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RESEARCH ARTICLE

Mathematical Chemistry

Computational analysis of diameter eccentricity based and hyper diameter eccentricity based indices for linear saturated monocarboxylic acids

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Abstract: Chemical graph theory deals with chemical graphs, which are used to represent chemical systems. Topological indices of molecular graphs are an important area of research in chemical graph theory. These indices are numerical values associated with compounds that aim to establish connections between chemical structures and physical attributes, chemical reactivity, and biological activity. Many graph polynomials have been proposed to compute various topological indices. Quantitative structure-property relationship (QSPR) analysis of chemical compounds involves several regression methods that rely on these topological indices. In this article, we utilize the newly introduced $\mathcal{D}\varepsilon$-polynomial to calculate the eccentricity-based indices such as the diameter eccentricity based and hyper diameter eccentricity based index values for nineteen linear saturated monocarboxylic acids. Quantitative structure-property relationship (QSPR) analysis is also performed for the seven thermodynamic properties of monocarboxylic acids. The relationship between thermodynamic properties and topological indices is explored using linear, quadratic and cubic regression models. The best fit curvilinear regression models were determined based on the R^2 and RMSE values of the models. To further investigate the statistical significance of our models, we also conducted chi-square goodness-of-fit tests to identify the best fit models.

Keywords: Diameter, eccentricity, monocarboxylic acids, QSPR, radius.

INTRODUCTION

Linear saturated carboxylic acids can be represented by the formula RCOOH, where R is a linear alkenyl group. One of the fundamental ideas in chemistry is that a molecule's qualities are inextricably linked to its structural characteristics. Chemical graph theory is a discipline in chemistry that deals with graphs. It involves working with chemical graphs, which are used to represent chemical systems (Kirmani *et al*., 2021). One of the most important fields of research in chemical graph theory is topological indices of molecular graphs. These studies are beneficial for determining the relationship between the molecular structure of a drug and its physicochemical properties (Basavanagoud & Praveen, 2020). For the quantitative structure -property relationship (QSPR) and quantitative structure-activity relationship (QSAR) analysis of chemical compounds, several regression methods based on topological indices have been used (Kulli, 2018; Shafiei, 2016).

A topological graph index, also known as a molecular descriptor, is a mathematical formula that may be applied to any graph that represents a chemical structure. This index may be used to assess mathematical values and

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further study a molecule's physical and other features. As a result, it is an effective means of eliminating costly and time-consuming laboratory studies (Baev, 2012). The topological index was first used by Harold Wiener (Wiener, 1947). He proposed the concept of the path number of a graph, which is the total of all the distances between pairs of carbon atoms in a molecule. The first generic Zagreb index was proposed by Gutman and Das (Gutman & Das, 2004). The Geometric-arithmetic (GA) index was established by Yuan *et al*. (Yuan *et al*., 2009) and contrasted with the well-known Randic index. The atom-bond connectivity index, sometimes known as the ABC index, was proposed by Estrada *et al*. (Estrada *et al*., 1988). Due to its relationship with the thermodynamic characteristics of alkanes, the ABC index is significant (Gutman *et al*., 2012). Eccentricity-based topological indices have also piqued the curiosity of several researchers. The eccentric connectivity index (ECI) was developed by Madan *et al*. in 2005 as a distance-based topological indicator and Ghorbani in 2012 provided new descriptions for the Zagreb indices by defining them in terms of the eccentricity of a molecular graph. The reverse ECI for a series of nanocones and fullerene structures was recently explored by Qudair Baig *et al*. in 2015.

In this study, we have considered the molecular structures of 19 monocarboxylic acids ranging from C2 − C20. To predict the thermodynamic properties of these monocarboxylic acids we have obtained the most relevant topological indices and developed curvilinear regression models. Shafiei (2015) established the values for the indices of Randic, Balaban, Szeged, and Harary for monocarboxylic acids. Havare (2019) analyzed QSPR models, to predict the thermodynamic characteristics of monocarboxylic acids using the forgotten topological index, forgotten coindex, max-min Rodeg index, and inverse sum Rodeg index.

Many graph polynomials have been proposed to compute various topological indices. The Hosoya polynomial (Hosoya 1988) is the most well-known polynomial to calculate distance-based topological indices such as the Wiener index and hyper Wiener index. The M-polynomial (Deutsch & Klavzar, 2015) is one of several algebraic polynomials published in 2015 that can be used to calculate a variety of degree-based topological indices. Recently, Mondal *et al*. (2021) proposed the neighbourhood M- polynomial. Their attention was on the neighbourhood indices that were based on degrees. The Padmakar-Ivan polynomial (PI polynomial) was initially introduced by Ashrafi *et al*. (2006) who also studied a few of its features. Our $\mathcal{D}\varepsilon$-Polynomial can be used to compute diameter eccentricity based and hyper diameter eccentricity based topological indices (Deepalakshmi & Desikan, 2023).

The following describes the structure of the paper: In the diameter eccentricity based and hyper diameter eccentricity based indices section, we present some fundamental concepts related to the newly introduced polynomial and indices. The Methodology and Illustration section presents the edge partition methodology for computing the $\mathcal{D}\varepsilon$-Polynomial for nineteen linear saturated monocarboxylic acids. An illustration for deriving the $\mathcal{D}\varepsilon$-Polynomial and the proposed indices for propanoic acid is also presented in this section. The curvilinear regression analysis of the monocarboxylic acid section shows the regression analysis of the indices vis-à-vis their thermodynamic properties to identify the best fit models. We discover that the cubic regression models, validated thorough R^2 and RMSE values, are the best fit models to predict the thermodynamic characteristics of monocarboxylic acids studied in this paper.

Diameter eccentricity based and hyper diameter eccentricity based indices

Let G be a simple, finite and connected graph with $V(G)$ as the vertex set and $E(G)$ as the edge set. Let d_p be the degree of a vertex p in G and ε_p the eccentricity of the vertex p. Let $\Delta(G)$ and $\delta(G)$ be the maximum and minimum degrees of the vertices of G, respectively.

Definition 1. (Deutsch & Klavzar, 2014). The eccentricity index for a graph G is defined as

$$\varepsilon(G) = \sum_{pq \in E} [\varepsilon_p + \varepsilon_q] \quad ...(1)$$

where ε_p denotes the eccentricity of the vertex p.

The Revan vertex degree of p in G is defined as $r_p = \Delta(G) + \delta(G) - d_p$ (Kulli, 2017, 2018). Based on this definition, we introduce a new type of vertex degree known as diameter eccentricity based vertex degree of p in G as

$$d\varepsilon_p = D(G) + 1 - \varepsilon_p$$

where $D(G)$ is the diameter of the graph G.

Example:

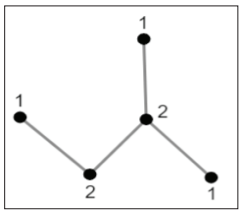

Figure 1: $\mathcal{D}\varepsilon$ —values for the molecular graph of propanoic acid P

The eccentricity of a vertex is a measure of its centrality. Diameter, on the other hand, may be considered as a measure of the spread of the graph. Our diameter eccentricity based vertex degree incorporates both these measures and specifies the relevance of a vertex in relation to the entire graph. Diameter eccentricity based and hyper diameter eccentricity based indices for each connected graph G are determined using the newly introduced polynomial named $\mathcal{D}\varepsilon$-Polynomial, defined as follows,

$$\mathcal{D}\varepsilon(G) = \sum_{i\leq j} \left(\text{number of edges pq such that } d\varepsilon_p = i, d\varepsilon_q = j\right)\alpha^i\beta^j$$

$$= \sum_{i\leq j} r\rho_{(i,j)}\alpha^i\beta^j \quad f(\alpha,\beta) \qquad ...(2)$$

where $r\rho_{(i,j)}$ signifies the number of edges in the edge partitions determined by the diameter eccentricity based vertex degrees of the end vertices of the edges of the graph while α and β are variables. Our $\mathcal{D}\varepsilon$-Polynomial is a function of α and β. In Table 1 we present our indices as functions of $d\varepsilon_p$ *and* $d\varepsilon_q$.

Table 1: Description of proposed indices

Indices	$f(d\varepsilon_p, d\varepsilon_q)$
First $\mathcal{D}\mathrm{R}\mathcal{E}$ Index $(\mathcal{D}R_1\mathcal{E})$	$d\varepsilon_p + d\varepsilon_q$
Second $\mathcal{D}\mathrm{R}\mathcal{E}$ Index $(\mathcal{D}R_2\mathcal{E})$	$d\varepsilon_p * d\varepsilon_q$
First Hyper $\mathcal{D}\mathrm{R}\mathcal{E}$ Index $(H\mathcal{D}R_1\mathcal{E})$	$(d\varepsilon_p + d\varepsilon_q)^2$
Second Hyper $\mathcal{D}\mathrm{R}\mathcal{E}$ Index $(H\mathcal{D}R_2\mathcal{E})$	$(d\varepsilon_p * d\varepsilon_q)^2$

Using our $\mathcal{D}\varepsilon$-polynomial, we can compute our diameter eccentricity based indices, $\mathcal{D}R_1\varepsilon$ and $\mathcal{D}R_2\varepsilon$, as well as our hyper diameter eccentricity based indices, $H\mathcal{D}R_1\varepsilon$ and $H\mathcal{D}R_2\varepsilon$. Table 2 shows the methodology for deriving our indices from the $\mathcal{D}\varepsilon$-polynomial.

Table 2: Derivation of proposed indices from $\mathcal{D}\varepsilon$-polynomial

Indices	Derivation from $\mathcal{D}\varepsilon(\mathcal{G})$
$\mathcal{D}R_1\mathcal{E}$	$(\partial_\alpha + \partial_\beta)(\mathcal{D}\varepsilon(G))\vert_{\alpha=1,\beta=1}$
$\mathcal{D}R_2\mathcal{E}$	$(\partial_\alpha * \partial_\beta)(\mathcal{D}\varepsilon(G))\vert_{\alpha=1,\beta=1}$
$H\mathcal{D}R_1\mathcal{E}$	$(\partial_\alpha + \partial_\beta)^2(\mathcal{D}\mathcal{E}(G))\vert_{\alpha=1,\beta=1}$
$H\mathcal{D}R_2\mathcal{E}$	$(\partial_\alpha * \partial_\beta)^2(\mathcal{D}\mathcal{E}(G))\vert_{\alpha=1,\beta=1}$

In Table 2,

$$\partial_\alpha \mathcal{D}\varepsilon(G) = \partial_\alpha f(\alpha,\beta) = \alpha\frac{\partial(f(\alpha,\beta))}{\partial\alpha},$$

$$\partial_\beta \mathcal{D}\varepsilon(G) = \partial_\beta f(\alpha,\beta) = \beta\frac{\partial(f(\alpha,\beta))}{\partial\beta}$$

METHODOLOGY AND ILLUSTRATION

We use the method of edge partitions and employ the newly introduced $\mathcal{D}\varepsilon$-Polynomial to compute our results for the molecular graphs of monocarboxylic acids. Let $r\rho_{(p,q)}$ denote the number of edges in the edge partition $(d\varepsilon_p, d\varepsilon_q)$ in the graph G. We make use of the diameter eccentricity based vertex degrees of the end vertices of the edges. The edge partitions for the 19-monocarboxylic acids are presented in Tables 3-21.

Table 3: $\mathcal{D}\varepsilon$ —Edge partitions of ethanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)
$r\rho_{(p,q)}$	3

From Table 3 we observe that the edges of ethanoic acid can be divided into 1 partition based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of ethanoic acid.

Table 4: $\mathcal{D}\varepsilon$ —Edge partitions of propanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,2)
$r\rho_{(p,q)}$	3	1

From Table 4 we observe that the edges of propanoic acid can be divided into 2 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of propanoic acid.

Table 5: $\mathcal{D}\varepsilon$ –Edge partitions of butanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)
$r\rho_{(p,q)}$	3	2

From Table 5 we observe that the edges of butanoic acid can be divided into 2 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of butanoic acid.

Table 6: $\mathcal{D}\varepsilon$ –Edge partitions of pentanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,3)
$r\rho_{(p,q)}$	3	2	1

From Table 6 we observe that the edges of pentanoic acid can be divided into 3 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of pentanoic acid.

Table 7: $\mathcal{D}\varepsilon$ –Edge partitions of hexanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)
$r\rho_{(p,q)}$	3	2	2

From Table 7 we observe that the edges of hexanoic acid can be divided into 3 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of hexanoic acid.

Table 8: $\mathcal{D}\varepsilon$ –Edge partitions of heptanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,4)
$r\rho_{(p,q)}$	3	2	2	1

From Table 8 we observe that the edges of heptanoic acid can be divided into 4 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of heptanoic acid.

Table 9: $\mathcal{D}\varepsilon$ –Edge partitions of octanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)
$r\rho_{(p,q)}$	3	2	2	2

From Table 9 we observe that the edges of octanoic acid can be divided into 4 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of octanoic acid.

Table 10: $\mathcal{D}\varepsilon$ –Edge partitions of nonanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,5)
$r\rho_{(p,q)}$	3	2	2	2	1

From Table 10 we observe that the edges of nonanoic acid can be divided into 5 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of nonanoic acid.

Table 11: $\mathcal{D}\varepsilon$ –Edge partitions of decanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)
$r\rho_{(p,q)}$	3	2	2	2	2

From Table 11 we observe that the edges of decanoic acid can be divided into 5 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of decanoic acid.

Table 12: $\mathcal{D}\varepsilon$ –Edge partitions of undecanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,6)
$r\rho_{(p,q)}$	3	2	2	2	2	1

From Table 12 we observe that the edges of Undecanoic acid can be divided into 6 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of undecanoic acid.

Table 13: $\mathcal{D}\varepsilon$ –Edge partitions of dodecanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)
$r\rho_{(p,q)}$	3	2	2	2	2	2

From Table 13 we observe that the edges of dodecanoic acid can be divided into 6 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of dodecanoic acid.

Table 14: $\mathcal{D}\varepsilon$ –Edge partitions of tridecanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)	(7,7)
$r\rho_{(p,q)}$	3	2	2	2	2	2	1

From Table 14 we observe that the edges of tridecanoic acid can be divided into 7 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of tridecanoic acid.

Table 15: $\mathcal{D}\varepsilon$ –Edge partitions of tetradecanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)	(7,8)
$r\rho_{(p,q)}$	3	2	2	2	2	2	2

From Table 15 we observe that the edges of tetradecanoic acid can be divided into 7 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of tetradecanoic acid.

Table 16: $\mathcal{D}\varepsilon$ –Edge partitions of pentadecanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)	(7,8)	(8,8)
$r\rho_{(p,q)}$	3	2	2	2	2	2	2	1

From Table 16 we observe that the edges of pentadecanoic acid can be divided into 8 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of pentadecanoic acid.

Table 17: $\mathcal{D}\varepsilon$ –Edge partitions of hexadecanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)	(7,8)	(8,9)
$r\rho_{(p,q)}$	3	2	2	2	2	2	2	2

From Table 17 we observe that the edges of hexadecanoic acid can be divided into 8 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of hexadecanoic acid.

Table 18: $\mathcal{D}\varepsilon$ –Edge partitions of heptadecanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)	(7,8)	(8,9)	(9,9)
$r\rho_{(p,q)}$	3	2	2	2	2	2	2	2	1

From Table 18 we observe that the edges of heptadecanoic acid can be divided into 9 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of heptadecanoic acid.

Table 19: $\mathcal{D}\varepsilon$ –Edge partitions of octadecanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)	(7,8)	(8,9)	(9,10)
$r\rho_{(p,q)}$	3	2	2	2	2	2	2	2	2

From Table 19 we observe that the edges of octadecanoic acid can be divided into 9 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of octadecanoic acid.

Table 20: $\mathcal{D}\varepsilon$ –Edge partitions of nonadecanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)	(7,8)	(8,9)	(9,10)	(10,10)
$r\rho_{(p,q)}$	3	2	2	2	2	2	2	2	2	1

From Table 20 we observe that the edges of nonadecanoic acid can be divided into 10 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of nonadecanoic acid.

Table 21: $\mathcal{D}\varepsilon$ –Edge partitions of eicosanoic acid

$(d\varepsilon_p, d\varepsilon_q)$	(1,2)	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)	(7,8)	(8,9)	(9,10)	(10,11)
$r\rho_{(p,q)}$	3	2	2	2	2	2	2	2	2	2

From Table 21 we observe that the edges of eicosanoic acid can be divided into 10 partitions based on the distance eccentricity based vertex degrees of the end vertices of the edges in the molecular graph of eicosanoic acid.

Illustration of $\mathcal{D}\varepsilon$- polynomial and $\mathcal{D}\varepsilon$ indices for propanoic acid

Let P denote the molecular graph of propanoic acid considered in Figure 1. It has 5 vertices and 4 edges.

Consider

$$\mathcal{D}\varepsilon(P) = \sum_{i\leq j} (r\rho_{(i,j)})\alpha^i\beta^j$$
$$= r\rho_{(1,2)}\alpha^1\beta^2 + r\rho_{(2,2)}\alpha^2\beta^2.$$

Using the edge partitions given in Table 4, it is clear that $r\rho_{(1,2)} = 3, r\rho_{(2,2)} = 1$.

Applying the values in $\mathcal{D}\varepsilon(P)$ we derive the $\mathcal{D}\varepsilon$-polynomial for propanoic acid as follows:

$$\mathcal{D}\varepsilon(P) = 3\alpha^1\beta^2 + 1\alpha^2\beta^2$$

We now compute the diameter eccentricity based and hyper diameter eccentricity based indices of the molecular graph of propanoic acid P using $\mathcal{D}\varepsilon$-Polynomial as follows:

$$\mathcal{D}R_1\varepsilon(P) = (\partial_\alpha + \partial_\beta)(\mathcal{D}\varepsilon(P))|_{\alpha=\beta=1}$$

$$= \left(\partial_\alpha \mathcal{D}\varepsilon(P) + \partial_\beta \mathcal{D}\varepsilon(P)\right)|_{\alpha=\beta=1}$$

$$= (\partial_\alpha(f(\alpha,\beta)) + \partial_\beta(f(\alpha,\beta)))|_{\alpha=\beta=1}$$

$$= ((\alpha \frac{\partial(3\alpha^1\beta^2+1\alpha^2\beta^2)}{\partial\alpha}) + (\beta \frac{\beta(3\alpha^1\beta^2+1\alpha^2\beta^2)}{\partial\beta}))|_{\alpha=\beta=1}$$

$$= (9\alpha^1\beta^2 + 4\alpha^2\beta^2)|_{\alpha=\beta=1} = 13.$$

Similarly, the other three indices can be obtained as follows:

$$\mathcal{D}R_2\varepsilon(P) = (\partial_\alpha * \partial_\beta)(\mathcal{D}\varepsilon(P))|_{\alpha=\beta=1}$$

$$= (\partial_\alpha * \partial_\beta)(f(\alpha,\beta))|_{\alpha=\beta=1}$$

$$= (6\alpha^1\beta^2 + 4\alpha^2\beta^2)|_{\alpha=\beta=1} = 10.$$

$$H\mathcal{D}R_1\varepsilon(p) = (\partial_\alpha + \partial_\beta)^2(\mathcal{D}\varepsilon(P))|_{\alpha=\beta=1}$$

$$= (\partial_\alpha + \partial_\beta)^2(f(\alpha,\beta))|_{\alpha=\beta=1}$$

$$= (27\alpha^1\beta^2 + 16\alpha^2\beta^2)|_{\alpha=\beta=1} = 43.$$

$$H\mathcal{D}R_2\varepsilon(p) = (\partial_\alpha * \partial_\beta)^2(\mathcal{D}\varepsilon(P))|_{\alpha=\beta=1}$$

$$= (\partial_\alpha * \partial_\beta)^2(f(\alpha,\beta))|_{\alpha=\beta=1}$$

$$= (12\alpha^1\beta^2 + 16\alpha^2\beta^2)|_{\alpha=\beta=1} = 28.$$

Similarly, we can obtain the proposed index values for the other monocarboxylic acid.

Curvilinear regression analysis of monocarboxylic acids

In this section, we will conduct a quantitative structure property relationship (QSPR) analysis on the topological indices listed in Table 1 for the seven thermodynamic properties of monocarboxylic acids (Shafiei, 2015; Shafiei, 2016; Havare, 2019): Thermal energy (TE kcal/mol), constant heat capacity of gas (CV cal/mol K), entropy of gas (EGS cal/mol K), enthalpy of formation of liquid (EFL kJ/mol), enthalpy of combustion of liquid (ECL kJ/mol), enthalpy of sublimation (ES kJ/mol) and Enthalpy of vaporization (EV kJ/mol).

We perform curvilinear regression analysis to identify the best fit models for predicting the seven thermodynamic properties of monocarboxylic acids using our proposed topological descriptors. We have performed linear, quadratic and cubic regression analysis given by the following equations:

$$P = \tilde{\alpha}_1(TI) + \tilde{\gamma} \quad ...(3)$$

$$P = \tilde{\alpha}_1(TI)^2 + \tilde{\alpha}_2(TI) + \tilde{\gamma} \quad ...(4)$$

$$P = \tilde{\alpha}_1(TI)^3 + \tilde{\alpha}_2(TI)^2 + \tilde{\alpha}_3(TI) + \tilde{\gamma} \quad ...(5)$$

where $\boldsymbol{P}$ is the thermodynamic property (dependent variable), $\tilde{\gamma}$ is the regression model constant, and $\tilde{\alpha_i}'s$ are the regression coefficients for the topological descriptors (TI), respectively.

We have derived and compared the linear, quadratic and cubic regression models based on $\boldsymbol{R^2}$ and RMSE values. We have taken into consideration models with $\boldsymbol{R^2 \geq 0.8}$ (as per International Academy of Mathematical Chemistry Guidelines).

We also performed χ^2-goodness of fit test to validate our models. The hypotheses which we considered for checking the goodness of fit of the regression models are:

H_0 : Proposed regression model is a good fit.
H_1 : Proposed regression model is not a good fit.

We have computed the values of the proposed indices for the 19-monocarboxylic acids. Tables 22 and 23 show the computed values for the proposed indices and the thermodynamic properties of monocarboxylic acids, respectively.

Table 22: Topological descriptor values of monocarboxylic acids

Name	$\mathcal{D}R_1\varepsilon$	$\mathcal{D}R_2\varepsilon$	$H\mathcal{D}R_1\varepsilon$	$H\mathcal{D}R_2\varepsilon$
Ethanoic acid	9	6	27	12
Propanoic acid	13	10	43	28
Butanoic acid	19	18	77	84
Pentanoic acid	25	27	113	165
Hexanoic acid	33	42	175	372
Heptanoic acid	41	58	239	628
Octanoic acid	51	82	337	1172
Nonanoic acid	61	107	437	1797
Decanoic acid	73	142	579	2972
Undecanoic acid	85	178	723	4268
Dodecanoic acid	99	226	917	6500
Tridecanoic acid	113	275	1113	8901
Tetradecanoic acid	129	338	1367	12772
Pentadecanoic acid	145	402	1623	16868
Hexadecanoic acid	163	482	1945	23140
Heptadecanoic acid	181	563	2269	29701
Octadecanoic acid	201	662	2667	39340
Nonadecanoic acid	221	762	3067	49340
Eicosanoic acid	243	882	3549	63540

Table 23: Thermodynamic property values of monocarboxylic acids

Acids name	CV	ECL	EFL	EGS	ES	EV	TE
Ethanoic acid	13.442	875.16	483.5	67.558	46.3	49.7	44.38
Propanoic acid	17.767	1527.3	510.8	74.612	50	56.1	64.578
Butanoic acid	22.163	2183.5	533.9	81.713	54.9	62.9	84.565
Pentanoic acid	26.538	2837.8	558.9	87.271	58.2	69	104.607
Hexanoic acid	30.927	3494.3	581.8	94.058	63	75	124.667
Heptanoic acid	35.421	4146.9	608.5	101.646	64.8	81.7	144.655
Octanoic acid	39.911	4799.9	634.8	109.25	69.4	86.9	164.637
Nonanoic acid	44.399	5456.1	658	116.353	72.3	93.6	184.621
Decanoic acid	48.889	6079.3	713.7	123.676	76.3	100.8	204.604
Undecanoic acid	53.378	6736.5	736.2	130.987	78.9	106.7	224.587
Dodecanoic acid	57.867	7377	775.1	138.293	82.2	115.9	244.57
Tridecanoic acid	62.255	8024.2	807.2	145.633	84.9	121.2	264.554
Tetradecanoic acid	66.844	8676.7	834.1	152.932	87.7	130.2	284.537
Pentadecanoic acid	71.627	9327.7	862.4	162.308	91.4	136.5	304.405
Hexadecanoic acid	75.73	9977.2	892.2	167.564	94.5	144.3	324.571
Heptadecanoic acid	80.216	10624.4	924.4	174.86	100.7	159.6	344.556
Octadecanoic acid	84.704	11280.1	947.4	182.181	102.8	164.7	364.539
Nonadecanoic acid	89.192	11923.4	984.1	189.486	105	172.9	384.522
Eicosanoic acid	93.681	12574.2	1012.6	196.113	109.9	179.2	404.506

CV: constant heat capacity; ECL: enthalpy of combustion of liquid; EFL: enthalpy of formation of liquid; EGS: enthalpy of gas; ES: enthalpy of sublimation; EV: enthalpy of vaporization; TE: thermal energy

RESULTS AND DISCUSSION

We observed that the cubic regression models were the best fit models with low RMSE values. From the cubic regression models, we concluded that the best index is $\mathcal{D}R_1\varepsilon$.

Best fit regression models

In this section we present the best fit cubic regression models based on $\mathcal{D}R_1\varepsilon$ for the seven thermodynamic properties of monocarboxylic acids.

$$CV = 5e-06\,(\mathcal{D}R_1\varepsilon)^3 - 0.0028(\mathcal{D}R_1\varepsilon)^2 + 0.726(\mathcal{D}R_1\varepsilon) + 9.004 \quad ...(6)$$

$$ECL = 0.0008(\mathcal{D}R_1\varepsilon)^3 - 0.4202(\mathcal{D}R_1\varepsilon)^2 + 107.3\,(\mathcal{D}R_1\varepsilon) + 243.2 \quad ...(7)$$

$$EFL = 2e-05\,(\mathcal{D}R_1\varepsilon)^3 - 0.0129(\mathcal{D}R_1\varepsilon)^2 + 4.305\,(\mathcal{D}R_1\varepsilon) + 452.8 \quad ...(8)$$

$$EGS = 7e-06\,(\mathcal{D}R_1\varepsilon)^3 - 0.0039(\mathcal{D}R_1\varepsilon)^2 + 1.12\,(\mathcal{D}R_1\varepsilon) + 60.65 \quad ...(9)$$

$$ES = 6e-06\,(\mathcal{D}R_1\varepsilon)^3 - 0.0028(\mathcal{D}R_1\varepsilon)^2 + 0.6204(\mathcal{D}R_1\varepsilon) + 43.3 \quad ...(10)$$

$$EV = 4e-06\,(\mathcal{D}R_1\varepsilon)^3 - 0.0025(\mathcal{D}R_1\varepsilon)^2 + 0.9176(\mathcal{D}R_1\varepsilon) + 45.54 \quad ...(11)$$

$$TE = 2e-05\,(\mathcal{D}R_1\varepsilon)^3 - 0.0128(\mathcal{D}R_1\varepsilon)^2 + 3.29\,(\mathcal{D}R_1\varepsilon) + 24.98 \quad ...(12)$$

Table 24: Statistical parameters for best fit model

Property	Curve equation	Best predictor	R^2	RMSE	χ^2
CV	(6)	$\mathcal{D}R_1\varepsilon$	0.9991	0.8063	0.622021
ECL	(7)	$\mathcal{D}R_1\varepsilon$	0.9989	131.8854	152.6476
EFL	(8)	$\mathcal{D}R_1\varepsilon$	0.9990	5.7997	1.117039
EGS	(9)	$\mathcal{D}R_1\varepsilon$	0.9993	1.2122	0.682761
ES	(10)	$\mathcal{D}R_1\varepsilon$	0.9957	1.3837	0.725426
EV	(11)	$\mathcal{D}R_1\varepsilon$	0.9972	2.3514	0.978772
TE	(12)	$\mathcal{D}R_1\varepsilon$	0.9990	3.9413	19.14061

The table value for χ^2 with degrees of freedom 18 at the 5% and 1% levels of significance are 28.869 and 34.809, respectively. From Table 24, we see that the calculated χ^2 values of the seven thermodynamic properties, except one property (enthalpy of combustion of liquid), were less than the table value at both levels of significance. Thus, we accept all the models except the model for ECL.

Figures 2 to 5 depict the regression plots for the properties versus the best predictor index.

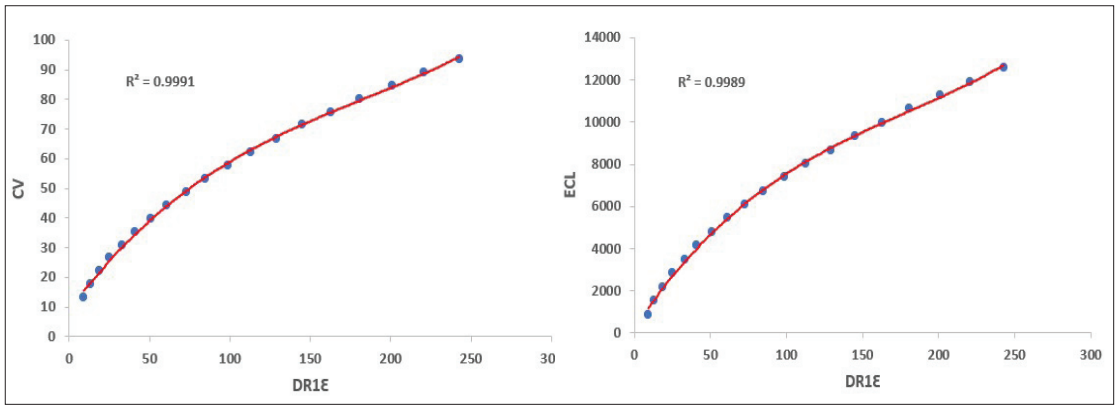

Figure 2: Cubic regression curve for CV and ECL against $\mathcal{D}R_1\varepsilon$

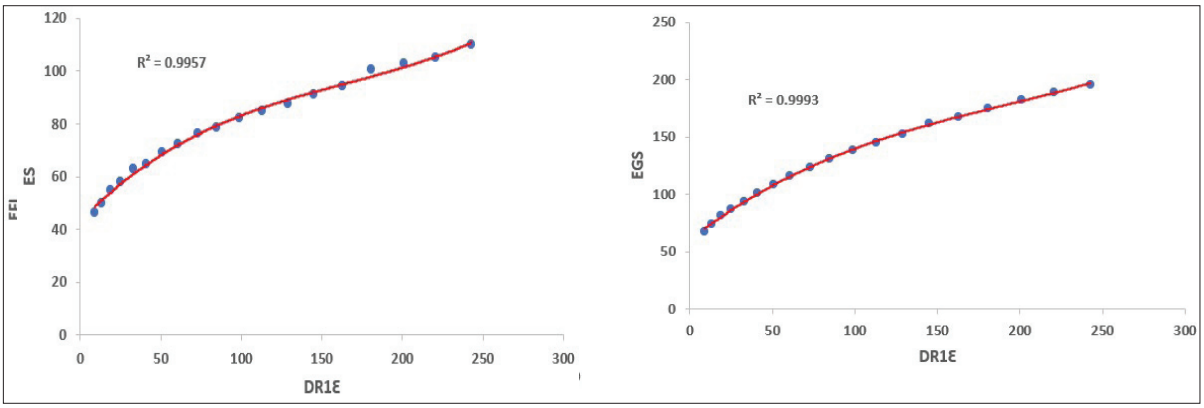

Figure 3: Cubic regression curve for EFL and EGS against $\mathcal{D}R_1\varepsilon$

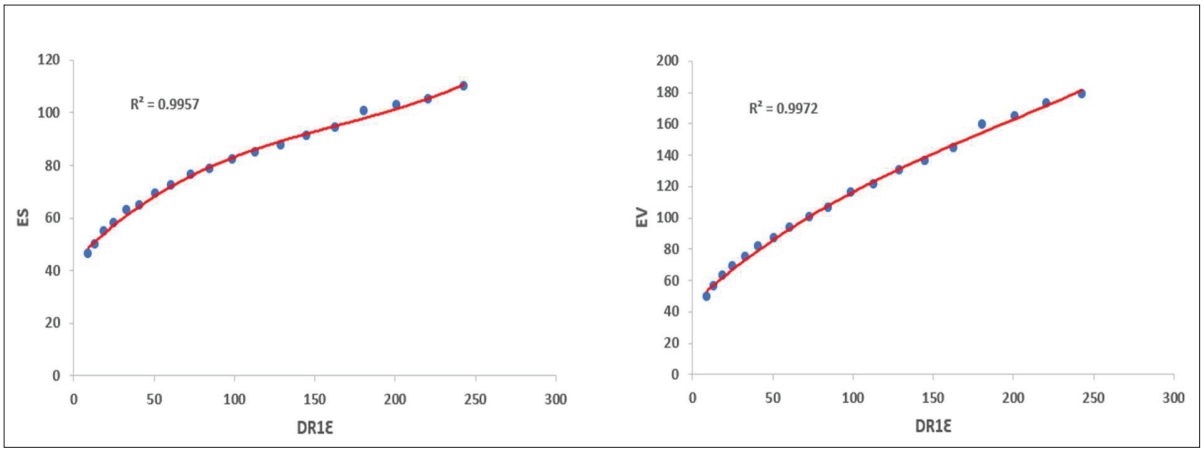

Figure 4: Cubic regression curve for ES and EV against $\mathcal{D}R_1\varepsilon$

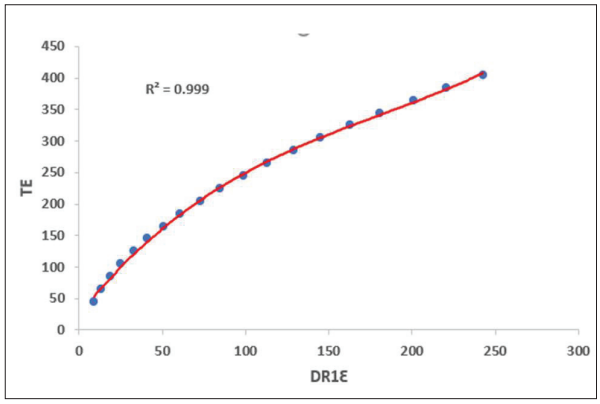

Figure 5: Cubic regression curve for TE against $\mathcal{D}R_1\varepsilon$

CONCLUSION

In this paper, we have utilized the newly introduced $\mathcal{D}\varepsilon$-Polynomial to derive the diameter eccentricity based and hyper diameter eccentricity based topological descriptors for nineteen linear saturated monocarboxylic acids. We conducted a QSPR analysis on seven thermodynamic properties of monocarboxylic acids using our proposed indices. We conclude that the cubic regression models based on our index $\mathcal{D}R_1\varepsilon$ provide the best fits for the thermodynamic properties in terms of R^2 and RMSE values. We also conducted chi-square goodness-of-fit tests to determine the statistical significance of our proposed models. The tests showed that the cubic regression models were a good fit for six of the thermodynamic properties, with the exception of enthalpy of combustion of liquid (ECL).

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