Communications on Applied Nonlinear Analysis
ISSN: 1074-133X
Vol 32 No. 4s (2025)

A Reduction Analysis of the Weiner Index on Predicting the Boiling Point of Hydrocarbons Using Graph Technique

R. Shankar[*], Varadha Raj Manivannan[1], M. Siva[2] & E. Padmavathy[3]

[*]Assistant Professor, Department of Mathematics, School of Arts and Science, Vinayaka Mission's Chennai Campus, Vinayaka Mission's Research Foundation (Deemed to be University), Paiyanoor-603 104, Tamil Nadu, India.

[1]Assistant Professor, Department of Mathematics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya (Deemed to be University), Kanchipuram-631 561, Tamil Nadu, India.

[2]Assistant Professor, Department of Mathematics, St. Joseph's Institute of Technology, OMR, Chennai-600 119, Tamil Nadu, India.

[3]Assistant Professor, Department of Mathematics, Vel Tech Rangarajan Dr. Sagunthala R&D Institute of Science and Technology, Avadi, Chennai-600 062, Tamil Nadu, India.

Email: rathinavelshankar@gmail.com, varadharaj.m219@gmail.com, sivam@stjosephstechnology.ac.in, padmavathyelu@gmail.com

Article History:

Received: *18-09-2024*

Revised: *23-11-2024*

Accepted: *31-11-2024*

Abstract:

Introduction: This study investigates the link between graph eccentricity and boiling points for nonanes and decanes, demonstrating graph theory's ability to predict the physical characteristics of organic compounds.

Objectives: Inspired by Wiener's work on topological indices, we create a novel power formula based on graph eccentricity to predict boiling points. This provides a more straightforward technique than typical wiener index computations.

Methods: Our findings show a substantial association between graph eccentricity and boiling temperatures, demonstrating the importance of structural characteristics in predicting chemical responses.

Results: This study advances chemical graph theory by proposing an alternate approach for estimating boiling points, underlining the importance of graph-based studies in understanding molecule structures and behaviours.

Conclusions: This research examines the molecular graph's eccentricity for 105 nonanes and decanes. Using a power formula, we discovered a substantial relationship between the boiling point and the eccentricity of the chemical structure.

Keywords: Molecular graph, Nonanes and Decanes, Winer index, Eccentricity, R-Programming Language.

1. Introduction

A graph G consists of a set called vertices v and edges e, such that each edge e_k is identified with an unordered pair of vertices. The number of vertices is called the order of the graph $|V| = n$ and the number of edges is called the size of the graph $|E| = m$ in [2].

In 1875, Arthur Cayley (as instance of [1]) introduced a method for representing molecules using graph theory. In this model, vertices represent atoms, and edges represent chemical bonds between them.

This molecular graph approach provided a foundational tool for visualizing and analyzing molecular structures through graph theory.

The Wiener index, introduced by Harold Wiener in [11], was the first graph metric applied in chemistry. The Wiener index (Wiener number) is a topological index of a molecule, defined as the sum of the lengths of the shortest paths between all pairs of vertices in the chemical graph representing the non-hydrogen atoms in the molecule (Harry Wiener, 1947). The Wiener index of G is the number $W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_G(i,j)$ is the entries of the distance matrix.

In his 1947 study, Harry Wiener explored how the structure of paraffins influences their boiling points. He found that an organic compound's boiling point and physical properties depend on the molecule's type, number, and arrangement of atoms. Wiener noted that differences in physical properties are due to changes in structural relationships, even though the number and type of atoms within an isomeric group remain constant. He also linked the Wiener polarity index to the Wiener index through a specific equation.

$$\Delta t = \frac{98}{n^2}\Delta w + 5.5\Delta pp \qquad (1)$$

where Δt is the boiling point of a group of isomers, $\Delta w = w_0 - w$, where $w_0 = \left(\frac{1}{6}\right)(n-1)(n)(n+1)$ distances between any two carbon atoms in a molecule, in terms of carbon-carbon bonds. We denote $\Delta p = p_0 - p$, where $p_0 = n - 3$ and p, the polarity number is defined as the number of pairs of carbon atoms separated by three carbon-carbon bonds.

A list of the detailed results obtained by applying this equation to the 37 paraffins from C_4H_{10} to C_8H_{18} and further extended this method for the boiling point data available for the nonanes and decanes. After Wiener, numerous researchers developed various techniques to determine physical and chemical properties from topological indices.

The polarity number p is the number of pairs of carbon atoms separated by three carbon-carbon bonds. He further defined the path number as the sum of the distances between two carbon atoms in a molecule in terms of carbon-carbon bonds. Later, these topological indices were named the Wiener index and the Wiener polarity index.

Following its introduction, researchers have developed extensions of the Wiener index and created other indices, such as the Hosoya index in [7], the Gutman and Schultz indices in [6], and many other distance-based topological indices in [4], to predict various molecular properties.

Figure 1: The Chemical Compound and Graph Structure

Shi, Kosari, Ahmad, Hameed, and Akhter's [9], examined topological indices based on vertex degree, particularly within flabellum graphs. Their study visualized these indices, offering insights into their behaviour within this graph class. Additionally, they applied the fuzzy first Zagreb index to analyze branching patterns in cyber flabellum graphs, contributing to understanding cybercrime.

A chemical graph is a labeled graph whose vertices correspond to the atoms of the compound and whose edges correspond to chemical bonds. Figure 1 shows a chemical compound's molecular graph and graph structure.

The eccentricity $e(v)$ of a vertex v in a connected graph G is $max\, dG(u,v)$ for all u in G. The minimum eccentricity is the radius and it is denoted by $r(G)$. The maximum eccentricity is the diameter and it is denoted by $diam(G)$. pKa-value is defined as a negative base-10 logarithm of the acid dissociation constant Ka of a solution is $pKa = log10\, Ka$.

Divya and Yamuna determined the pKa value of local anaesthesia with similar structures and properties, such as boiling point, melting point, and vapour pressure, which are compressed by compressing the drug graph and reducing the calculation in [5]. Some more researchers investigated and determined the problem using various types of topological indices in [8], [10], and [12].

This paper analyses the molecular graph and graph eccentricity for the hydrocarbons. Using a power formula, our observations reveal a strong correlation between the boiling point and the eccentricity of the chemical structure. This formula can be applied to estimate the boiling point of a chemical based on its molecular structure. We also calculate the correlation coefficients between boiling point and Wiener index and between boiling point and eccentricity.

2. Results

In chemical graph theory, the Wiener index (also Wiener number) is a topological index of a molecule, defined as the sum of the lengths of the shortest paths between all pairs of vertices in the chemical graph representing the non-hydrogen atoms in the molecule. Let G be a graph with n vertices. For each pair i, j of vertices, let d_{ij} denote the distance between i and j. The Wiener Index of G is the number $W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_G(i,j)$. An example of calculating the Wiener index for 2,3-dimethyl hexane is shown in Figure 2.

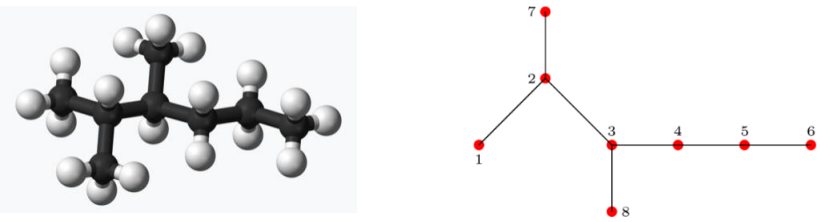

Figure 2: 2,3-dimethyl hexane Structure and Graphical Representation

We observe that while calculating the Wiener index for a graph G with n vertices, we need to determine the distance between every pair of vertices. $W(G) = \frac{1}{2}(20 + 14 + 12 + 14 + 18 + 24 + 20 + 18) = 70$. Moreover, we have to create $n * n$ matrix and determine the row sums. If a boiling point can be determined by using any other graph property that involves less calculation, then it becomes simple to

determine the physical properties, which is attempted in this article. We recollect that the structural arrangement of atoms and variations in physical properties are related. To satisfy this, Wiener defined a topological index based on distance between vertices. Using this property, we try to simplify the calculation process involved in determining the topological index. Moreover, while defining this index care has been taken to include all the vertices of G.

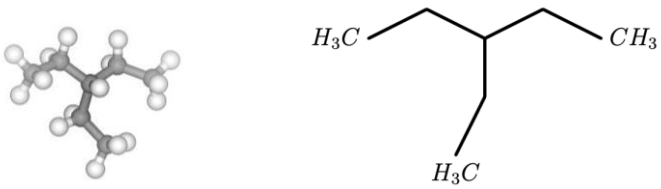

Figure 3. 3-ethyl pentane Structure and Graphical Representation

Graph eccentricity is a graph property that involves distance and can be defined on every vertex of G. Graph eccentricity given for any molecular structure. Determine the molecular graph. Find the eccentricity of all the vertices of the molecular graph. We define the sum of the eccentricity of all the vertices has the eccentricity of the graph. The example for calculation of eccentricity of 3- Ethyl pentane as shown in Figure 4.

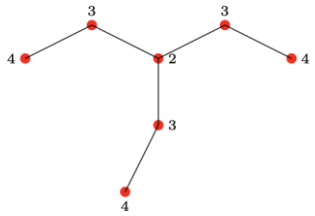

Figure 4. The Eccentricity value is 23 for 3-ethyl pentane

2.1 Determination of Power Formula

An equation of the form $B = \alpha W^{\beta}$ relating the boiling point B and the Wiener index WThis is an approximated power formula determined by Colin Adams and Robert Franzosa in [3], shown in Equation (2). We try to develop a similar kind of formula using the eccentricity of any given molecular graph.

$$B = 181 \times W^{0.1775} \quad (2)$$

Figure 5 displays a graph showing the correlation between the original boiling point and eccentricity.

We observe that a strong correlation between boiling point and eccentricity of the chemical structure can be approximated by an increasing curve. Fitting a power equation $B = \alpha E^{\beta}$ and find that the relation between the boiling point B and eccentricity E for the data in Table 1 is approximated by

$$B = 82 \times E^{0.15} \quad (3)$$

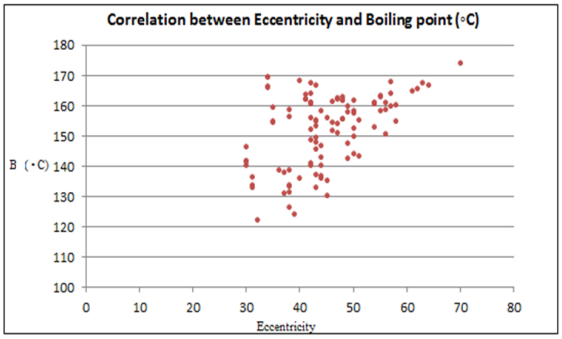

Figure 5. A scatter diagram of the original boiling point and eccentricity index

Table 1: The Boiling Points for Nonanes and Decanes using Power Formula

SI.No	Name	Wiener Index	Eccentricity	Original Boiling point ($°C$)	Calculated Boiling Point ($°C$) from power formula $B_p = 181W^{0.1775}$	Calculated Boiling Point ($°C$) from power formula $B_E = 82E^{0.15}$
1	n-Nonane	120	56	150.8	150.25	149.9
2	2-methyoctane	114	51	143.3	146.85	147.2
3	3-methyoctane	120	50	144.2	150.25	147.4
4	4-methyoctane	108	49	142.5	142.85	147
5	3-Ethylheptane	104	44	143	139.85	144.6
6	4-Ethylheptane	102	42	141.2	138.15	143.6
7	2,2-Dimethylheptane	104	45	130.5	139.85	145.1
8	2,3-Dimethylheptane	102	44	140.5	138.15	144.6
9	2,4-Dimethylheptane	102	43	133	138.15	144.1
10	2,5-Dimethylheptane	104	44	136	139.85	144.6
11	2,6-Dimethylheptane	108	45	135.2	142.85	145.1
12	3,3-Dimethylheptane	98	43	137.3	135.25	144.1
13	3,4-Dimethylheptane	98	42	140.5	135.25	143.6
14	2-Methyl-3-ethylhexane	96	38	139	133.85	141
15	2,2,3-Trimethylhexane	92	38	133.4	130.85	141

16	2,2,4-Trimethylhexane	94	38	126.5	131.85	141
17	2,2,5-Trimethylhexane	98	39	124.1	135.35	142
18	2,3,3-Trimethylhexane	90	37	138	129.15	140
19	2,3,5-Trimethylhexane	96	38	131.4	133.85	141
20	2,4,4-Trimethylhexane	92	37	131	130.85	140
21	3,3,4-Trimethylhexane	88	36	139	127.85	140.3
22	3,3-Diethylpentane	88	30	146.5	127.85	137
23	2,2-Dimethyl-3-ethylpentane	88	31	133.8	127.85	137.2
24	2,3-Dimethyl-3-ethylpentane	86	30	142	125.85	136.5
25	2,4-Dimethyl-3-ethylpentane	90	31	136.7	129.15	137.2
26	2,2,3,3-Tetramethylpentane	82	30	140.2	122.85	136.5
27	2,2,3,4-Tetramethylpentane	86	31	133	125.85	137.2
28	2,2,4,4-Tetramethylpentane	88	32	122.3	127.85	137
29	2,3,3,4-Tetramethylpentane	84	30	141.5	123.85	136.5
30	n-Decane	165	70	174	174.85	155
31	2-Methylnonane	158	64	166.8	170.85	153
32	3-Methylnonane	153	63	167.8	168.85	152.7
33	4-Methylnonane	150	62	165.7	167.35	152.3
34	5-Methylnonane	149	61	165.1	166.85	152
35	2,4-Dimethyloctane	142	54	153.2	163	149
36	2,5-Dimethyloctane	143	56	159	163.6	150
37	2,6-Dimethyloctane	146	57	160	165.2	150.4
38	2,7-Dimethyloctane	151	58	160.2	167.8	151
39	3,3-Dimethyloctane	138	56	161.2	160.85	150
40	3,6-Dimethyloctane	141	54	160.8	162.85	149.2
41	4,5-Dimethyloctane	135	54	161	158.85	149.2
42	4,n-Propylheptane	138	48	161.7	160.85	147
43	4-Isopropylheptane	131	44	158.6	156.85	145

44	2-Methyl-5-ethylheptane	138	50	158.4	160.85	147.5
45	2,2,4-Trimethylheptane	131	44	147	156.25	145
46	2,2,6-Trimethylheptane	145	42	148.9	164.85	144
47	2,3,3-Trimethylheptane	127	49	160	154.85	147
48	2,3,6-Trimethylheptane	136	51	155.3	159.85	148
49	2,4,4-Trimethylheptane	127	47	151	154.85	146.1
50	2,4,6-Trimethylheptane	135	49	147.6	158.85	147
51	2,3,5-Trimethylheptane	131	50	152.8	156.85	147.5
52	3,4-Diethylhexane	125	42	160.7	153.35	144
53	2,2-Diehtyl-4-ethylhexane	126	43	148	153.85	144.2
54	2,2,3,4-Tetramethyhexane	118	38	156.5	148.85	142
55	2,2,4,5-Tetramethylhexane	124	43	145.8	152.85	144.2
56	2,2,5,5-Ttramethylhexane	127	44	136.8	154.85	145
57	3,5-Dimethylheptane	100	40	136	136.85	142.6
58	2-methyl-4-ethylhexane	98	38	134	135.25	141
59	3-Ethyloctane	145	57	168	160.85	150.4
60	4-Ethyloctane	141	55	163.6	162.85	150
61	2,2-Dimethyloctane	146	58	155	165.25	150.8
62	2,3-Dimethyloctane	143	57	164	163.85	150.4
63	3,4-Dimethyloctane	137	55	163	159.85	150
64	3,5-Dimethyloctane	138	55	158.6	160.85	150
65	4,4-Dimethyloctane	134	54	161	158.85	149.2
66	2-Methyl-3-ethylheptane	134	50	161.9	158.85	147.5
67	2-Methyl-4-ethylheptane	134	45	156	158.85	145.1

68	3-Methyl-4-ethylheptane	129	47	154.17	155.85	146.1
69	3-Methyl-5-ethylheptane	88	43	155	127.85	144.2
70	4-Methyl-3-ethylheptane	130	48	163.1	155.85	146.6
71	4-Methyl-4-ethylheptane	126	46	151.8	153.85	145.6
72	2,2,3-Trimethylheptane	130	50	157.6	155.85	147.5
73	2,2,5-Trimethylheptane	134	50	150	158.85	147.5
74	2,3,4-Trimethylheptane	128	48	161.7	154.85	146.6
75	2,3,5-Trimethylheptane	131	49	157.9	156.85	147
76	2,4,5-Trimethylheptane	130	48	155.7	155.25	146.6
77	3,3,4-Trimethylheptane	123	47	162.8	151.85	146.1
78	3,3,5-Trimethylheptane	126	48	155.8	153.85	146.6
79	3,4,4-Trimethylheptane	122	46	161.4	151.85	145.6
80	3,4,5-Trimethylheptane	125	47	162.2	153.35	146.1
81	3-Methyl-3-isopropylhexane	124	43	166.7	152.85	144.2
82	3,3-Diethylhexane	121	42	167.6	150.85	144
83	2,2-Dimethyl-3-ethylhexane	122	43	155.2	151.85	144.2
84	2,3-Dimethyl-3-ethylhexane	119	42	164.1	149.85	144
85	2,3-Dimethyl-4-161.1ethylhexane	123	42	161.2	152.03	144
86	2,4-Dimethyl-4-ethylhexane	122	42	161.1	151.85	144
87	2,4-Dimethyl-3-ethylhexane	122	38	159	151.85	142
88	2,5-Dimethyl-3-ethylhexane	127	43	153.5	154.85	144.2

89	3,3-Dimethyl-4-ethylhexane	118	41	162.1	148.85	143.1
90	3,4-Dimethyl-3-ethylhexane	117	41	162.1	148.35	143.1
91	2,2,3,3-Tetramethylhexane	115	42	161.3	147.05	144
92	2,2,3,5-Tetramethylhexane	123	43	149.4	152.05	144.2
93	2,2,4,4-Tetramethylhexane	119	42	152.4	149.85	144
94	2,3,3,4-Tetramethylhexane	115	41	163.9	147.05	143.1
95	2,3,3,5-Tetramethylhexane	120	46	154.5	150.25	146
96	2,3,4,4-Tetramethylhexane	116	41	162.2	147.65	143.1
97	2,3,4,5-Tetramethylhexane	121	42	156.2	150.85	144
98	3,3,4,4-Tetramethylhexane	111	40	168.4	144.85	143
99	2,4-Dimethyl-3-isopropylpentane	117	35	154.9	148.25	140
100	2-Methyl-3,3-diethylpentane	114	34	169.5	146.35	139.2
101	2,2,3-Trimethyl-3-ethylpentane	110	34	166.6	143.65	139.2
102	2,2,4-Trimethyl-3-ethylpentane	115	35	154.5	147.05	140
103	2,3,4-Trimethyl-3-ethylpentane	112	34	169.4	145.05	139.2
104	2,2,3,3,4-Pentamethylpentane	108	34	166.1	142.35	139.2
105	2,2,3,4,4-Pentamethylpentane	111	35	159.6	144.85	139.8

3. Results and Discussion

The molecular graph's eccentricity for 105 nonanes and decanes. Using a power formula, we discovered a substantial relationship between the boiling point and the eccentricity of the chemical structure in Table 1. The molecular graph comparison Figure 6 between the original boiling point Vs boiling point calculated from determined power formula in Equation 3.

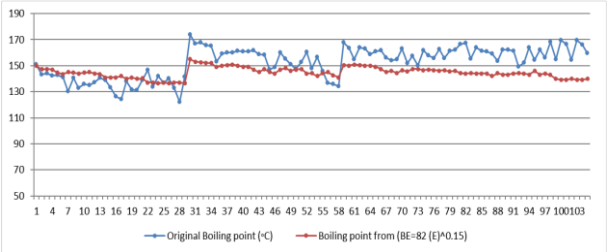

Figure 6. Comparision on Original Boiling Point and Determinate Power Formula

We observe that the power formula developed can be used to determine the approximate boiling point of any chemical whose molecular structure is known. Let B_W, B_P and B_E denote the boiling points of nonanes and decanes using formulas (1), (2), (3) respectively. The following Figure 7 and Figure 8 provides an R program for determining the correlation coefficient between B_W, B_E and B_P, B_E respectively.

```
> Bw=c(150.8,143.5,144.2,141.8,142.5,140,131.4,140,134.5,136.9,136.3,135.2,140.7,138.3,133.4,124.8,12
4.2,136.5,132.8,127.9,139.6,145.1,134.1,142.7,136.5,137.8,131.7,112.1,140.2,174,167.1,167.1,164.8,16
3.8,157,157,160.9,160.3,158.5,161.5,161.1,158.5,157.2,158.5,146.2,148.5,158.8,156.6,147.8,150.1,151.
7,162.3,146.8,155.4,144.8,136.8,137.6,135.2,165.4,161.4,155.4,163.4,163.1,158.5,154.6,160.1,154.6,16
0.7,159.1,161.7,157.8,156.2,149.1,159.7,157.2,156.2,160.3,152.3,159.4,162.3,155.8,163.9,153.9,161.9,1
60.3,159.4,153.9,153.3,160.9,165.5,158,149.3,139.9,163.5,151.9,159,158.4,165.1,154.5,168,164.1,152.5
,166.1,162.1,148.6)
> Be=c(149.9,147.2,147.4,147,144.6,143.6,145.1,144.6,144.1,144.6,145.1,144.1,143.6,141,141,141,142,14
0,141,140,140.3,137,137.2,136.5,137.2,136.5,137.2,137,136.5,155,153,152.7,152.3,152,149,150,150.4,1
51,150,149.2,149.2,147,145,147.5,145,144,147,148,146.1,147,147.5,144,144.2,142,144.2,145,142.6,141
,150.4,150,150.8,150.4,150,150,149.2,147.5,145.1,146.1,144.2,146.6,145.6,147.5,147.5,146.6,147,146.6
,146.1,146.6,145.6,146.1,144.2,144,144.2,144,144,144,142,144.2,143.1,143.1,144,144.2,144,143.1,146,
143.1,144,143,140,139.2,139.2,140,139.2,139.2,139.8)
> fit=lm(Bw~Be)
> fit

Call:
lm(formula = Bw ~ Be)

Coefficients:
(Intercept)           Be
    -74.565        1.561
```

```
> Bp=c(150.25,146.85,150.25,142.85,139.85,138.15,139.85,138.15,138.15,139.85,142.85,135.25,135.25,1
33.85,130.85,131.85,135.35,129.15,133.85,130.85,127.85,127.85,127.85,125.85,129.15,122.85,125.85,1
27.85,123.85,174.85,170.85,168.85,167.35,166.85,163,163.6,165.2,167.8,160.85,162.85,158.85,160.85,
156.85,160.85,156.25,164.85,154.85,159.85,154.85,158.85,156.85,153.35,153.85,148.85,152.85,154.85,
136.85,135.25,160.85,162.85,165.25,163.85,159.85,160.85,158.85,158.85,158.85,155.85,127.85,155.85,
153.85,155.85,158.85,154.85,156.85,155.25,151.85,153.85,151.85,153.35,152.85,150.85,151.85,149.85,
152.03,151.85,151.85,154.85,148.85,148.35,147.05,152.05,149.85,147.05,150.25,147.65,150.85,144.85,
148.25,146.35,143.65,147.05,145.05,142.35,144.85)
> Be=c(149.9,147.2,147.4,147,144.6,143.6,145.1,144.6,144.1,144.6,145.1,144.1,143.6,141,141,141,142,14
0,141,140,140.3,137,137.2,136.5,137.2,136.5,137.2,137,136.5,155,153,152.7,152.3,152,149,150,150.4,1
51,150,149.2,149.2,147,145,147.5,145,144,147,148,146.1,147,147.5,144,144.2,142,144.2,145,142.6,141
,150.4,150,150.8,150.4,150,150,149.2,147.5,145.1,146.1,144.2,146.6,145.6,147.5,147.5,146.6,147,146.6
,146.1,146.6,145.6,146.1,144.2,144,144.2,144,144,144,142,144.2,143.1,143.1,144,144.2,144,143.1,146,
143.1,144,143,140,139.2,139.2,140,139.2,139.2,139.8)
> fit=lm(Bp~Be)
> fit
Call:
lm(formula = Bp ~ Be)

Coefficients:
(Intercept)           Be
   -216.807        2.528
```

Figure 7. The Correlation Coefficient Between B_W, B_E and B_P, B_E

Figures 9 and 10 show a good correlation between the formulas. From this, we understand that the graph eccentricity can be used instead of the Wiener index for determining the boiling point of nonanes and decanes.

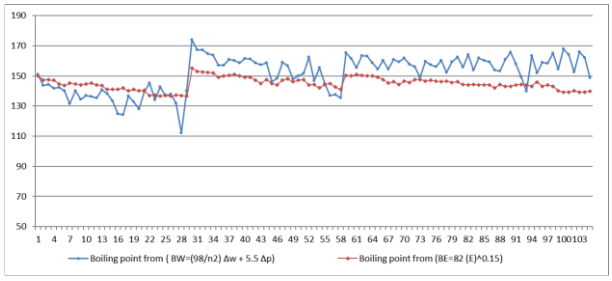

Figure 9. The Correlation Coefficient Between B_W, B_E

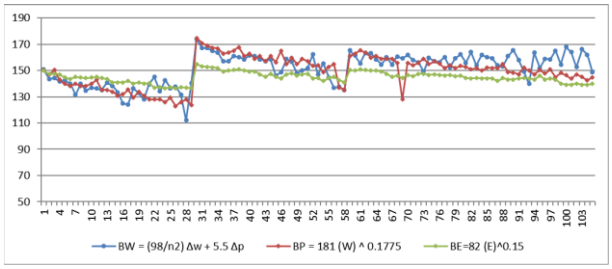

Figure 10. The Correlation Coefficient Between B_W, B_P, B_E

4. Conclusion

This research examines the molecular graph's eccentricity for 105 nonanes and decanes. Using a power formula, we discovered a substantial relationship between the boiling point and the eccentricity of the chemical structure. This formula may be used to predict the boiling point of a chemical based on its molecular structure, where $(n^2 - n)$ calculations are reduced. We also calculate the correlation coefficients between the boiling point and the Wiener index and the boiling point and eccentricity.

5. Acknowledgement

The authors would like to express their sincere gratitude to the management and faculty members of the *School of Arts and Science, Vinayaka Mission's Chennai Campus, Vinayaka Mission's Research Foundation (Deemed to be University), Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya (Deemed to be University), St. Joseph's Institute of Technology*, and *Vel Tech Rangarajan Dr. Sagunthala R&D Institute of Science and Technology* for their encouragement and support throughout this research.

We especially thank our colleagues for their valuable suggestions, and we extend our heartfelt thanks to the reviewers for their constructive feedback, which helped refine this paper.

Conflict of interest statement: The authors declared no conflict of interest in the manuscript.

References

[1] Burch KJ, Wakefield DK, Whitehead EG. Boiling point models of alkanes. MATCDY. 2003; 47: 25-52.
[2] Chartrand G, Lesniak L. Graphs and Digraphs, Chapman and Hall, CRC, fourth ed., 2005.
[3] Colin Adams, Robert Franzosa. Introduction to Topology, Pearson Education. 2008.
[4] Dankelmann P, Mukwembi S. The distance concept and distance in graphs. In Distance in Molecular Graphs Theory (eds. Gutman, I. and Furtula, B). 2012; 3-48.
[5] Divya T, Yamuna M. Drug. pKa value prediction from compressed graph. Innovare Journal of Engineering and Technology. 2019; 7(5): 1-6. https://journals.innovareacademics.in/index.php/ijet/article/view/29034
[6] Gutman, I. Selected properties of the schultz molecular topological index. Journal of Chemistry Information Computer Science. 1994; 1087-1089.
[7] Nikolić S, Trinajstić N, Mihalić Z. The wiener index: development and applications, Croat.Chem. Acta. 1995; 68(1): 105-129.
[8] Rücker G, Rücker C. On topological indices, boiling points and cycloalkanes, Journal of chemical information and computer sciences. 1999; 39(5): 788-802.
[9] Shi X, Kosari S, Ahmad U, Hameed S, Akhter S. Evaluation of various topological indices of flabellum graphs. Mathematics. 2023. 11(19): 41-67. https://doi.org/10.3390/math11194167
[10] Wardecki, Dawid, Ma lgorzata Do lowy, Katarzyna Bober-Majnusz. Evaluation of the usefulness of topological indices for predicting selected physicochemical properties of bioactive substances with anti-androgenic and hypouricemic activity. Molecules. 2023; 28(15).
[11] Wiener H. Structural determination of paraffin boiling points. J.Am.Chem.Soc. 1947; 69: 17-20.
[12] Yuede Ma, Matthias Dehmer, Urs-Martin K¨unzi, Shailesh Tripathi, Modjtaba Ghorbani, Jin Tao, Frank Emmert-Streib. The usefulness of topological indices. Information Sciences. 2022; 606: 143-151.