

Mathematical-Computational Optimization Methods on Primary Molecular Effect Model for Selected High Temperature Superconductors with Electronics Physics Applications

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ABSTRACT

Article Info

Volume 8, Issue 2

Page Number : 159-167

Publication Issue :

March-April-2022

Article History

Accepted: 20 March 2022

Published: 31 March 2022

In previous series of contributions, Inverse Least Squares (ILS) Numerical Optimization, 3D/4D Interior Optimization, 3D/4D Graphical Optimization software and algorithms-programming were presented. The BCS theory Isotope Effect applications on superconductors TC dual/multiobjective optimization was the main subject. This contribution deals with the Molecular Effect Model for High Temperature Superconductors (HTSCs), in primary hypothesis stages. Selected group of HTSCs is Sn-Sb-Te-Ba-Mn-Cu-O . Namely, classical Inverse Least Squares, 2D Interior Optimization, and 2D Graphical Optimization techniques are applied. Results comprise Tikhonov Regularization algorithms and mathematical methods for this HTSCs group. Mathematical-programming findings to optimize this Type II HTSCs are presented with ILS outcoming data in Matlab and GNU-Octave. Rulings present an hypothesis of new 'Molecular Effect' model/algorithm, intended be proven for this HTSCs group. In this Molecular Effect optimization, Inverse Least Squares and Inverse Least Squares polynomial methods are applied with acceptable Numerical and 2D Graphical Optimization solutions. Results show accuracy with low programming residuals that confirm these findings. Solutions comprise two strands, the modelling for Molecular Effect, and the Inverse Least Squares improved programming methods with confidence intervals and statistical images. Hypothesis in Electronics Physics applications for Superconductors and High Temperature Superconductors emerge from findings. Modelling-hypothesis applications in Superconductor Theory turn up from the numerical and imaging data obtained.

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.

I. INTRODUCTION

The Interior Optimization Method (IO) was presented and demonstrated [3-5] for superconductors model optimization. It is a separation of variables method combined with Graphical Optimization 3D imaging/graphs.

Interior Optimization is not designed exclusively for finding out exclusively an specific global minimum. Instead, for designer's choice, the searched optimal parameter could be a local minimum, partial-global minimum or variants of these singular parameters according to experimental-theoretical convenience. Not always in Engineering and Physics is necessary to find optimal values for a group of equations conditioned to particular constraints of a laboratory/industrial/specific problem. Then, IO provides with the facility to select desired optimal parameters in subsequent stages ordered and set applying the method of separation of variables.

High-Temperature Superconductors are those ones whose T_c is approximately higher than 80 K—exactly 77 K [3-5, 12-15]. They have usually complex molecular composition/weight and a number of groups/varieties. HTSCs are usually Type II ones. In BCS classical superconductors theory, the Isotope Effect model for uni-element superconductors equation reads,

$$[M_i]^{\alpha} T_c - K \cong 0; \\ \text{for } i = 1, \dots, n; \quad (1)$$

where K is a constant, M Atomic Element Mass (AMU) of an element with (n) isotopes, T_c is critical temperature (Kelvin). (i) is the corresponding isotope for the element.

In this study, the Molecular Effect Model for HTSCs is hypothesized and numerically-graphically presented [Casesnoves, 2020].

The Isotope Effect Model is based on the mathematical correlation between atomic mass of every superconductor-element isotope and the Critical Temperature T_c . That model has proven be acceptable with some inaccuracies [3-5, 12-15]. In this study, the Molecular Effect hypothesis, [Casesnoves, 2020], that is mathematical-theoretically presented and numerically simulated, is based on a similar modelling mathematical-criterion. That is, HTSCs show a number of chemical groups whose molecular composition/formulation diverge in proportion of valences/elements [1-9,12-15]. From this theoretical base, it is primarily guessed that when deviations of molecular weight due to proportion/isotopic-variation in the molecule, there may be a mathematical model to predict the T_c magnitude change for every HTSC-group element.

In summary, the improved-study shows an advanced contribution for the Interior Nonlinear Optimization Method previously presented in [3-5, 12-15] on superconductors BCS theory applied on HTSCs modelling. It is focused on ILS model-programming software and computational 2D imaging results both in Matlab and GNU-Octave. The scheme of the method is proven, with proofs in applications at the Electronics Physics Type II HTSCs field. The most important innovation is the Molecular Effect Model [Casesnoves, 2020].

II. MATHEMATICAL METHOD AND SOFTWARE IMPLEMENTATION DATA

The problem approached is to try an extrapolation of the BCS Isotope Effect to HTSCs similar modelling. As it was previously explained, [3-5, 12-15] for scientific clarity, inclusion of the algorithm development is in this section. The Type II group of HTSCs modelled is Sn-Sb-Te-Ba-Mn-Cu-O group whose T_c values are over 0° centigrade. Table 1 shows the chemical-physical data for computational ILS optimization.

NUMERICAL OPTIMIZATION DATA FOR Sn-Sb-Te-Ba-Mn-Cu-O GROUP [HT-SUPERCONDUCTOR, MOLECULAR EFFECT HYPOTHESIS]	
FORMULATION	MOLECULAR WEIGHT (UAM) / APPROXIMATE T _c (Kelvin)
Sn10SbTe9Ba2MnCu21O42+	4.7940e+003 / +187 C
Sn9SbTe8Ba2MnCu19O38+	4.3565e+003 / +187 C
Sn8SbTe7Ba2MnCu17O34+	3.9190e+003 / +167 C
Sn7SbTe6Ba2MnCu15O30+	3.4816e+003 / +155 C
Sn10SbTe4Ba2MnCu16O32+	3.6778e+003 / +141 C
Sn9SbTe4Ba2MnCu15O30+	3.4635e+003 / +136 C
Sn8SbTe4Ba2MnCu14O28+	3.2493e+003 / +129 C
Sn9SbTe3Ba2MnCu14O28+	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 [12-15].

For this Molecular Model, the constraints values for parameters are shown in Tables 1-3. The algorithms set for ILS Molecular Effect, with a polynomial $p(MO)$ reads,

minimize Tikhonov functional $J(\alpha)$,
with $\alpha_1=0$ and L_2 Norm

$$J_{\alpha}(u)_{u \in \mathbb{R}^n} = \|Au - p(MO)\|_2^2 + [\alpha_1] J(u);$$

Hence minimize

$$\|T_{ci} - p(MO_i)\|_2^2,$$

for $i = 1, \dots, n$

subject to ,

$$a \leq MO_i \leq a_1;$$

$$b \leq T_{ci} \leq b_1;$$

(2)

where MO is the molecular weight of the HTSC selected (i) within a HTSC group with (i) elements

and [a-b] are constraints intervals. T_{ci} is critical temperature (Kelvin) for every (i) member of HTSCs group. The figure α_1 is a constant specific Tikhonov Regularization Parameter. The constraints [a-b] are applied for optimization. OF was selected with ILS programming in Matlab without algorithmic-linearization, and variations depending on program results accuracy, Figures 1-2. Algorithm programming with imaging-processing results are shown in Figure 2. 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. These numerical data, although significant for verification, were not included in publication.

III. MOLECULAR EFFECT ILS OPTIMIZATION RESULTS

The numerical results with acceptable residuals are shown in Tables 2-3 (Appendix). The Molecular Model formula is a parabolic-shaped curve when taking a polynomial ILS method of 4 degrees, Matlab Figure 1, GNU-Octave Figure 3. If the model is linearized, the results is presented in Figure 2.

Residuals can be considered acceptable at both equations obtained. The time consuming for designing program is about 5-10 seconds, depending on graphics options. In engineering practice, this simulation is a significant advantage that gives many options for fast on-site HTSCs superconductivity T_c approximate-predictions.

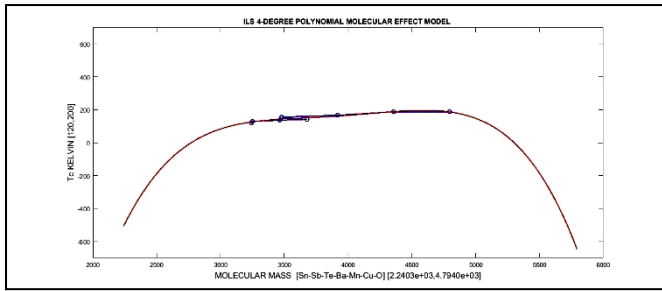


Fig. 1.- First 4-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (red) and experimental data (blue). The model is a parabolic equation, approximately. The numerical results with acceptable residuals are shown in Tables 2-3 (Appendix).

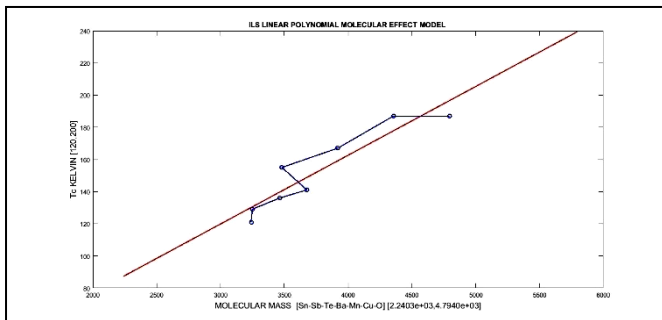


Fig. 2.- A simple linear model ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (red) and experimental data (blue). The simplification of model is a linear equation with slope (gradient) of low value. The numerical results with acceptable residuals are shown in Tables 2-3 (Appendix).

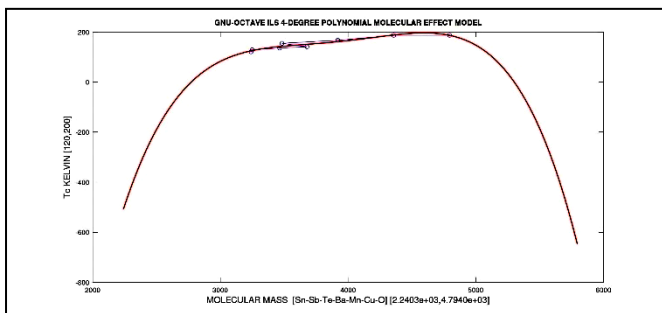


Fig. 3.- GNU-Octave First 4-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (red) and experimental data (blue). The model gives also a parabolic equation, approximately. The imaging processing program is similar to Matlab one with acceptable results. Specific changes for GNU-Octave patterns and subroutines were compulsory.

IV. DISCUSSION AND CONCLUSIONS

The objective of this research was to prove/show the results for Molecular Effect Model in HTSCs group Sn-Sb-Te-Ba-Mn-Cu-O . For this HTSCs group, a ILS hypothesis of Molecular Effect was approached and numerically analyzed. The rationale of this Molecular Effect sets on the base of the molecules similar atomic weights (isotopes variation in molecular composition and/or molecular approximate proportion/composition for any constituent element) for this HTSC group [1-9].

Results can be classified into numerical and 2D graphical. Numerical results for HTSC group Molecular Effect Algorithms [Casesnoves, 2020], can be considered acceptable with low residuals. The approximations with 4 and 1 degree ILS polynomial methods rulings are useful for T_c predictions.

2D Graphical Optimization results both in Matlab and GNU-octave are considered acceptable. Software improvements with specific subroutines and patters for each system showed clear/acceptable images.

In summary, 2D ILS Graphical Optimization methods have verified the primary theoretical hypothesis. Extrapolation of this Molecular Effect Model to several groups of HTSC appear to be useful and feasible in initial approximations subject to improvements.

V. SCIENTIFIC ETHICS STANDARDS

2D/3D Graphical Optimization Methods were created by Dr Francisco Casesnoves in 3rd November 2016, and Interior Optimization Methods in 2019. 2D/3D/4D Graphical and Interior Optimization Methods were created by Dr Francisco Casesnoves in 2020. This article has previous papers information, whose inclusion is essential to make the contribution understandable. The 2D Graphical Optimization in Matlab and GNU-Octave constitutes a software engineering improvement from previous contributions [3-9]. The 2D/3D/4D Interior Optimization method is original from the author (August 2020-1). This study was carried out, and their contents are done according to the European Union Technology and Science Ethics. Reference, 'European Textbook on Ethics in Research'. European Commission, Directorate-General for Research. Unit L3. Governance and Ethics. European Research Area. Science and Society. EUR 24452 EN [37-40]. And based on 'The European Code of Conduct for Research Integrity'. Revised Edition. ALLEA. 2017. This research was completely done by the author, the computational-software, calculations, images, mathematical propositions and statements, reference citations, and text is original for the author. When a mathematical statement, proposition or theorem is presented, demonstration is always included. The article is exclusively scientific, without any commercial, institutional, academic, religious, religious-similar, non-scientific theories, personal opinions, political ideas, or economical influences. When anything is taken from a source, it is adequately recognized. Ideas and some text expressions/sentences from previous publications were emphasized due to a clarification aim [37-40].

VI. REFERENCES

- [1]. Aditya M. Vora. Modified Transition Temperature Equation for Superconductors. Chin.Phys.Lett. Vol. 25, No. 6 (2008) 2162.
- [2]. Abramowitz, Stegun. Handbook of Mathematical Functions. Applied Mathematics Series. 55.1972.
- [3]. Casesnoves, F "Interior Optimization Methods with Electronics Applications", International Journal of Scientific Research in Science, Engineering and Technology (IJSRSET), Online ISSN : 2394-4099, Print ISSN : 2395-1990, Volume 7 Issue 3, pp. 428-436, May-June 2020.
- [4]. Casesnoves, F. "Advanced Interior Optimization Methods with Electronics Applications", International Journal of Scientific Research in Science, Engineering and Technology (IJSRSET), Online ISSN : 2394-4099, Print ISSN : 2395-1990, Volume 7 Issue 5, pp. 97-110, September-October 2020. DOI : 10.32628/IJSRSET207518.
- [5]. Casesnoves, F. "Multiobjective Interior Optimization Computational Methods for Electronics BCS Superconductivity", International Journal of Scientific Research in Computer Science, Engineering and Information Technology (IJSRCSEIT), ISSN : 2456-3307, Volume 6 Issue 5, pp. 280-293, September-October 2020. Available at DOI : 10.32628/CSEIT206556.
- [6]. Casesnoves, F. Mathematical Models and Optimization of Erosion and Corrosion. Ph.D. Thesis, Taltech University, Tallinn, Estonia. 14 December. 2018. ISSN 25856898.
- [7]. Casesnoves, F. Die Numerische Reuleaux-Methode Rechnerische und Dynamische Grundlagen mit Anwendungen (Erster Teil); Scientia Scripts: 2019; ISBN-13: 978-620-0-89560-8, ISBN-10: 6200895600.
- [8]. Casesnoves, F. Primary Modelling for Electromagnetic Waves Transmission in Extreme Weather Conditions. Inter-national

- Journal of Innovative Research in Science, Engineering, and Technology. Volume 7, Issue 10, 2018. ISSN Online: 2319-8753. DOI: 10.15680/IJIRSET.2018.0710022.
- [9]. Casesnoves, F. The Numerical Reuleaux Method, a computational and dynamical base with applications. First Part. Lambert Academic Publishing. ISBN-10 3659917478. 2019.
- [10]. Darwin, C. The origin of species. Barnes & Noble Classics. 2004.
- [11]. Haupt, R, Haupt, S. Practical Genetic Algorithms. Wiley. Second Edition. 2004.
- [12]. Kazufumi, I; Bangti, J. Inverse Problems, Tikhonov Theory and Algorithms. Series on Applied Mathematics Volume 22. World Scientific. 2015.
- [13]. Plakida, N. High-Temperature Cuprate Superconductors Experiment, Theory, and Applications. Springer Series in Solid-State Sciences ISSN 0171-1873. 2010.
- [14]. Alexandrev, A S. Theory of Superconductivity, From Weak to Strong Coupling. Series in Condensed Matter Physics. Institute of Physics Publishing Philadelphia. 2003.
- [15]. Khare, N. Handbook of High-Temperature Superconductor. Marcel Dekker USA. ISBN: 0-8247-0823-7. 2003.
- [16]. Casesnoves F, Suzenkov A. Mathematical Models in Biotribology with 2D-3D Erosion Integral-Differential Model and Computational-Optimization/Simulation Programming. International Journal of Scientific Research in Computer Science, Engineering and Information Technology. 2017 IJSRCSEIT | Volume 2 | Issue 3 | ISSN : 2456-3307.
- [17]. Casesnoves F, Antonov M, Kulu P. Mathematical models for erosion and corrosion in power plants. A review of applicable modelling optimization techniques. IEEE Xplore database and will be cross referred in SCOPUS. Proceedings of RUTCON2016 Power Engineering Conference.2016. Riga Technical University.
- [18]. Casesnoves, F. 2D computational-numerical hardness comparison between Fe-based hardfacings with WC-Co reinforcements for Integral-Differential modelling. Key Engineering Materials Journal. Trans Tech publications 2018. Vol 762, pp 330-338. DOI: 10.4028/www.scientific.net/KEM.762.330.ISSN: 1662-9795. 2018.
- [19]. Casesnoves F, Surzhenkov A. Inverse methods for computational simulations and optimization of erosion models in power plants. IEEE Proceedings of RUTCON2017 Power Engineering Conference.Riga Technical University. IEEEExplore Publication in 5th December 2017. DOI:10.1109/RTUCON.2017.8125630. Electronic ISBN: 978-1-5386-3846-0. USB ISBN: 978-1-5386-3844-6.Print on Demand (PoD) ISBN: 978-1-5386-3847-7.
- [20]. Casesnoves, F. 'Computational Simulations of Vertebral Body for Optimal Instrumentation Design'. ASME Journal of Medical Devices (Research Paper). Author: F Casesnoves .Journal of Medical Devices. June 2012. Volume 6. Issue 2/021014.11 pages.<http://dx.doi.org/10.1115/1.4006670>.
- [21]. Casesnoves,F.'Large-Scale Matlab Optimization Toolbox (MOT) Computing Methods in Radiotherapy Inverse Treatment Planning'. High Performance Computing Meeting. Nottingham University. January 2007.
- [22]. Casesnoves, F. 'A Monte-Carlo Optimization method for the movement analysis of pseudo-rigid bodies'. 10th SIAM Conference in Geometric Design and Computing, Texas, San Antonio, USA. Contributed Talk. November 2007.
- [23]. Casesnoves, F. 'Applied Inverse Methods for Deformable Solid Dynamics/Kinematics in Numerical Reuleaux Method (NRM)'.

- International Journal of Numerical Methods and Applications. volume 9(2) 2013 .pages 109-131. peer-reviewed International Mathematical/Computation Journal Article. print/Online.http://www.pphmj.com/abstract/7688.htm. This article is specially innovative in Inverse Problems applications for deformable solids kinematics/dynamics, further publications are included in United States Congress Library and Nu-merical Reuleaux Method is accepted by scientific community as an innovative dynamics method in deformable solids with mechanical, biomechanical and aerospace applications. New applications of this method will be probably found significantly in future.
- [24]. Casesnoves, F. Nonlinear comparative optimization for biomaterials wear in artificial implants technology. Pre-sented in Applied Chemistry and Materials Science RTU2018 Conference Proceedings. 2018.
- [25]. Huang X. Does the isotope effect of mercury support the BCS theory?. Condensed Matter. 2011.
- [26]. Hummel, R E. Electronic Properties of Materials.
- [27]. Kasap F, P. Capper (Eds.), Springer Handbook of Electronic and Photonic Materials, DOI 10.1007/978-3-319-48933-9_50ourth Edition. Springer. 2000.
- [28]. Kessel W.On a General Formula for the Transition Temperature of Superconductors. Naturforsch. 29 a, 445 — 451. 1974.
- [29]. Kulou P, Casesnoves F, Simson T, Tarbe R. Prediction of abrasive impact wear of composite hardfacings. Solid State Phenomena, Proceedings of 26th International Baltic Conference on Materials Engineering. 2017. Solid State Phenomena Submitted: 2017-06-12. ISSN: 1662-9779, Vol. 267, pp 201-206. DOI:10.4028/www.scientific.net/SSP.267.201 2017 Trans Tech Publications, Switzerland Online: 2017-10-10.
- [30]. Luenberger, G D. Linear and Nonlinear Programming. Fourth Edition. Springer. 2008.
- [31]. Moysés Luiz, Adir. Superconductivity – Theory and Applications, Edited by ISBN 978-953-307-151-0. 2010.
- [32]. Reynolds C A, Serin, Nesbitt. The Isotope Effect in Superconductivity. I. Mercury. The Isotope Effect in Superconductivity'. Mercury. Physical review volume 84, Number 4, November. 1951.
- [33]. Seri B., C. A. Reynolds, and B. Nesbitt. Mass Dependence of the Superconducting Transition Temperature of Mercury. Letters to Editor. Phys. Rev 80-761. Page 761. 1950.
- [34]. Todinov, M. Reliability and Risk Models. Wiley. 2005.
- [35]. Vidyasagar M. Nonlinear Systems Analysis. Second Edition. Prentice Hall.1993.
- [36]. Wesche, R. Chapter 50. High-Temperature Superconductors. Springer Handbook of Electronic and Photonic Materials. 2017.
- [37]. 'European Textbook on Ethics in Research'. European Commission, Directorate-General for Research. Unit L3. Governance and Ethics. European Research Area. Science and Society. EUR 24452 EN.
- [38]. The European Code of Conduct for Research Integrity. Revised Edition. ALLEA. 2017.
- [39]. Good Research Practice. Swedish Research Council. ISBN 978-91-7307-354-7. 2017.
- [40]. Ethics for Researchers. EU Commission. Directorate-General for Research and Innovation. Science in society /Capacities FP7. 2013.

VII. AUTHOR'S BIOGRAPHY

Dr Francisco Casesnoves earned the Engineering and Natural Sciences PhD by Tallinn 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-

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nonlinear-optimization [books 2019-2020], The series of Radiotherapy Improvements for AAA superposition-convolution model, the Graphical and Interior Optimization Methods [2016-8], the new Computational Dissection-Anatomical Method, [2020] and invention of Forensic Robotics [2020-2021]. Dr Casesnoves scientific service since 2016 to the Free and Independent Republic of Estonia for technological development (and also at Riga technical University, Power Electrical and Electronics Department) is about 35 physics-engineering articles, two books series, and 1 industrial radiotherapy project associated to Europe Union EIT Health Program (Tartu University, 2017).

Cite this article as :

Francisco Casesnoves , "Mathematical-Computational Optimization Methods on Primary Molecular Effect Model for Selected High Temperature Superconductors with Electronics Physics Applications", International Journal of Scientific Research in Computer Science, Engineering and Information Technology (IJSRCSEIT), ISSN : 2456-3307, Volume 8 Issue 2, pp. 159-167, March-April 2022. Available at doi : <https://doi.org/10.32628/CSEIT228220>
Journal URL : <https://ijsrcseit.com/CSEIT228220>

APPENDIX

Table 2.- Numerical results for Molecular Effect Model with 4-degree polynomial and approximated equation.

ILS MOLECULAR EFFECT MODEL (4-DEGREE)			
COEFFICIENT	VARIABLE X	COEFFICIENT APPROX	VARIABLE X SELECTED
-19.7073349721385e+003	CONSTANT	-19.7073e+003	CONSTANT
20.3782639010116e+000	X	20.3783e+000	X
-7.83958167010360e-003	X ²	-7.8396e-003	X ²
1.33736190239691e-006	X ³	0	X ³
-85.1472747658128e-012	X ⁴	0	X ⁴
RESIDUAL = 4.29102685700562e+000			
APPROXIMATE POLYNOMIAL			
Tc = [-19.7073e+003] + [20.3783e+000] MO+ [-7.8396e-003] MO²			

Table 3.- Numerical results for Molecular Effect Model with 1-degree linear polynomial and approximated equation.

ILS MOLECULAR EFFECT LINEAR MODEL (1-DEGREE)			
COEFFICIENT	VARIABLE X	COEFFICIENT APPROX	VARIABLE X SELECTED
-8.46948713440384e+000	CONSTANT	[-8.4695]	CONSTANT
42.7657510130286e-003	X	[42.7658e-003]	X
RESIDUAL = 4.96771361838260e+000			
APPROXIMATE POLYNOMIAL			
Tc = [-8.4695]+ [42.7658e-003] MO			