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COMPUTER SCIENCE AND INFORMATION TECHNOLOGY - ADVANCES AND APPLICATIONS

Research Based Book Chapter

INTERIOR OPTIMIZATION METHODS WITH ELECTRONICS APPLICATIONS EXAMPLES. PART II: MOLECULAR EFFECT MODEL IMPROVEMENTS AND FOUNDATIONS

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RESEARCH BASED BOOK CHAPTER

INTERIOR OPTIMIZATION METHODS WITH ELECTRONICS APPLICATIONS EXAMPLES. PART II: MOLECULAR EFFECT MODEL IMPROVEMENTS AND FOUNDATIONS

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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, and actually is Director of Independent Bioengineering Laboratory. Dr. Casesnoves earned MSc-BSc, Physics/Applied-Mathematics (Public Eastern-Finland-University, MSc Thesis in Radiotherapy Treatment Planning Optimization, which was developed after graduation in a series of Radiation Therapy Optimization-Modelling publications [2007-present]). Dr. Casesnoves earned Graduate-with-MPhil, in Medicine and Surgery [1983] (Madrid University Medicine School, MPhil in Radioprotection Low Energies Dosimetry [1985]). Casesnoves resigned definitely to his original nationality in 2020 for ideological reasons, anti-monarchy-corruption, democratic-republican ideology, and ethical-professional reasons, and does not belong to Spain Kingdom anymore. His constant service to the International Scientific Community and Estonia Republic technological progress involves about 100 DOI articles, more than 120 total publications, and about 5 books. Recent advances published are in Superconductors Mathematical Modelling and Radiotherapy Brain Neurobiological Models, 3D-AI Isodosezones and Isodoselines. Among Dr. Casesnoves inventions and scientific creations are:

1. Numerical Reuleaux Method.
2. Radiotherapy Omega Factor correction for AAA model wedge filters dose delivery.
3. Integral-Differential materials erosion model.
4. Graphical Optimization.
5. Interior Optimization Methods.
6. Superconductors Molecular Effect Model.
7. Superconductors Multifunctional Transmission Line.
8. BED radiotherapy model GA and Graphical Optimization Isodoselines and Isodosezones.
9. Aerospace Turbulence Energy Absorbing System
10. The radiotherapy Fluence Foils Method (FFM) for AAA model.

Preface

This chapter-booklet is focused on Interior Optimization Methods, and specifically for Molecular Effect Model (MEM). Superconductivity is an extensive research multidisciplinary-field where physics, chemistry, materials science, electromagnetism and other areas overlap one another. Therefore, it is crucial to assert that this text is based on computational intelligence optimization methods to obtain as much accurate as possible equations that define HTSC critical temperature—MEM algorithms, simple, with approximations. The practical-database text objective is to gather foremost MEM results developed during a number of previous publications. Sections 1-2 deal with introductions and generalizations. After that there are two subparts, the first one, Sections-[3-5], is a compendium of all numerical database from previous selected papers for two cutting-edge superconductors types-compounds. Namely, Cuprates and Sn groups with different optimization methods. Expressly, Sections 3-[Cuprates-MEM Genetic Algorithms], 4-[Cuprates-MEM Interior-Polynomial 2D-3D Graphical Optimization and Carnot Factor], and 5-[Sn-MEM 2D Polynomial and Genetic Algorithms Optimization]. Those all are used actually in industrial/research electronics with many applications, the most commonly Cuprates category. Along these sections Electronics Physics/Engineering applications for those groups with numerical optimization improvements for the MEM model are mathematically-2D-3D-graphically demonstrated. Second subpart comprises Section 6-[Advances for the most important Hg Isotope Effect aspects], with Hg review-improvements Isotope Effect with 2D-3D Graphical-interior Optimization. In that Section 6, Hg Isotope Effect model optimization algorithms for data development, which is almost exact, is taken in and extensively explained. This Hg and other superconducting chemical elements for Isotope Effect were included in the First Book [9(2)]. Hg Isotope Effect was in conjunction with the first book, [9(2)], and here, for its importance, is improved in numerical accuracy and 3D image-processing. Therefore, the whole Book Chapter is centered to offer a large electronics-physics practical database, previously checked, and show several improvements from precedent contributions. That is, since MEM is in development, its exactness can be applied practically for Critical Temperature acceptable approximate predictions—respectively for cuprates and Tin category. In general, the engineered software shows progression compared to the first book [9(2)]. That is, a better essential physics-parameter data-processing when using superconductors. References are divided into four groups. First one comprises the foremost Cuprates literature. The second one constitutes the Author's selected articles series, for fast search. The third shows a series of the most important references of superconductors publications/literature. Group fourth deals with essential mathematical-computational books. Therefore, the notation of the references is as follows: [reference-number(references-1-group), reference-number(references-2-group), reference-number (references-3-group), reference-number (references-4-group)….].

Keywords
Interior Optimization Methods (IO), Graphical Optimization (GO), Systems of Nonlinear Equations, Electronics Superconductors, Interior Optimization (IO) Methods, Graphical Optimization, Molecular Effect Model (MEM), Tikhonov Regularization (TR), Inverse Least Squares (ILS), Critical Temperature (T_C), Temperature Superconductors (HTSC), BCS Theory, Isotope Effect, (IO), Pareto-Multiobjective Optimization (PMO), Computational Intelligence Methods, Genetic Algorithms (GA).

'To the pursuit of the Truth for itself'

1. General Introduction

When the MEMs where initially tried, [1(2), 2(2)], the foundation failed because it was taken an exponential-algorithm based on Isotope Effect model. The first errors gave rather miscalculations and inconsistencies. Instead, after several tentatives a quasi-polynomial fit was more suitable, and was improved in successive numerical-graphical methods steps. Then, when doing so, 2D-3D Interior Optimization, Graphical Optimization, and Evolutionary Algorithms techniques were applied. The results were some specific superconductors, such as Hg-Cuprates, fitted approximately well for a specific range of Critical Temperatures, while other showed higher errors and lower ranges of accuracy. Refinements, however, were useful to decrease errors. The main conclusion for the MEM construction was that Electronics Physics deep review of the MEM is needed in next stages to reach totally accurate MEMs. That constitute electronically and electromagnetism a theoretical difficult challenge. The main types of superconductors are divided into sections and foremost algorithms/formulations, errors and predictions are also included. Selected 2D-3D image processing charts are shown at every Section with convenient clarifications. Among the number of advances included combined with all sections are the following:

1. 2D-3D Graphical Optimization
2. 2D-3D Interior Optimization, developed from [1(2)-2(2)] mainly
3. 2D-3D Inverse Optimization Methods for a number of Objective Functions, mainly applying the L_1 Chebyshev Norm for Tikhonov Regularization
4. 2D-3D Pareto-Multiobjective Computational Intelligence based on Evolutionary Algorithms Methods
5. 2D-3D Graphical and Interior Optimization based on Pareto-Multiobjective algorithms and software

From these topics in the list, emphasis for their efficacious-modernity and importance can be Pareto-Multiobjective Methods-results, 2D-3D Genetic Algorithms Graphical Optimization and 2D-3D Interior Optimization. Image processing techniques are and were essential for publication series. Programming Systems for software-engineering design were Matlab, Freemat, and GNU-octave. Sometimes Fortran and F# for parallel numerical results checking. The series of research work are extensive and can be consulted using the Further Reading References Section. Extensive formulation is included in Section 5. The reader can get sufficient numerical dataset for implementing specific different software, especially for (T_C) approximate predictions, usually in Kelvin scale. The Author's paper series are set apart from general references. As it is the scientific community ethical criterion of the Casesnoves' Bioengineering Laboratory, almost all those articles are open access.

2. General Mathematical and Computational Methods

Along these publication series, [1(2)-17(2)], a number of mathematical, [2(4)-4(4)], software-engineering, and original algorithms methods were used mainly with MATLAB and GNU-Octave. First and foremost, it is a must to set clearly the main method:

Definition 1.-Interior-Graphical Optimization Method, [Casesnoves, 2018, 9(2)] is a type of Nonlinear Optimization that combines separation of variables method with stages of Graphical Optimization, [Interior Graphical-Optimization Methods were created by Francisco Casesnoves on 3rd November 2018, while he was preparing his Doctoral Thesis Defence. First implementation of algorithms and computational-verification of simulations were carried out in the morning of April 1st, 2020]. The method is based on the classical technique of separation of variables widely used in Differential, and Partial Differential Equations Theory .

What is done in mathematical concepts, is to apply the partial differential equations classical separation of variables method. With separation of variables, it is possible to optimize all the parameters in subsequent stages of 3D graphical optimization plots. At every plot, it is selected the desirable local, global, or semi-local minimum for the variable of convenience. This was done in previous publications for accurate calculations, [2(4)-

4(4)], of Isotope Effect in some essential superconducting elements, such as for instance Hg .

In brief, the method can be synthesized as follows: the initial Graphical Optimization begins with 3 variables, namely, first, second and objective function. An optimal value is determined. The following stage one parameter with two variables is decomposed, and it is taken the optimal values, and so on. Therefore, it is easy to prove, through the multi-selection of local and approximate minima at Graphical Optimization sets, that in general the multiobjective solution for a system of nonlinear equations is not unique. In other words, it is demonstrated from 3D visualization and separation of variables, this classical mathematical assertion. Roughly speaking, one by one the optimal parameters are extracted from the multiparameter objective function to obtain the desirable values. These do not have necessary to be global or local minima, because in practical work, sometimes different magnitudes, neither local nor global minima are needed.

Numbers of graphs required depend on the number of variables of the nonlinear system of equations. As said, the determination of optimal values not necessarily has to be minimal. Optimal values taken depend of the engineering requirements for laboratory optimization, devices manufacturing, experimental plan, or similar tasks. The advantage is that the software engineering gives a fast tool to find necessary data immediately with short time consuming. Some important selected examples of the mathematical-computational methods contained in this booklet are briefed in the following.

1. Inverse Optimization algorithm example, usually with Tihkonov and Chevyshev methods [2(4-4(4)]. The Tikhonov regularization theory constituted an essential method for Isotope Effect articles series, and were also applied for MEM optimization software. Details are included at all Sections, and as an example, the simplest objective function form reads:

For this Superconductor Molecular Model, namely MEM, the constraints values for parameters are shown, for instance, in Equation 1, Section 2, or Equation 1 Section 3. The algorithms set for Tikhonov Inverse Least Squares, [2(4)-4(4)], (ILS) Molecular Effect, with a polynomial p(MO) reads,

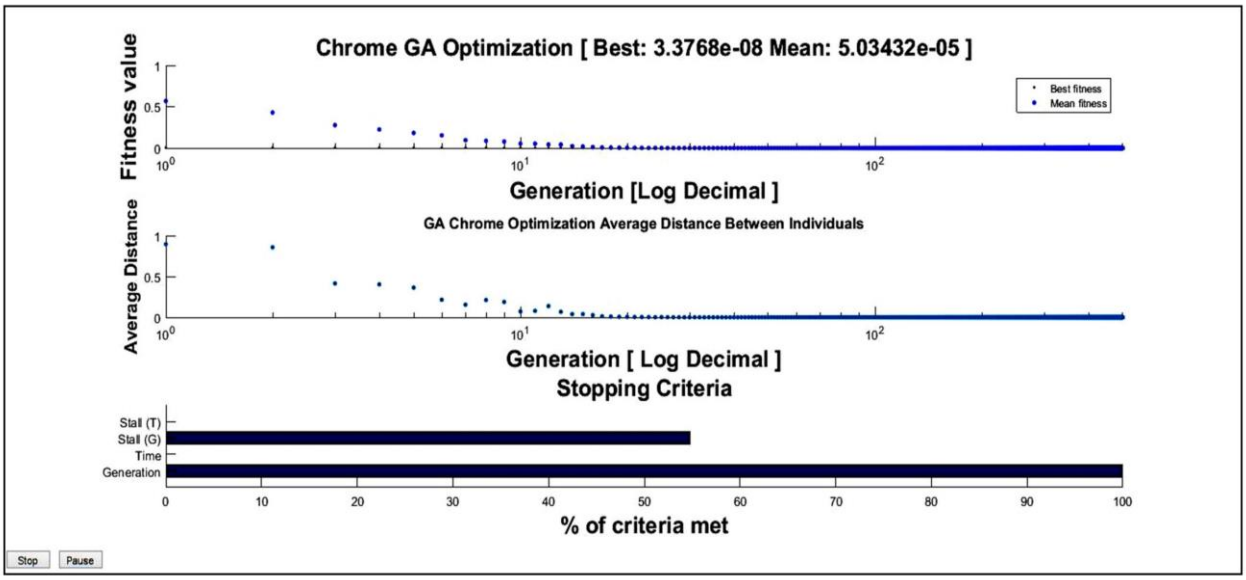
$$
\begin{aligned}
&APPLIED\ TIKHONOV\ FUNCTIONAL;\\
&minimize\ functional\ J\,(\alpha)\\
&with\ \alpha_1 = 0\ and\ L_2\ Norm,\\
&J_\alpha\,(U)_{U\in\Re} = \|\ AU\ -\ P(MO)\ \|_2^2 + [\,\alpha_1\,]\,J_\alpha(U)\,;\\
&Hence\ minimize,\\
&\|\ T_{Ci}\ -\ P(MO_i)\ \|_2^2\ ,\\
&for\ i = 1.....n\\
&subject\ to,\\
&a\ \leqq\ MO_i\ \leqq\ a_1\ ;\\
&b\ \leqq\ T\ \leqq\ b_1\ ;
\end{aligned}
$$

Equation 1
where,
Ja (u) : Functional with regularization parameter alpha.
R : Real space.
u : Searched parameter solution.
MOi : Molecular mass for HTSC Sn class. Section 5, Table 1.
P(MOi) : Polynomial optimization parameter matrix. HTSC Sn range, [Section 6].
a1 : Constant parameter. Tikhonov Regularization Parameter, selected null.
| • |: L_2 Chevyshev Norm (at algorithm software absolute value).
a,a1 : Constraint range specified at Table 1 for HTSC Sn class.
b, b1 : Constraint range specified at Table 1 for HTSC Sn class.

(Example 1. Casesnoves Bioengineering Laboratory. Software. 11347)

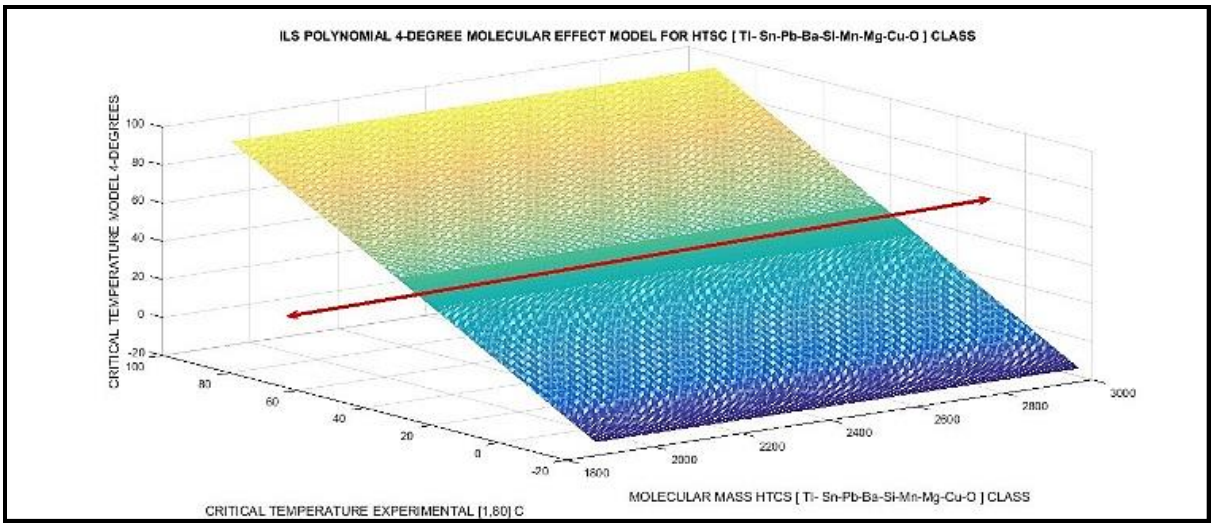
As detailed, MO is the molecular weight of the HTSC selected (i) within a HTSC group with (i) elements and [a-b] are constraints intervals. TCi (= U), is critical temperature (Kelvin) for every (i) member of HTSCs group. Note the matrix (A= 1). The figure a1 is a constant specific Tikhonov Regularization Parameter. The constraints [a-b] are applied for optimization. OF was selected with ILS programming in Matlab or GNU-Octave without algorithmic-linearization, and variations depending on program results accuracy,

2. Computational Intelligence Optimization example, developed through Genetic Algorithms, both graphical and numerical. For example:



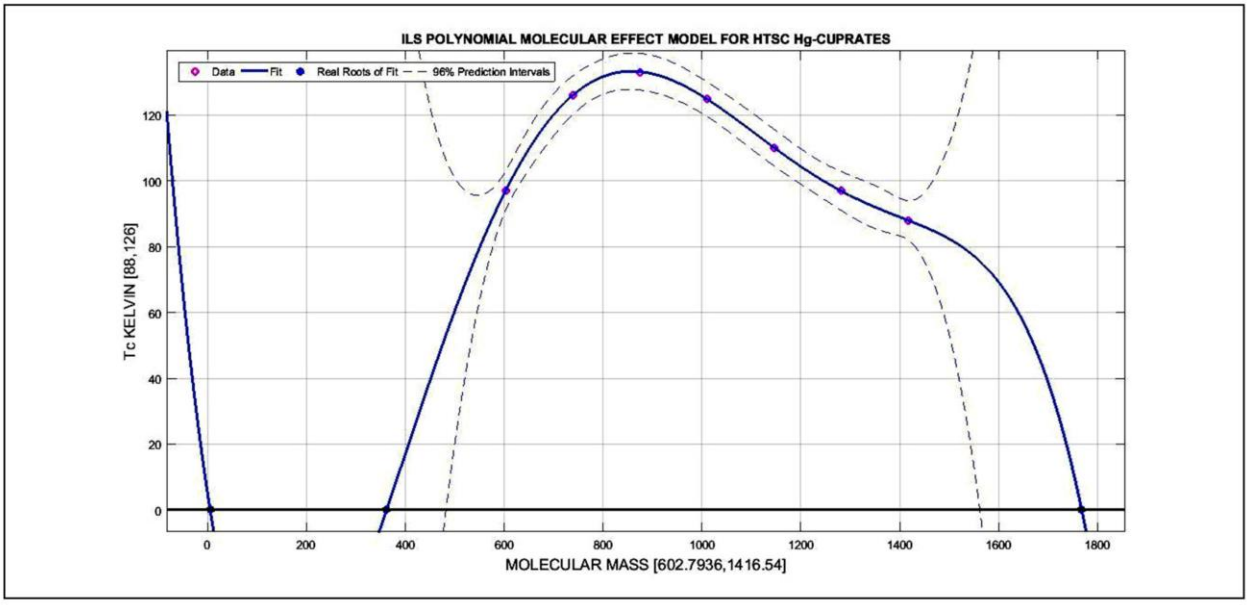
(Example 2. Casesnoves Bioengineering Laboratory. Software. 11348)

3. 3D Imaging Processing Methods Example to obtain the better precise, sharp and specific graphics. For example:



(Example 3. Casesnoves Bioengineering Laboratory. Software. 11349)

4. 3D Imaging Processing Methods Example to obtain the better precise, sharp and specific graphics. For example:



(Example 4. Casesnoves Bioengineering Laboratory. Software. 11350)

3. Hg-Cuprates Superconductors MEM with Evolutionary Algorithms

Abstract

Two different methods are used for Molecular Effect Model Artificial Intelligence Optimization in HTSC Cuprates class—namely, Hg-Cuprates HTSCs, [Hg-Ba-Ca-Cu-O] with [T_C > 0°] . First one is an Inverse Least Squares polynomial numerical technique. Second, Genetic Algorithms (GA) Artificial Intelligence (AI) software is applied in 3D Graphical and Interior Optimization MEM modelling methods. This category is among the most important HTSC. Results comprise both improvements and evaluation with Tikhonov Regularization Functionals algorithms without using objective function logarithmic changes. Determinations also prove the small magnitude differences between these two optimization methods. Outcomes confirm Cuprates Molecular Effect Model (MEM) previously developed hypothesis/equations, and curve shapes. Solutions got show a series of 2D imaging process charts complemented with a group of numerical results. Electronics Physics applications for Superconductors and High Temperature Superconductors and Medical Technology emerge from the study and are specified for MEM.

Keywords
Genetic Algorithms (GA), Molecular Effect Model (MEM), Interior Optimization (IO), Graphical Optimization (GO), Systems of Nonlinear Equations, Critical Temperature (Tc). Tikhonov Regularization (TR), Inverse Least Squares (ILS), Electronics Superconductors, High-Temperature Superconductors (HTSC), BCS Theory, Cuprates HTSCs [Hg-Ba-Ca-Cu-O], Molecular Mass (MO), BCS Theory.

3.1. Introduction and Objectives

The objective of this Section study is to apply Artificial Intelligence in Molecular Effect Model by using ILS- Polynomial and Evolutionary Algorithms for modelling of several important compounds of Cuprates HTSCs class. Namely, Hg-Cuprates, [Hg-Ba-Ca-Cu-O] constrained to [TC > 0°]. The methods applied are 2D Graphical-Interior Polynomial Optimization and Genetic Algorithm techniques. All the software developed constitutes improvements/applications of previous research publications [3(2)-14(2)], not limited to Superconductors field. Along the GA optimization series published, [1(2)-14(2)], Evolutionary Algorithms have proven be accurate and practical, with many programming options. Given any HTSCs class, if differences of molecular weight as a result of proportion/isotopic-variation in the molecule occur, the MEM T_C predictions could be eficacious. As an hypothesis to approximate/predict this T_C magnitude changes MEM has shown be accurate for specific HTSC categories [1(1)-6(1)]. MEM was initially conceived/created on the basis of largely proven Isotope Effect. Inverse Methods, and a number optimization algorithms, [2(4)-3(4)], could also be applied to select a desired T_C subject to an optimal molecular weight composition. The innovations of this following research are given by the software for ILS Polinomial and GA methods. As was presented in [4(2)], and Section 4, further advance consists in setting at Z axis the absolute difference between MEM T_C and experimental T_C. However, in this Section-3, 2D methods are demonstrated exclusively. The software method applied in this study is set with GNU-Octave and Matlab ILS Polynomial and GA Matlab tools, together with 2D Imaging Processing programming in both systems. Results cogency involves a series of 2D charts for ILS Polynomial and GA MEM for Hg-Cuprates. These show the acceptable programming/patterns performance, and final T_C polynomial predictive equations, [Casesnoves Bioengineering Laboratory. Software. 11360].

Succinctly, the Section shows ILS Polynomial and evolutionary algorithm methods with 2D Graphical Optimization for Cuprates HTSC class. The aim is to continue the improvements

for MEM in search for refinements and precision. Applications in Electronics Physics new materials are explored.

3.2. Mathematical and Computational Methods

At Table 1, the software programming setting data for Equation 1, and Section 1]. The programming algorithm made [1(1)-5(1), 4(2)-10(2), 14(2), 3(4), 2(4)-4(4)]. The Tikhonov Functional is implemented/improved with Chebyshev L1 norm from those previous researches. As in [14(2)], the difference with next Section 4 is the 3D setting of MEM algorithm objective function at Z axis [abs (TC Experimental-TC MEM])—that is, upgrade from 2D to 3D. For this Section, the first stage method, Figure 1, comprises the polynomial fit to obtain approximations for subsequent GA further programming patterns/constraints. Secondly, for Evolutionary Method, the results-dataset and GA parameters are shown in single and/or multifunctional charts. That is, both used methods are interactive. Reserved for next Section-3, is the more difficult third stage. It consists in the implementation of GA results into 3D Graphical optimization charts. With 2D GA program, the refinements to obtain the 3D MEM optimal surfactal-fitness will be got in next Section-3. Equation 1 shows the polynomial algorithm based on Tikhonov Regularization, [4(3)-4(4)]. For GA algorithms applied here in the subsequent optimization stage, see Section 6. Equation 1 can be implemented both with GNU-Octave and Matlab, among various computational systems. In those systems, there are several subroutines and methods to get optimal/acceptable results, Table 2.

NUMERICAL OPTIMIZATION DATA FOR Hg-CUPRATES

FORMULATION	MOLECULAR WEIGHT (UAM)	APPROXIMATE T_C (Kelvin)
$HgBa_2CuO_4$	602.7936	97
$HgBa_2CaCu_2O_6$	738.42	126
$HgBa_2Ca_2Cu_3O_8$	874.0432	133
$HgBa_2Ca_3Cu_4O_{10}$	1009.7	125
$HgBa_2Ca_4Cu_5O_{12}$	1145.3	110
$HgBa_2Ca_5Cu_6O_{14}$	1280.9	97
$HgBa_2Ca_6Cu_7O_{16}$	1416.54	88

Table1. Numerical Data for Cr and HTSC Hg-Cuprates. Note the 97 Kelvin temperature corresponds to two different compounds. This fact gives to the 2D and 3D MEM plots a parabolic-like analytic geometry shape. Hg-Cuprates T_C is expressed in Kelvin usually.

$$
\begin{aligned}
&APPLIED\ POLYNOMIAL\ TIKHONOV\ FUNCTIONAL;\\
&minimize\ functional\ J\,(\alpha)\\
&with\ \alpha_1 = 0\ and\ L_2\ Norm,\\
&J_\alpha\,(U)_{U\in\Re} = \|\ AU\ -\ P(MO)\ \|_2^2\ +\ [\,\alpha_1\,]\,J_\alpha(U)\,;\\
&Hence\ minimize,\\
&\|\ \textstyle\sum_{i=1}^{i=n}\ [\,T_{Ci}\ -\ \sum_{m=0}^{m=j}\ K_m\ P(MO_i)^m\ ]\ \|_2^2\ ,\\
&for\ i = 1.....n\ ;\ and\ \ m = 1.....j\ ,\\
&subject\ to,\\
&a_1\ \leqq\ MO_i\ \leqq\ a_n\ ;\ Supercondutor\ Category\ Molecular\ Masses;\\
&b_1\ \leqq\ T_{Ci}\ \leqq\ b_n\ ;\ Superconductor\ Category\ Critical\ Temperatures\,;\\
&K_0\ \leqq\ K_m\ \leqq\ K_j\ ;\ ParametersforPolynomialILSMethod\ [as\ selected\ degree\ j]\,;
\end{aligned}
$$

[Casesnoves Bioengineering Laboratory. Algorithms-Software. 113]

Equation 1

where,

Ja (u) : Functional with regularization parameter alpha.
R : Real space.
u : Searched parameter solution.
MOi : Molecular mass for HTSC Sn class. Section 5, Table 1.
P(MOi) : Cuprates Polynomial optimization parameter matrix. For HTSC Sn class range, see [Section 5].
a1 : Constant parameter. Tikhonov Regularization Parameter, selected null.
| • | : L_2 Chevyshev Norm (at algorithm software absolute value).
i : Number of compounds in every category with corresponding Critical temperatures .
a1,an : Constraint range specified at Table 1 for HTSC class (in this case Cuprates).
b1, bn : Constraint range specified at Table 1 for HTSC class.
m0, mj : Selected Polynomial Degree power number with corresponding coefficients.

The programming techniques are related to previous research [3(2)-9(2), 14(2), 48(3)-51(3)] and dual-program design. In [14(2), 15(2)], software and imaging processing details with explanations are included. With the 2D polynomial fit data, it is possible to get approximations for further setting of GA constraints and lower/upper boundaries. Sketch 1 shows the software method base.

BASIC SKETCH OF MATHEMATICAL PROGRAMMING METHOD	
STAGE	**REASON**
1 MAKE A 2D POLYNOMILA FIT TO SELECT THE BEST POLYNOMIAL MEM DEGREE	GET PRECISION WHEN APPLYING GA CONSTRAINTS
2 SET THE OPTIMAL BOUNDARIES AND CONSTRAINTS WITHING GA SOFTWARE	ONCE THE DATA AND 2D ANALYTIC GEOMETRY IS GOT, SET GA BOUNDARIES AND CONSTRAINTS
3 EVALUATE ALL THE RESIDUALS GOT AND SELECT THE BEST MEM EQUATION	CHOSE THE OPTIMAL FINAL FORMULA FOR THAT HTSC CLASS

Sketch 1. Programming method that was applied in the study. From polynomial ILS method, once getting approximate optimal coefficients, to Evolutionary Algorithms technique. [Casesnoves Bioengineering Laboratory. Software. 11371].

3.3. 2D Imaging-Processing Results

2D graphical results for Hg-Cuprates are presented in Figs 1-7. By observing and guessing data from the figures series, it is easy going to learn and deduce all the graphical and numerical results. Hg- Cuprates MEM show gets the most accurate results at present hypothesis stage, [14(2)].

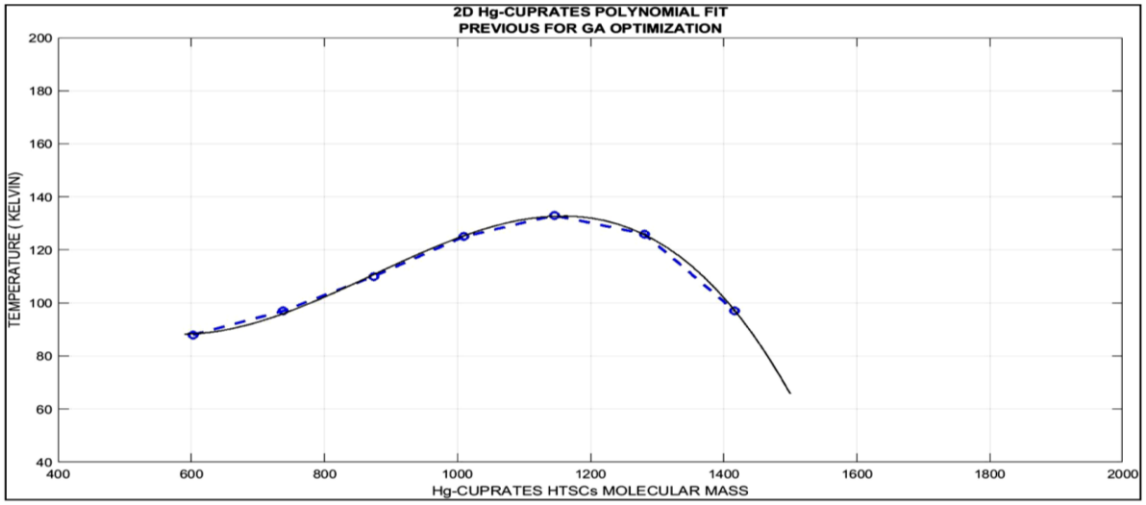


Figure 1. Among all the HTSCs studied in publication series, Hg-Cuprates MEM shows the best analytic geometry results. Note the close coincidence among splines and polynomial model. The GA programming multifunctional 2D graph. 2D Sn polynomial fit parameters intervals set into GA program with Matlab. As it was found in previous contributions, for Sn class the MEM shows in [5(2), 6(2), 13(2), 14(2), 15(2)] an approximate 2D parabolic shape [8(2)]. But Thallium class has a 2D sigmoid analytic geometry, [8(2)].

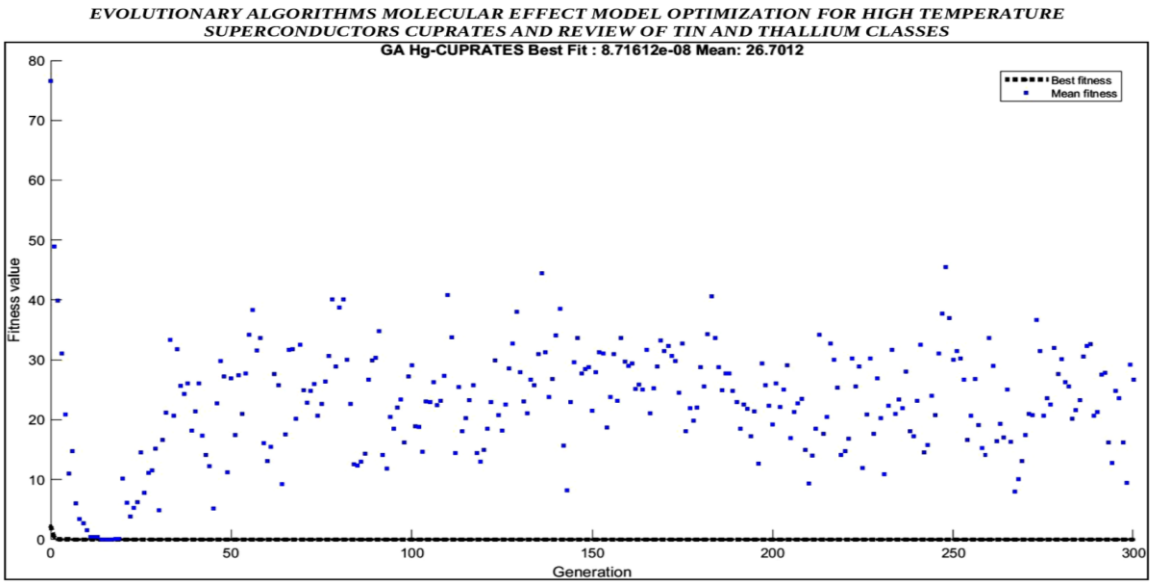


Figure 2. Matlab GA tool best fit chart, with 5 optimization parameters obtained from polynomial data, the most important chart of GA method. Generations Number is 300. As it was found in previous contributions, for Sn and Thallium classes the MEM shows in [8(2)] an approximate 2D parabolic shape in 2D charts. [Casesnoves Bioengineering Laboratory. Software. 11373]

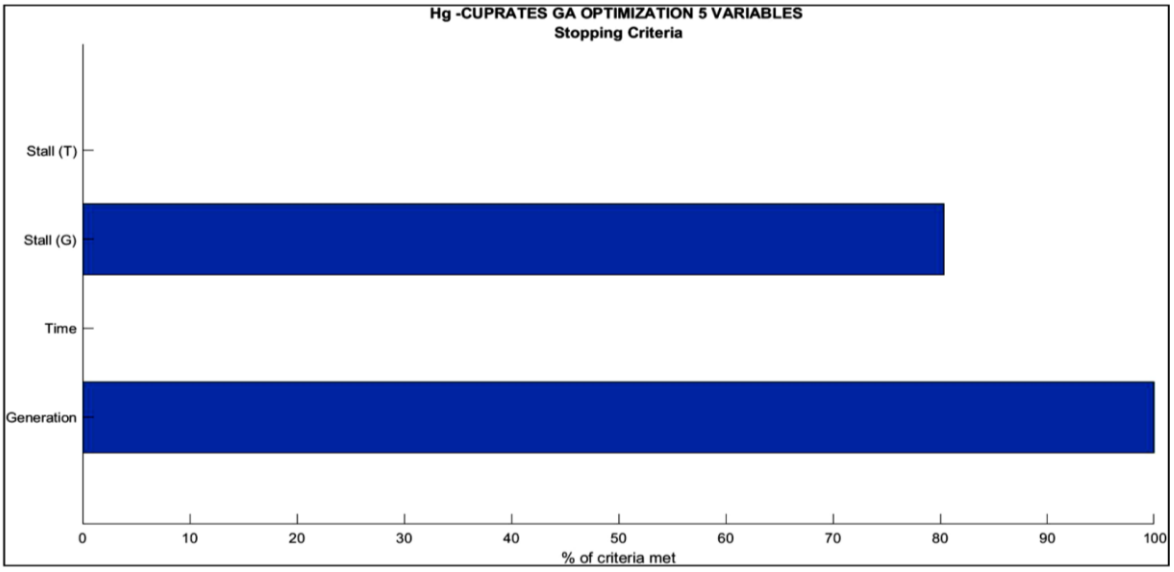


Figure 3. The second most important 2D GA programming graph, note (% criteria met). Generations Number is 300. As it was found in previous contributions, for Sn and Thallium classes, the MEM shows in [7(2), 8(2), 11(2)] acceptable results.

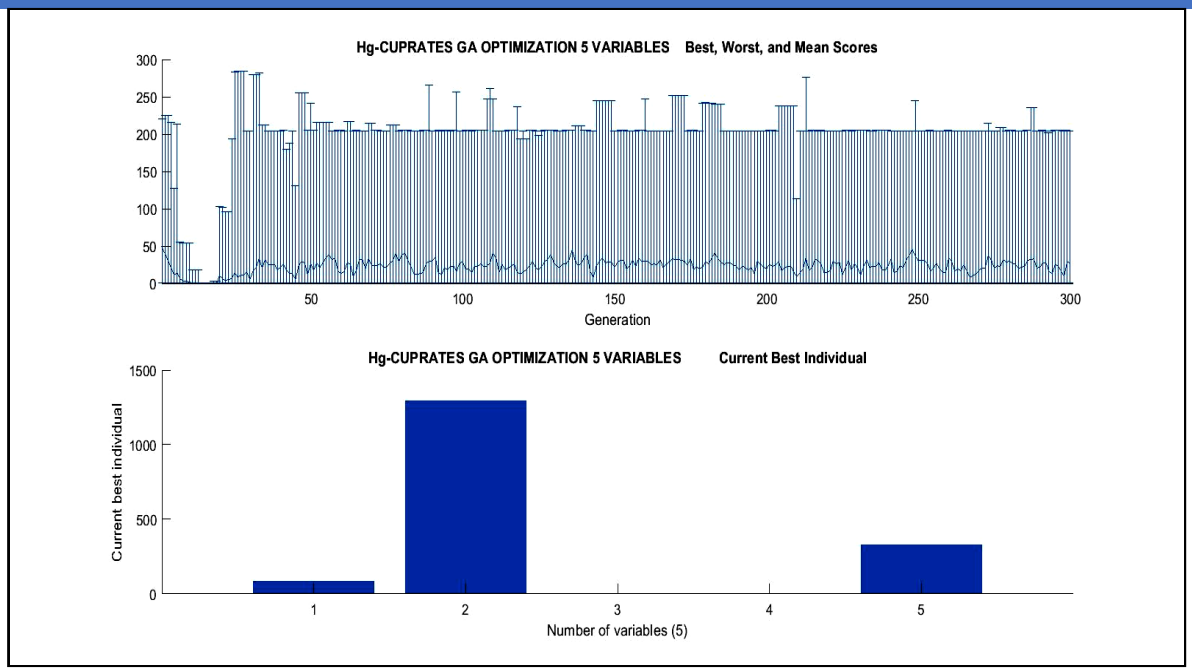


Figure 4. A multifunctional 2D GA programming graph. Generations Number is 300. Complementary data for scores and best individuals. For 2 variables, the result is the most optimal.

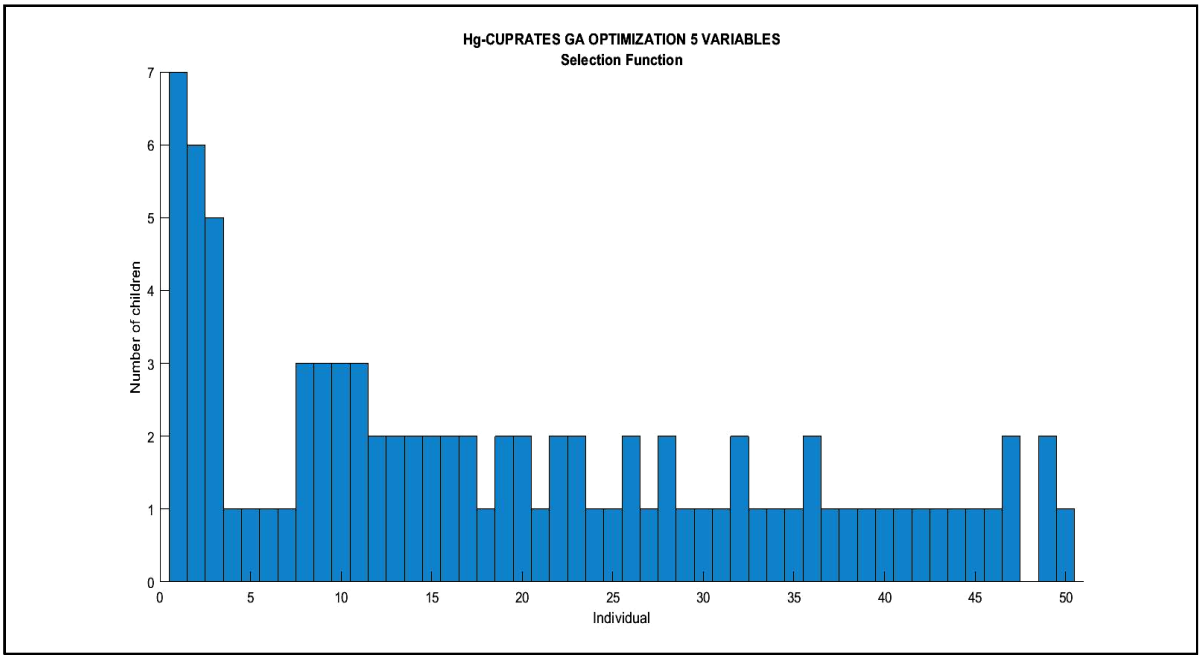


Figure 5. A 2D GA programming graph. Generations Number is 300. Complementary data for children generations and best individuals. For GA Matlab tool, the 2D imaging processing quality is very good. [Casesnoves Bioengineering Laboratory. Software. 11374].

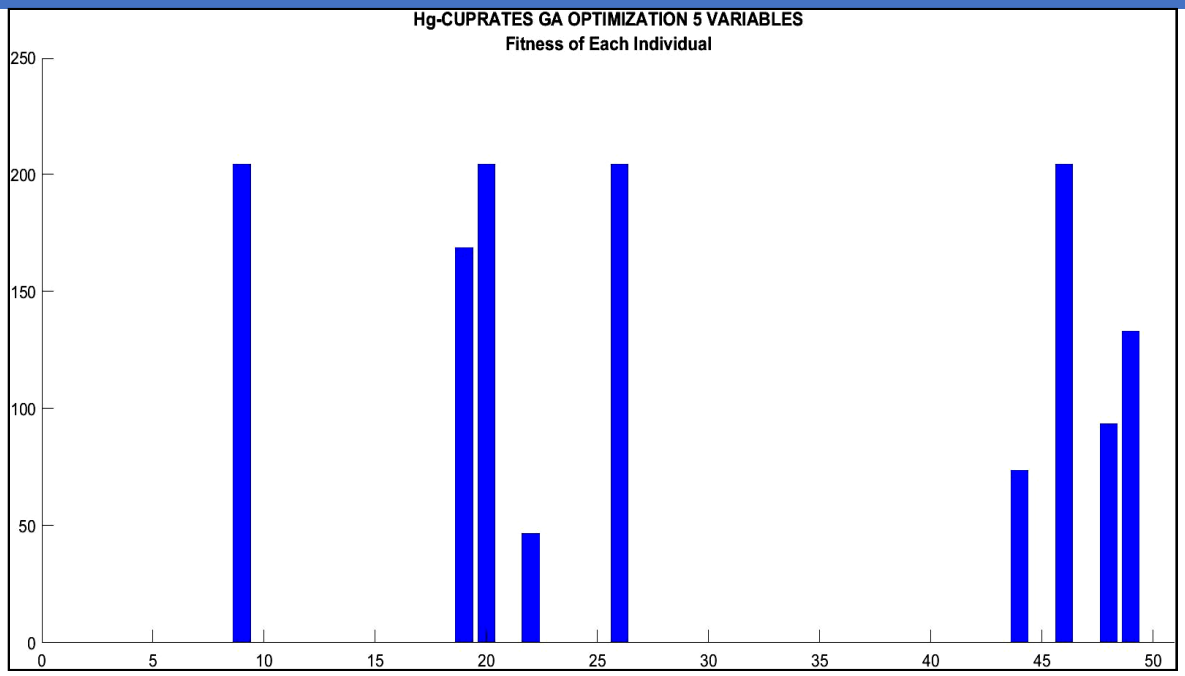


Figure 6. A 2D GA programming complementary graph showing fitness of every individual. Generations Number is 300.

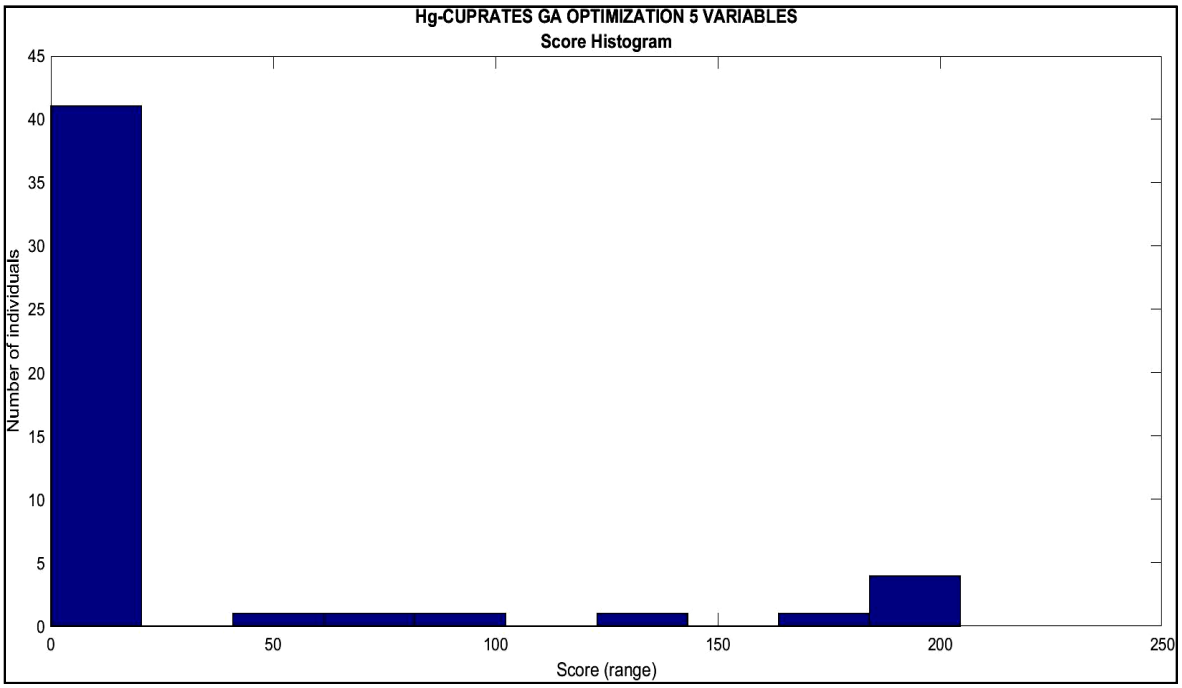


Figure 7. The second most important 2D GA programming graph, note (Score Histogram). Generations Number is 300.

3.4. Numerical Results for Hg-Cuprates

Tables 5-6 show all the dual numerical results with errors for every HTSCs classes. Hg-Cuprates formula is almost quadratic. Errors can be considered acceptable. Number of GA generations is 300-800. Usually, polynomial coefficients of magnitude order about 10^{-9} are discarded for setting algorithms.

Hg-CUPRATES GA OPTIMIZATION RESULTS		
STAGE	EQUATION	COMMENTS
STAGE 1 POLYNOMIAL EQUATION	$T_C = (-478.78e\text{-}009)\ X^3 + (1.25e\text{-}003)\ X^2 - (976.86e\text{-}003)\ X + (326.61)$	Very small numerical differences with GA
STAGE 2 GENETIC ALGORITHMS EQUATION (5 OPTIMIZATION PARAMETERS)	$T_C = (-478.78e\text{-}009)\ X^3 + (1.23e\text{-}003)\ X^2 - (977.00e\text{-}003)\ X + (328.67)$	5 optimization parameters were set, small differences, cubic coefficient almost null, therefore the equation can be considered almost quadratic

Table 5. From [8(2)], brief of Numerical results for cuprates HTSCs classes MEM optimization (3-Degree polynomial ILS) and 2D Graphical GA implementation of software. For Sn and Thallium categories, [Section 5 [8(2), 14(2)] , error is higher in GA because for GA those programs were done for 800 generations, and for polynomial fit was made for 200 functions—so residuals increase, [1(2)-14(2)] .

3.5 Electronics Physics Applications Briefing

Table 3 shows overview of applications for MEM one. Molecular Effect and Isotope Effect applications are guessed and developed from experimental literature database [1(2)-14(2)]. From Table 3, the following points can be considered important,

1 Every HTSCs class shows get a proper 2D algorithm according to Molecular Mass.

2 The most frequent analytic geometry shape obtained is inverse-parabolic.

3 Inverse methods can be applied for engineering design of Superconducting Multifunctional Transmission Lines [12(2)].

4 Applications are at this stage theoretically deduced. MEM usages were also detailed in previous contributions.

SUPERCONDUCTING MOLECULAR EFFECT MODEL APPLICATIONS BRIEFING		
TYPE	**USAGE**	**ADVANTAGES COMMENTS**
General 2D T_c / Molecular Mass curve shape.	For catching up the approximate variation of T_c related to Molecular Mass. This is useful for guess of possibility of T_c predictions	Every HTSC class shows get a proper 2D shape. Usually parabolic inverse, but sigmoid can occur also
Transmission power cable	Power transmission with low loss and large capacity	Electrical and Power Engineering important usage, Low voltage, large current and high transmission power density. Small occupied urban space .
When there are several isotopes types in different proportions in the sample that cause variations in Molecular Mass	In this case, approximations/predictions for T_c could be got from the 2D curve equation	Approximations to be confirmed by following experimental data
When there are several isotopes types in different valences in the sample that cause a different Molecule within the HTSC class	In this case, approximations/predictions for T_c could be got from the 2D curve equation	Approximations to be confirmed by following experimental data. More difficult
When both phenomena happen. Different valences, and isotopes proportions in the prospective HTSC experimental work.	In this case, approximations/predictions for T_c could be got from the 2D curve equation	Much more difficult
Inverse Optimization of isotopes proportion to obtain a desirable T_c	Precision to reach an optimal T_c	This is a theoretical approach

Table 3. Brief of applications for the MEM that were explained in former contribution series. Isotope Effect applications can also be guessed, [1(2)-14(2)].

3.6. Discussion and Conclusions

This research objective was multiple. Firstly, to apply the ILS Polynomial Optimization on Hg-Cuprates HTSCs class, following the former studies. Secondly, the usage/implementation of the Polynomial dataset for getting more accuracy with Genetic algorithm method. Finally, analyze/compare both 2D graphical and numerical results. Therefore, as in [8(2)], the innovation of this study is the GA application following results got in previous contributions [7(2), 8(2), 14(2)]. The GA optimization for Hg-Cuprates was performed with 5 parameters. Results comprise initially Hg-Cuprates HTSCs class 2D MEM polynomial Objective Function Graphical and Numerical Optimization database. Secondly a GA series of graphics for Evolutionary method. This 2D imaging processing prove close similarities in MEM with the Tin class approximately parabolic-shaped curvatures and numerical- graphical extrapolations

for T_C —see Section 5. The best results, both numerical and curve-shape for MEM are got with the Hg-Cuprates group. This is significative to prove MEM, because Cuprates category is widely used today in superconductivity engineering/physics.

Numerical results for both methods are approximately acceptable, Table 2. These HTSC groups MEM [Casesnoves, 2020], 2D analytical geometry shapes and 3D MEM Objective Functions curvatures can be considered approximately satisfactory with low residuals, Figures 1-7 Electronics Physics applications for MEM are explained, Table 3.

Advantages of this GA software method are the 2D improved mathematical and geometrical numerical analysis for the MEM optimization. Further, the numerical coincidence with 2D polynomial fits proves the cogency of the Artificial intelligence method. Inconvenients with GA programming multifunctional 2D imaging processing was the increasing running time, about 2-4 minutes, when several GA optimization parameters and numerical statistics are implemented in a unique graph. However, the Matlab GA tool for this modern technique type gives wide information about the optimization process. The higher number of generations, the longer running gradient time in GA compared to other optimization Inverse Least Squares Polynomial methods used previously. Therefore, MEM hypothesis algorithms are at secondary development stage.

Software and programming methods are based on previous contributions. Sketch 1 shows the basic technique stages, [7(2), 8(2),14(2)] . The programming for Figures 1-7 requires arranging of GA special commands, patterns, loops, optimal running time choice, and setting precise upper and lower boundary limits for constraints.

Grosso modo, a 2D improved-comparative ILS Polynomial and GA methods for MEM subject to Hg-Cuprates is demonstrated/developed for MEM. Primary applications in Electronics/ Electromagnetics are included.

4. Hg-Cuprates Superconductors with Carnot Factor

Abstract

From previous publication series, the Molecular Effect Model (MEM) with Interior and Graphical Optimization is presented. Those studies comprised Type I and Type II superconductors materials, both classical and modern ones. However, this Section shows 2D-3D advances in MEM for important Hg-Cuprates, HTSC Type II, and new applications of MEM to determine-compute the thermodinamical Carnot Factor. Imaging-processing in 2D-3D and numerical results with two systems, GNU-Octave and Matlab, are proven and detailed. Software-engineering results are shown in single or multifunctional graphics,

complemented with numerical tables. Applications in Electronics Physics Superconductors modelling are explained.

Keywords

Molecular Effect M (MEM), Interior Optimization (IO) Methods, Polynomial Fitting (PF), Graphical Optimization (GO), Systems of Nonlinear Equations, Tikhonov Regularization (TR), Inverse Least Squares (ILS), Electronics Superconductors, High-Temperature Superconductors (HTSC), BCS Theory, Carnot Factor (CF).

4.1. Introduction

This Section continues superconductivity Cuprates mathematical modelling, but upraised for 2D-3D Interior and Graphical Optimization [5(2)-7(2), 12(2)-16(2)]. Today, SC and HTSC constitute a research field/applications framework with quite unpredictable practical/theoretical rapid advances. The Critical Temperature predictions in function of material composition for engineering/manufacturing applications are an important part of the SC and HTSC efficacious usage.

HTSC Hg-Cuprates category is one of the first Type II class discovered/applied in superconductivity, [1(1)-6(1)]. From [1(1), 5(1)], the Cuprates Critical Temperature is above the liquid-nitrogen boiling point [≈77.3 K]. Roughly speaking, Hg-type compounds general-chemical formula [Hgx1-Bax2-Cax3-Cux4-Ox5], where the subindices [1-5] can vary. Those are the subject of the study. Their important applications are varied. Namely, [5(1)], power engineering, production of high-field magnets in the range of [5–10] T, superconducting tapes and cables, rotating machines, fault current limiters, etc. In Electronics, for example, passive and active microwaves devices, digital circuits, and many other. At References 7.1, important books related specifically for HTSC Cuprates are [1(1)-6(1)]. For References 7.3 further reading, it is recommended [1(3), 8(3)-10(3), 42(3)-44(3)]. Since the superconductivity research field is multidisciplinary, to understand the electromagnetism area and proofs of superconductors theory could be difficult. Some electromagnetism references, [50(3)], deal with electrostatics, electrodynamics, magnetism and related equations-proofs that are applied/indispensable in basic superconductivity theory. The foremost mathematical applied framework along Author's Further Reading References 7.2, can be found [1(4)-5(4)]. For a fast catch-up of initial investigations/experimental of superconductors Type I at [10(1)-11(1)].

Related to Cuprates optimal industrial applications, classical Carnot Factor (CF), is commonly used in thermal-power engineering. That is, to minimize the industrial costs when using superconductors. The Carnot Cycle theory belongs Thermodynamic Physics branch. However today, for refrigerator cycles, there is a large variety of thermodinamical cycles, [1(1), 13(1), 17(2)]. This subject is developed in the second Section.

4.2. Fundamental Concepts

The determination of critical temperature (TC) in superconductors Type I and Type II is crucial for power engineering, physics, and industrial applications [1(1)-6(1), 9(2)]. The superconductivity research field is an open area whose new advances and applications number is increasing recently. Along a series of articles and a book, [1(2)-9(2)], 3D Interior Optimization mathematical methods were developed for modelling the classical-exponential BCS equation for classical Type I (TC) determination. Inspired mathematically from Isotope Effect, but with a different modeling technique, the Molecular Effect Model (MEM) for Type II High Temperature Superconductors was primarily built up. In that research line, 2D-3D Interior and Graphical Optimization modeling-methods were applied for MEM in cuprates, Example-Figure 1 .

Therefore, this new contribution presents advances for MEM model in HTSC cuprates, one of the most important families in HTSC. In addition, the practical Carnot Factor, [1(1), 13(1)], applied on superconductivity for cuprates, is optimized in 2D-3D imaging-processing and numerical data.

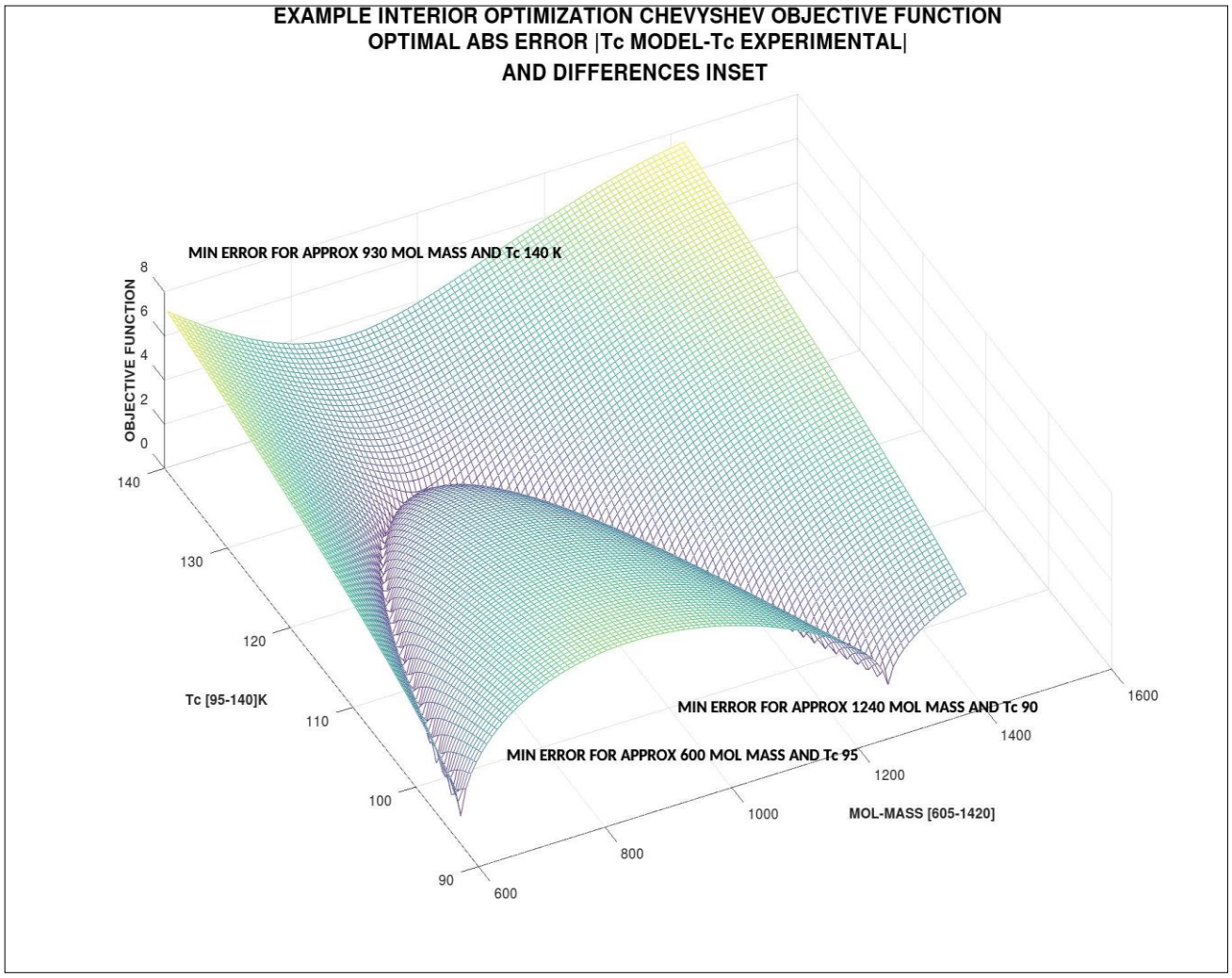
Results comprise a database of BCS and MEM (TC) values for Type I and Type II superconductors. The challenges for future SC and HTSC research are described in Table 1, [Casesnoves, 2021, author's proposal]. Then, some views in this field for the future superconductivity advances are also included at Tables 1-2, [7(1)]. Consequently, the article has two main strands. Namely, the improvements for MEM in HTSC cuprates, and Carnot Factor 2D-3D Graphical Optimization. Additionally, an extended/complemented review of Hg Isotope Effect, 2D-3D Graphical/Interior Optimization, set in simplified concepts/graphs, is presented. Future trends and research lines/areas for HTSC are shown in Tables 1-2. Engineering and Physics applications are briefed.

SUPERCONDUCTORS POWER-ENGINEERING FUTURE CHALLENGES [Author's Proposal]			
Overview Type	**Advance**	**Limitation**	**Additional**
Copper and classical line transmissions. For example: single triaxial HTS cable operating at 13 kV and transferring 69 MVA of power [Refs-9, 49].	Substitution of classical transmission lines (TL) with savings of common metal materials.	Length of TL And materials/energy cost for cooling superconductors.	The new Type II HTSC might overcome some or several of those technical hurdles.
Classical line transmissions substitution. Superconductivity in the Future Electric Grid for short-distances.	Increase of savings in space and underground conduction space. Reduce electricity costs through intracontinental power marketing. Specially power engineering super-computer demands.	According to ground, land, urban surroundings, safety conditions, etc. However refrigeration issues make long distances connections difficult.	Cost of staff, designers, refrigeration technology, additional power-plant engineering changes derived of the new system.
High-Voltage Transmission Lines.	Theoretical projects advances. From [Refs-9, 49] : '*within the superconducting layer of the new 2G superconductors, current densities are typically more than 10,000 times higher than those possible in copper*'.	Several, as High-Voltage TL are much longer and transmit high-power energy. High magnetic field that should be shielded.	The more progress in new SC and HTSC materials, the better possibilities. The bureaucratic work is reduced since one HTSC TL takes less volume-space. Reduction thermal and electromagnetic contamination field (EMF) for population surrounding underground infrastructure.
Energy efficiency and loss savings.	Theoretically extremely high savings and efficiency. Conventional transformers replacement, [Refs-9, 49]. Functional optimization to substitute the necessary conventional transformers exclusively. Then, from [Refs-9, 49], significant energy losses occur in conventional transformers as a result of the iron in the core (no-load losses) and the copper in the windings (load losses).	Limited by construction costs, cooling devices, underground construction, etc. Conversion technology phases could result in high cost.	The more progress in new SC and HTSC materials, the better efficacy in savings possibilities.
Intense magnetic Field generated surrounding neighborhood. Magnetoradioprotection problem.	How can be taken advantage of this magnetic field and at the same time avoid magnetoradioprotection risks? .	Explore this engineering energy approach possibility. Resulting magnetic energy could be extracted? .	The magnetic field generated by SC is intense. Shielding is necessary at some places. For example cardiological damage possibility to vulnerable surrounding people etc.

Table 1. Improved-modified from a previous conference publication, [7(1)], Author's proposal about future superconductivity, strategic research lines according Overview of possible future developments/applications for SC and HTSC applications in transmission lines.

SUPERCONDUCTORS POWER-ENGINEERING AND ELECTRONICS SOME FUTURE STRATEGIC RESEARCH LINES [From 49, Sarrao, J ; Nault, R. (2006). Basic research needs for superconductivity.]	
PRIORITY [Directly From 49, Sarrao, J ; Nault, R. (2006)]	**REASONS AND OBJECTIVES**
Identifying simplified criteria for screening materials and implementing them into Computational Algorithms	Elaboration of screens for new-potential superconductors will enable this search, because it will allow identification of the most likely materials with faster/slower conductivity. Then, substitution of classical SC with more reliable and operational ones.
Integrating Synthesis and Surface-Sensitive Characterization Techniques	There are new laboratory techniques to be used for these objectives, such as molecular beam epitaxy (MBE), applicable for films of various complex oxides.
Computational Libraries of Potential Superconductors	Efficacious and efficient techniques/methods for creating materials libraries that which could be used for new properties.
Developing Reliable and Fast Methods to Determine the Surface Structure	This is an important point as it saves laboratory time for characterization of potential new superconductors, and therefore increases probabilities of advances.
Enabling materials for superconductor utilization	Materials apparently unable to show superconducting properties could get that characteristics by using modifications.
Low-temperature Insulators	Insulators are essential to reach optimal critical temperatures. That involves both mechanical improvements and thermal properties research.
Magnets and Dielectrics	More efficacious and efficient transformers for more optimal magnetic fields and capacitors.
Control Systems	For example, MOSFETs, capacitors, inductors with better cryogenic properties given by new materials.
Maximize Refrigeration Efficiency	That is a field of convergence for several branches, namely, Chemistry, Mechanics, Thermodynamics and Thermo-Physics.

Table 2. From a previous conference publication, [4(2)] future strategic research lines according [1(7), Sarrao, J; Nault, R. (2006)]. This is a briefing of future investigation areas. Those are basic research needs for superconductivity] criteria. Note: that is an overview and brief resume with data of a prestigious institution among other conferences about SC and HTSC research institutes.



Example-Figure 1. Molecular Effective Model got for Cuprates with minimum error. For example, inset, according to Table 3, [Abs-Error ≤ 8 K] for approx [605, 1420] molecular mass and Tc around [95,140] K. That is, the approximation of MEM matches published experimental Tc [15(2)]. Note that in this tentative program imaging-processing the surface graphical optimization is rather complicated but fits approximately experimental results. Observe the shape similarities between the 3D surface parabolic geodesics and the 2D parabolic curves of Figure 1. The Table 3 Cuprates shows a parabolic-numerical-shape with approximately the same TC for low molecular masses, and high ones, while for intermediate molecular mass magnitudes the TC values are the highest. Just that is proven at this MEM computational-graphical optimization [Casesnoves Bioengineering Laboratory. Software. 11378].

4.3. Research Objectives

Research objectives with Cuprates are mainly two. The first one is to improve the Molecular Effect Model for cuprate HTSC from previous publications, [5(2)-7(2), 12(2)-16(2)]. Secondly, to begin the study of Carnot factor for HTSC by using Cuprates MEM models, [14(1)]. Based on these methods/software, complementary and higher-accuracy purpose, developed in Section 6, will be to review the precision obtained with Interior Optimization Method for Hg, which is useful as Hg is a chemical element whose isotopes show a varied statistical composition in this natural element, [5(2)-7(2), 12(2)-16(2)]. Applications for HTSC electronics physics are briefed.

Grosso modo, this article shows improvements for Molecular effect Model for Cuprates and findings for 2D-3D Graphical optimization Cuprates Carnot Factor. Electronics physics applications are detailed.

4.4. Mathematical and Computational Methods

The programming techniques are related to previous research [1(2)-17(2)] and dual-multiple-programs design. Along those articles, software and 2D-3D imaging processing details with explanations are included. With the 2D polynomial fit data, it is possible to get approximations for further setting of Genetic Algorithms constraints and lower/upper boundaries, but that is not the study objective.

4.5. Interior Optimization

Interior Optimization is a method, [9(2)], that was developed computationally mainly for electronics physics applications, although is a mathematical-computational general method. Specifically was published, [1(2), 2(2)], for Isotope Effect in several SC elements. Here was used for getting the best polynomial algorithm in the selected, Table 3, HTSC cuprates.

4.6. Graphical Optimization

Graphical Optimization method was developed by Author in 2016, mainly for metal hardness mathematical modelling, [12(3)]. Later on, in publication series for several research areas, [22(3)]. Basically, this method involves the numerical fit of the objective function set in a 3D surface to find with precision the global, local, partial, desired-selected, or approximated minima. Here it is used to get the accurate difference in Kelvin degrees between Tc experimental, Table 3, and Tc of the model, results at Table 4. Note that since the 2D and 3D imaging-processing charts, Figures 1-4, give large numerical

values at prompt; it is possible guess the prediction of Tc for a different cuprate compound whose isotope composition makes difference from the standard experimental dataset, Table 3. That is in fact the objective-usage of the present study here.

4.7. HTSC Cuprates Computational Dataset

There are several Cuprates HTSC major categories. Namely, Hg-Ba-Ca-Cu (the subject of this study), Thallium-based cuprates, those compounds formed when Tl is substituted by Bi or when Ba is replaced by Sr, and some of them with Rare Earths. This study is based on Hg-Ba-Ca-Cu-O compounds/family, as it is widely used in industry, Table 3. In that data-table HTSC cuprates show a parabolic-shape distribution with approximately the same TC , Example Figure 1, for low molecular masses, and high ones. Instead, for intermediate places molecular mass magnitudes for corresponding TC values are the highest, Figure 1, Table 3. In such a way, the relative-numerical links among molecular masses and Tc was used for creating the Molecular Effect Model. It is inspired from classical Isotope Effect one [10(1)-11(1)]. Hg-Cuprate compounds show a very useful/practical Tc, and as an instance, it is about the night temperature of the moon, [16(2)].

CUPRATES COMPUTATIONAL SOFTWARE DATASET [Mainly from Hott et al. , 2005; and Superconductors.org, 2025 ; Tetragonal Crystal Lattice]			
Cuprate Type	**Molecular Weight**	**T_c [Kelvin, K]**	**Additional**
HgBa2 Ca6 Cu7 O16	1416.5400	88	Minimum T_c
HgBa2 Ca5 Cu6 O15	1312.8960	107	Decreasing T_c
HgBa2 Ca5 Cu6 O14	1280.9000	97	Decreasing T_c
Hg2 Ba2 Ca3 Cu4 O12	1242.2420	114	Decreasing T_c
HgBa2 Ca4 Cu5 O13	1161.2750	110	Decreasing T_c
Hg Ba2 Ca4 Cu5 O12	1145.3000	110	Decreasing T_c
(Hg0.8Tl0.2)Ba2Ca2Cu3O8.33	1096.1000	138	Maximum T_c
HgBa2 Ca3 Cu4 O11	1025.6530	127	IncreasingT_c
Hg Ba2 Ca3 Cu4 O10	1009.7000	125-126	Double point for optimization
Hg2 Ba2 Ca2 Cu3 O10	1106.6000	45	N/A, T_c difference too high
Hg2 Ba2 CaCu2 O8	971.0000	44	N/A, T_c difference too high
HgBa2 Ca2 Cu3 O9	890.0300	134	IncreasingT_c but low Molecular Mass
Hg Ba2 Ca2Cu3 O8	874.0432	133-135	Double point for optimization
HgBa1.8 Tl0.2 Ca2 Cu3 O10	804.6400	138	IncreasingT_c
HgBa2 CaCu2 O7	754.4100	128	IncreasingT_c
Hg Ba2 CaCu2 O6	738.4200	126	IncreasingT_c
HgBa2(Ca1-xSrx)Cu2O6+	738.4100	123-125	For (x=0), Double point for optimization
HgBa2 Cu1 O5	618.7900	97	Approximated Minimum T_c
Hg Ba2 Cu O4	602.7936	97	Approximated Minimum T_c

Table 3. Software programming selected data with references for Cuprates Hg-Ba-Ca-Cu-O group [1(1)-6(1), 14(1)]. The criterion for ordering data was increasing molecular mass. Details are included.

For the 2D-3D computational development, a number of algorithms are applied [see Section 6, Algorithms 1-6]. For example, one foremost among these reads,

INTERIOR OPTIMIZATION MULTIOBJECTIVE ALGORITHM, (SIMPLEST TECHNIQUE):

$$
\begin{aligned}
&if\ optimization\ stage\ is,\\
&minimize,\\
&f(\overrightarrow{X}) = f\,[x_1, x_2, ...x_N]\\
&by\ using\ similar\ partial\ differential\ method\\
&of\ separation\ of\ variables,\ for\ instance,\\
&if\ it\ is\ at\ principal\ function, a\ product,\ such\ as,\\
&x = x_1 \bullet x_2\ ,\\
&it\ is\ grouped\ for\ a\ 3D\ axis\ imaging - processing\ as,\\
&x_{1s} = x_1 \bullet x_2\ ,\\
&and\ so\ one;
\end{aligned}
$$

(1)

where,

f(X) : Vectorial principal function. X is a vector of one sub-function.

f(xi) : Sub-function component of principal function vector or matrix, every xi is a variable-vector.

N : Number of matrix functions.

xi : A variable-vector. S is the number of sub-functions.

4.8. Carnot Factor Optimization

Carnot Factor (CF), is commonly used to optimize the industrial cost of superconductivity usage [1(1)]. It is based on the classical Carnot Cycle in Thermodynamic Physics. For refrigerator cycles, there is a large variety of thermodinamical ones. Most applied theoretical cycles are the Carnot and Claude cycles, however the options are varied. The refrigerator whether liquid or gas constitutes an essential part of the cooling system. A classical refrigerator was liquid nitrogen, [77 K], [1(1), 13(1)]. Recently, most applied for superconducting lines are liquid hydrogen (Tc = 20 K), liquid nitrogen, [77 K], liquid helium for Low Temperatures Superconductors [T= 4.2 K]. For superconductivity below [T =39 K], both helium gas and liquid nitrogen.

Therefore, today Carnot Factor for thermodynamical efficiency continues being used effectively. In general, at [T = 4.2 K], the superconducting energy has not an economically optimal cost [1(1),13(1)]. The so-called Operation Temperature is fundamental parameter for Carnot Factor determination. An example is shown at [1(1)], namely ' to remove a heat input of 1 W an ideal, reversible refrigerator consumes at room temperature a power of 70 W for Top = 4.2 K, whereas this power is only 2.9 W for operation at 77 K '. Critical current is another important constraint for the economic cost of superconductor devices, but not the focus of this study.

In brief, the second objective of this research is to optimize in 2D-3D the CF for HTSC cuprates of Table 3. Hence the CF algorithm, [1(1)], reads,

$$Carnot\ Factor\ (CF)\ Fundamental\ Equation,$$
$$CF = \frac{300\ K - T_{operating}}{T_{operating}};$$

(2)

where,

CF : Carnot Factor (adimensional).
K: Kelvin.
Tcold = 300 K (usually). Note that in Figures 5-8, it is set at programs in intervals [275,326].
Toperating: Operating temperature of the superconductor device (K). In Figures-software is set at [20,120] or [0,120] K.
This formula is applied for 2D-3D numerical determinations in two ways. In 2D, first one is setting a range of Toperation interval [0 , 120] K, and at the second, but computationally more difficult, implementing simultaneously a Tcold interval of [275 , 325], Figure 5 . Just the same second method was used for 3D CF surface, Figures 5-8.

4.9. 2D-3D Graphical-Interior Optimization and Numerical Results

Based on publications series, [1(2)-17(2)], the software-programming results for these methods, graphical and numerical, are demonstrated /shown in the following, Figures 1-8, Table 4.

4.10. 2D-3D Graphical Cuprate MEM Optimization

The graphical-interior simulations in 2D-3D are done by using and improving previous publications superconductivity software, [17(2)], mainly. According to Example Figure 1, the first step is to order database of Table 3 for programming. After that, a regression polynomial fit is designed in four phases to obtain a final continuous 3-degree optimal polynomial of Tc in function of the molecular mass, Figure 1. It was found no significant numerical precision difference between a 3-degree and a 4-degree fit. The initial polynomial equation is set with further software to obtain a continuous model, through these successive steps, Figure 1, Equation (2). Both GNU-Octave and Matlab systems were/could be used for 2D-3D graphics, and in most of cases programs are equivalent with few differences, Figures 1-4. Proven Molecular Effect Model : The parabolic shape of Figure 1 is extrapolated to Figure 2 , inset, red polygon, and model efficacy is demonstrated.

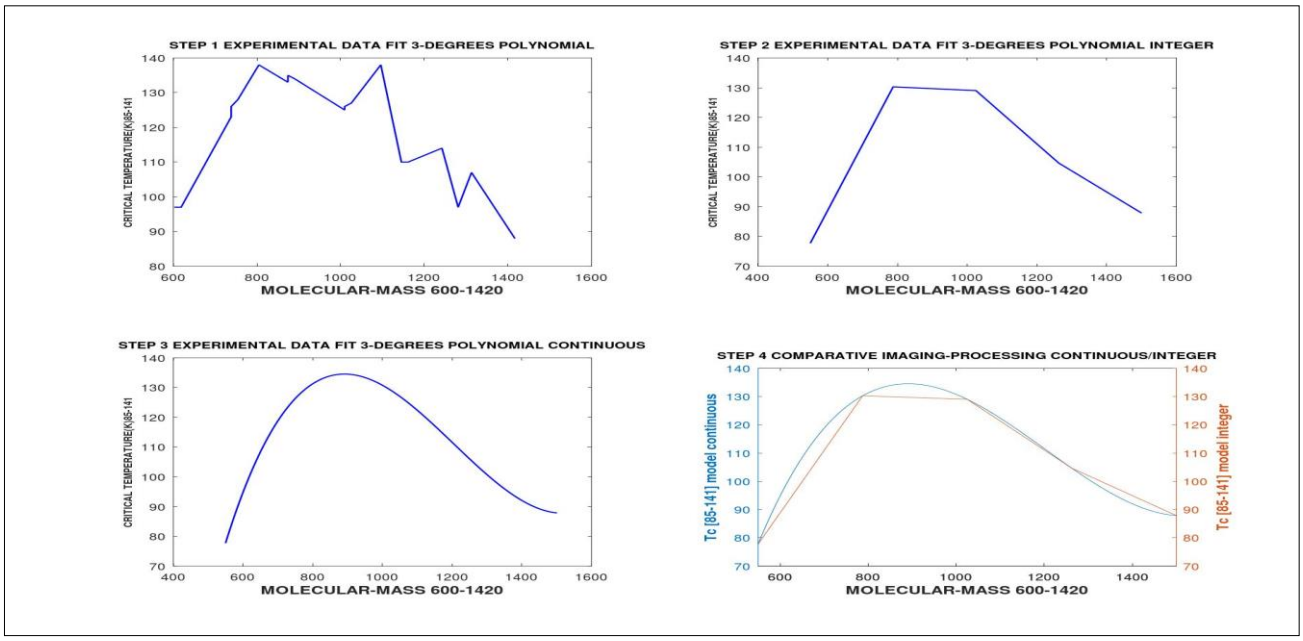


Figure 1. GNU-Octave 2D Molecular Effective Model for Cuprates programming-construction with minimum error, four stages. As in Example Figure 1, these 2D approximations of MEM match published experimental Tc, Table 3 . From step 1 to step 4, it is demonstrated the efficacy of the polynomial fit, Equation (2). Note in this tentative program imaging-processing that the geodesic surface of Example Figure 1 indeed contains/shows these curves or integer approximations. Every curve shape from step 1 to step 4 has different fitting software, and to obtain those stage by stage is rather complicated/laborious. The Table 3 Cuprates shows a parabolic-shape with

approximately the same TC for low molecular masses, and high ones, while for intermediate molecular mass magnitudes the TC values are the highest. Just that is proven at this 2D MEM computational-graphical optimization. Matlab programs for this 2D imaging-processing are almost equivalent. Next Figure 2 demonstrates these parabolic shapes reproduced with precision at 3D MEM model. It is a rather laborious program. [Casesnoves Bioengineering Laboratory. Software. 11379].

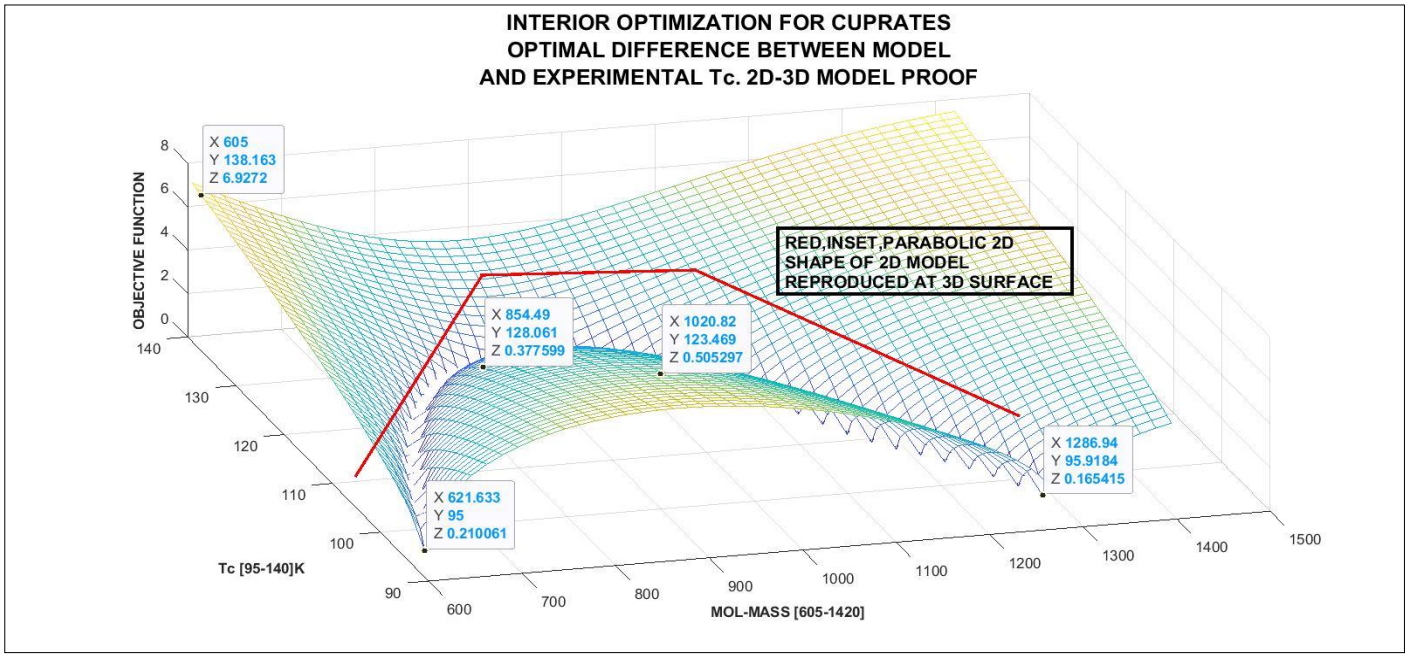


Figure 2 .- Matlab 3D Molecular Effective Model for Cuprates with minimum error, marked inset numerical data. As in Example Figure 1, those 2D approximations of MEM match published experimental Tc. A polygon resembling the parabolic shape of the Figure 1, (inset, in red), shows the geodesic similarities with 2D curves of Figure 1. Note the low absolute errors (Z values) got with the polynomial MEM model, Equation (2). The matrices software to obtain this image-processing is rather difficult, not for program length, but for matrices congruence [Casesnoves Bioengineering Laboratory. Software. 11381].

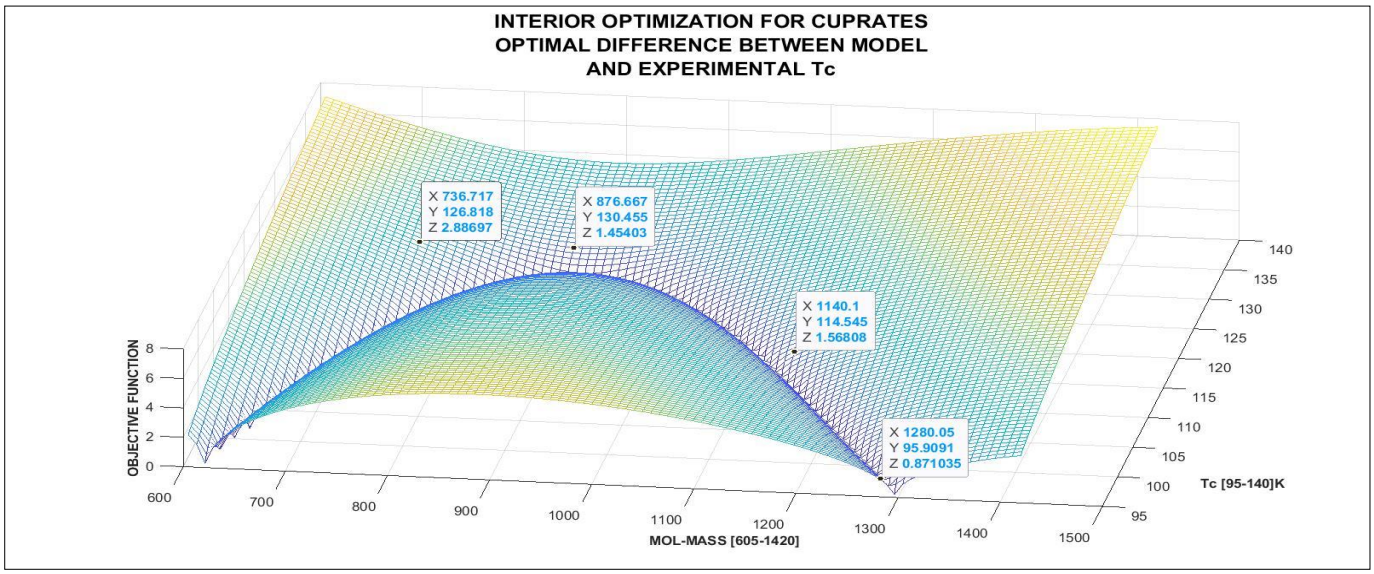


Figure 2.1 .- Matlab 3D Molecular Effective Model for Cuprates with Table 4 extracted dataset. It is intended to prove the absolute error improvements for the MEM model. Absolute error, according to this image and Table 4, is : 2D-3D abs errors (K) ; [0 ≤ Abs Error ≤ 8] (K). Marked inset, numerical data. As in Example Figure 1, those 2D approximations of MEM match published experimental Tc. Note more clearly the low absolute errors (Z values) got with the polynomial MEM model, Equation (2). As in Figure 2, the matrices software to obtain this image-processing is rather difficult, not for program length, but for matrices congruence [Casesnoves Bioengineering Laboratory. Software. 11382].

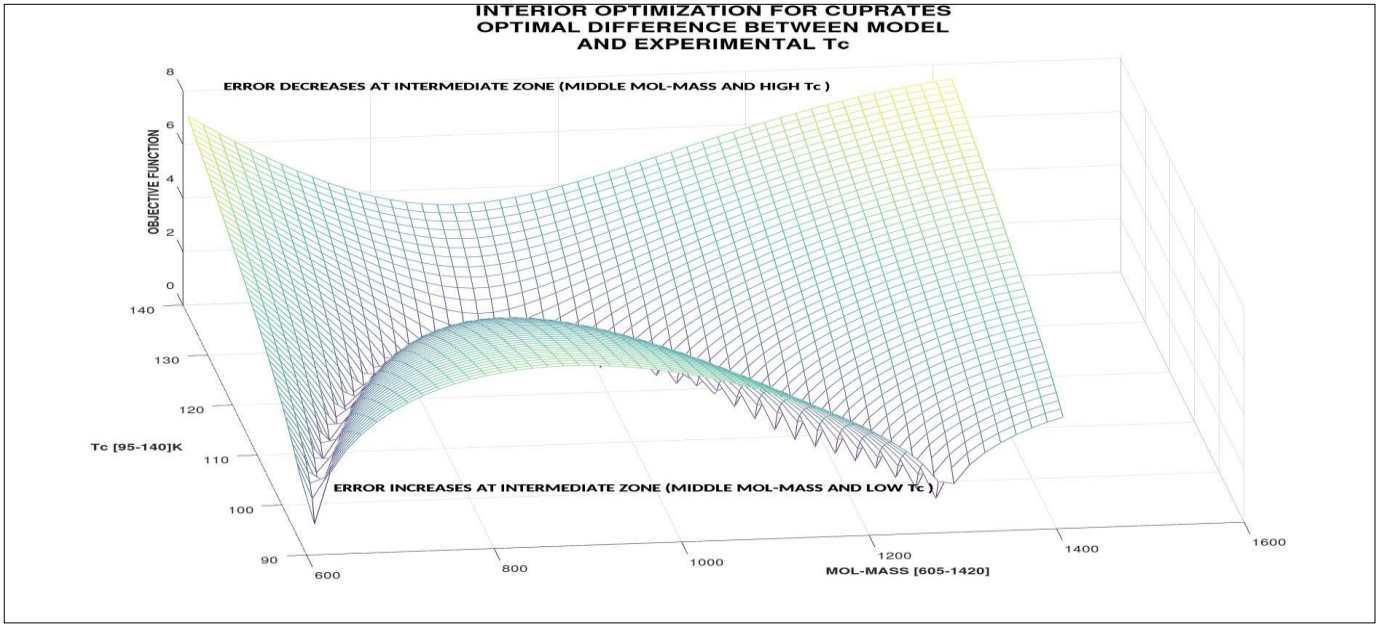


Figure 3 .- GNU-Octave 3D Molecular Effective Model for Cuprates with Table 3 extracted dataset. It is intended to show the absolute error improvements and error distribution along the surface (Notes inset). Absolute error, decreases at posterior surface part, and

increases at anterior one. According to this image and Table 4, is: 2D-3D abs errors (K) ; [0 ≤ Abs Error ≤ 8] (K) . As in Matlab imaging-processing Figures 2, 2.1 the matrices software to obtain this image-processing is rather difficult, not for program length, but for matrices congruence. The GNU-Octave image processing quality is acceptable but Matlab is better [Casesnoves Bioengineering Laboratory. Software. 11382].

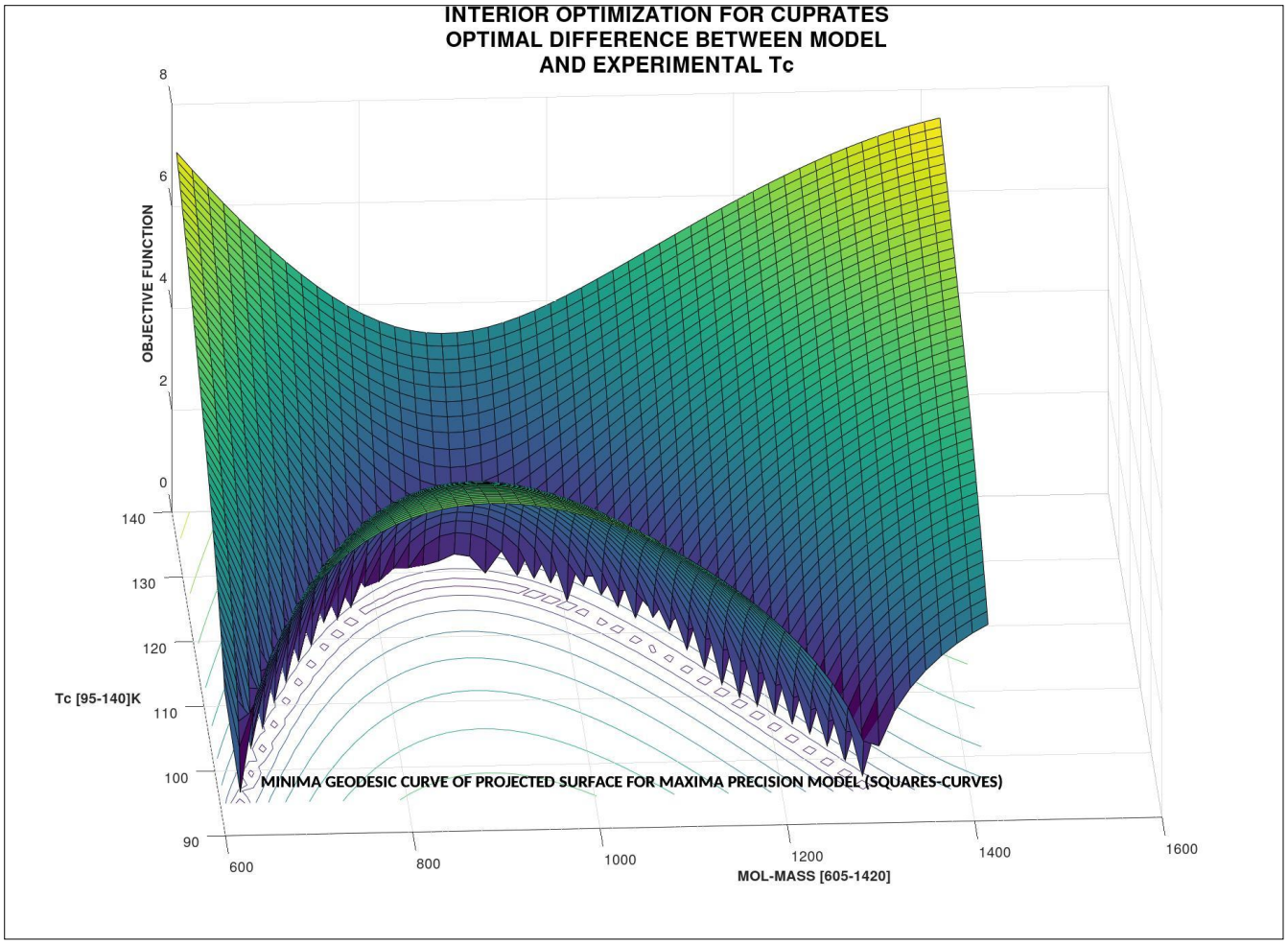


Figure 4. This GNU-Octave image was programmed for showing clearly the geodesic error projections and surface curves marking the minima (squares or small polygons) curve from where the surface begins to get higher Z-coordinates at the posterior. That is, the minima geodesic projections where the surface begins to grow towards posterior and anterior directions are shown with those small squares. The image-processing subroutine at pattern is different from Figure 3 [Casesnoves Bioengineering Laboratory. Software. 11383].

4.11. 2D-3D Graphical Cuprate Carnot Factor (CF) Optimization

According to Equation (1), CF constitutes a practical numerical reference for functional manufacturing and operating of SC and HTSC devices. Figure 5 was designed with 2D software-engineering inspired in [1(1)], but with variable intervals for both Toperation and Tcold (blue for fixed Tcold at 300 K, and red-dashed or black for variable intervals of Toperation and Tcold. It is proven that, even separating the curves (second chart right, x+10, y+10), the shapes are almost coincident. That is corroborated at 3D implementation, Figures 6-8.

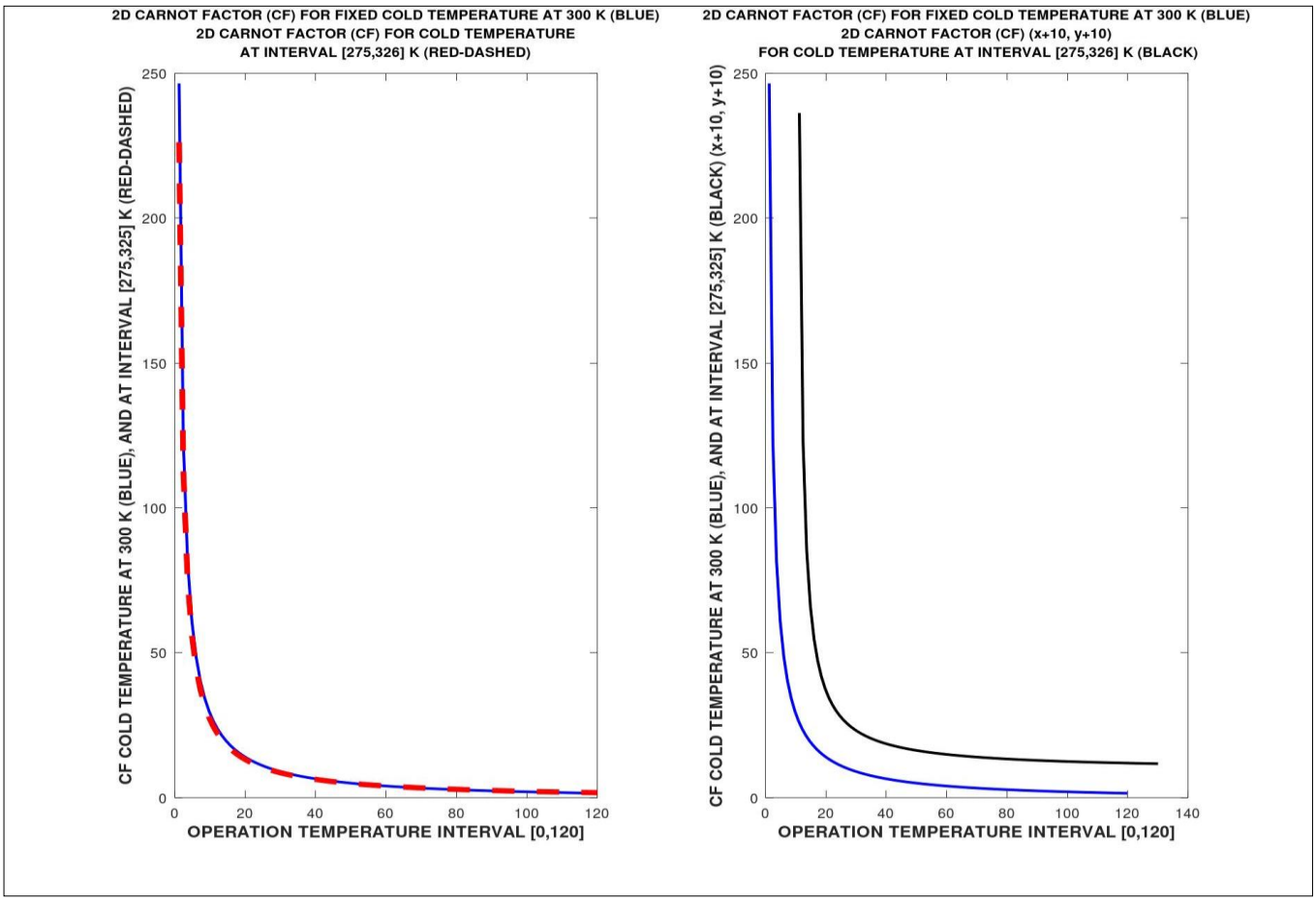


Figure 5.- GNU-Octave 2D Carnot Factor for Cuprates with two programming techniques. Matlab programs for this 2D imaging-processing are almost equivalent. Red dashed-line, inset left, shows variable intervals for both Toperation [0,120] K, and Tcold fixed at 300 K, while the blue coincident line correspond to CF with Tcold [275,326] and Toperation [0,120]. At right, both curves are separated to prove almost total coincidence, that is, blue curve is for fixed Tcold at 300 K, and black one shows CF for Tcold interval [275,326]. For better visualization, the second methods, inset black, shows a small translation (second

black curve, x+10, y+10), the shapes are almost coincident. This program seems be simple, but is rather laborious [Casesnoves Bioengineering Laboratory. Software. 11384].

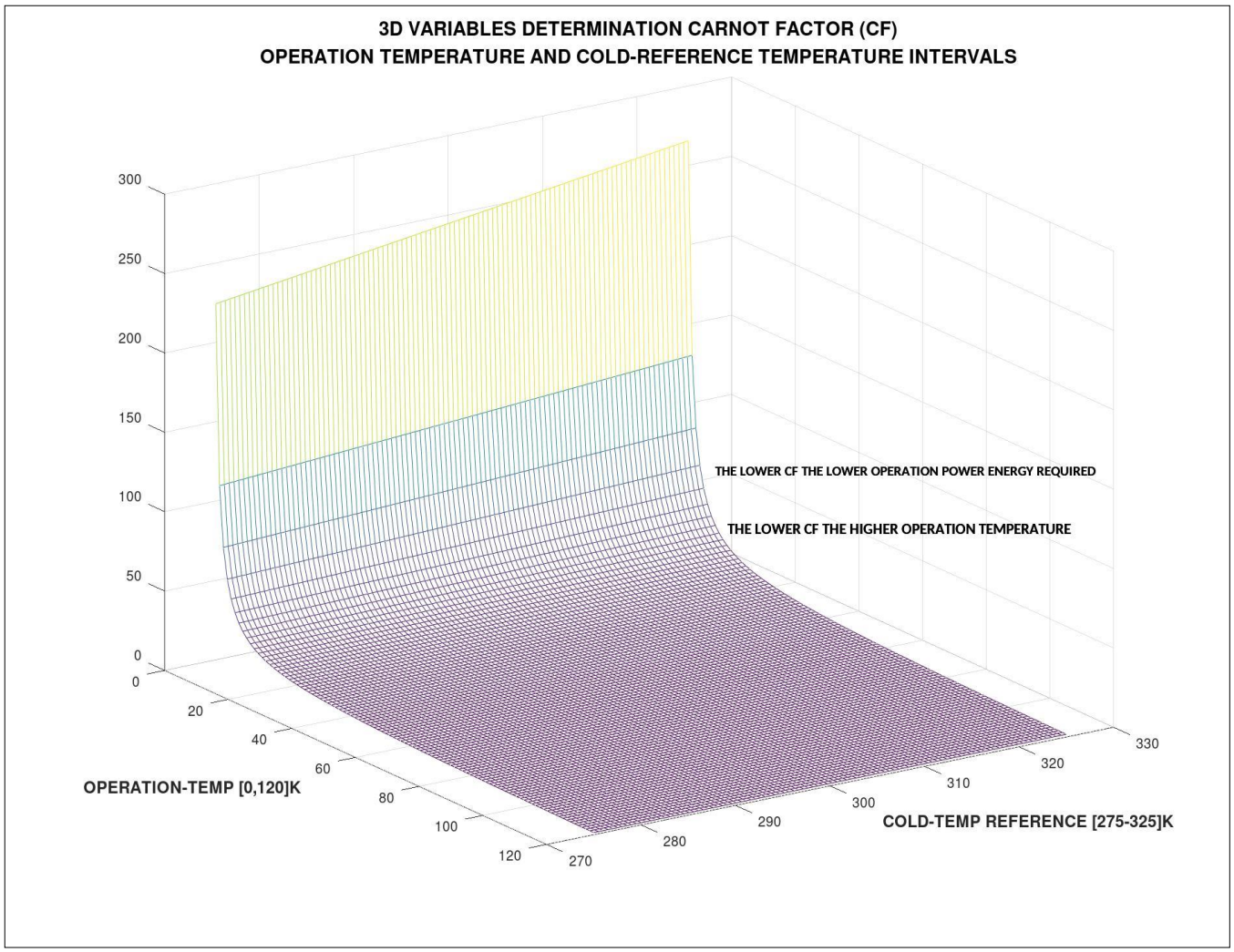


Figure 6 .- GNU-Octave 3D Carnot Factor model for Cuprates with Tcold interval [275,325] and Tcold one [0,120]. Minimum error. Marked inset, the minimum CF zone, and the maximum Cf area. Matrices at program patterns have to be calculated precisely [Casesnoves Bioengineering Laboratory. Software. 11385].

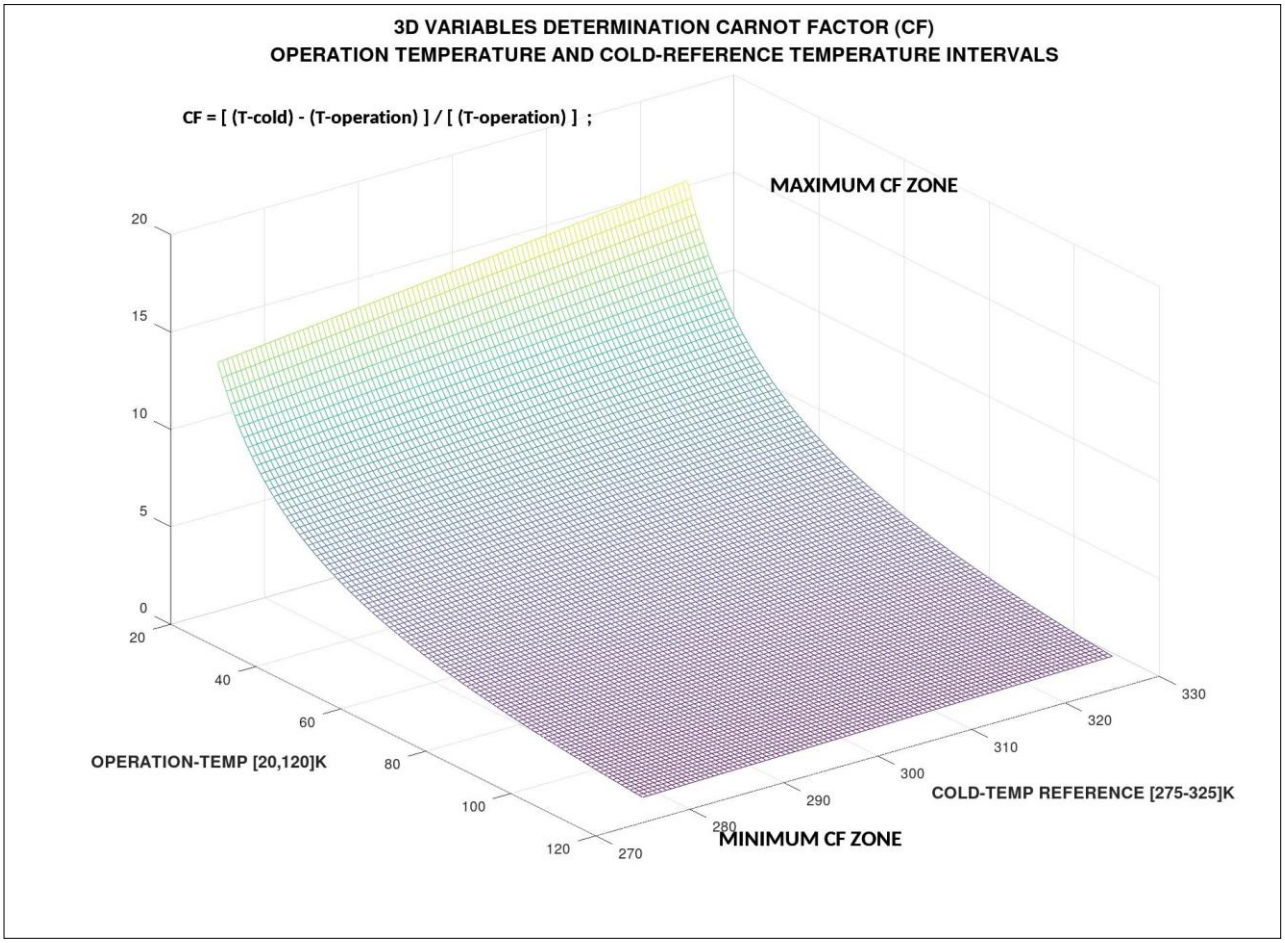


Figure 7.- GNU-Octave 3D Carnot Factor model for Cuprates with Tcold interval [275,325] and Tcold one [0,120]. Minimum error. Marked inset, the minimum CF zone, and the maximum Cf area. Matrices at program patterns have to be calculated precisely [Casesnoves Bioengineering Laboratory. Software. 11386].

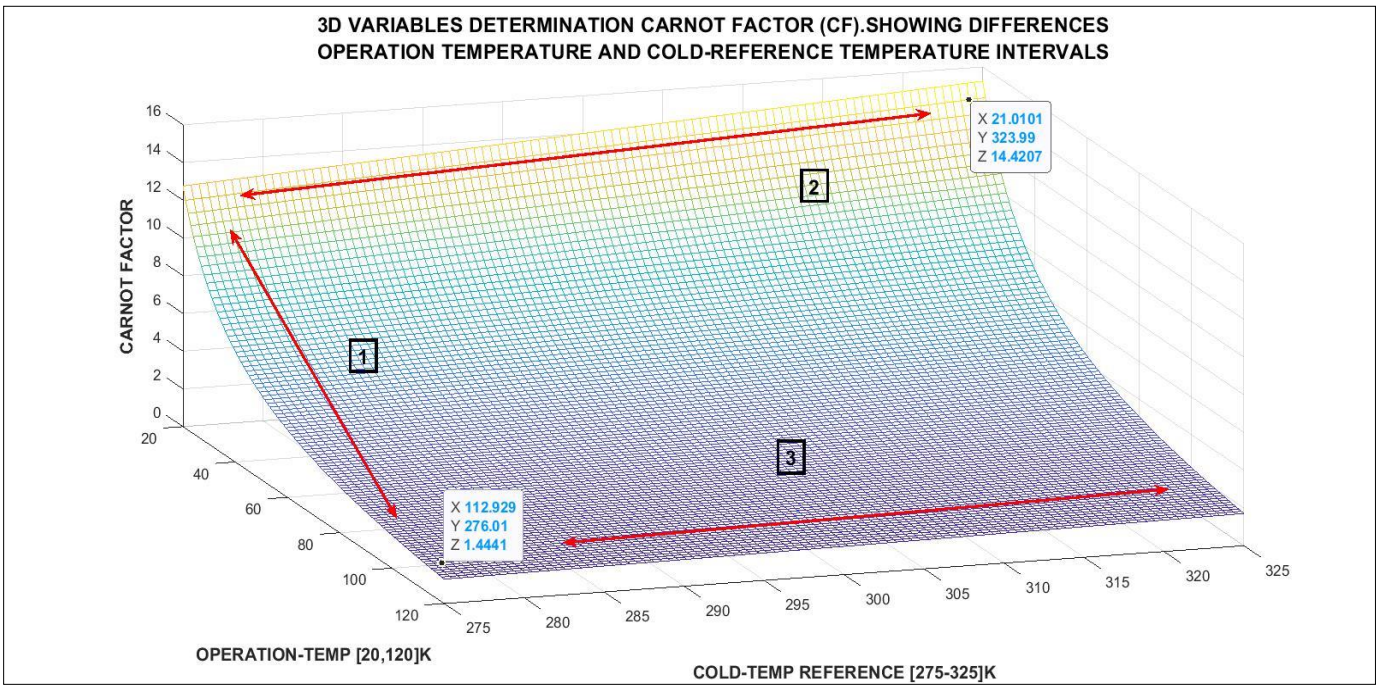


Figure 8.- Matlab 3D Carnot Factor model for Cuprates with Tcold interval [275,325] and Tcold one [0,120]. Minimum error. Marked inset with red-lines directions, the variable gradients. The lower CF, the lower operation power energy required. Besides, the lower CF, the higher operation temperature. Some numerical data are shown for illustration. Direction (1) proves the lower CF, the higher operation temperature at low Tcold (about 275 K). Direction (2) shows the higher Tcold, the higher CF, at low Toperation (about 20 K). Direction (3) proves the higher Tcold, the higher smoothly CF, at high Toperation (about 120 K) [Casesnoves Bioengineering Laboratory. Software. 11387].

4.12. Numerical Results

The numerical results have two strands. The first one is the MEM model equation that was used for Tc predictions in function of cuprates HTSC molecular mass. That is, the main algorithm since some variants was applied in specific programs. The second is the comparative numerical results that can be got from the Matlab and GNU-Octave 2D-3D plots. In Matlab it is easier and the cursor at prompt/display can give more numerical information. Table 4 shows some numerical-comparative results. The main algorithm obtained by polynomial fit reads,

$$The Critical Temperature, T_C\,(M),\ for Cuprates Molecular Effect Model,$$
$$T_C = (3.816905454232244e-07)\ M^3 + (-1.378534024981543e-03)\ M^2 + (1.547508999519298)\ M + (-4.198839134235919)\ 10^2 - (420.980091430742)^{0.46}\ ;$$

(3)

where,

Tc (M) : Function of Critical Temperature (Tc) as function of Cuprates Molecular Mass (M) from Table 3 dataset polynomial optimization [Casesnoves Bioengineering Laboratory. Algorithms-Software. 11386].

NUMERICAL RESULTS AND ERRORS			
Graphical-Optimization Method for Error Boundaries Calculations: From 2D-3D model curves and surfaces, Figures, 1-5, the magnitude values of Table 3 are tentatively sought with GNU-Octave (2D) and Matlab (3D) cursors. Then, the figures given by the 2D and 3D dataset are used to calculate tentatively the maximum and minimum errors among the experimental Tc and the model Tc. The highest differences between Table 3 experimental data and model values are taken to determine the global error boundaries. The final calculation is done with a simple Matlab or GNU-Octave program.			
3D NUMERICAL RESULTS, EXAMPLES			
MOLECULAR MASS EXPERIMENTAL [APPROXIMATED TO Table 3]	Tc EXPERIMENTAL (K) [Table 3]	Tc MOLECULAR EFFECT MODEL CONTINUOUS MODEL PREDICTION (K) [Figure 2.1]	3D ABS ERROR (K) ; [0 ≤ Abs Error ≤ 8] (K) Average 3D Error= 4.0633 K ; (Figures 2-4) [Although some errors are high, the statistical mode is low, then average error results be about 4 K]
736.7170	123-125	126.8180	~ 0
876.6670	133-135	130.455	~ 0
1140.1000	110	114.5450	1.57
1280.0500	97	95.9091	0.87
2D NUMERICAL RESULTS, EXAMPLES			
MOLECULAR MASS EXPERIMENTAL [Table 3]	Tc EXPERIMENTAL (K) [Table 3]	Tc MOLECULAR EFFECT MODEL CONTINUOUS MODEL PREDICTION (K) [Figure 1]	2D ABS ERROR (K) ; [0 ≤ Abs Error ≤ 8] (K) Average 2D Error= 4.0633 K ; (Figure, from step 3-4) [Although some errors are high, the statistical mode is low, then average error results be about 4 K]
602.7936	97	95.93	1.07
738.4100	123-125	124.34	~ 0
874.0432	133-135	134.68	~ 0
1025.6530	127	129.04	2.04
1241.2420	114	106.73	7.27
1280.9000	97	101.04	4.04
1416.5400	88	91.00	3.00

Table 4.-2D-3D Cuprates MEM model with errors according to Figures 1-4. Absolute Error is [0 ≤ Abs Error ≤ 8] (K). Average 2D-3D Error= 4.0633 K ; (Figures 1-4). Results are improved from previous publications [5(2)-17(2)].

4.13. Discussion and Conclusions

The objectives of the study were to improve the Molecular Effect Model for HTSC Cuprates by using 2D-3D Interior and Graphical Optimization. The MEM model built was based on an initial 3-degree polynomial fit taking Critical Temperatures related to HTSC Cuprates (Hg-Ba-Ca-Cu-O) Molecular Masses. Second objective was to determine Carnot Factors 2D-3D imaging-processing dataset for up-to-date current cuprates.

Results comprise a low-error MEM improved for Cuprates. 2D-3D abs errors (K); [0 ≤ Abs Error ≤ 8] (K). Average 2D-3D, Error= 4.0633 K ; (Figures 1-4). Although some errors are high, the statistical mode is low, then average error results be about 4 K. All errors are proven in 2D-3D imaging series, with corresponding numerical results. The Carnot Factor calculations are shown in 2D-3D charts, Figures 5-8, for different Operating Temperature magnitudes. Those Carnot Factor results match almost exactly the literature, [1(1)]. As a result from the software methods used, a series of new programs were got for software advances in Graphical and Interior Optimization.

Therefore, MEM presented shows errors [0 ≤ Abs Error ≤ 8] (K). These can be considered an advance from previous contributions. Efficacious utility of this MEM predictions for a range of isotopes are detailed in Tables 3-4 .

In summary, Molecular Effect Model improvements were got with Tc predictions for possible proportion variants in molecule isotopes composition. Secondly Carnot Factor for cuprates was optimized and presented in 2D-3D chart series. Electronics Physics applications are explained.

5. Sn Superconductors Group

Abstract

Sn HTSC constitutes an important group with multiple electronics physics applications—it belongs to the generic Cuprates class. This Part shows the MEM most important results obtained along a Sn-HTSC publications series. 2D-3D optimization and imaging-processing methods are mainly two. The first one is Inverse Least Squares (ILS) 2D polynomial Numerical/Graphical Optimization for Molecular Effect model as presented. The Sn-MEM predictions for this group of [Sn-Sb-Te-Ba-Mn-Cu-O] compounds gives a regular 2D-3D polynomial dataset, namely with a quasi-parabolic shape similar to HTSC-MEM cuprates group in Parts 1-2 . This group also constitutes a recent materials innovation of HTSCs with an auspicious [T_C > 0°]. As a result, constitute important recent/prospective electronics physics applications. The polynomial algorithms used comprise Tikhonov Regularization techniques and ILS mathematical methods. The second method applied is Evolutionary Algorithms, with its corresponding software. Findings for these two MEM optimizations, based on these, demonstrate/show acceptable theoretical Numerical and 2D-3D Graphical/Interior Optimization solutions with low residuals. The 2D imaging-processing polynomial curves show a quasi-parabolic shape. Solutions comprise several parts, distributed along publications series. Namely, the modeling for T_C MEM predictions, and the Inverse Least Squares improved programming methods with 95% confidence intervals and statistical images. For Genetic Algorithms results, the optimal polynomial MEM equation coefficients do not differ too much in magnitude order compared to ILS polynomial fit. Proposed Electronics Physics applications for Superconductors and High Temperature Superconductors turn up from all these numerical/graphical results.

Keywords Interior Optimization (IO) Methods, Graphical Optimization, Systems of Nonlinear Equations, Tikhonov Regularization (TR), Inverse Least Squares (ILS), Electronics Superconductors, High-Temperature Superconductors (HTSC), BCS Theory, [Sn-Sb-Te-Ba-Mn-Cu-O] Molecular HTSC Group, Molecular Mass (MO).

5.1. Introduction and Objectives

In superconductors research series, ILS method was widely applied [3-6, 39-49]. Evolutionary or Genetic Algorithms (GA) method was applied on Hg-Cuprates HTSC class [3-5, 48, 49] with acceptable results. GA have proven be useful and efficacious in optimization and large-scale optimization [3-9]. Comparative optimization algorithms and methods constitute a practical tool for getting theoretical/experimental results confirmed [3-6, 39-49].

For superconductors with Sn, such as classical Nb3Sn, some important parameters related to critical temperature can be determined with theoretical-experimental polynomial algorithms, [51(1)]. For example, the volumetric specific capacity γC in the vicinity of its critical temperature Tc, [18.3 K], or thermal conductivity. However, those formulas polynomial are specific for boundary intervals in the vicinity of critical temperature [51(1)]. Therefore, the initial approach of MEM for critical temperature in function of molecular mass has approximate numerical sense.

In this contribution, the Molecular Effect Model predictions for HTSCs [Sn-Sb-Te-Ba-Mn-Cu-O] category group are presented and numerically-graphically shown [Casesnoves, 2020]. The Isotope Effect Model, [Eq. (4), Section 6], is a simple algorithm that works based on element-atomic mass of a Type 1 superconductor-element isotope and the Critical Temperature Tc. That is, two main parameters and a constant to be determined experimental-numerically. That model simplicity has proven be acceptable with some inaccuracies [1(1)-5(1), 10(1), 11(1), 1(2)-5(2), 14(2), 15(2)]. In this study, the Molecular Effect hypothesis, [Casesnoves, 2020], is optimized for getting TC predictions.

Thus, [Sn-Sb-Te-Ba-Mn-Cu-O] chemical group whose molecular composition/formulation diverge in proportion of valences/elements, [1(1)-1(5), 12(1)], is optimized with ILS polynomial model. From this theoretical-model base, predictive values of TC are presented. When deviations of molecular mass due to proportion/isotopic-variation in the molecule, the MEM mathematics can predict approximately the TC magnitude change for every HTSC-group compound may be useful/efficacious—some HTSC categories are better than other for this technique. In previous studies, primary optimization for recent HTSCs with TC > 0° centigrade was presented [1(2)-15(2)]. The definition of High Temperature Superconductors [1(1)-5(1)] is those specific Superconductors whose Tc is approximately higher than 80 K—exactly 77 K . Their chemical molecular composition is complex with rather high molecular mass/weight and a number of groups/varieties, [1(15) shows HTSC classes briefed and clearly] . The fast improvements in HTSCs class research make a steady increasing number of new compounds, physical-chemical properties, and innovative/unpredictable applications, for instance, [16(2)]. These HTSCs belong to so-called Type II ones. In consequence, for this Section 5, the Molecular Effect Model predictive equation for HTSCs [Sn-Sb-Te-Ba-Mn-Cu-O] group are calculated/analyzed and graphically examined. In other words, both Isotope Effect and MEM result be useful for TC

prediction equations in Superconductors and HTSCs. However, the second one is still hypothetical.

The software method applied in this study is dual. The first program is a 2D polynomial fit to obtain approximate polynomial coefficients boundaries and confirm the MEM analytic geometry shape. Then, with this data the refinement and confirmation of the numerical results are got through a GA second program. The main advantage of this method is making sure of the numerical results cogency.

Results comprise MEM for these Sn class 2D charts, 2D GA Graphics of program performance, and final TC polynomial predictive equations. The novelty of this study, is therefore, the GA application in contrast with previous contributions [1(2)-4(2)].

In summary, the Section shows a 2D numerical-dual-graphical ILS Polynomial and Genetic Algorithm Optimization study for the hypothesis of MEM set on [Sn-Sb-Te-Ba-Mn-Cu-O] HTSCs class. Algorithms are implemented with GNU-Octave and Matlab systems software and 2D Graphical model plots are developed. Both 2D ILS numerical polynomial results and Genetic Algorithms software show low errors and residuals. The model analytic geometry shape results are approximately quasi-parabolic curves.

5.2. Numerical Dataset for Computational Methods

The selected Sn compounds criterion is restricted for total elements equality in the complete chemical formula. Namely, Sn-Sb-Te-Ba-Mn-Cu-O category. Table 1 shows composition, and approximate Critical Temperature for everyone. The Sn group is large, [12(1)], and several lattices are involved among different sub-categories. For example, (a (Z+12)212 structure), (a (Z+4)212 structure), [12(1)]. However, those chemical-chrystal special-characteristics are beyond the scope of this text.

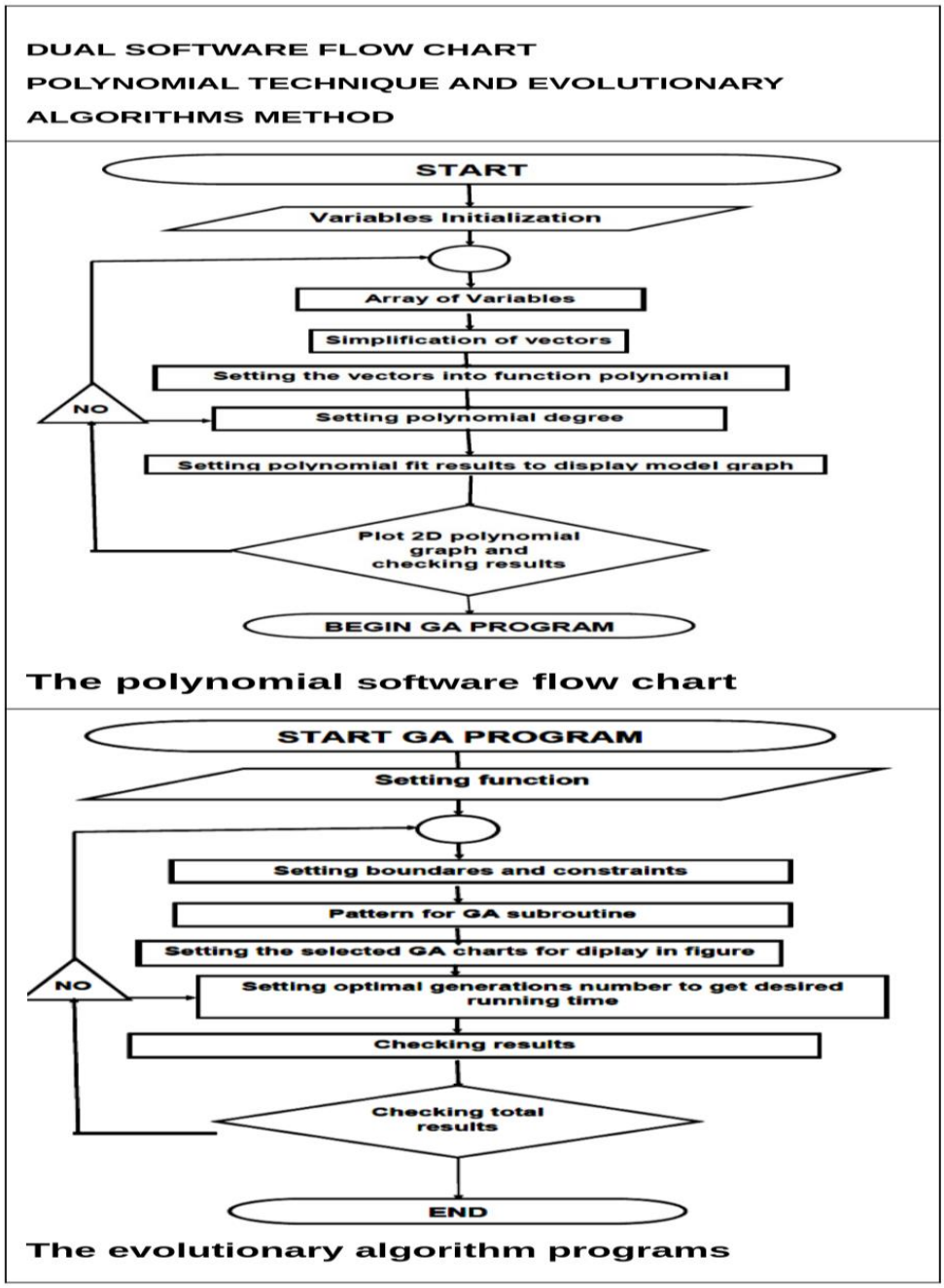
What is needed is to set the Molecular Effect model for [Sn-Sb-Te-Ba-Mn-Cu-O] HTSC group was the molecular masses (MO) and the experimental T_C values, Table 1. The method is similar to [1(2)-6(2),12(1)], but in this study T_C predictions are obtained with software and graphical 2D statistical programming. Algorithm is based on Tikhonov Regularization Theory [5(2)].

NUMERICAL OPTIMIZATION DATA FOR Sn-Sb-Te-Ba-Mn-Cu-O GROUP [HT-SUPERCONDUCTOR, MOLECULAR EFFECT HYPOTHESIS]	
FORMULATION	**MOLECULAR WEIGHT (UAM) / APPROXIMATE Tc (Kelvin)**
$Sn_{10}SbTe_9Ba_2MnCu_{21}O_{42+}$	4.7940e+003 / +187 C
$Sn_9SbTe_8Ba_2MnCu_{19}O_{38+}$	4.3565e+003 / +187 C
$Sn_8SbTe_7Ba_2MnCu_{17}O_{34+}$	3.9190e+003 / +167 C
$Sn_7SbTe_6Ba_2MnCu_{15}O_{30+}$	3.4816e+003 / +155 C
$Sn_{10}SbTe_4Ba_2MnCu_{16}O_{32+}$	3.6778e+003 / +141 C
$Sn_9SbTe_4Ba_2MnCu_{15}O_{30+}$	3.4635e+003 / +136 C
$Sn_8SbTe_4Ba_2MnCu_{14}O_{28+}$	3.2493e+003 /+129 C
$Sn_9SbTe_3Ba_2MnCu_{14}O_{28+}$	3.2403e+003 / +121 C

Table 1. The development of optimization of parameters for Sn-Sb-Te-Ba-Mn-Cu-O group implemented in this study [12(1), 1(2), 2(2), 5(2)]. Selected superconductors have the same chemical elements.

5.3. Mathematical and Computational Methods

Sketch 1 shows two programming flow charts. The first is for ILS-polynomial method and the second one for GA technique.



Sketch 1. Software flow chart for both methods, polynomial and genetic algorithms.

5.4. Results

Results are divided into several groups, depending of the method, or whether they are 2D graphical or numerical. All of them belong to the series of Sn-cuprates articles previously published with some improvements/clarifications, [5(2)-8(20, 13(2)-16(2)]

5.4.1. 2D Graphical Results

The first series of results shows the 2D polynomial graphics for 3 and 4 polynomial degrees. The numerical results are shown in some of them after images.

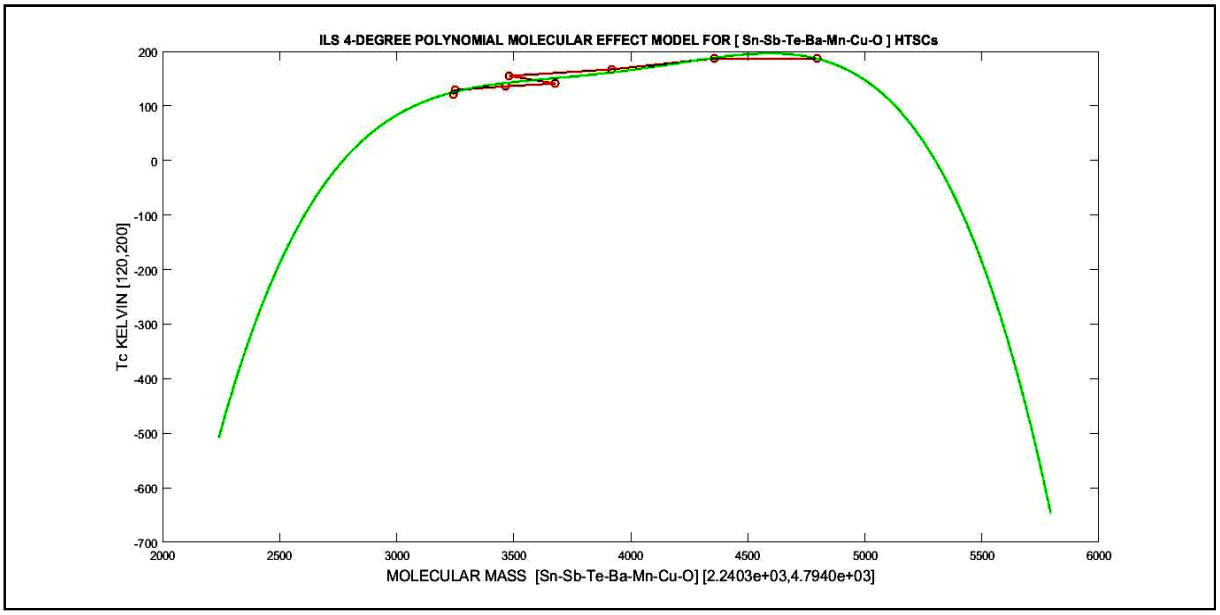


Figure 1. Matlab 4-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modeled curve (green), and inset experimental data (red points). The model is a parabolic equation, approximately. As it was found in previous contributions, for Sn class the MEM shows get an approximate parabolic shape. Green extrapolated model, red, experimental dataset [Casesnoves Bioengineering Laboratory. Software. 11390].

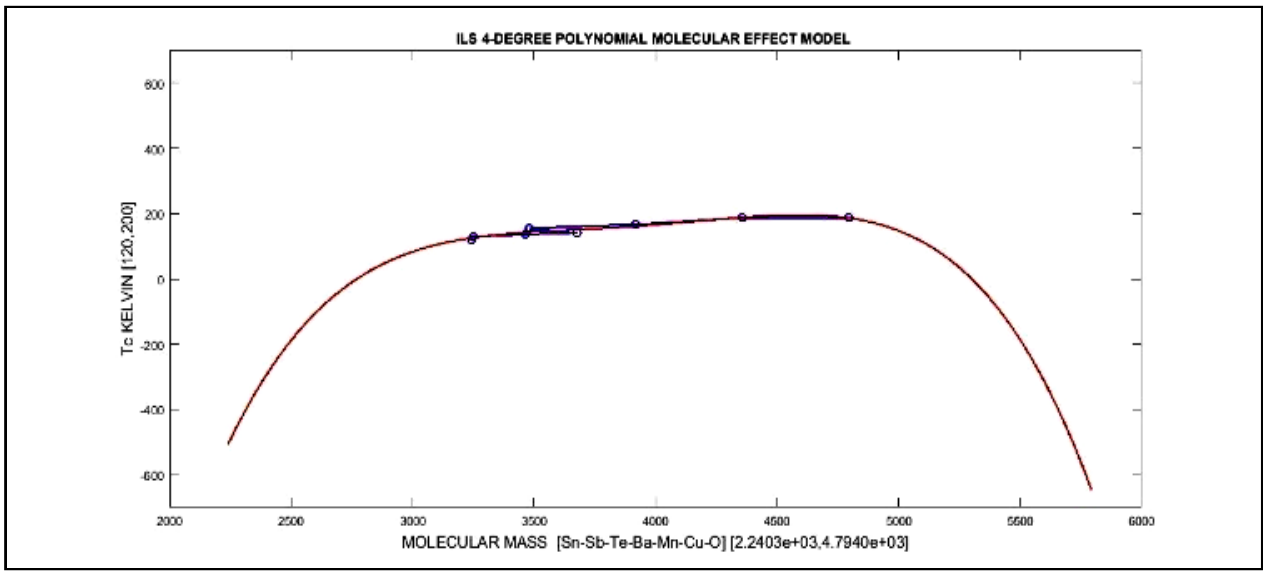


Figure 2. Other variant for Matlab First 4-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (red) and experimental data (blue). The model is a parabolic equation, approximately. The numerical results with acceptable residuals are shown in Tables 2-3 [Casesnoves Bioengineering Laboratory. Software. 11391].

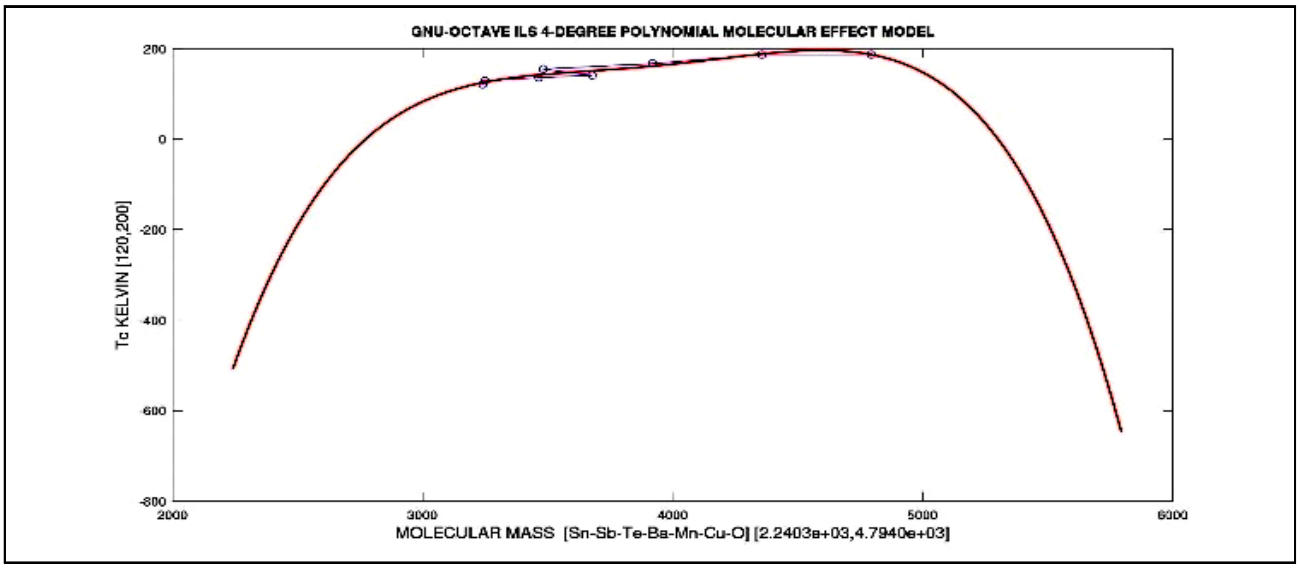


Figure 3. GNU-Octave First 4-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (red) and experimental data (blue). The model confirms also the parabolic equation, approximately. The imaging processing program is similar to Matlab one with acceptable results. Specific changes for GNU-Octave patterns and subroutines were compulsory, Sketch 1 [Casesnoves Bioengineering Laboratory. Software. 11392].

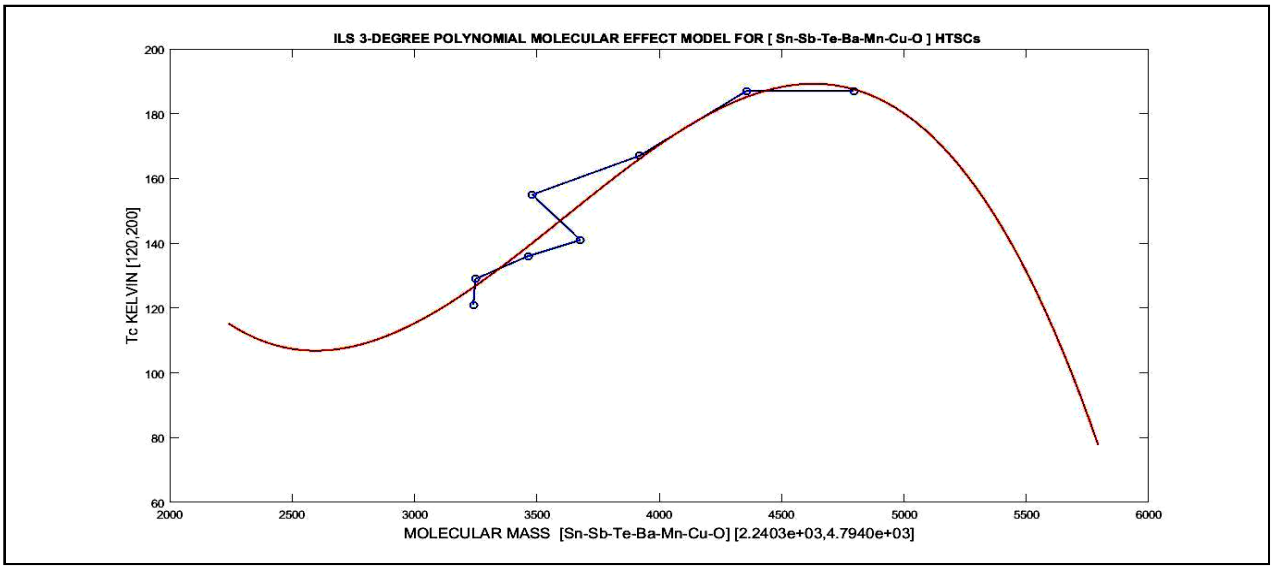


Figure 4. Matlab comparative 3-Degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Matlab Extrapolated modelled curve (red) and experimental data (blue). The model results to resemble a parabolic equation, approximately [Casesnoves Bioengineering Laboratory. Software. 11303].

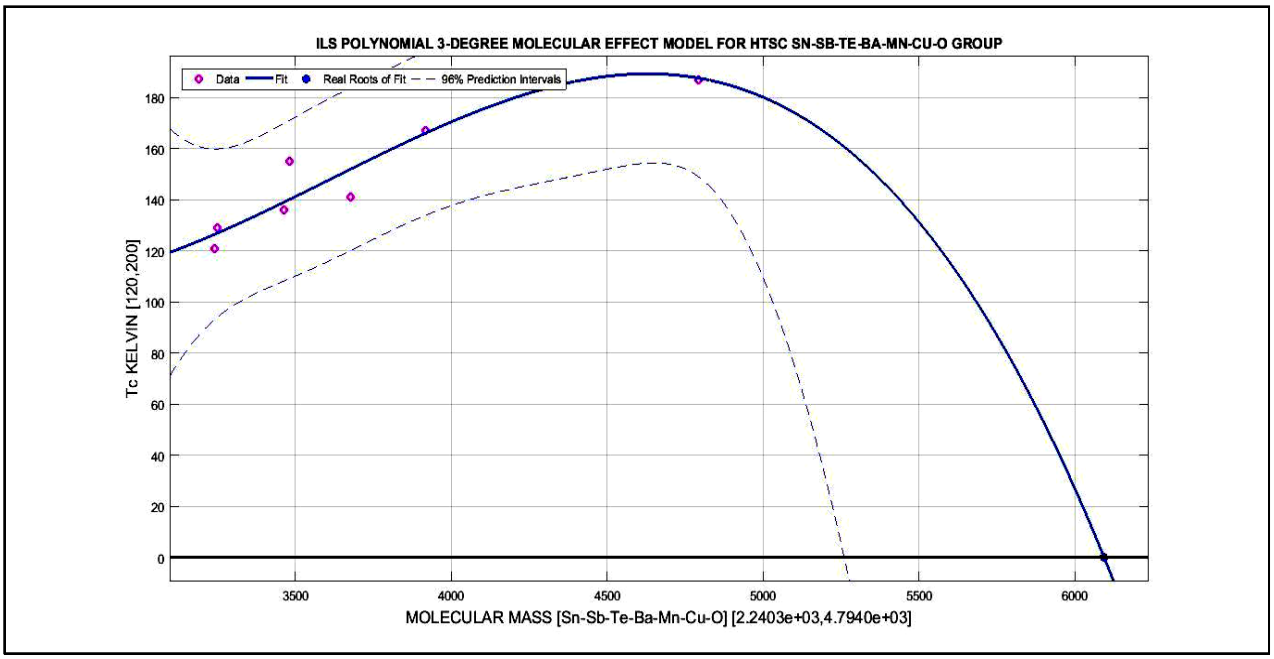


Figure 5. Matlab 3-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (blue), confidence intervals (blue-dashed), and experimental data (red points). The model is a parabolic equation, approximately. Confidence Interval, blue-dashed-lines inset, is 95%, marked in dashed blue-lines parallel to model [Casesnoves Bioengineering Laboratory. Software. 11394].

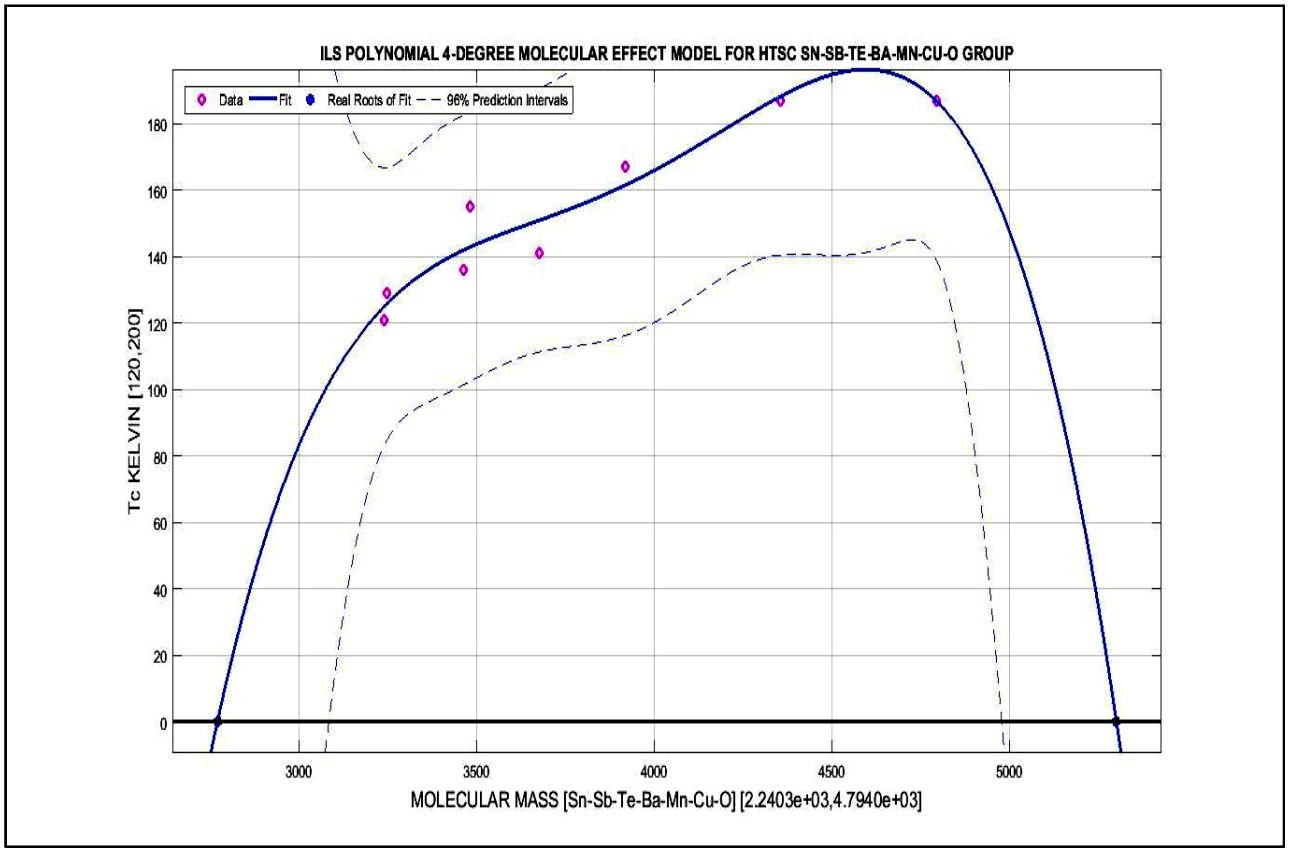


Figure 6. Matlab second 4-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (blue), confidence intervals (blue-dashed), and experimental data (red points). The model is a parabolic equation, approximately. Confidence Interval, blue-dashed-lines inset, is 95%, marked in parallel to model [Casesnoves Bioengineering Laboratory. Software. 11395].

5.4.2. Numerical Results

Tables 2-4 show comparative polynomial numerical results with predictions and residuals. Table 5 presents complete equations results for ILS Polynomial method and GA model.

OPTIMIZATION PREDICTIONS Tc MOLECULAR MODEL FOR [Sn-Sb-Te-Ba-Mn-Cu-O]	
MOLECULAR MASS	Tc EXPERIMENTAL
4794	187
4356.5	187
3919	167
3481.6	155
3677.8	141
3463.5	136
3249.3	129
3240.3	121
Tc PREDICTED	ERROR [RESIDUAL 4.44320233780593]
187.568123561098	-0.568123561098332
185.151755901108	1.848244098892
166.040208798827	0.959791201172607
140.069834151831	14.9301658481686
151.939414878914	-10.939414878914
138.991341832237	-2.991341832237
126.857143024242	2.14285697575804
126.382177851734	-5.38217785173424

Table 2. Numerical T_C predictions for ILS 3-degree model with errors ([TC Experimental]-[TC Predicted]). The software-development of parameters optimization for [Sn-Sb-Te-Ba-Mn-Cu-O] group requires appropriate patterns, loops and arrays. Data obtained can be considered acceptable. Note the numerical differences with ILS 4-degree model in Table 3, both in errors and residual.

OPTIMIZATION PREDICTIONS Tc MOLECULAR MODEL FOR [Sn-Sb-Te-Ba-Mn-Cu-O]	
MOLECULAR MASS	Tc EXPERIMENTAL
4794	187
4356.5	187
3919	167
3481.6	155
3677.8	141
3463.5	136
3249.3	129
3240.3	121
Tc PREDICTED	ERROR [RESIDUAL 4.29102685700562]
186.827561856328	0.17243814367248
188.185961473922	-1.18596147392236
161.470460729484	5.52953927051567
142.816812530255	12.1831874697455
150.930540120149	-9.9305401201490 9
141.913885803682	-5.91388580368221
125.917530213279	3.08246978672105
124.937247272766	-3.9372472727664

Table 3. Numerical T_C predictions for ILS 4-degree model with errors with errors ([T_C Experimental]-[T_C Predicted]). The software-development of optimization of parameters for Sn-Sb-Te-Ba-Mn-Cu-O group requires appropriate patterns, loops and arrays. Data obtained can be considered acceptable. Numerical differences with ILS 3-degree model show lower error magnitudes and residual.

ILS MOLECULAR EFFECT MODEL (4-DEGREE)			
COEFFICIENT	VARIABLE X	COEFFICIENT APPROX	VARIABLE X SELECTED
-19.70733497213 85e+003	CONSTANT	-19.7073e+003	CONSTANT
20.37826390101 16e+000	X	20.3783e+000	X
-7.83958167010 360e-003	X^2	-7.8396e-003	X^2
1.33736190239 691e-006	X^3	0	X^3
-85.14727476581 28e-012	X^4	0	X^4
RESIDUAL = 4.29102685700562e+000			
APPROXIMATE POLYNOMIAL			
Tc = [-19.7073e+003] + [20.3783e+000] MO+ [-7.8396e-003] MO^2			

Table 4. Numerical results for Molecular Effect Model with 4-degree polynomial and approximated equation. MO is the Sn compound weight. This numerical TC MEM for ILS 4-degree polynomial model with residual error and approximations [discard polynomial coefficients ≤ 10-12]. The software-development of parameters optimization for [Sn-Sb-Te-Ba-Mn-Cu-O] category requires appropriate patterns, loops and arrays. Data obtained can be considered acceptable. For 3-degree ILS polynomial results, [15(2)].

5.4.3. Genetic Algorithms Optimization

Results Stage 2, Genetic Algorithm, Figure 7 proves the GA program performance in a multifunctional chart. The most important parts are the Best fit that gives the fitness value, and the percentage of criteria met. The other parts show complementary information, such as best, worst and mean scores, stopping criteria and children number evolution. This type of software was initially developed in [5(2)].

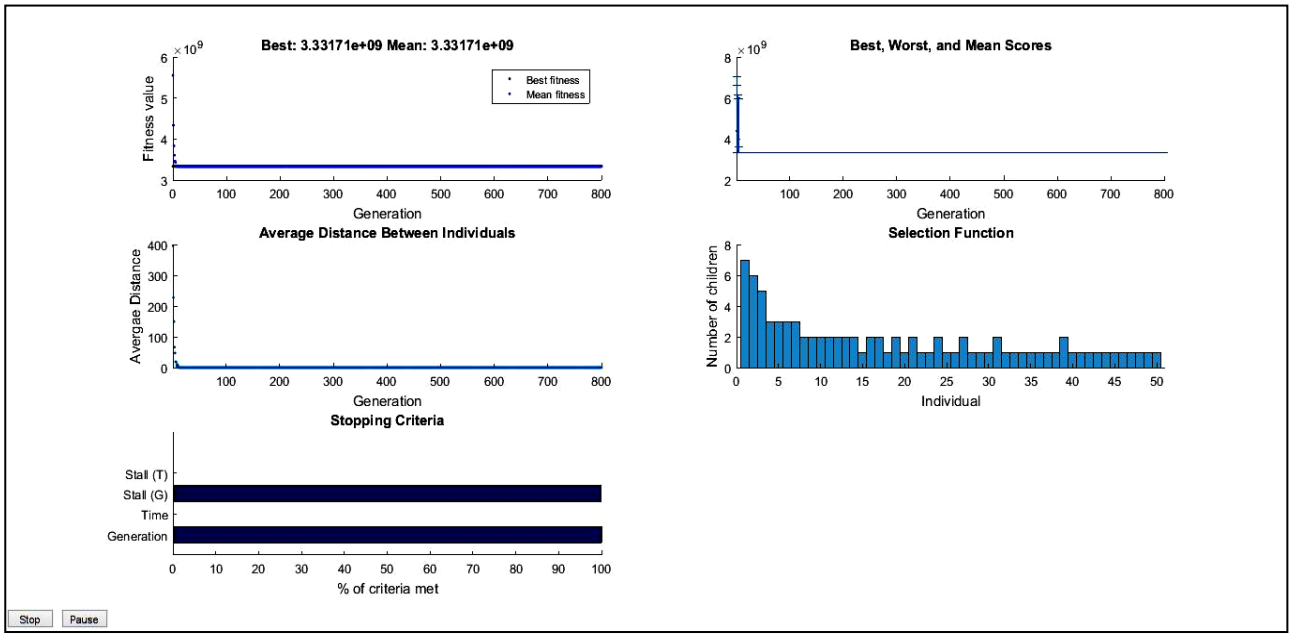


Figure 7. The Second stage. 2D polynomial fit parameters intervals set into GA program with Matlab. Generations Number is 800. As it was found in previous contributions, for Sn class the MEM shows get an approximate 2D parabolic shape. Percentage of criteria is met at 100 % [Casesnoves Bioengineering Laboratory. Software. 11396].

5.5. Numerical Comparisons

Table 2 shows all the dual numerical results with errors. Errors can be considered acceptable. Note the 800 number of GA generations.

NUMERICAL RESULTS		
PROGRAMMING STAGE	**METHOD**	**COMMENTS**
FIRST	Polynomial fit Inverse Least Squares. Tihkonov Functional algorithms.	Program and 2D graphics patterns. Curves quasi parabolic shapes.
SECOND	Genetic Algorithm from ILS Tikhonov Functional. It is more complicated software.	Program and GA Multigraphics patterns, parameters and dataset.
POLYNOMIAL MEM EQUATION		
Tc = [-21.7822e-006] + [216.4114e-003] MO + ... +[-347.6922] MO^2		**ERROR [200 functions] = 4.5173e+000**
GENETIC ALGORITHM MEM EQUATION		
Tc = [-20.7821e-006] + [217.4114e-003] MO + ... +[-346.6922] MO^2		**ERROR [800 generations] = 57.7211e+003** **Note the small numerical differences with ILS polynomial**

Table 5. Brief of Numerical results for optimization stage 1 (polynomial) and stage 2 (GA implementation) of software. Error is higher in GA because for GA the program was done for 800 generations, and for polynomial fit was made for 200 functions.

5.6. Applications

A briefing of applications in Electronics Physics and Power Engineering are shown at Table 7. Table 8 deals with Isotope Effect review of applications, also related to Type II HTSC, [1(2)-5(2)].

SUPERCONDUCTING MOLECULAR EFFECT APPLICATIONS
[HYPOTHESIS BRIEFING FOR ELECTRONICS PHYSICS AND POWER ENGINEERING]

TYPE	USAGE	COMMENTS
General 2D T_c / Molecular Mass curve shape	For catching up the approximate variation of T_c related to Molecular Mass. This is useful for guess of possibility of T_c predictions	Every HTSC class shows gets a proper 2D/3D shape. Usually parabolic inverse, (Hg-cuprates and Sn-categories), but quasi-sigmoid can occur also
Electrical Motors	Higher efficiency and small size	Reduced energy loss and occupied area. Improved efficiency
Fault current limiter	Zero resistance in normal state and enhanced stability of the grid. Large impedance in fault state. Combination of detection, trigger and limiting current. Fast response. No harmful effect on power grid	Improved reliability of power supply. Protected electrical apparatus. Reduced cost of construction and retrofit. Increased transmission capacity of the grid
When there are several isotopes types in different proportions in the sample that cause variations in Molecular Mass	In this case, approximations/predictions for T_c could be got from the 2D curve equation, or 3D optimization surface	Approximations to be confirmed by following experimental data
Electrical generators	High capacity density. Low loss, small size and light weight. Low synchronous reactance. High overload ability	Reduced energy loss and occupied area. Improved stability of the power system. Compensated reactive power, improved. power quality and stability of grid
When there are several isotopes types in different valences in the sample that cause a different Molecule within the HTSC class	In this case, approximations/predictions for T_c could be got from the 2D curve equation	Approximations to be confirmed by following experimental data. More difficult
Superconducting Magnetic Energy Storage	Regulation of power quality and stability of the grid	Specific varied application not for electric engineering. Fast power compensation.Enhanced dynamic stability of the grid. Improved power quality. Improved reliability of power supply
When both phenomena happen. Different valences, and isotopes proportions in the prospective HTSC experimental work	In this case, approximations/predictions for T_c could be got from the 2D curve equation	Much more difficult, but some new model algorithms are being validated
Current lead	Low thermal conductivity. High current density	Low heat leakage. High efficiency
Inverse Optimization of isotopes proportion to obtain a desirable T_c	Precision to reach an optimal T_c	This is a theoretical approach

Table 6. Applications of the MEM that was developed in contribution series, [14(2), 15(2)]. Several power engineering ideas are referred to [Wang, Y, 51(3)].

ISOTOPE EFFECT BCS MODEL RELATED APPLICATIONS		
APPLICATION TYPE	**METHOD**	**COMMENTS**
Usage of dataset for more different T_C formulas/algorithms.	Those other models are less simple. Isotope Effect model is fast and accurate.	Dataset for one model could be useful for other model in first instance
Mixed element with different isotopes proportions	Optimization for the best T_C magnitude	This can be done with different optimization methods/algorithms
Element with unique isotope compound	Optimization for the best T_C magnitude for that exclusive isotope	This can be done with several optimization methods/algorithms
Combined simulations for 2-3 isotope/elements types	Predictions for group-approximated T_C magnitudes	Various algorithms with Interior Optimization

Table 7. Review and improved similarities of MEM applications and Isotope Effect superconductivity.

5.7. Discussion and Conclusions

The research subject was to prove/show the prediction results for Molecular Effect Model in HTSCs group [Sn-Sb-Te-Ba-Mn-Cu-O]. This HTSCs materials are of interest because of their electronical-thermodynamical property and future applications with TC > 0°. For this HTSCs category, Molecular Effect model was graphically and numerically studied.

Results have two strands, numerical-predictions for TC and 2D graphical for model curves. First stage of numerical-predictions are based on polynomial ILS 2D Graphical Optimization. Those numerical results for this HTSC category Molecular Effect Algorithms, can be considered acceptable with low residuals, Tables 2-5. Approximations with 3 and 4 degree ILS polynomial methods results have proven get low errors and residuals, Tables 2-3. For 4-degrees, Prediction Error interval is ≈[-4 , 13]. However, average magnitude error is lower ≈ [5.24]. Second stage deals with the implementation of those ILS results withing

Genetic algorithms programs to try more accurate results and explicit 2D graphical database.

Software and programming was based on previous contributions [1(2)-9(2), 15(2)-16(2)]. Specific subroutines and patters for every graph and numerical predictions table were built. The programming for Figs 2 and 4 requires statistical and confidence intervals patterns.

Hg-Cuprates HTSCs class 2D/3D MEM polynomial Objective Function Graphical and Numerical Optimization database prove close similarities in MEM with the Sn group approximately quasi-parabolic shaped curvatures and numerical-graphical extrapolations for TC . However, as proven in Sections 3-4, the best results for MEM are got with the Hg-Cuprates category. Numerical results for both applied methods are approximately acceptable, Tables 2-5. In this HTSC Sn group MEM, 2D analytical geometry shapes and 2D MEM Objective Functions curvatures are satisfactory with low residuals, Figures 1-7. Electronics Physics applications for MEM are explained, Tables 6-7.

Advantages of the GA software method are the 2D improved mathematical and geometrical numerical analysis for the MEM optimization. That is, for instance, generations number, average distance between individuals, percentage of criteria met, etc. Further, the numerical coincidence with 2D polynomial fits proves the cogency of the GA Artificial Intelligence method. Inconvenients with GA programming multifunctional 2D imaging processing are the increasing running time, about 2-4 minutes, when several GA optimization parameters and numerical statistics are implemented in a unique multigraph. The higher number of generations, the longer running gradient time in GA compared to other optimization Inverse Least Squares techniques used.

Software and programming methods are based on previous contributions [3-9, 48-51]. Sketch 1 shows the basic technique stages. The programming for Figures 1-7 requires arranging of ILS and GA special commands, patterns, loops, optimal running time choice, and setting precise upper and lower boundary limits for constraints in GA method.

A number of applications for MEM and basic Isotope Effect BCS model are explained, Tables 6-7 with comparisons.

GNU-Octave and Matlab software methods and programming are based on previous contributions [14(2)-16(2)]. In both systems, specific subroutines and patters for every graph and numerical predictions table are built. There are few differences between the two systems for these objectives. The programming for Figure 7 requires arranging of GA special patterns loops, and setting precise upper and lower boundary limits for constraints.

Applications of these 2D MEM simulations are within/related to the field of the BCS theory of superconductivity in the isotope effect model. It is important to remark that further prospective applications for the molecular effect model in the HTSC groups of compounds are primarily considered for TC predictions when HTSCs show several chemical groups whose molecular composition/formulation differs in proportion to the valences/elements.

Succintly, a 2D ILS polynomial and GA methods for HTSCs category [Sn-Sb-Te-Ba-Mn-Cu-O] are presented for MEM. Applications in Electronics Physics Electromagnetics are included and emerge from the study findings.

6. Isotope Effect Interior Optimization Precision-Briefing

Abstract

Along previous publications, [1(2)-4(2), 9(2), 17(2)], Hg optimization of Isotope Effect was computationally developed. At this chapter Section, higher precision both in numerical and 3D imaging-processing for Hg element Isotope Effect is shown. Results from previous contributions are improved, especially in 3D imaging-processing model. Numerical results for Hg Critical temperature coincide with other Author's literature, and at 3D model graphs show be consistent—small magnitude differences are demonstrated. Interior Multiobjective Optimization algorithms for general Isotope Effect computations are extensively perfected/refined and their formulations explained.

Keywords

Isotope Effect (IE), Hg, Molecular Effect Model (MEM), Interior Optimization (IO) Methods, Polynomial Fitting (PF), 3D Graphical Optimization (GO), Systems of Nonlinear Equations, Tikhonov Regularization (TR), Inverse Least Squares (ILS), Electronics Superconductors, High-Temperature Superconductors (HTSC), BCS Theory.

6.1. Introduction

As explained in previous Sections, a superconductor can be defined as any material type whose electrical resistance is approximately null under specific thermodynamic and electromagnetic conditions. The essential thermodynamic conditions needed to reach the superconductivity state are given by a critical temperature TC, beyond which, toward lower temperatures, a superconductivity effect takes place and interactions with magnetic fields constitute an important modifying factor. The TC magnitude is around absolute zero Kelvin for conventional superconductors and approximately 100 degrees higher for high-temperature ones. Apart from this crucial condition, there are other physical ones. Namely, the maximum critical current, lower critical magnetic field H, and upper critical magnetic field H. Other factors are pressure and resistivity [1(1)–1(5)]. In general, the large variety of models and formulations within the theory of superconductivity, cause a multiple factor dependence that constrains the material superconductivity transition/effect. The superconductor's principal physical-engineering advantage is its zero-energy loss for electrical currents. However, this excellent property for saving energy is not electromagnetically optimal. The benefit of null-conductivity energy loss is reduced by the necessary energy to cool the material to −273◦ [Centigrade]. These

antagonist constraints have to be optimized to obtain the most efficient total energy savings.

The current research/theoretical advances in superconductivity are profuse and wide ranging [1(1)–14(1), 1(2), 6(2), 8(2), 9(2), 10(2), 31(3)-34(3), 36(3), 38(3), 51(3)]. Their mathematical background is extensive with several theoretical models, approximations, and equation variants. At the atomic and molecular level, quantum mechanics and chemistry play a significant role in the basis for the theory of superconductivity. High-temperature superconductors are those whose TC is higher than 80 K. They have an unusually complex molecular composition and several varieties. In the classical BCS theory of superconductivity, the isotope effect model equation algorithm is shown at Equation 4.

Therefore, this is a review about the fundamentals of Interior Optimization Method [Refs-8, 9, text-paragraphs and some images], focused on Hg Isotope Effect accuracy-precision improvements. The objective is to improve Isotope Effect equations for the classical superconductor Hg with Interior Optimization. The study is focused on classical Hg SC Type I Hg, but the method is general along superconductors-elements of Type I. As said in plain language, [9(2)], Interior Optimization is a numerical computational-graphical method based on graphical variables separation techniques, which are applied in subsequent 3D imaging stages, which could be also 2D. That is, the analytical partial differential equations method basis is used to make a graphical-optimal numerical determination-selection through 3D/2D imaging-stages in order to select the best/desired values of any several variables algorithm. In this briefing, the mathematical and computational fundamentals of the method are shown with Hg Isotope Effect results. Initially, these techniques were designed for superconductor modelling optimization, specifically BCS Isotope Effect optimization, the Molecular Effect Model (MEM), and Superconducting Multifunctional Transmission Lines Project [12(2)]. All these optimization approaches can be utilized for any science branch that could demand this necessary type of mathematical-computational methods.

In summary, this accuracy-review shows an advanced contribution for the Interior Nonlinear Optimization Method previously presented/developed for Hg. Mathematical and computational base is explained/proven for the classical superconductor Hg Type I. A number of algorithms are set for sharp mathematical learning. 3D imaging processing graphics with two systems, namely GNU-Octave and Matlab, are profusely included. Electromagnetism and electronics Physics applications are thorough.

6.2. Mathematical Methods and Algorithms with Matrix Algebra

Linear systems are included in this study as nonlinear ones with exclusively Unitarian power and without nonlinear operations among parameters. Consider the multiobjective problem with constraints,

CLASSICAL MULTIOBJECTIVE OPTIMIZATION ALGORITHM, (SIMPLEST):

$$
\begin{aligned}
&minimize,\\
&f(\overrightarrow{X}) = F\left[f_1(\overrightarrow{x}_1), f_2(\overrightarrow{x}_2), \ldots\ldots\ldots f_N(\overrightarrow{x}_N)\right],\\
&subject\ to,\\
&\overrightarrow{a}_1 \leqq \overrightarrow{x}_1 \leqq \overrightarrow{b}_1\ ;\\
&\overrightarrow{a}_2 \leqq \overrightarrow{x}_2 \leqq \overrightarrow{b}_2\ ;\\
&.\\
&.\\
&.\\
&\overrightarrow{a}_N \leqq \overrightarrow{x}_N \leqq \overrightarrow{b}_N\ ;\\
&Further\ linear\ and\ nonlinear\ constraints\ can\ be\ added;
\end{aligned}
$$

[Casesnoves Bioengineering Laboratory. Algorithms-Software. 11390] **(1)**

where,

f(X) : Vectorial principal function. X is a vector of sub-functions.

f(xi) : Sub-function component of principal function vector or matrix, every xi is a vector . Such as,

F(X) = [f(xi),..... f(xN)] i = 1.....N.

ai : Lower boundary constant. (i = 1.....N).

bi : Upper boundary constant. (i = 1…..N) .

N : Number of matrix functions.

This (1) is an equation of several variables that has not, in general, unique solution. If the objective function becomes an [i] number of nonlinear functions. Hence,

INTERIOR OPTIMIZATION MULTIOBJECTIVE ALGORITHM, (SIMPLEST APPLIED):

$$
\begin{aligned}
&for\ i = 1.....N\ ,\\
&minimize,\\
&f(\overrightarrow{X}) = F\,[x_{i1}, x_{i2}, ...x_N]\\
&subject\ to,\\
&\overrightarrow{a}_{i1} \leqq \overrightarrow{x}_{i1} \leqq \overrightarrow{b}_1\ ;\\
&\overrightarrow{a}_{i2} \leqq \overrightarrow{x}_{i2} \leqq \overrightarrow{b}_{i2}\ ;\\
&.\\
&.\\
&.\\
&\overrightarrow{a}_{iN} \leqq \overrightarrow{x}_{iN} \leqq \overrightarrow{b}_{iN}\ ;\\
&Further\ linear\ and\ nonlinear\ constraints\ can\ be\ added;
\end{aligned}
$$

[Casesnoves Bioengineering Laboratory. Algorithms-Software. 11391] **(2)**

where,

f(X) : Vectorial principal function. X is a vector of sub-functions.

f(xi) : Sub-function component of principal function vector or matrix, every xi is a variable-vector. Such as,

f(X) = F [xi1, xi2…. xiN] i = 1…..N. The is a sub-function of N variables, everyone is a vector.

ai : Lower boundary constant. (i = 1…..N).

bi : Upper boundary constant. (i = 1…..N).

N : Number of matrix functions.

Therefore, it is a system of nonlinear equations functions with several variables, [5(4)], that in general case do not have to be equal in number to the parameters. If there are terms with operations among parameters, and roots, the unique solution is even more difficult to

be find out. Optimization algorithms and software can find usually a local minimum, semi-global minimum, or a local minimum according to constraints. A classical method is Monte-Carlo programs, such as GEANT type, [28(3)], classically used in IMRT-IMPT radiotherapy, although there are options for Monte-Carlo and Quasi-Monte-Carlo software available. Jacobian and classical Newton-Raphson methods are, for example, used to find an approximate solution. Number of methods to find solution/approximate solutions for a system of nonlinear equations is extent, and it is not the specific focus of this contribution. Monte-Carlo method can be considered methods to find solution/approximate solutions for a system of nonlinear equations are extent. Monte-Carlo method can be considered good, because the program usually, taking continuous random values, search for an optimal solution of variables, no matter how many they are. Genetic Algorithms constitutes a stochastic method that has proven be very useful and precise nowadays. Given this algorithm, the Graphical and Interior Optimization Methods can be applied starting for grouping variables step by step. The technique is an extrapolation of the classical partial equations method of separation of variables. That is,

INTERIOR OPTIMIZATION MULTIOBJECTIVE ALGORITHM,
(SIMPLEST TECHNIQUE):

$$
\begin{aligned}
&if\ optimization\ stage\ is,\\
&minimize,\\
&f(\overrightarrow{X}) = f\,[x_1, x_2, ...x_N]\\
&by\ using\ similar\ partial\ differential\ method\\
&of\ separation\ of\ variables,\ for\ instance,\\
&if\ it\ is\ at\ principal\ function, a\ product,\ such\ as,\\
&x = x_1 \bullet x_2\ ,\\
&it\ is\ grouped\ for\ a\ 3D\ axis\ imaging - processing\ as,\\
&x_{1s} = x_1 \bullet x_2\ ,\\
&and\ so\ one;
\end{aligned}
$$

[Casesnoves Bioengineering Laboratory. Algorithms-Software. 11392] **(3)**

where,

f(X) : Vectorial principal function. X is a vector of one sub-function.

f(xi) : Sub-function component of principal function vector or matrix, every xi is a variable-vector.

N : Number of matrix functions.

xi : A variable-vector. S is the number of sub-functions.

Or just the same parameters-grouping for sums, exponentials, etc. Thus, the technique begins with a 3D graph of two selected parameters, at Z axis the objective function. The optimal/desired values are fixed at that graph. Those fixed values are taken for the subsequent 3D graph that involves the following two parameters, and so on.

What is done in mathematical concepts is to apply the partial differential equations classical separation of variables method. With separation of variables, it is possible to optimize all the parameters in subsequent stages of 3D graphical optimization plots. At every plot, it is selected the desirable local, global, or semi-local minimum for the variable of convenience.

In such a way that the initial Graphical Optimization begins with 3 variables, namely, first, second and objective function. An optimal value is determined. The following stage one parameter with two variables is decomposed, and it is taken the optimal values, and so on.

Therefore, it is easy to prove, through the multi-selection of local and approximate minima at Graphical Optimization sets, that in general the multiobjective solution for a system of nonlinear equations is not unique. In other words, it is demonstrated from 3D visualization and separation of variables, this classical mathematical assertion.

Number of graphs required depends on the number of variables of the nonlinear system of equations. The determinations of optimal values not necessarily have to be minimal. Optimal values taken depend of the engineering requirements for laboratory optimization, devices manufacturing, experimental plan, or similar tasks. The advantage is that the software engineering gives a fast tool to find necessary data immediately with short time consuming.

6.3. Optimization Algorithms for Superconductors Isotope Effect

In this section a brief summary of Superconductivity towards the Transition Equation and the Isotope Effect in BCS Theory is presented. The Superconductivity Theory framework is rather extent and with large mathematical background. It involves Quantum Theory, Molecular Chemistry, Materials Physics and other science and engineering branches. All

these areas converge together in Superconductors theory and applications. Which is useful to prove Interior Optimization Method is the simple equations of Transition-Temperature-Critical and Isotope Effect? The classical-simple Critical Temperature Equation for superconductors reads,

ISOTOPE EFFECT MULTIOBJECTIVE ALGORITHM,
(SIMPLEST FORMULATION):

$$for\ i = 1.....N\ , number\ of\ element\ isotopes,$$
$$[M_i]^{\alpha}\ T_{Ci}\ -\ K \cong 0\ ,$$
$$for\ i\ =\ 1, ...N\ ;$$
$$Further\ linear\ and\ nonlinear\ modifications/constraints\ can\ be\ added;$$

[Casesnoves Bioengineering Laboratory. Algorithms-Software. 11393] **(4)**

where,

K : Sub-function component of principal function vector or matrix, every xi is a vector . Such as,

Mi = Atomic mass of every isotope. AMU.

$\boldsymbol{\alpha}$: Isotope effect constant power parameter. Adimensional.

Tci : Critical Temperature of every isotope. Kelvin.

i : Isotope number for everyone of them.

From the stage when the solid reaches critical temperature, the superconductivity effect begins. TC varies for every isotope element within a defined mass element, although not excessively in magnitude.

This equation, although simple, remains useful today. It was taken to illustrate Interior Optimization Method in simple way. The evolution of this equation, for example, [1(1)-5(1)], involves extent mathematical background and mathematical-physics theory. It is sufficient to prove the Interior Optimization Method with this classical equation.

Just note that taking decimal or Neperian logarithms the equation (6) can be linearized for setting graphics related to different isotopes with corresponding atomic proper mass.

To set the simplest nonlinear system of equations, for Hg Isotope Effect Interior Optimization, the algorithm selected with 100 equations reads,

$$
\begin{aligned}
&\text{ISOTOPE EFFECT MULTIOBJECTIVE}\\
&\text{OBJECTIVE FUNCTION ALGORITHM,}\\
&\text{CHEBYSHEV L1 NORM,}\\
&\text{(SIMPLEST FORMULATION):}\\
&for\ i = 1.....N\ , number\ of\ element\ isotopes,\\
&everyone\ with\ proper\ T_C\ ,\\
&minimize,\\
&\|[M_i]^{\alpha}\ T_{Ci}\ -\ K_i\|_{L_1}\ ;\\
&subject\ to\ ,\\
&a\ \leqq\ M_i\ \leqq\ a_1\ ;\\
&b\ \leqq\ T_{Ci}\ \leqq\ b_1\ ;\\
&c\ \leqq\ K_i\ \leqq\ c_1\ ;\\
&d\ \leqq\ \alpha\ \leqq\ d_1\ ;\\
&NOTE:\ At\ imaging-processing\ it\ is\ also\\
&implemented\ Objective\ Function\ as,\\
&OF\ =\ [M_i]^{\alpha}\ T_{Ci}\ -\ K_i\ ,\\
&Further\ linear\ and\ nonlinear\ modifications/constraints\ can\ be\ added;
\end{aligned}
$$

[Casesnoves Bioengineering Laboratory. Algorithms-Software. 11394] **(5)**

where,

Ki : Isotope Effect constant for every isotope.

Mi = Atomic mass of every isotope. AMU.

$\boldsymbol{\alpha}$: Isotope effect constant power parameter. Adimensional.

Tci : Critical Temperature of every isotope. Kelvin.

i : Isotope number for everyone of them.

a , a1 : Lower and upper boundary constant for Mi. (i = 1…..N). AMU.

b, b1 : Lower and upper boundary constant for Tci. (i = 1…..N). Kelvin.

c, c1 : Lower and upper boundary constant for every Ki at implemented interval. (i = 1…..N).

d, d1 : Lower and upper boundary constant for every $\boldsymbol{\alpha}$i at implemented interval. (i = 1…..N) . Adimensional.

N : Number of isotopes.

|| || L1 : Chevyshev norm.

where i is the corresponding number within the range of simulations. For example, in range of simulations for Hg, M [10(1)-11(1)] is,

M ϵ [199.5 , 203.4]

[Casesnoves Bioengineering Laboratory. Algorithms-Software. 11395] **(6)**

In the same way, range of constraints can be seen in axes ranges of Figures 1-5. Therefore, with Equations 1-6, a nonlinear system of equations is set. The variables are to get optimized. The method is Interior-Graphical Optimization, that is proven accurate and useful [9(2), 17(2)]. It was taken Hg superconductivity values from literature [1(1)-5(1), 10(1)-11(1)]. Extrapolation to large and complicated Electronic Physics equations, Electronics, or any type of system can be guessed from this application.

6.4 Software Engineering Dataset

The software developed for this contribution had some easy parts and not a few programming difficulties to adapt the programs on Chebyshev L1 norm for objective function, Equations 1-6. Additional complications were the algebra changes in the subroutines to get functional the program for surface Graphical Optimization visualization. This requires mathematical changes-background.

The software was developed in GNU-Octave and Matlab and is almost equivalent for Freemat also. These numerical data are all for this contribution. In previous contributions, higher values were taken for high-accuracy. Graphical Optimization programs were designed for double precision, since were based on engineering software of extent number of previous publications.

To check complementarily the numerical results, both Fortran and F# subroutines in optimization were used. While Fortran proved to match the Graphical Optimization results, F# showed restrictions and obviously, limits that discarded this type of language for accurate results in nonlinear optimization. None of these F# numerical data were included in publication.

INTERIOR OPTIMIZATION SOFTWARE DATASET Hg ISOTOPE EFFECT [From Refs-7, 10 -11, experimental data]	
PARAMETER	**MAGNITUDE INTERVAL PROGRAMMING IMPLEMENTED**
M, Isotope Atomic Mass (AMU)	[199.5,203,4] AMU
Experimental Alpha	[0.30,0.60]
Experimental Critical Temperature Tc, (K)	[4.146, 4.185] K
K constant calculation from experimental data	[50.00,60.00]
The Figures show imaging processing patterns with/without L1 Chevyshev norm for explicit clarity to prove the global minima	

Table 5. Dataset implemented in programs for Hg Interior Optimization. That is a classical experimental foundation of Hg superconductivity, [10(1) -11(10, experimental]. Dataset is at software patterns in intervals.

6.5. Computational Graphical-Interior Optimization and Numerical Results

The results are shown in Tables and Graphics. Numerical results match values in the literature for natural Hg. However, alpha value is lower than the classical magnitude of 0.5, from [Refs-7, 10-11].

Residuals can be considered acceptable, although not of high-precision accuracy. The time consuming for designing program is extremely short. The time for selecting optimal values is also very short with the Matlab graphical cursor. In engineering practice, this is a significant advantage that gives many options for fast on-site superconductivity data management at laboratory. Results confirm useful utility of Equations 1-6.

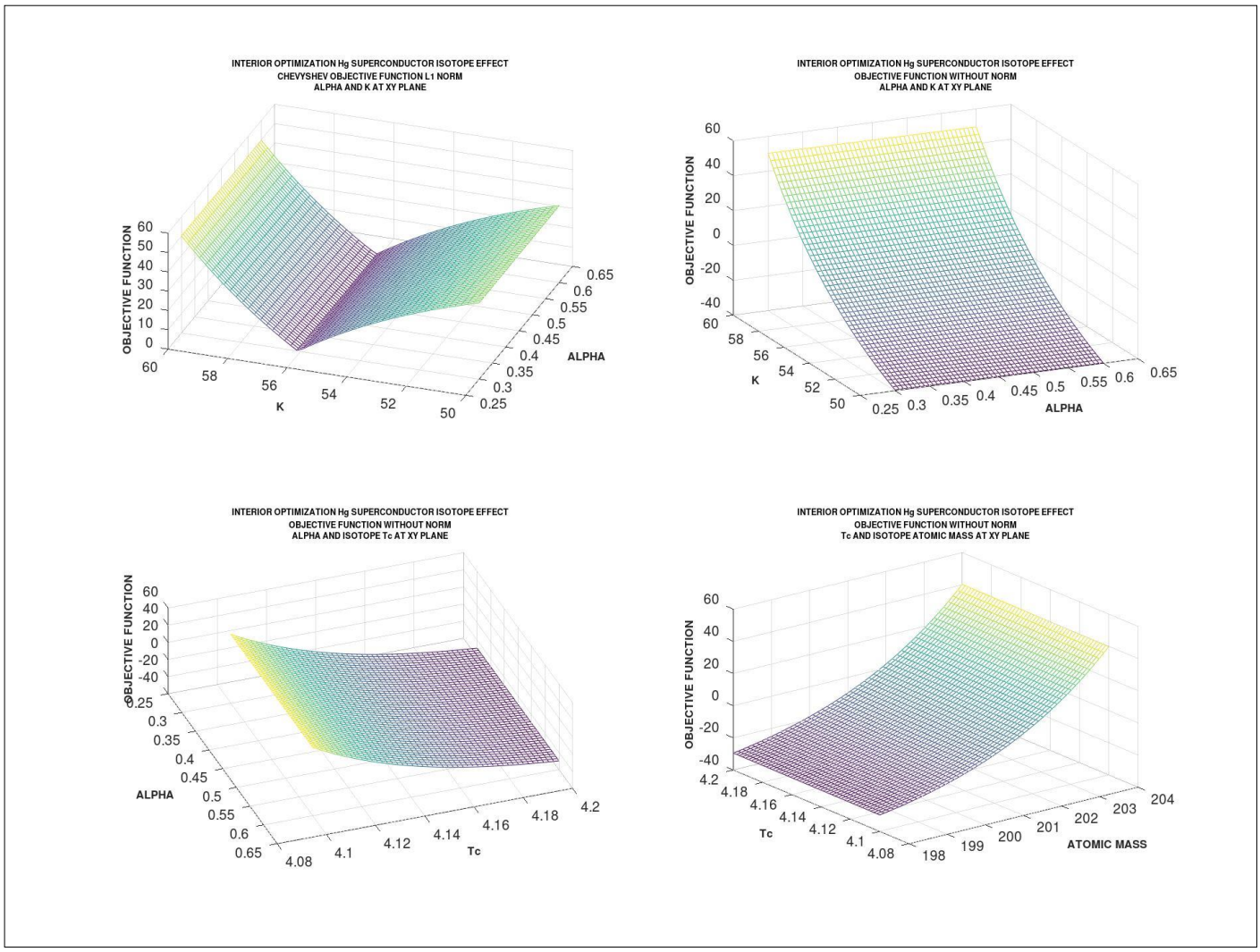


Figure 1. GNU-Octave multiple imaging-processing for Hg advanced Interior-Graphical optimization. It was graphically determined the optimal K value and the power magnitude for constant a. First image is got with L1 Chevyshev norm. The others are set with simple OF. The first image shows intersection line of global minima line for alpha and K at XY plane. The others set at XY plane the alpha-Tc and Tc-Atomic-Mass numerical functions. At Z=0, can be sharply seen the global minima proof. Running time is about 2-4 seconds. [Casesnoves Bioengineering Laboratory. Algorithms-Software. 11398].

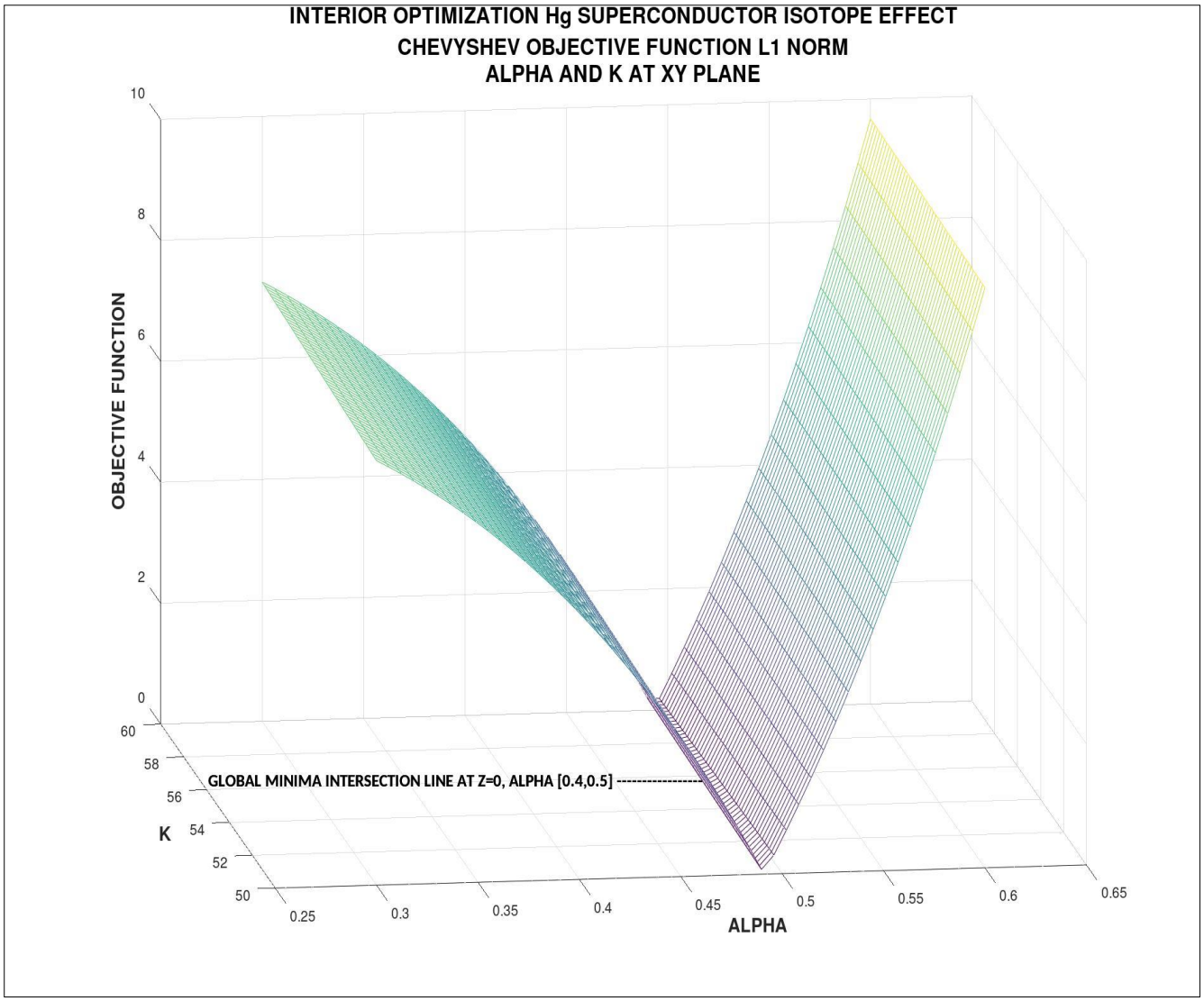


Figure 2. GNU-Octave imaging-processing for Hg advanced Interior-Graphical optimization. It was graphically determined the optimal K value and the power magnitude for constant a, inset marked global minima line. Image is got with L1 Chevyshev norm. It shows intersection line of global minima line for alpha and K at XY plane. Running time is about 2 seconds [Casesnoves Bioengineering Laboratory. Algorithms-Software. 11399].

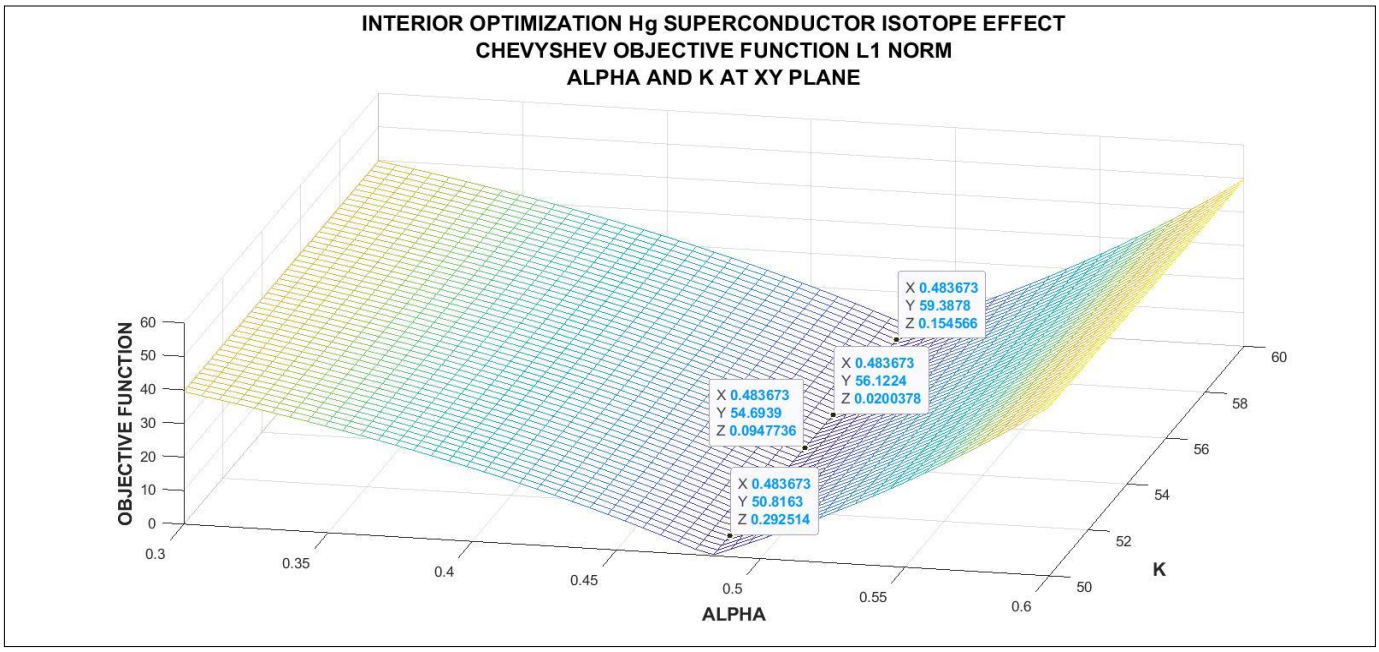


Figure 3. Matlab imaging-processing for Hg advanced Interior-Graphical optimization. It was graphically determined the optimal K value and the power magnitude for constant a, inset marked global minima line. Image is got with L1 Chevyshev norm. It shows intersection line of global minima line for alpha and K at XY plane. Dataset, inset, is used for numerical results graphical calculations. Running time is about 2 seconds [Casesnoves Bioengineering Laboratory. Algorithms-Software. 113100].

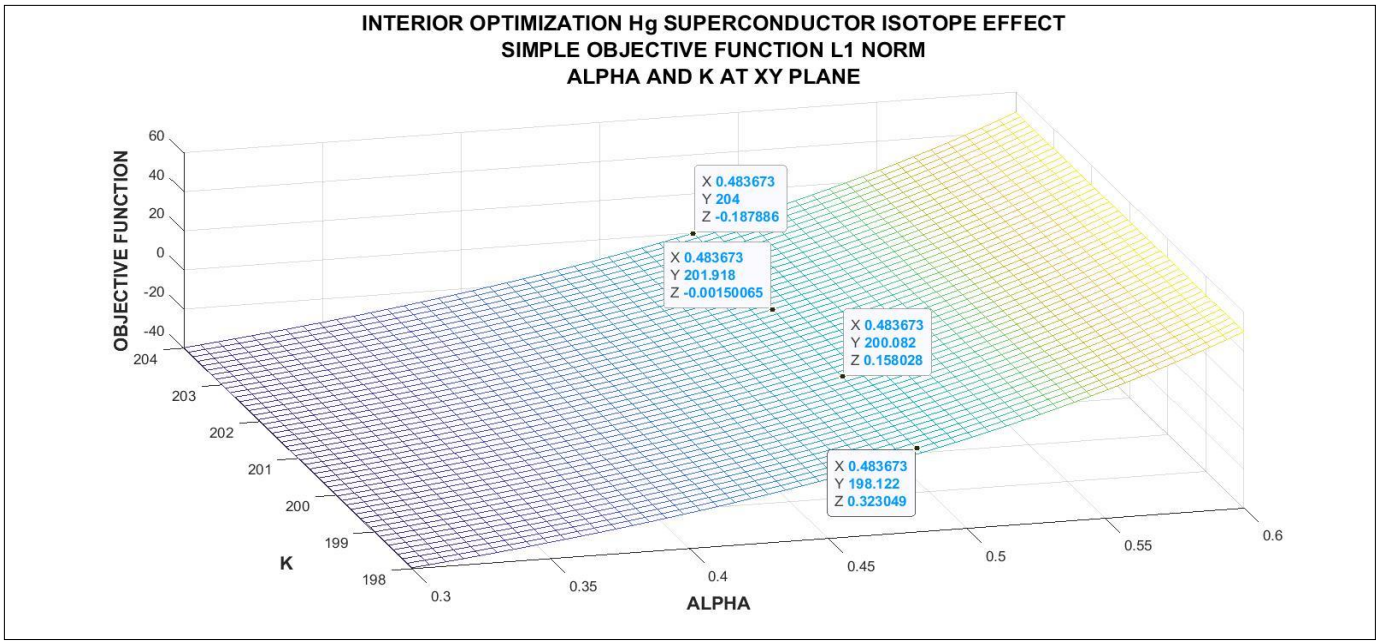


Figure 4. Matlab imaging-processing for Hg advanced Interior-Graphical optimization. It was graphically determined the optimal K value and the power magnitude for constant a, inset marked global minima line. Image is got without L1 Chevyshev norm. It shows of global minima points-line for alpha and K at XY plane. Dataset, inset, is used for numerical

results graphical calculations. Running time is about 2 seconds. At GNU-Octave graphics, the usual magnitude of alpha was around [0.490] [Casesnoves Bioengineering Laboratory. Algorithms-Software. 113101].

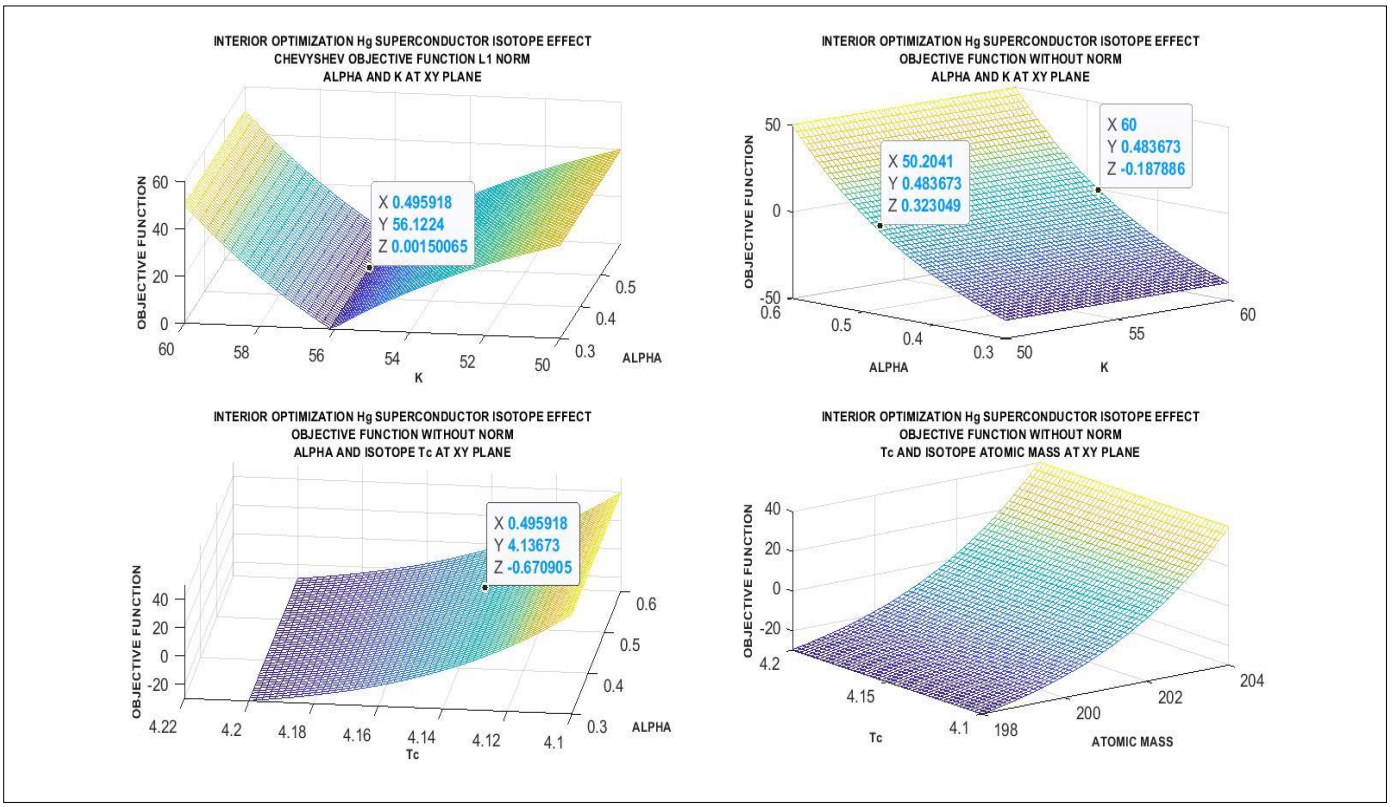


Figure 5. Matlab multi-imaging-processing for Hg advanced Interior-Graphical optimization. It was graphically determined the optimal K value and the power magnitude for constant a, inset marked global minima line. First image is got with L1 Chevyshev norm, the others without. It is shown of global minima points-line for alpha and K at XY plane, alpha and Tc, and Tc and Atomic Mass. Dataset, inset, is used for numerical results graphical calculations. Running time is about 1-3 seconds. OF residuals at Z axis are low. [Casesnoves Bioengineering Laboratory. Algorithms-Software. 113102].

INTERIOR OPTIMIZATION NUMERICAL RESULTS Hg ISOTOPE EFFECT [From Refs-7, 10 -11, experimental data]	
PARAMETER	**OPTIMAL INTERVAL FOR ALL ISOTOPE AMU** (Data obtained from Interior-Graphical Optimization)
M, Isotope Atomic Mass (AMU)	[201.0,201,0] AMU (For any other OF parameter)
Experimental Alpha	[0.480,0.495] (For any other OF parameter)
Experimental Critical Temperature Tc, (K)	[4.125, 4.140] K (For any other OF parameter)
K constant calculation from experimental data	[56.30,56.40] (For any other OF parameter)
The Figures show imaging processing patterns with/without L1 Chevyshev norm for explicit clarity to prove the global minima	

Table 6. 2D-3D Interior-Graphical optimal results got from imaging-processing series. Results are sligthly lower than publications for Hg, [10(1)-11(10]. Correction: 'Experimental Alpha' must be read ' Computational Improved Alpha magnitude'.

6.6. Discussion and Conclusions

The objective of the research is to improve the Isotope Effect classical model for Hg and obtain an alpha constant preciser magnitude. It was got by using 2D-3D Interior and Graphical Optimization. This update-review of Isotope Effect classical model was enhanced from previous contributions [1(1)-6(1), 10(1)-11(1), 9(2)].

3D imaging-processing software is upgraded from previous studies in loops, patterns, and subroutines. Results of this progress-refined programming and imaging-processing for Hg Isotope Effect can be considered acceptable. Consequently, Interior Optimization demonstrates advances both in 3D Graphical and numerical results. This improved-review proves programming method precision/accuracy that matches literature database,

namely [10(1)-11(1)], and demonstrates the efficacious software implemented and mathematical method. The numerical magnitude precision for Hg SC Type I alpha constant, namely, [0.480 , 0.495], is got with higher-precision at Table 6, can be considered/proven slightly lower than literature publications, [10(1)-11(11)]. It could be questioned that those experimental alpha-parameter Hg-Isotope Effect BCS equations/determinations are relatively the first ones, and the proportion of Hg isotopes could be/chosen not constant/equal at experimental work.

The 2D-3D imaging processing results with both systems, GNU-Octave and Matlab can be considered good/satisfactory. The Matlab imaging-processing and visual tools is better than GNU-Octave one. It was intended to explain with notes, inset images, the most important findings/concepts at every graphics.

Therefore, Hg Isotope Effect database presented shows low errors, according to 3D Graphical-interior Optimization. This can be considered an advance from previous contributions. Efficient utilities of these Hg isotope Effect for Type I superconductors predictions are detailed in Tables 3-4.

In summary, Hg Isotope Effect Model improvements were got with Tc predictions for possible isotope-proportion variant composition. Electronics Physics applications emerge from this progression-review of the Hg Isotope Effect.

7. References and Suggested Further Reading

The text references are divided into several groups for reader's better learning. The first group is related to the first and foremost Isotope Effect element discovery, that is, Hg. And for the essential cuprates HTSC. Author's references are set apart for fast consultation. The last general references section involves mathematical and optimization methods, Sn HTSC references and other HTSC important groups.

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8. Scientific Ethics Standards

According to European Union and International Scientific Ethics [45(3)-47(3)]. All the software/algorithms were done by Author. No artificial intelligence (AI) was used for programming or any article-part. If were so, it is declared, both in tools/systems for software anyway, and AI browsers-direct-information. In this Part II article series, the essential purposive equations/measurements applied/obtained by other Authors are properly recognized. When any mathematical statement, algorithm/proposition/theorem is presented, proofs and parameters/units are detailed/referred. Earlier research database, algorithms/images, are selected from prior publications in order to sharp reading with further references included. If any inconsistency is found, it is clarified in subsequent publications. Any citation such as [Casesnoves, 'year'], is intended to clarify intellectual property at current times, without intention to brag. Article is exclusively scientific, without persuasive commercial, institutional, academic influences, deliberate obfuscation, religious/religious-influences, non-scientific theories, personal opinions, political ideas, or economical-conflict links. Author has no conflict of interest.

9 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, MSc Thesis in Radiotherapy Treatment Planning Optimization, which was developed after graduation in a series of Radiation Therapy Optimization-Modelling publications [2007-present]). Dr. Casesnoves earned Graduate-with-MPhil, in Medicine and Surgery [1983] (Madrid University Medicine School, MPhil in Radioprotection Low Energies Dosimetry [1985]). Casesnoves resigned definitely to his original nationality in 2020 for ideological reasons, anti-monarchy-corruption, democratic-republican ideology, and ethical-professional reasons, and does not belong to Spain Kingdom anymore. His constant service to the International Scientific Community and Estonia Republic technological progress involves about 80 articles, more than 100

total publications, and about 4 books. Recent advances published are in Superconductors Mathematical Modelling and Radiotherapy Brain Neurobiological Models, 3D-AI Isodosezones and Isodoselines. Among Dr. Casesnoves inventions and scientific creations are:

1. Numerical Reuleaux Method.
2. Radiotherapy Omega Factor correction for AAA model wedge filters dose delivery.
3. Integral-Differential materials erosion model.
4. Graphical Optimization.
5. Interior Optimization Methods.
6. Superconductors Molecular Effect Model.
7. Superconductors Multifunctional Transmission Line.
8. BED radiotherapy model GA and Graphical Optimization Isodoselines and Isodosezones.
9. Aerospace Turbulence Energy Absorbing System

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To Natashka Kamarova, the best of my life, always with me

Authors Contributions

The author is solely responsible for conceptualization, computational validation, dataset implementation, formal mathematical programming analysis, visualization, funding, methodology, formal algorithms analysis, investigation, writing—original draft, writing—review. The author has read and agreed to the published version of the manuscript. AI Declaration : The author confirms that no AI tools were used to generate any content of this manuscript.

Conflict of Interest

Author declares no conflict of interest, all was made by Author.