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RECIPROCAL STATUS-DISTANCE INDEX OF GRAPHS

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Abstract. *Reciprocal Status-Distance (RSD) Index* , $RSD(G)$ of a connected graph G is defined as,

$$RSD(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)},$$

where, $\sigma_G(u) = \sum_{v \in V(G)} d_G(u,v)$ is the status of a vertex u in $V(G)$.

This research study focuses on a newly developed Reciprocal Status-Distance (RSD) Index of graphs and its bounds. In addition, the RSD Index of some well-known class of graphs is derived. The regression analysis of RSD, DD, and RDD index is carried out with the properties of some Paraffin hydrocarbon molecules. The correlation analysis found that the RSD index is better than the degree distance and reciprocal degree distance index for predicting some properties of hydrocarbon molecules.

1. Introduction

Chemical graph theory is a branch of mathematical chemistry that explores the connection between molecules and graphs. In a graph, points are called vertices, and lines as edges. When we turn molecules into graphs, atoms become vertices, and bonds become edges. This representation is called a molecular graph. Typically, hydrogen atoms are excluded, and the remaining graph is known as the carbon graph of the molecule.

A topological graph index is a numerical measure that shows a correlation between chemical composition and various physical properties, chemical reactivity, or biological activity. Over the last few decades, numerous topological indices have

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been developed and used for chemical documentation, isomer classification, molecular complexity analysis, chirality, similarity/dissimilarity, QSAR/QSPR, drug design, database selection, lead optimization, and more.

Let G be a graph of order n and size m. Let $V(G)$ be the vertex set and $E(G)$ be the edge set of G. The edge between the vertices u and v is denoted by uv. The *degree* $d_G(u)$ of a vertex u is the number of edges incident to it. The *distance* between two vertices u and v, denoted by $d_G(u,v)$, is the length of the shortest $u-v$ path in G. The maximum distance between any pair of vertices in G is called the *diameter* of G and is denoted by $diam(G)$ or simply D. The *status* $\sigma_G(u)$ of a vertex u in graph G is the total sum of distances between u and all the other vertices. We refer to the books [**23, 12**] for graph theoretic terminology.

The Wiener index $W(G)$ of a connected graph G is defined as [**14**],

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v) = \frac{1}{2}\sum_{v\in V(G)} \sigma_G(u).$$

One can find further information about the Wiener index by referring to [**25, 6, 22, 36**].

The Harary index of G is defined as the sum of reciprocals of distances between all unordered pairs of vertices of a connected graph [**9**],

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d_G(u,v)}.$$

To learn more about the Harary index, one can refer [**7, 10, 26, 27, 29**].

The most important graph indices are the first and second Zagreb indices introduced by I. Gutman and Trinajstic, [**20**]. They are denoted as $M_1(G)$ and $M_2(G)$ and were defined as:

$$M_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)],\ M_2(G) = \sum_{uv\in E(G)} [d_G(u)d_G(v)].$$

One can locate chemical applications and explore the mathematical properties of Zagreb indices in [**28, 8, 34, 35**].

The first and second Zagreb coindices of a graph G are defined as [**38**],

$$\overline{M}_1(G) = \sum_{uv\notin E(G)} [d_G(u) + d_G(v)],\ \overline{M}_2(G) = \sum_{uv\notin E(G)} [d_G(u)d_G(v)].$$

Recent findings related to Zagreb coindices in the literature [**3, 4, 16, 17**].

The degree distance index of a graph G was introduced independently by Dobrynin, Kochetova [**1**] and Gutman [**19**],

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} [d_G(u) + d_G(v)]d_G(u,v).$$

For more about degree distance, one can refer [**30, 41, 5, 21**].

Hongbo Hua and Shenggui Zhang introduced a new graph invariant named reciprocal degree distance, which can be seen as a degree-weight version of the Harary index as [**15**],

$$RDD(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d_G(u) + d_G(v)}{d_G(u, v)}.$$

Recent findings concerning reciprocal degree distance can be found in the literature [**39, 13, 40, 37**].

Inspired by the work on reciprocal degree distance index, the reciprocal status-distance index (RSD) is defined as[**31**],

$$RSD(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u, v)} \tag{1.1}$$

where, $\sigma_G(u) = \sum_{v\in V(G)} d_G(u, v)$ is the status of a vertex u in $V(G)$ [**11**].

Recent findings related to the status can be found in the literature [**32, 33, 18, 2**].

Example: Let G be a graph shown in Figure 1.

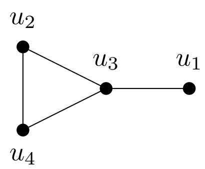


FIGURE 1. Graph G

Here, $\sigma_G(u_1) = 5, \quad \sigma_G(u_2) = 4, \quad \sigma_G(u_3) = 3 \quad \text{and} \quad \sigma_G(u_4) = 4.$

$$\begin{aligned} RSD(G) &= \sum_{\{u,v\}\subseteq V(G)} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u, v)} \\ &= \frac{\sigma_G(u_1) + \sigma_G(u_2)}{d_G(u_1, u_2)} + \frac{\sigma_G(u_1) + \sigma_G(u_3)}{d_G(u_1, u_3)} + \frac{\sigma_G(u_1) + \sigma_G(u_4)}{d_G(u_1, u_4)} \\ &\quad + \frac{\sigma_G(u_2) + \sigma_G(u_3)}{d_G(u_2, u_3)} + \frac{\sigma_G(u_2) + \sigma_G(u_4)}{d_G(u_2, u_4)} + \frac{\sigma_G(u_3) + \sigma_G(u_4)}{d_G(u_3, u_4)} \\ RSD(G) &= 39. \end{aligned}$$

The paper is organized as follows: The bounds for the *RSD* are computed in the next section. Section 3 calculates the *RSD* Index of a well-known class of graphs. Section 4 computes the *RSD* Index of Cluster graphs. The last section deals with the correlation between *RSD*, *DD*, and *RDD* index with the boiling point (*BP*), molar volume (*MV*), molar refractions (*MR*), and critical pressures (*CP*) of some paraffin hydrocarbon molecules.

2. Bounds for the reciprocal status-distance index

In this section, we obtained the bounds for the *RSD* index of graphs and characterized the equality of these bounds.

THEOREM 2.1. *Let G be a graph of order n, size m, and diameter D. Then,*

$$RSD(G) \geqslant \frac{4(n-1)}{D}\Big(\binom{n}{2} + m(D-1)\Big) - \frac{1}{D}[DM_1(G) + \overline{M}_1(G)].$$

Equality holds if and only if $D \leqslant 2$.

PROOF. For any vertex u of G, there are $d_G(u)$ vertices which are at a distance one from u, and the remaining $(n-1-d_G(u))$ vertices are at a distance at least 2. Thus,

$$\sigma_G(u) \geqslant d_G(u) + 2(n-1-d_G(u)) = 2(n-1) - d_G(u) \tag{2.1}$$

Moreover, equality holds if and only if $D \leqslant 2$. Then,

$$\begin{aligned}
RSD(G) &= \sum_{\{u,v\}\subseteq V(G)} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)} \\
&= \sum_{uv\in E(G)} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)} + \sum_{uv\notin E(G)} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)} \qquad (2.2)\\
&\geqslant \sum_{uv\in E(G)} \big(4n-4-[d_G(u)+d_G(v)]\big) + \sum_{uv\notin E(G)} \frac{4n-4-[d_G(u)+d_G(v)]}{D}, \\
&\qquad\qquad \because \frac{1}{d_G(u,v)} \geqslant \frac{1}{D} \\
&= m(4n-4) - M_1(G) + \Big(\binom{n}{2} - m\Big)\Big(\frac{4n-4}{D}\Big) - \frac{\overline{M}_1(G)}{D}
\end{aligned}$$

$$RSD(G) \geqslant \frac{4(n-1)}{D}\Big(\binom{n}{2} + m(D-1)\Big) - \frac{1}{D}[DM_1(G) + \overline{M}_1(G)].$$

For equality: The right-hand summand of (2.2) is zero if and only if $D = 1$. For $uv \notin E(G)$, $\frac{1}{d_G(u,v)} = \frac{1}{D}$ iff $D = 2$. Hence, by (2.1), equality holds iff $D \leqslant 2$. □

THEOREM 2.2. *Let G be a graph of order n, size m, and diameter D. Then,*

$$RSD(G) \leqslant D(n-1)\Big(\binom{n}{2} + m\Big) - \frac{D-1}{2}\Big(2M_1(G) + \overline{M}_1(G)\Big).$$

Equality holds if and only if $D \leqslant 2$.

PROOF. For any vertex u of G there are $d_G(u)$ which are at distance 1 from u and the remaining $(n-1-d_G(u))$ vertices are at distance at most D. Thus,

$$\sigma_G(u) \leqslant D(n-1) - (D-1)d_G(u) \text{ and equality holds if and only if } D \leqslant 2. \tag{2.3}$$

Then,

$$RSD(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)}$$

$$(2.4) \qquad = \sum_{uv\in E(G)} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)} + \sum_{uv\notin E(G)} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)}$$

$$\leqslant \sum_{uv\in E(G)} \Big(2D(n-1)-(D-1)[d_G(u)+d_G(v)]\Big)$$

$$+ \sum_{uv\notin E(G)} \frac{2D(n-1)-(D-1)[d_G(u)+d_G(v)]}{2},$$

$$\Big| \because \frac{1}{d_G(u,v)} \leqslant \frac{1}{2}, \text{ if } uv\notin E(G)$$

$$(2.5) \qquad = 2mD(n-1)-(D-1)M_1(G)+D\Big(\binom{n}{2}-m\Big)(n-1)$$

$$- \frac{(D-1)}{2}\overline{M}_1(G)$$

$$RSD(G) \leqslant D(n-1)\Big(\binom{n}{2}+m\Big) - \frac{(D-1)}{2}\Big(2M_1(G)+\overline{M}_1(G)\Big).$$

For equality: The right-hand summand of (2.4) is zero if and only if $D = 1$. For $uv \notin E(G)$, $\frac{1}{d_G(u,v)} = \frac{1}{2}$ iff $D = 2$. Hence, by (2.3), equality holds iff $D \leqslant 2$. □

3. *RSD* index of a well known class of graphs

PROPOSITION 3.1. (1) *For a complete graph K_n, $RSD(K_n) = n(n-1)^2$.*

(2) *For a complete bipartite graph $K_{p,q}$,*

$$RSD(K_{p,q}) = (p^3+q^3)+(p+q)-2(p^2+q^2)+pq\left[\tfrac{7}{2}(p+q)-5\right].$$

(3) *Let For a path P_n of n vertices,*

$$RSD(P_n) = \frac{2}{3}n(n^2-1)H_{n-1} - \frac{(n-1)}{18}(13n^2-2n-12)$$

where H_k is the harmonic series $1+\frac{1}{2}+\frac{1}{3}+....+\frac{1}{k}$

(4) *For a cycle C_n of length n,*

$$RSD(C_n) = \begin{cases} \frac{n^2}{2}H(C_n), & \text{if } n \text{ is even} \\ \frac{n^2-1}{2}H(C_n), & \text{if } n \text{ is odd.} \end{cases}$$

PROOF. (1) For any vertex u of K_n, $\sigma_G(u) = (n-1)$. Thus, $RSD(K_n) = n(n-1)^2$.

(2) Let V_1 and V_2 be the partite sets of $K_{p,q}$, where $|V_1| = p$ and $|V_2| = q$. Then, $\forall\, u \in V_1$, $\sigma_G(u) = q+2(p-1)$, $\forall\, v \in V_2$, $\sigma_G(v) = p+2(q-1)$. Partition the set of all pairs of vertices in $V(K_{p,q})$ into three sets,

$$X_1 = \{\{u,v\} \subseteq V | \{u,v\} \in V_1)\}, \quad |X_1| = \binom{p}{2}$$
$$X_2 = \{\{u,v\} \subseteq V | \{u,v\} \in V_2)\}, \quad |X_2| = \binom{q}{2}$$
$$X_3 = \{\{u,v\} \subseteq V | u \in V_1 \text{ and } v \in V_2\}, \quad |X_3| = pq. \text{ Now,}$$

$$RSD(K_{p,q}) = \sum_{X_1} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)} + \sum_{X_2} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)} + \sum_{X_3} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)}$$
$$RSD(K_{p,q}) = \sum_{X_1} \frac{2(q+2(p-1))}{2} + \sum_{X_2} \frac{2(p+2(q-1))}{2} + \sum_{X_3} \frac{(p+q)+2(p+q-2)}{1}$$
$$RSD(K_{p,q}) = (p^3+q^3)+(p+q)-2(p^2+q^2)+pq\left[\frac{7}{2}(p+q)-5\right].$$

(3) Let P_n be a path with n vertices which are labeled as, $u_1, u_2, ..., u_n$, where u_{i-1} is adjacent to u_i, $i = 2, 3, ..., n$. Then,

$$\sigma(u_i) = i-1+i-2+...+1+1+2+...+n-i = \frac{n(n+1)}{2} + (i-n-1)i$$

$$RSD(P_n) = \sum_{1 \leqslant i < j \leqslant n} \frac{\sigma_G(u_i)+\sigma_G(u_j)}{d_G(u_i,u_j)} = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{\sigma_G(u_i)+\sigma_G(u_j)}{d_G(u_i,u_j)}$$
$$= \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{\frac{n(n+1)}{2} + (i-n-1)i + \frac{n(n+1)}{2} + (j-n-1)j}{j-i}$$
$$= \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left[\frac{n(n+1)+(i-n-1)i}{j-i} + j + i + \frac{i^2}{j-i} - (n+1)\left(1 + \frac{i}{j-i}\right)\right]$$
$$= \sum_{i=1}^{n-1} \left[(n(n+1)+2i^2-2i(n+1))H_{n-1} + \frac{(n-i)}{2}(3i-(n+1))\right],$$

where H_{n-i} is the harmonic series $1 + \frac{1}{2} + \frac{1}{3} + ... + \frac{1}{n-i}$. We have

$$\sum_{i=1}^{n-1} H_{n-1} = \sum_{i=1}^{n-1}\sum_{j=1}^{n-i} \frac{1}{i} = nH_{n-1} - (n-1)$$
$$\sum_{i=1}^{n-1} iH_{n-1} = \sum_{i=1}^{n-1}\sum_{j=1}^{n-i} \frac{j}{i} = \frac{n}{2}(n+1)H_{n-1} - \frac{(n-1)}{4}(3n+2)$$
$$\sum_{i=1}^{n-1} i^2 H_{n-1} = \sum_{i=1}^{n-1}\sum_{j=1}^{n-i} \frac{j^2}{i} = \frac{n}{6}(2n^2+3n+1)H_{n-i} - \frac{(n-1)}{36}(22n(n+1)+3(n+2)).$$

Hence,

$$RSD(P_n) = n(n+1)\left[nH_{n-1} - (n-1)\right] + 2\left[\frac{n(2n^2+3n+1)}{6}H_{n-1}\right.$$

$$-\frac{n-1}{36}(22n^2+25n+6)\Big]-2(n+1)\Big[\frac{n(n+1)}{2}H_{n-i}-\frac{n-1}{4}(3n+2)\Big]$$

$$RSD(P_n)=\frac{2}{3}n(n^2-1)H_{n-1}-\frac{(n-1)}{18}(13n^2-2n-12).$$

(4) Let C_n be a cycle with n vertices which are labeled as, $u_1, u_2, ..., u_n$ such that $u_iu_{i+1}, u_1u_n \in E(C_n)$, $1 \leqslant i \leqslant n-1$.

Case 1: C_n is an even cycle.

$$\sigma_G(u_i) = 2\sum_{j=1}^{\frac{n}{2}-1} j + \frac{n}{2} = \frac{n^2}{4}, \qquad 1 \leqslant i \leqslant n.$$

$$RSD(C_n) = \sum_{\{u_i,u_j\}\subseteq V(C_n)} \frac{\sigma_G(u_i)+\sigma_G(v_j)}{d_G(u_i,u_j)} = \sum_{\{u_i,u_j\}\subseteq V(C_n)} \frac{\frac{n^2}{4}+\frac{n^2}{4}}{d_G(u_i,u_j)}$$

Hence,

$$RSD(C_n) = \frac{n^2}{2}H(C_n)$$

Case 2: C_n is an odd cycle.

$$\sigma_G(u_i) = 2\sum_{j=1}^{\frac{n-1}{2}} j = \frac{n^2-1}{4}, \qquad 1 \leqslant i \leqslant n.$$

$$RSD(C_n) = \sum_{\{u_i,u_j\}\subseteq V(C_n)} \frac{\sigma_G(u_i)+\sigma_G(v_j)}{d_G(u_i,u_j)}$$

$$= \sum_{\{u_i,u_j\}\subseteq V(C_n)} \frac{\frac{n^2-1}{4}+\frac{n^2-1}{4}}{d_G(u_i,u_j)} = \frac{n^2-1}{2}H(C_n),$$

where

$$H(C_n) = \begin{cases} n\big(\sum_{i=1}^{\frac{n}{2}}\frac{1}{i}\big)-1, & if\ n\ is\ even \\ n\big(\sum_{i=1}^{\frac{n-1}{2}}\frac{1}{i}\big), & if\ n\ is\ odd. \end{cases}$$

□

A Wheel W_{n+1} is a graph obtained from the cycle C_n, $n \geqslant 3$ by adding a new vertex and making it adjacent to all the vertices of C_n. The degree of a central vertex of W_{n+1} is n, and the degree of all other vertices is 3.

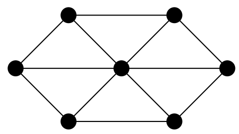
W_7 :


FIGURE 2. Wheel graph, W_7

Proposition 3.2. *For a Wheel graph W_{n+1}, $n \geqslant 3$. Then,*

$$RSD(W_{n+1}) = n^3 + \frac{n^2}{2} - \frac{3n}{2} + 2m_2 n - 3m_2.$$

Proof. Let u_0 be the center of W_{n+1} then . Partition the set of all pairs of vertices in $V(W_{n+1})$ into two sets,

$$X_1 = \{(u_0, v)|v \in V_1\}, \quad |X_1| = n$$

$$X_2 = \{(u, v)|(u, v) \in V_1\}, \quad |X_2| = \frac{n(n-1)}{2}, \; m_2 = uv \in E(X_2).$$

We have,

$$\sigma_G(u_0) = n$$

$$\sigma_G(u) = 3 + 2(n-3) = 2n - 3, \quad u \in V(W_{n+1}) - \{u_0\}$$

Then,

$$RSD(W_{n+1}) = \sum_{X_1} \frac{\sigma_G(u_0) + \sigma_G(v)}{d_G(u, v)} + \sum_{X_2} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u, v)}$$

$$RSD(W_{n+1}) = n[n + (2n-3)] + \sum_{uv \in X_2} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u, v)} + \sum_{uv \notin X_2} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u, v)}$$

$$RSD(W_{n+1}) = n^3 + \frac{n^2}{2} - \frac{3n}{2} + 2m_2 n - 3m_2$$

□

A friendship graph (or Dutch windmill graph) F_n,n$\geqslant$ 2 is constructed by coalescence n copies of the cycle C_3 length 3 with a common vertex. It has $2n + 1$ vertices and $3n$ edges. The degree of a coalescence vertex of F_n is $2n$, and the degrees of all other vertices are 2.

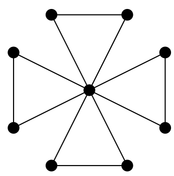


Figure 3. Friendship graph, F_4

Proposition 3.3. *For a friendship graph F_n,n$\geqslant$ 2. Then,*

$$RSD(F_n) = 8n^3 - 2n^2 + 4m_2 n - 2m_2.$$

Proof. Let $u \in V_1 = V(F_n) - \{u_0\}$,partition the set of all pairs of vertices of F_n into two sets,

$$X_1 = \{(u_0, v)|v \in V_1\}, \quad |X_1| = n \tag{3.1}$$

$$X_2 = \{(u,v)|u,v \in V_1\}, \quad |X_2| = \binom{2n}{2}, \; m_2 = uv \in E(X_2) \tag{3.2}$$

We have,

$$\sigma_G(u_0) = 2n, \quad \sigma_G(u) = 2 + 2(2n-2) = 4n-2, \quad u \in V(F_n) - \{u_0\}, \tag{3.3}$$

$$RSD(F_n) = \sum_{X_1} \frac{\sigma_G(u_0) + \sigma_G(v)}{d_G(u,v)} + \sum_{X_2} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)}$$

$$RSD(F_n) = \sum_{X_1} \frac{\sigma_G(u_0) + \sigma_G(v)}{d_G(u,v)} + \sum_{uv \in X_2} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} + \sum_{uv \notin X_2} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)}. \tag{3.4}$$

Substituting equations 3.1, 3.2, and 3.3 in 3.4. Thus,
$RSD(F_n) = 8n^3 - 2n^2 + 4m_2n - 2m_2$.

□

4. *RSD* index of some graphs obtained from the complete graph.

Proposition 4.1. *Let e_i, $i = 1, 2, ..k$, $1 \leqslant k \leqslant n-2$, be the distinct edges of a complete graph K_n, $n \geqslant 3$, all being incident to a single vertex. The graph $Ka_n(k)$ is obtained by deleting e_i, $i = 1, 2, ..., k$ from K_n. Then,*

$$RSD(Ka_n(k)) = n^3 - 2n^2 + n + 2nk - k^2 - 3k - \frac{\overline{M}_1(Ka_n(k))}{2}.$$

Proof. Let e_i, $i = 1, 2, ..k$, $1 \leqslant k \leqslant n-2$, be the distinct edges of a complete graph K_n, $n \geqslant 3$, all being incident to a vertex u_0. Partition the set of all edges in $E(Ka_n(k))$ into four sets,

$$X_1 = \{uv|\ d_G(u) = n-1-k, d_G(v) = n-1\}, \ |X_1| = (n-k-1), \tag{4.1}$$

$$X_2 = \{uv|\ d_G(u) = n-2, d_G(v) = n-2\}, \ |X_2| = \frac{k(k-1)}{2}, \tag{4.2}$$

$$X_3 = \{uv|\ d_G(u) = n-2, d_G(v) = n-1\}, \ |X_3| = k(n-1-k) \tag{4.3}$$

$$X_4 = \{uv|\ d_G(u) = n-1, d_G(v) = n-1\}, \ |X_4| = \frac{(n-k-1)(n-k-2)}{2} \tag{4.4}$$

We have,

$$\sigma_G(u) = 2(n-1) - d_G(u),$$
$$\sigma_G(v) = 2(n-1) - d_G(v),$$
$$\sigma_G(u) + \sigma_G(v) = 4(n-1) - (d_G(u) + d_G(v)), \tag{4.5}$$

$$RSD(Ka_n(k)) = \sum_{\{u,v\} \subseteq V(Ka_n(k))} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)}$$

$$= \sum_{X_1} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} + \sum_{X_2} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} + \sum_{X_3} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)}$$

$$+ \sum_{X_4} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} + \sum_{uv \notin E(Ka_n(k))} \frac{4(n-1) - (d_G(u) + d_G(v))}{d_G(u,v)}. \tag{4.6}$$

By using equations 4.1 to 4.5 in 4.6. Thus,

$$\begin{aligned}RSD(Ka_n(k)) &= (n-k-1)[2(n-1)+k] + k(k-1)n + k(n-k-1)(2n-1)\\ &\quad + (n-1)(n-k-1)(n-k-2) + \frac{4(n-1)k}{2} - \frac{\overline{M}_1(Ka_n(k))}{2}\\ &= n^3 - 2n^2 + n + 2nk - k^2 - 3k - \frac{\overline{M}_1(Ka_n(k))}{2}.\end{aligned}$$

□

PROPOSITION 4.2. *Let $f_i, i-1,2,...,k, 1 \leqslant k \leqslant \left[\frac{n}{2}\right]$ be independent edges of the complete graph $K_n, n \geqslant 3$. The graph $Kb_n(k)$ is obtained by deleting $f_i, i = 1,2,...,k$ from K_n. Then*

$$RSD(Kb_n(k)) = n^3 - 2n^2 + n + 2kn + 4k - 8k^2 - \frac{\overline{M}_1(Kb_n(k))}{2}$$

PROOF. Let $f_i, i-1,2,...,k, 1 \leqslant k \leqslant \left[\frac{n}{2}\right]$ be independent edges of the complete graph $K_n, n \geqslant 3$. The set of all edges of $E(Kb_n(k))$ can be partitioned into three edge sets,

(4.7) $X_1 = \{uv \mid d_G(u) = n-2 \text{ and } d_G(v) = n-1\}$, $|X_1| = 2k(n-2k)$,

(4.8) $X_2 = \{uv \mid d_G(u) = n-1 \text{ and } d_G(v) = n-1\}$, $|X_2| = \dfrac{(n-2k)(n-2k-1)}{2}$,

(4.9) $X_3 = \{uv \mid d_G(u) = n-2 \text{ and } d_G(v) = n-2\}$, $|X_3| = \dfrac{2k(2k-1)}{2} - k$

We have,

$$\sigma_G(u) = 2(n-1) - d_G(u),\ \sigma_G(v) = 2(n-1) - d_G(v) \tag{4.10}$$

$$\sigma_G(u) + \sigma_G(v) = 4(n-1) - (d_G(u) + d_G(v)). \text{ Then,} \tag{4.11}$$

$$RSD(Kb_n(k)) = \sum_{\{u,v\}\subseteq V(Kb_n(k))} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)}$$

$$\begin{aligned}RSD(Kb_n(k)) = &\sum_{X_1} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)} + \sum_{X_2} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)} + \sum_{X_3} \frac{\sigma_G(u)+\sigma_G(v)}{d_G(u,v)}\\ &+ \sum_{uv\notin E(Ka_n(k))} \frac{4(n-1)-(d_G(u)+d_G(v))}{d_G(u,v)}.\end{aligned} \tag{4.12}$$

After using equations 4.7, 4.8, 4.9, and 4.11 in 4.12, the result is obtained:

$$RSD(Kb_n(k)) = n^3 - 2n^2 + n + 2kn + 4k - 8k^2 - \frac{\overline{M}_1(Kb_n(k))}{2}.$$

□

PROPOSITION 4.3. *Let V_k be a k-element subset of the vertex set of the complete graph $K_n, 2 \leqslant k \leqslant n-1, n \geqslant 3$. The graph $Kc_n(k)$ is obtained by deleting from K_n all the edges connecting pairs of vertices from V_k. Then,*

$$RSD(Kc_n(k)) = n^3 - 2n^2 + n - k^3 + 2k^2 + 2kn - 3k - \frac{\overline{M}_1(Kc_n(k))}{2}$$

PROOF. Let V_k be a k-element subset of the vertex set of the complete graph $K_n, 2 \leqslant k \leqslant n-1, n \geqslant 3$.The set of all edges of $E(Kc_n(k))$ can be partitioned into two edge sets,

$$X_1 = \{uv|\ d_G(u) = n-k \ and \ d_G(v) = n-1\},\ |X_1| = (n-k)k \tag{4.13}$$

$$X_2 = \{uv|\ d_G(u) = n-1 \ and \ d_G(v) = n-1\},\ |X_2| = \frac{(n-k)(n-k-1)}{2}. \tag{4.14}$$

We have,

$$\sigma_G(u) = 2(n-1) - d_G(u), \tag{4.15}$$

$$\sigma_G(v) = 2(n-1) - d_G(v), \quad \sigma_G(u) + \sigma_G(v) = 4(n-1) - (d_G(u) + d_G(v)), \tag{4.16}$$

$$RSD(Kc_n(k)) = \sum_{\{u,v\} \subseteq V(Kc_n(k))} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} \tag{4.17}$$

$$\begin{aligned} RSD(Kc_n(k)) = & \sum_{X_1} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} + \sum_{X_2} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} \\ & + \sum_{uv \notin E(Ka_n(k))} \frac{4(n-1) - (d_G(u) + d_G(v))}{d_G(u,v)}. \end{aligned} \tag{4.18}$$

Using equations 4.13, 4.14, and 4.16 in equation 4.18. Thus,

$$RSD(Kc_n(k)) = n^3 - 2n^2 + n - k^3 + 2k^2 + 2kn - 3k - \frac{\overline{M}_1(Kc_n(k))}{2}.$$

□

PROPOSITION 4.4. *Let $3 \leqslant k \leqslant n, n \geqslant 5$. The graph $Kd_n(k)$ is obtained by deleting from K_n the edges of a $k-$ membered cycle. Then,*

$$RSD(Kd_n(k)) = n^3 - 2n^2 + 2nk - 6k - \frac{\overline{M}_1(Kd_n(k))}{2}$$

PROOF. Let $3 \leqslant k \leqslant n, n \geqslant 5$. The set of all edges of $E(Kd_n(k))$ can be partioned into three edge sets,

$$X_1 = \{uv|\ d_G(u) = n-3 \ and \ d_G(v) = n-3\}, |X_1| = [\binom{k}{2} - k], \tag{4.19}$$

$$X_2 = \{uv|\ d_G(u) = n-3 \ and \ d_G(v) = n-1\}, |X_2| = (n-k)k \tag{4.20}$$

$$X_3 = \{uv|\ d_G(u) = n-1 \ and \ d_G(v) = n-1\}, |X_3| = \frac{(n-k)(n-k-1)}{2} \tag{4.21}$$

$$\begin{aligned} RSD(Kd_n(k)) = & \sum_{X_1} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} + \sum_{X_2} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} + \sum_{X_3} \frac{\sigma_G(u) + \sigma_G(v)}{d_G(u,v)} \\ & + \sum_{uv \notin E(Kd_n(k))} \frac{4(n-1) - (d_G(u) + d_G(v))}{d_G(u,v)}. \end{aligned} \tag{4.22}$$

To obtain the result, substitute equations 4.19 to 4.21 into equation 4.22. Thus

$$RSD(Kd_n(k)) = n^3 - 2n^2 + 2nk - 6k - \frac{\overline{M}_1(Kd_n(k))}{2}$$

□

5. Obtained correlation between *RSD*, *DD* and *RDD* indices with the properties of paraffin molecules.

The properties of Graphs can be used in the study of the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) of the molecules [**24**]. The properties of the molecules are listed in Table 1. This section studied the correlation between the boiling points (BP) $^\circ C$, molar volume (MV) cm^3, molar refractions (MR) cm^3, and critical pressures (CP) atm of the paraffin hydrocarbons with the reciprocal status distance, degree distance and reciprocal degree distance index, of the corresponding molecular graphs.

R No.	**Molecules**	**RSDs**	**DDs**	**RDDs**
1	3-methylpentane	180.166667	95	33.8333
2	2,2 -dimethylbutane	159.166	82	36
3	2,3 dimethylbutane	173.333	86	34.666
4	2,2 dimethylpentane	275	142	46.1666
5	3,3 dimethylpentane	291.5	134	46.9166
6	n-octane	531.283	280	49.785
7	3-methylheptane	521.96	234	58.686
8	3-ethylhexane	496.9	228	53.3
9	2,2-dimethylhexane	494.733	222	55.2
10	2,4 dimethylhexane	514.8833	226	55.7333
11	2-methyl, 3-ethylpentene	478.5	212	57.1666
12	2,2,4-trimethylpentene	486.833	194	54.833

TABLE 1. RSD, DD and RDD index of paraffin molecules.

From Tables 1 and 2, one can obtain the correlation coefficient and regression equations of *RSD*, *DD*, and *RDD* indices with some properties of the paraffin molecules. From Table 3, one can notice that the correlation between *RSD* with the properties of paraffin molecules is obtained and compared with the correlation achieved from other indices.

R No.	**Properties of Molecules**	**Regression Equations**	R^2
1	Boiling Point (BP)	$y = 2.5x - 56.08$	0.81896733
2	Molar Volume (MV)	$y = 3.45x - 349.17$	0.594349346
3	Molar Refraction (MR)	$y = 13x - 295.05$	0.908109456
4	Critical Pressure (PC)	$y = -25.93x + 890.61$	0.817207108

TABLE 5. The observation shows the correlation analysis between DD index with certain properties of paraffin molecules.

R No.	**Molecules**	**BP**($^\circ C$)	**MV**(cm^3)	**MR**(cm^3)	**CP(atm)**
1	3-methylpentane	62.9	129.7	29.8	30.8
2	2,2 -dimethylbutane	50	148.7	29.93	30.7
3	2,3 dimethylbutane	57.9	130.2	29.81	31
4	2,2 dimethylpentane	79	34.62	148.7	28.4
5	3,3 dimethylpentane	86	144.5	34.33	30
6	n-octane	125	162.6	39.19	24.64
7	3-methylheptane	118	144.5	39.1	25.6
8	3-ethylhexane	118	164.3	38.94	25.74
9	2,2-dimethylhexane	107	160.1	39.25	25.6
10	2,4 dimethylhexane	108	163.1	39.13	25.8
11	2-methyl, 3-ethylpentene	116	174.5	43.46	25.96
12	2,2,4-trimethylpentene	99	165.1	39.26	25.5

TABLE 2. Properties of paraffin molecules.

R No.	**Indices**	**BP**	**MV**	**MR**	**PC**
1	RSDs	0.968606	0.777507	0.939561	-0.981
2	DDs	0.976755	0.737975	0.896882	-0.96955
3	RDDs	0.904968	0.770941	0.952948	-0.904

TABLE 3. Correlation coefficient of *RSD*, *DD*, and *RDD* with the some properties of paraffin molecules.

R No.	**Properties of Molecules**	**Regression Equations**	R^2
1	Boiling Point (BP)	$y = 5.7x - 151.37$	0.938197212
2	Molar Volume (MV)	$y = 8.39x - 900.07$	0.604517823
3	Molar Refraction (MR)	$y = 31.45x - 761.35$	0.882775418
4	Critical Pressure (PC)	$y = -59.34x + 2010.7$	0.962361937

TABLE 4. The observation shows the correlation analysis between the RSD index with certain properties of paraffin molecules.

R No.	**Properties of Molecules**	**Regression Equations**	R^2
1	Boiling Point (BP)	$y = 0.32x + 18.86$	0.81896733
2	Molar Volume (MV)	$y = 0.49x - 26.98$	0.594349346
3	Molar Refraction (MR)	$y = 1.89x - 20.32$	0.908109456
4	Critical Pressure (PC)	$y = -3.31x + 139.34$	0.817207108

TABLE 6. The observation shows the correlation analysis between the RDD index with certain properties of paraffin molecules.

From Tables 4,5 and 6, one can notice that the regression analysis was done by using *RSD*, *DD*, and *RDD* indices.

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