Restricted Detour Index of Some Graph Operations with Chemical Application: A Review

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Abstract:

The concept of the Wiener distance is considered one of the fundamental pillars in chemical graph theory, having served over the past decades as the foundation from which numerous distance-based measures-and consequently, various topological indices-have emerged. These indices are widely used in analyzing and predicting the physical properties of a wide range of chemical compounds.

Among these concepts is the restricted detour distance, defined as the length of the longest induced path between two vertices u and v in a connected graph G, such that the set of vertices P forming this path induced a subgraph of G i.e., $\langle V(P)\rangle = P$. The corresponding restricted detour index is defined as the sum of the restricted detour distance over all unordered pairs of distinct in the graph G.

This paper presents a historical review of the concept of restricted detour distance, its associated index, and the corresponding polynomial. We also highlight the most significant research papers that have addressed the computation of this index for certain types of graph operations, particularly those that result in straight chain graphs. In addition, we explore a practical application involving the use of the restricted detour index to identify a correlation with the boiling point of a group of hexagonal carbon compounds.

***Key words*:** chain graphs, chemical graphs, graph operations, restricted detour index.

الخلاصة:

يُعتبر مفهوم مسافة وينر أحد الركائز الأساسية في نظرية البيان الكيميائية، حيث شكل على مدى العقود الماضية الأساس الذي انبثقت منه العديد من المقاييس القائمة على المسافة، وبالتالي، ادلة طوبولوجية مختلفة. تُستخدم هذه الادلة على نطاق واسع في تحليل وتوقع الخصائص الفيزيائية لمجموعة واسعة من المركبات الكيميائية.

ومن بين هذه المفاهيم، مسافة الانحراف المقيدة(restricted detour distance)، التي تُعرَّف بأنها طول أطول درب مُستحث بين رأسين u و vفي البيان متصلG ، بحيث ان مجموعة الرؤوس Pالتي تُشكل هذا الدرب تولد بيان جزئي مستحث من البيانG ، أي V(P))=P.يُعرّف دليل الانحراف المقيد (restricted detour index) بأنه مجموع مســـافة الانحراف المقيدة لجميع ازواج الرؤوس المختلفة في البيان.G

تقدم هذه الورقة مراجعة تاريخية لمفهوم مسافة الانحراف المقيدة و دليل الانحراف المقيد ومتعددة حدود الانحراف المقيدة. كما نُسلِّط الضوء على أهم الاوراق البحثية التي تناولت حساب هذا الدليل لأنواع مُعيَّنة من العمليات على البيانات، وخاصةً تلك التي تُنتج بيان سلسلة مستقيمة. بالإضافة إلى ذلك، نستعرض تطبيقًا عمليًا يتضمن استخدام دليل الانحراف المُقيَّد للكشف عن علاقة الارتباط بينه وبين درجة غليان مجموعة من مركبات الكاربون السداسية

1. Introduction:

The concept of distance in graph theory has gained significant importance following its application in mathematical chemistry, particularly after Wiener discovered a correlation between the boiling points of alkane compounds and the topological structure of their molecular graphs [21]. In this representation, each vertex in the graph corresponds to an atom in the molecular compound, while the edges represent the chemical bonds connecting these atoms. The distance between any two vertices u and v in a vertex set $V(G)$ of a graph G is defined as the minimum number of edges in any path connecting u and v. The Wiener index, denoted by $W(G)$, is defined as the sum of the distances $d(u,v)$ between all pairs of distinct vertices in G , i.e.

$$W(G) = \sum_{\{u,v\}\in V(G)} d(u,v) \ .$$

In 1988, Hosoya introduced the Hosoya polynomial, denoted as $H(G;x)$ and defined it as follows [16]:

$$H(G;x) = \sum_{\{u,v\}\in V(G)} x^{d(u,v)}.$$

The Wiener index can be obtained by differentiating the Hosoya polynomial with respect to x and then substituting $x = 1$ in to the result, i.e.

$$W(G) = \frac{d}{dx} H(G; x)|_{x=1} .$$

Subsequently, several new types of distances were introduced in graph theory, each giving rise to a corresponding index. Some of these indices are either derived directly from the distance definitions or formulated through associated distance-based polynomials. Notably, many of these indices have demonstrated significant applicability not only in modeling the chemical and physical properties of various compounds[17], but also in analyzing the structural architecture and connectivity patterns of networks [12]. Among the most prominent of these distances are the Steiner distance [11], the communicability distance [13], the resistance distance [9], restricted detour distance [10] , and detour distance [14].

In this paper, we present a historical overview of one of these distance types, known as the restricted detour distance on graphs, through a series of special graph operations. This concept has notable applications in chemistry.

In 1993, Chartrand, Johns, and Tain were the first to define the detour distance in graphs under the condition that $\langle V(P)\rangle = P$, where $\langle V(P)\rangle$ denotes the subgraph induced by the vertices of a longest path P [10]. The detour distance between two vertices u and v, subject to this restriction, is now called the restricted detour distance.

A restricted detour path (induced detour path) between two vertices u and v is defined as an induced $u - v$ path of maximum length, denoted by $D^*(u, v)$. A connected graph G is said to be a restricted detour graph if $D^*(u, v) = d(u, v)$ for every pair of distinct vertices in G, such as trees, complete and bipartite graphs.

In contrast, every cycle of order $p \geq 5$ fails to meet this condition and is not a restricted detour graph [10].

The ***restricted detour distance*** is differs from the detour distance which define as the length of a longest $u - v$ path between two vertices $u,v \in V(G)$, and denoted $D(u, v)$, [4]. Accordingly, the detour index of a graph G, denoted by $D(G)$, is defined as the sum of all detour distances between every pair of distinct vertices in G, [14]. that is:

$$D(G) = \sum_{\{u,v\}\subseteq V(G)} D(u, v).$$

The ***restricted detour index*** of a graph G, denoted by $dd^*(G)$, is defined by the following, [4]:

$$dd^*(G) = \sum_{\{u,v\}\subseteq V(G)} D^*(u,v).$$

It is worth noting that Trinajstić, et al. employed an exponential relation involving the Wiener index and the detour index to achieve a better prediction of the boiling point for a number of chemical compounds. This relation is expressed as:

$$b.p. = A + B\big(D(G)W(G)\big)^C \qquad \ldots(1)$$

where $b.p.$ denotes the boiling point and $A = -169.62 \pm 5.91, B = 93.00 \pm 4.86, C = 0.13066 \pm 0.00391$. further details of this study can be found in [22].

This relation will be utilized in a alter section of this paper to examine the potential of the restricted detour index in predicting boiling points.

In 2012, Mohammed-Saleh introduced a ***restricted detour polynomial*** denoted by $D^*(G;x)$ and defined as:

$$D^*(G;x) = \sum_{\{u,v\}\subseteq V(G)} x^{D^*(u,v)}.$$

We can also obtain the index for this type of distance by differentiating the polynomial above and substituting the value of x by one.

Numerous research papers have studied the restricted detour distance, its corresponding index, and polynomial [1-4,7,15,18,19]. However, in this review paper, we focus on operations that generate chain graphs.

Several methods exist for constructing a chain graph, including edge identification between two or more graph, the edge-introducing, or identification of a vertex in one graph with a vertex in another. These operations resemble the bonding patterns found in chemical compounds, such as the connections between carbon rings-whether hexagonal, pentagonal, or otherwise-ultimately leading to the formation of interconnected cyclic compounds that are both stable and structurally complex. As these compounds become increasingly intricate, studying their physical properties becomes more challenging. Accordingly, this study seeks to investigate whether the restricted detour index exhibits a strong correlation with boiling point, which could allow it to serve as an effective tool for analyzing the physical properties of cyclic compounds, also includes a discussion of the theorems presented in the selected research papers.

2. Edges Identification Operation:

In this section, we present a review of restricted detour index for straight chain graphs resulting from the identification of an edge or edges between two or more graphs, such as hexagonal ring chains, quadrilateral chains, and straight wheel chains.

2.1 Hexagonal chain graph (J_m) [4]:

Ali and Mohammed-Saleh [4] proposed a general formula for computing the restricted detour polynomial of a hexagonal chain graph J_m consisting of m hexagons $(h_1, h_2, \dots, h_m)$, where $m \geq 1$. The following illustrates the general structure of this graph.

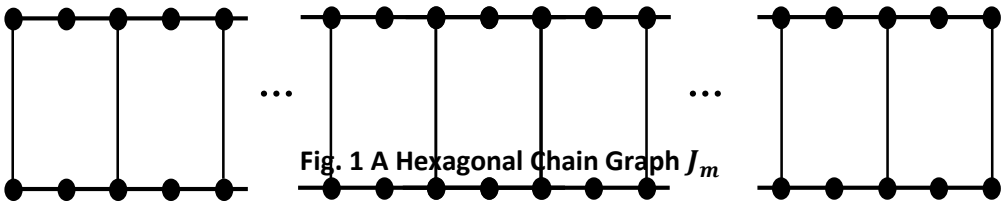

Fig. 1 A Hexagonal Chain Graph J_m

Theorem 2.1.1 [4]: For $m \geq 4$,

$D^*(J_m; x) = 4m + 2 + (5m-1)x + 3mx^3 + 6mx^4 + (2m-2)x^5 + (6m-6)x^6 + (8m-10)x^7 + (2m-2)x^8 + (6m-12)x^9 + (8m-16)x^{10} + 8(x+1)\sum_{k=4}^{m}(m+1-k)x^{3k}$.

Corollary 2.1.2 [4]: For $m \geq 4$, the restricted detour index of J_m is given by:

$$dd^*(J_m) = 8m^3 + 28m^2 - 2m + 9.$$

We will use the relation (1) mentioned in the introduction, which is taken from [22], along with Theorem 2.1.2, on a group of polyacene compounds whose molecular structures topologically resemble the hexagonal chain graph (J_m). We will also require the boiling point values of the polyacene compounds, which will be taken from reference [17].

Table 1 some properties of $C_{4n+2}H_{2n+4}, n = 1, 2, \dots, 9$, [17]

	Compound name	Molecular Weight	Melting Point (°C):	Boiling Point (°C):	Density (g/cm3 at 25°C)	Molar Volume (cm3/mol): (25°C)	Compound shape
1	Benzene. C6H6	78.112	5.49	78.8±7.0	0.9 ± 0.1	89.4±3.0	
2	Naphthalene C10H8	128.171	77-82	221.5±7.0	1.0 ± 0.1	123.5±3.0	
3	Anthracene C14H10	178.229	78.09	337.4±9.0	1.1 ± 0.1	157.7±3.0	
4	Tetracene C18H12	228.288	135.96	436.7±12.0	1.2 ± 0.1	191.8±3.0	
5	Pentacene C22H14	278.346	180.52	524.7±17.0	1.2 ± 0.1	225.9±3.0	
6	Hexacene C26H16	328.405	231.70	604.1±22.0	1.3 ± 0.1	260.0±3.0	
7	Heptacene C30H18	378.474	264.86	677.0±22.0	1.3 ± 0.1	294.1±3.0	
8	Octacene C34H20	428.499	297.98	744.7±27.0	1.3 ± 0.1	328.2±3.0	
9	Nonacene C38H22	478.594	331.10	753.68	1.3 ± 0.1	362.4±3.0	

By using the relation (1), but applying the product of the Wiener index and the restricted detour index for this compounds, and comparing it with the boiling points listed in the table above, we obtain the following results:

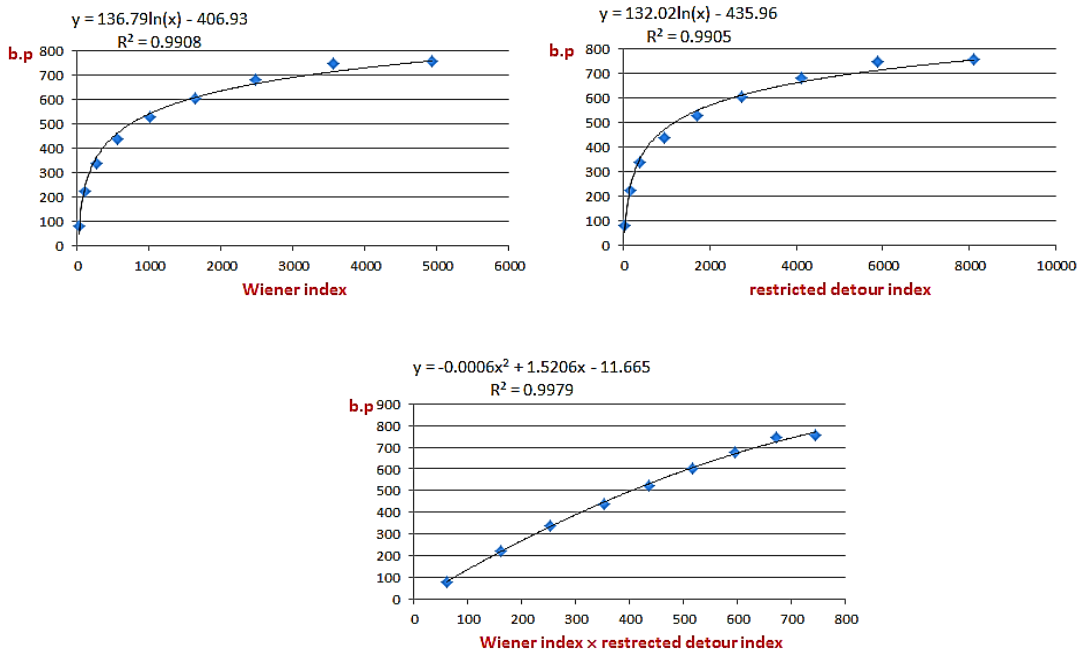

Fig. 2 Wiener index and restricted detour indices with boiling point ($b.p$) of $C_{4n+2}H_{2n+4}, n = 1, 2, \dots, 9$

It is observed that the correlation coefficient reaches 0.9979, indicating a very strong relationship. This result provides clear evidence of the effectiveness of using the product of the restricted detour index and the Wiener index in predicting the boiling points of this class of cyclic carbon compounds.

2.2 The Ladder (L_n) [4] (Square chain):

A ladder graph L_n is the result of the Cartesian product of the complete graph K_2 and a path graph $P_n, n \geq 2$ that is $L_n = K_2 \times P_n$, as showing in Fig. 3.

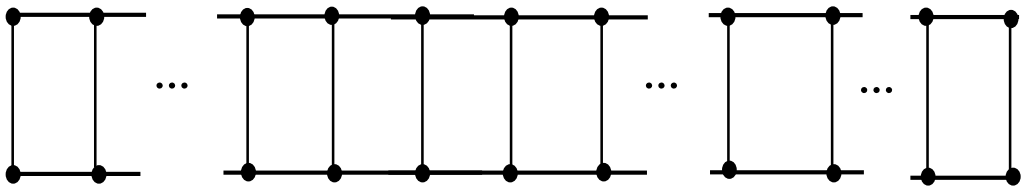

Fig. 3 A Ladder Graph L_n

Theorem 2.2.1 [4]: For $n \geq 3$,

$$D^*(L_n; x) = 2n + (3n-2)x + 2(n-1)x^2$$

$$+2\sum_{k=2}^{n-1}(n-k)x^k\left(x^{2\left\lceil\frac{k-1}{4}\right\rceil} + x^{1+2\left\lfloor\frac{k}{4}\right\rfloor}\right).$$

Corollary 2.2.2 [4]: For $n \geq 2$, we have:

$$dd^*(L_n) = \begin{cases} \frac{1}{2}n(2n^2+n-2), & \text{for even } n \\ \frac{1}{2}(2n^3+n^2-6n+5) + 4\left(\left\lceil\frac{n-2}{4}\right\rceil + \left\lfloor\frac{n-1}{4}\right\rfloor\right), & \text{for odd } n \end{cases}$$

The previous theorem for the restricted detour index of ladder chain graphs may be applied to organic compounds with linearly fused four-membered rings, such as n-ladderanes, where n represents the number of rings. These structures resemble quadrilateral chains, making the restricted detour index a potentially valuable topological descriptor for their physicochemical analysis.

The references [1,3] present theoretical results concerning the restricted detour index and its polynomial for straight chains of wheel graphs as well as k −wheel chains, without addressing any chemical or structural applications. This highlights a promising opportunity for future research to

investigate whether such graph structures have analogs in molecular systems or within network theory, potentially extending the practical relevance of these theoretical findings.

3. Vertex Identified Operation:

Let G_1 and G_2 be two disjoint graphs, and let $u \in V(G_1)$ and $v \in V(G_2)$ be designated vertices in G_1 and G_2, respectively. The vertex identifying graph, denoted by $G_1 \bullet G_2$, is the graph obtained by identifying the vertices u and v into a single vertex, thereby combining the two graphs at that vertex. The edge interdicting graph, denoted by $G_1 : G_2$, is the graph fromed by adding a new edge between the vertices u and v, thereby introducing a connection between G_1 and G_2 without identifying any vertices.

In his work [18], Mohammed-Saleh generalized the vertex identifying operation to include a family of m finite and connected graphs. He then found the restricted detour polynomial corresponding to the resulting graph from generalized operation.

Consider a family of pairwise disjoint, connected graphs $G_1, G_2, \dots, G_m$, where each graph G_i has an order $p_i \geq 2$ for $i = 1,2,3, \dots m$. Let u_i, v_i be two distinct vertices in each G_i. The straight chain of identifying graphs, denoted by $\mathcal{G}_m$, is constructed by identifying vertex u_{i+1} in G_{i+1} with v_i in G_i for all $i = 1,2,3, \dots, m-1$, that is[18]

$$\mathcal{G}_m = \mathcal{G}_{m-1} \bullet G_m = (\mathcal{G}_{m-2} \bullet G_{m-1}) \bullet G_m = G_1 \bullet G_2 \bullet \dots \bullet G_{m-1} \bullet G_m$$

Fig. 4 shown $\mathcal{G}_m$ graph, where $v_i = u_{i+1}$.

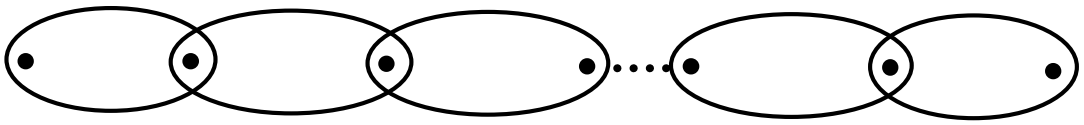

Fig. 4 The Straight Chain Of Identifying Graphs $\mathcal{G}_m$

Theorem 3.2 [18]: For $m \geq 2$,

$$D^*(\mathcal{G}_m; x) = D^*(\mathcal{G}_{m-1}; x) + D^*(G_m; x) + D^*(u_m, G_m; x) D^*(v_{m-1}, \mathcal{G}_m; x) - D^*(u_m, G_m; x) - D^*(v_{m-1}, \mathcal{G}_{m-1}; x)$$

Where

$$D^*(v_{m-1}, \mathcal{G}_{m-1}; x) = \sum_{i=1}^{m} \left\{ x^{\sum_{j=i+1}^{m-1} \gamma(i)} (D^*(v_i, G_i; x) - 1) \right\} + 1$$

In which $\gamma(i) = D^*_{G_j}(u_j, v_j)$

The next theorem represents a special case of the previous one, through which a polynomial expression is derived to compute the restricted detour distance of the graph G when repeated m times, reflecting a mathematical simplification of the problem in the case of repeated graph.

Theorem 3.3 [18]: For $m \geq 2$,

$$D^*(\mathcal{G}_m; x) = D^*(\mathcal{G}_{m-1}(G); x) + D^*(G; x) - D^*(u, G; x)$$

$$+[D^*(u, G; x) - 1]\left\{[D^*(v, G; x) - 1] \sum_{i=1}^{m-1} x^{(m-i-1)D_G(u,v)} + 1\right\}$$

As demonstrated in the preceding theorem, Mohammed-Saleh [18] formulated a general rule for vertex identification applicable to any set of graphs. Theorems 3.5 and 3.6 present the general formulas for pentagonal and hexagonal chains (as shown in Fig. 5), respectively. These theorems constitute the practical application of the theoretical results, enabling the study of the structural properties of various types of carbon ring chains, Particularly the pentagonal and hexagonal ones.

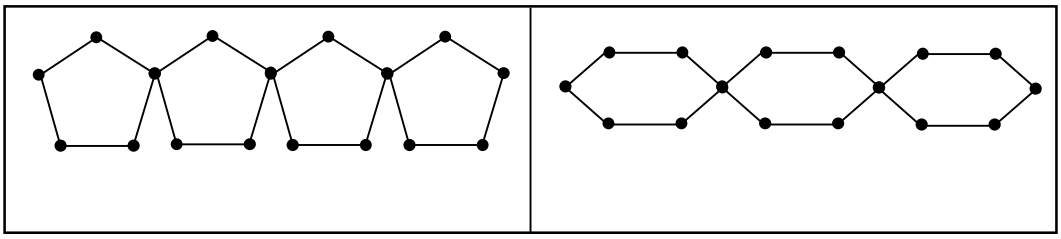

Fig. 5 Pentagonal and Hexagonal Chain Graphs

Theorem 3.5 [18]: for $m \geq 2$

$$D^*(\mathcal{G}_m(C_6); x) = m(5 + 6x + 3x^3 + 6x^4) + 1 + (2x + x^3 + 2x^4)^2 \sum_{j=1}^{m-1} \sum_{i=1}^{m-j} x^{3(m-i-j)}.$$

Theorem 3.6 [18]: for $m \geq 2$

$$D^*(\mathcal{G}_m(C_5); x) = 1 + m(4 + 5x + 5x^3) + (2x + 2x^3)^2 \sum_{j=1}^{m-1} \sum_{i=1}^{m-j} x^{3(m-i-j)}.$$

corollary 3.7 [18]: for $m \geq 2$

(1) $dd^*\left(\mathcal{G}_m(C_6)\right) = \frac{5}{2}m^2(5m+1) - m,$

(2) $dd^*\left(\mathcal{G}_m(C_5)\right) = 8m^3 + 8m^2 + 4m.$

4. Edge-Introducing Operation:

Let $G_1, G_2, \ldots, G_m$ be a family of m (where $m \geq 2$) pairwise disjoint and connected graphs. For each graph G_i, let u_i and v_i be distinct vertices. The straight chain of edge – introducing graphs, denoted as $\mathcal{J}_m$, is formally defined as the graph constructed by introducing $m-1$ new edges, specifically $u_{i+1}v_u$, for each i ranging from 1 to $m-1$, connecting the graphs G_1 through G_m. It's clear that

$$\mathcal{J}_m = \mathcal{J}_{m-1} : G_m = G_1 : G_2 : \ldots : G_m.$$

The graph $\mathcal{J}_m, m \geq 3$ is shown in Fig. 6.

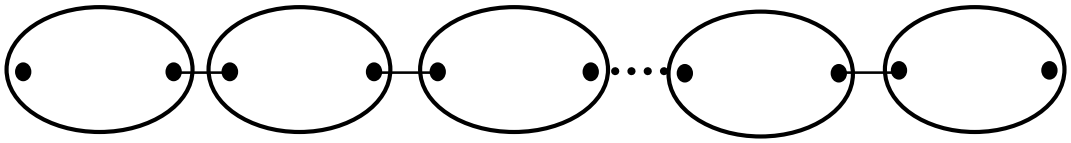

Fig. 6 The Straight Chain Of Edge-Introducing Graphs $\mathcal{J}_m$

Theorem 4.2 [18]: for $m \geq 2$,

$D^*(\mathcal{J}_m; x) = D^*(\mathcal{J}_{m-1}; x) + D^*(G_m; x)$

$$+xD^*(u_m, G_m; x)D^*(v_{m-1}, \mathcal{J}_{m-1}; x),$$

where

$D^*(v_{m-1}, \mathcal{J}_{m-1}; x) = \sum_{i=1}^{m-1}\left\{x^{m-i-1}\, x^{\sum_{j=i+1}^{m-1}\gamma(j)} D^*(v_i, G_i; x)\right\}.$

In which $\gamma(j) = D^*_{G_j}(u_j, v_j)$

Theorem 4.2 provides a polynomial expression for computing the restricted detour distance resulting from the edge-introducing graph operation applied to m copies of the graph G, as a Corollary 4.3 presents an application of this theorem to a set of chemical compounds.

Theorem 4.3 [18]: For $m \geq 2$,

$$D^*(\mathcal{J}_m; x) = mD^*(G; x)$$

$$+x\, D^*(u, G; x)D^*(v, G; x)\left\{\sum_{j=1}^{m-1}\sum_{i=1}^{m-j} x^{(m-i-j)\left(1+D_G^*(u,v)\right)}\right\}\blacksquare$$

It is clear that research papers [4,18] provide direct and relevant applications in the field of mathematical chemistry.

In 2017, Ivan D. Ali and Herish O. Abdullah computed the restricted detour polynomials resulting from the edge identification of two wheel graphs and determined their corresponding restricted detour indices [7].

In recent studies, two new definitions derived from the restricted detour index-namely, the average restricted detour distance and restricted detour median graph-have been introduced in two papers [3, 15]

5. Conclusion:

After reviewing several research papers and applying the edge identification operation to hexagonal ring graphs, obtained a series of graphs that mimic the topological structure of polyacene compounds. By using relation (1), where the exponential term includes the product of the restricted detour index and the Wiener index, obtained a very strong correlation with a value of $R = 0.9979$. This result indicates the efficiency and effectiveness of the restricted detour index as a topological descriptor for predicting the boiling point of polycyclic carbon-based compounds.

6. Suggestions for Future Works:

- Establishing explicit formulas or inequalities that relate the restricted detour index to other well-known graph invariants for special graphs, such as the Wiener index or D-index, similar to the relationships researched in tree graphs [8] and regular complete graphs[6].
- A research on the restricted detour index under several additional graph operations, aiming to generalize its behavior and identify patterns or bounds across diverse structural transformations.
- Further investigating the correlation between the restricted detour index and various physicochemical properties of chemical compounds in order to evaluate its effectiveness as a molecular descriptor.

- Research on the graphs that represent the upper and lower bounds of the restricted detour index.
- A research to assess the applicability and relevance of the restricted detour index in network theory may serve as a valuable direction for future research.

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