr Francisco Casesnoves in 3rd November 2016, and Interior Optimization Methods in 2019. 2D/3D/4D Graphical and Interior Optimization Methods were created by Dr Casesnoves in 2020. This article has previous papers information, from [1, 4-6], whose inclusion is essential to make the contribution understandable. The 2D Graphical Optimization in Matlab constitutes a software engineering improvement from previous contributions [1,3-9]. The 2D/3D/4D Interior Optimization method is original from the author (August 2020-1). This study was carried out, and their contents are done according to the International Scientific Community and European Union Technology and Science Ethics [38-41]. References [40,41] and [38,39]: '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 [37-40]. And based on 'The European Code of Conduct for Research Integrity'. Revised Edition. ALLEA. 2017. This research was completely done by the author, the computational-software, calculations, images, mathematical propositions and statements, reference citations, and text is original for the author. When a mathematical statement, algorithm, proposition or theorem is presented, demonstration is always included. If any results inconsistency is found after publication, it is clarified in subsequent contributions. The article is

exclusively scientific, without any commercial, institutional, academic, religious, religious-similar, non-scientific theories, personal opinions, political ideas, or economical influences. When anything is taken from a source, it is adequately recognized. Ideas and some text expressions/sentences from previous publications were emphasized due to a clarification aim [38-41].

Author's Biography

Dr Francisco Casesnoves earned the Engineering and Natural Sciences PhD by Talllinn University of Technology (started thesis in 2016, thesis Defence/PhD earned in December 2018, official graduate Diploma 2019). He works as independent research scientist in computational-engineering/physics. Dr Casesnoves earned MSc-BSc, Physics/Applied-Mathematics (Public Eastern-Finland-University, 2001, MSc Thesis in Radiotherapy Treatment Planning Optimization, approved on 3rd November 2001, which was developed after graduation in a series of Radiation Therapy Optimization-Modelling publications and radiotherapy Biological Models [2007-present]). Dr Casesnoves earned Graduate-with-MPhil, in Medicine and Surgery [1983] (Madrid University Medicine School, MPhil in Radioprotection Low Energies Dosimetry [1985]). He studied always in public-educational institutions, was football player 1972-78 (defender and midfielder, Madrid Football Young-League) and as Physician, supports healthy life and all sports activities. Casesnoves resigned definitely to his original nationality in 2020 for ideological reasons, democratic-republican ideology, and ethical-anti-corruption-professional reasons, and does not belong to Spain kingdom anymore. His constant service to the International Scientific Community and Estonian technological progress (2016-present) commenced in 1985 with publications in Medical Physics, with further specialization in applied optimization methods in 1997 at Finland—at the moment approximately 100 recognized publications with approximately 65 DOI papers. His main branch is Computational-mathematical Nonlinear/Inverse Methods Optimization. Casesnoves best-achievements are the Numerical Reuleaux Method in dynamics and nonlinear-optimization [books 2019-2020], The series of Radiotherapy Improvements for AAA superposition-convolution model, the Graphical and Interior Optimization Methods [2016-8], the new Computational Dissection-Anatomical Method, [2020], invention of Forensic Robotics [2020-2021], and Molecular Effect Model for High Temperature Superconductors [2020]. Dr 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 39 physics-engineering articles, two books series, and 1 industrial radiotherapy project associated to Europe Union EIT Health Program (Tartu University, 2017).

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