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Accurate Empirical Fractional-Order Electrical Models of Young and Old Dentines

Norbert Herencsar¹, *Senior Member, IEEE*, Aslihan Kartci¹, *Member, IEEE*,
and Oguzhan Cicekoglul², *Member, IEEE*

Abstract—Electrical impedance spectroscopy (EIS) is a fast, non-invasive, and safe technique for bioimpedance measurement. In dental research, EIS has been used to detect tooth cracks and caries with higher accuracy than visual and radiographic methods. Recently, a study has been reported on effect of age on impedance measurements for two age groups by employing EIS. The aim of that study was to demonstrate the usefulness of fractional calculus in equivalent circuit modeling. In proposed double dispersion Cole impedance (C-C) models, both resistance and pseudo-capacitance values were found to be significantly different for both age groups. However, in our study, the first time it was found out that proposed models' total pseudo-capacitance values of both young and old dentines can be reduced by 34% and 7.5%, respectively, if recurrent electrical impedance model for $n = 2$ bifurcations to be used. Secondly, new empirical fractional-order electrical models of human tooth using the optimized Valsa network with EIA standard compliant RC values are reported that provide better understanding of the structure of dentine from resistance and capacitance point of view.

I. INTRODUCTION

The electrical impedance of biological and biomedical tissues so-called bioimpedance is a complex quantity, which varies with the tissue's composition and the frequency of the electrical signal applied for impedance measurement. Therefore, its impedance is found as a frequency dependent complex function in a form $Z(j\omega) = \text{Re}(Z) + j \cdot \text{Im}(Z)$, where the real (Re - resistance R (Ω)) and imaginary (Im - reactance X (Ω)) parts of the complex impedance are calculated as $R = |Z|\cos\theta$ and $X = |Z|\sin\theta$, respectively. The electrical impedance spectroscopy (EIS) is a powerful technique that measures the variation of electrical impedance of an analyzed tissue by applying an electrical stimulus (a known noise signal, sinusoidal signal, or binary multifrequency signals of voltage or current) at different frequencies and then to observe the resulting current or voltage [1]. EIS is used in a broad range of applications. For instance, in dentistry, it has been used to detect cracks and caries in enamel and dentine, because early detection of dental caries poses a major challenge to modern dentistry. As it is known, dentine structure is considered as a complex hydrated

composite and it constitutes the bulk of a human tooth and has unique ability to undergo structural changes [2]. It has been shown [3]–[8], in several *in vitro* and *in vivo* studies to be better than existing methods of caries diagnosis.

The interest in applications of the fractional calculus (FC) in modeling complex biomedical phenomena has increased significantly in recent decades, because best fitting accuracy is achieved between experimental and optimization results when constant phase elements (CPEs) are used in models [9]. Nowadays, Caputo definition of fractional-order differential operator describing CPE behavior is the most used, because the derivative of a constant is zero and the initial conditions are described in the same form as in the integer-order differential equations [10]. Caputo's derivative is described as ${}_0^C D_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{f^{(n)}(\tau)}{(t-\tau)^{\alpha-n+1}} d\tau$, where $\Gamma(\cdot)$ is the gamma function and $n-1 \leq \alpha \leq n$. Applying the Laplace transform to Caputo's derivative yields $\mathcal{L}\{{}_0^C D_t^\alpha f(t)\} = s^\alpha F(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} f^{(k)}(0)$, where $f(0)$ is the initial condition. Therefore, the impedance of a fractional-order element is proportional to s^α and then it is possible to define the impedance expression for a capacitor, resistor, and inductor, respectively. One of the first attempts on applying FC in dentistry can be found in [11] when authors investigate the effect of dentine age (young and old) on impedance and equivalent double dispersion Cole impedance (C-C) model for each age group are proposed. However, up to date, no empirical teeth models have been reported that would provide better understanding of the structure of dentine from resistance and capacitance point of view. Therefore, in this paper, EIA standard compliant lumped parameter-based empirical models of teeth using recurrent electrical model for $n = 2$ bifurcations are proposed that show minimum 99.988% fit accuracy with 34% or 7.5% less total pseudo-capacitance in comparison with models reported in [11].

II. MATERIALS AND METHODS

A. Dentine Samples Preparation, Data Collection, and Bioimpedance Model

In brief, freshly extracted un-erupted human third molars were used to avoid the effect of attrition due to age. Two age groups were selected in the investigation; 20 (± 1) and 50 (± 1) years old and five dentine samples were collected from each age group. Bioimpedance measurements were carried out at 20 °C using a Solartron Analytical SI 1260 Impedance Gain-Phase Analyzer over the frequency range 10 mHz to 10 MHz. More details of the sample preparation,

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¹Brno University of Technology, Department of Telecommunications, Technicka 3082/12, 616 00 Brno, Czech Republic {herencsn; kartci}@feec.vutbr.cz. ²Bogazici University, Department of Electrical and Electronics Engineering, Bebek, Istanbul, 34342, Turkey cicekoglul@boun.edu.tr.

TABLE I: Parameter Values for the Components of the Equivalent Circuit Models for Each Age Group.

Components	Elements	Cole-Cole Model Mean Values [11]		Proposed Model with Random Values		Proposed Model with EIA Standard Compliant RC Values	
		Young Dentine	Old Dentine	Young Dentine	Old Dentine	Young Dentine	Old Dentine
Saline solution	R_{-ss} (Ω)	71.5	72.1	71.5	72.1	71.5	72.3
Smear layer	CPE_{T-s} ($\mu F \cdot s^{-0.5}$)	23.8	14.6	15.64	13.52	15.6	13.5
	CPE_{P-s} (-)	0.5					
	$R-s$ (Ω)	244	128.1	564.3	149.38	562	150
Dentine	CPE_{T-d} ($\mu F \cdot s^{-0.5}$)	45.6	182.8	30.23	169.34	30.1	169
	CPE_{P-d} (-)	0.5					
	$R-d$ ($k\Omega$)	43.1	60.9	42.78	60.88	43	60.4
Total pseudo-capacitance ($\mu F \cdot s^{-0.5}$)		69.4	197.4	45.87	182.86	45.7	182.5
Total resistance ($k\Omega$)		43.42	61.1	43.42	61.1	43.63	60.62

sample holder, physiological saline solution, and impedance of a control electrical are given in [11]. It was found out that C-C model using Warburg impedances (order of CPEs is 0.5) provides the best fit accuracy. The electrical component values of proposed circuit model depicted in Fig. 1(a) for each age group is shown in Table I. As it can be observed, the smear layer over the dentine surface and dentine itself have their own resistance (respectively $R-s$, $R-d$) and pseudo-capacitance (CPE_{T-s} , CPE_{T-d}), while the saline solution resistance $R-ss$ only. However, proposed models' [11] total pseudo-capacitance values of both age groups can be significantly reduced, as shown below.

B. Statistical Analysis

Standard and widely used statistical analyses [1] such as relative error of magnitude of CPEs, phase angle error of CPEs, relative error of real and imaginary parts of the complex bioimpedances, and the determination coefficients (R_R^2 , R_X^2) of the fitted models with random values and via EIA standard compliant RC values and standard deviation (Std. Dev.) were calculated in the next section for estimating the accuracy of the proposed models.

III. RESULTS AND DISCUSSION

A. Proposed Empirical Fractional-Order Electrical Model of Teeth with Reduced CPEs

The recurrent electrical impedance model for $n = 2$ bifurcations is shown in Fig. 1(b) [10]. This model again consists of three resistors and two CPEs, hence it ensures modeling of the resistance and pseudo-capacitance of smear layer and dentine as well as the saline solution resistance. Assuming usage of Warburg impedances (equal order labeled as $CPE_{P-s} = CPE_{P-d} = \alpha$), the impedance of of this model is described by:

$$Z(s) = R_{-ss} + \frac{1}{s^\alpha \cdot CPE_{T-s} + \frac{1}{R-s + \frac{1}{s^\alpha \cdot CPE_{T-d} + \frac{1}{R-d}}}}, \quad (1)$$

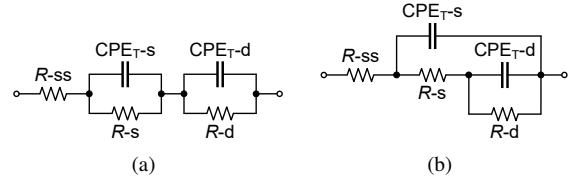


Fig. 1: (a) Double dispersion Cole impedance model, (b) recurrent electrical impedance model for $n = 2$ bifurcations.

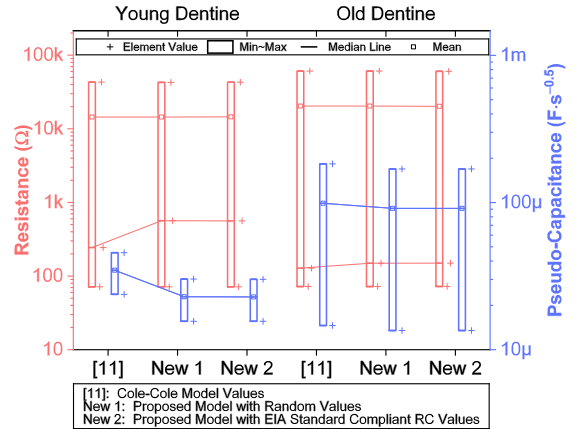
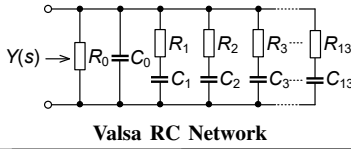


Fig. 2: Comparison of resistance and pseudo-capacitance values in [11] and proposed circuit models of teeth.

where $s = j\omega$. The complex impedance of (1) can be expressed by applying theory [12], but here it is not given due to page constraints. The recurrent electrical impedance model parameters were obtained by applying [12] and numerically re-analyzing the complex impedance of C-C model for each age group. The component values for both random values and via EIA standard compliant RC values are listed in Table I. Here it is worth noting that while the total resistance remained nearly the same, the total pseudo-capacitance are reduced by 34% and 7.5% for young and old dentines, respectively, in comparison with models reported in [11]. This is also evident from comparison of resistance and pseudo-capacitance values shown in Fig. 2.

TABLE II: Standard EIA Compliant RC Values Used in Proposed CPEs of Orders 0.5 via Valsa Network and Error Analysis.

Elements	 Valsa RC Network			
	Young Dentine		Old Dentine	
	CPE _{T-s}	CPE _{T-d}	CPE _{T-s}	CPE _{T-d}
	$15.6 \mu F \cdot s^{-0.5}$	$30.1 \mu F \cdot s^{-0.5}$	$13.5 \mu F \cdot s^{-0.5}$	$169 \mu F \cdot s^{-0.5}$
C_0 (F) / R_0 (Ω)	680 p / 787 k	10.2 p / 383 k	562 p / 887 k	6.8 n / 73.2 k
C_1 (F) / R_1 (Ω)	2.61 n / 38.3	1.8 μ / 6.34 k	12.1 n / 232	66.5 n / 7.68
C_2 (F) / R_2 (Ω)	6.2 n / 86.6	3.74 n / 12	29.4 n / 536	11.8 μ / 1.37 k
C_3 (F) / R_3 (Ω)	30 n / 470	2.43 n / 1.8	66.5 n / 1.27 k	4.99 μ / 590
C_4 (F) / R_4 (Ω)	13.7 n / 205	8.66 n / 30.9	158 n / 2.94 k	28 n / 3.3
C_5 (F) / R_5 (Ω)	909 n / 13.3 k	21.5 n / 73.2	365 n / 6.98 k	13.7 n / 1.1
C_6 (F) / R_6 (Ω)	42.2 μ / 374 k	4.32 μ / 15.4 k	35.7 μ / 442 k	66.5 μ / 7.68 k
C_7 (F) / R_7 (Ω)	1.33 n / 12.7	52.3 n / 180	5.23 n / 100	374 n / 43.2
C_8 (F) / R_8 (Ω)	178 n / 2.4 k	309 n / 1.07 k	887 n / 16 k	909 n / 102
C_9 (F) / R_9 (Ω)	14 μ / 178 k	76.8 μ / 187 k	2.32 n / 41.2	28 μ / 3.24 k
C_{10} (F) / R_{10} (Ω)	2.26 μ / 29.4 k	25.5 μ / 88.7 k	2.05 μ / 38.3 k	158 n / 18.2
C_{11} (F) / R_{11} (Ω)	75 n / 1.02 k	127 n / 442	1.1 n / 14	2.15 μ / 249
C_{12} (F) / R_{12} (Ω)	402 n / 5.9 k	10.5 μ / 36.5 k	12 μ / 215 k	464 μ / 36.5 k
C_{13} (F) / R_{13} (Ω)	5.76 μ / 69.8 k	750 n / 2.61 k	4.99 μ / 88.7 k	154 μ / 18.2 k
Relative magnitude error (%) / Phase angle error (Deg.)				
Max	1.15 / 0.62	1.19 / 0.56	1.08 / 0.61	1.19 / 0.53
Mean	0.47 / 0.25	0.49 / 0.28	0.42 / 0.24	0.48 / 0.24
Median	0.42 / 0.24	0.47 / 0.3	0.38 / 0.24	0.46 / 0.24
Std. Dev.	0.3 / 0.15	0.29 / 0.14	0.27 / 0.14	0.31 / 0.13

B. Proposed Empirical Models of CPEs via Valsa Network

For better understanding of the structure of dentine from resistance and capacitance point of view, the CPEs in Fig. 1(b) fitted to EIA standard compliant values were realized via Valsa RC network [13]. CPEs were optimized using approach [14] powered by genetic algorithm, which based on defined fitness function provides a phase optimization in the desired bandwidth (10 mHz to 10 MHz) with determined branch number (13 in this work) without any complex mathematical analysis. Table II lists the standard EIA compliant RC values used in proposed CPEs with desired pseudo-capacitances and orders via Valsa network. Example of phase variation of proposed CPEs for the young dentine and ideal and simulated phase and magnitude responses vs. frequency as an inset are shown in Fig. 3. The fitted equations using power and linear regressions for the magnitudes and for the phases, respectively, are given inside figure. Distribution of resistance and capacitance values for both age groups are depicted in Fig. 4. From the obtained results it is evident that the maximum relative magnitude errors for young and old dentine are $\pm 1.19\%$ with maximum phase angle error $\pm 0.62^\circ$ and $\pm 0.61^\circ$, respectively, in defined frequency range.

C. Comparison of Bioimpedance Models

For biological and biomedical tissues, the relationship between R and X of the complex impedance can be described

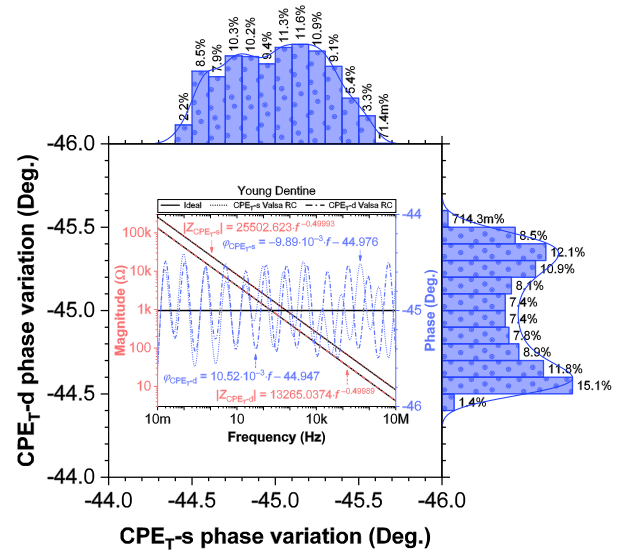


Fig. 3: Example of phase variation of proposed CPEs of orders 0.5 via Valsa RC network with phase and magnitude responses vs. frequency as an inset for the young dentine.

with a circular arc in the Nyquist plot. These plots of simulated [11] and proposed fitting circuit models of teeth are shown in Fig. 5. Plotted zooms as insets for young

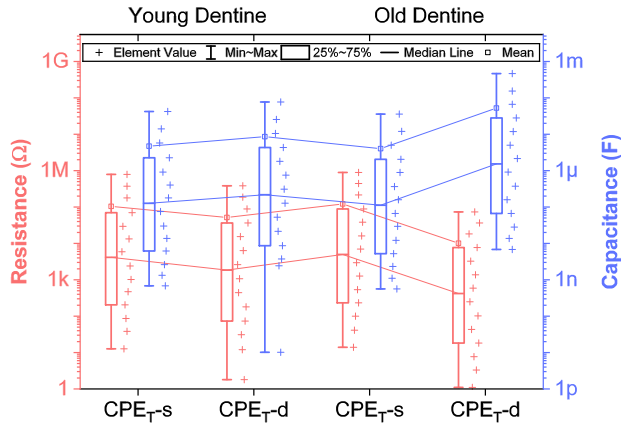


Fig. 4: Distribution of resistance and capacitance values in Valsa RC network for realizing CPEs of orders 0.5.

and older dentine show similar appearances for both age groups. Statistical analysis results are given in Tab. III. From the obtained results it is evident that the maximum relative errors of R and X of the complex impedance varies from 0.9% to 1.82%, respectively, over frequency range from 10 mHz to 10 MHz. Note that the corresponding coefficients of determination of $R_{R,X}^2$ between the initial C-C model and proposed electrical equivalent circuit models for fitting show 99.988% to 100% fit accuracy with low standard deviation.

IV. CONCLUSIONS

Fractional-order bioimpedance circuit models provide a better fit accuracy for impedance data of any tissues over their integer-order counterparts. These models, while lacking in commercial unavailability of CPEs, empirical equivalents employing EIA standard compliant RC values providing an explanation of their structures, are still very useful in practical applications.

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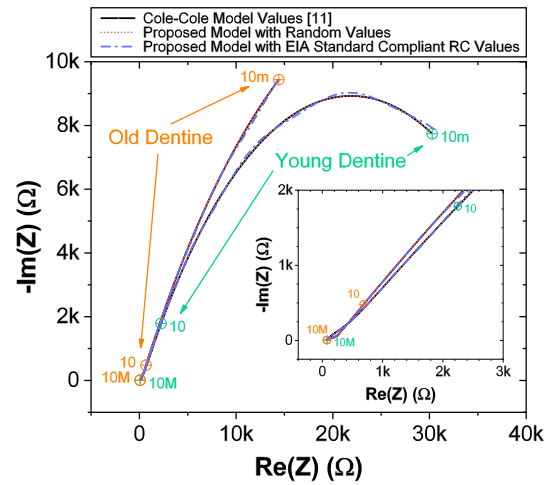


Fig. 5: Nyquist plots of simulated [11] and proposed models of young and old dentine with zoom at high frequency region as an inset. Selected frequencies are highlighted.

TABLE III: Comparison of Results of Proposed Models Fitted to Data of [11] and Indexes of Fit Accuracy.

Evaluation Criteria	Proposed Model with Random Values		Proposed Model with EIA Standard Compliant RC Values	
	Young Dentine	Old Dentine	Young Dentine	Old Dentine
Relative $Re(Z)$ error (%) / Relative $-Im(Z)$ error (%)				
Max	0 / 0	0 / 0	1.05 / 1.82	0.9 / 1.58
Mean			0.33 / 0.62	0.35 / 0.61
Median			0.27 / 0.58	0.31 / 0.59
Std. Dev.			0.27 / 0.39	0.21 / 0.4
R_R^2 (%)	100	100	99.997	99.997
R_X^2 (%)			99.989	99.988
Std. Dev. (Ω)	0		52.46	29.03

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