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Stress-Difference Index for Graphs

R. Rajendra, P. Siva Kota Reddy and C. N. Harshavardhana

ABSTRACT: The stress of a vertex is a node centrality index, which has been introduced by Shimbel (1953). The stress of a vertex in a graph is the number of geodesics (shortest paths) passing through it. A topological index of a chemical structure (graph) is a number that correlates the chemical structure with chemical reactivity or physical properties. In this paper, we introduce a new topological index for graphs called stress-difference index using stresses of vertices. Further, we establish some inequalities, prove some results and compute stress-difference index for some standard graphs. Also, we found that there is a positive correlation between the stress-difference index and some physical properties of lower alkanes.

Key Words: Graph, Neighborhood of a vertex, stress of a vertex, path, geodesic, topological index.

Contents

1. Introduction

For standard terminology and notion in graph theory, we follow the text-book of Harary [2]. The non-standard will be given in this paper as and when required.

Let $G = (V, E)$ be a graph (finite and undirected). The distance between two vertices u and v in G, denoted by $d(u, v)$ is the number of edges in a shortest path (also called a graph geodesic) connecting them. We say that a graph geodesic P is passing through a vertex v in G if v is an internal vertex of P (i.e., v is a vertex in P, but not an end vertex of P).

The concept of stress of a node (vertex) in a network (graph) has been introduced by Shimbel as centrality measure in 1953 [12]. This centrality measure has applications in biology, sociology, psychology, etc., (See [3,11]). The stress of a vertex v in a graph G, denoted by $\mathrm{str}_G(v)$ $\mathrm{str}(v)$, is the number of geodesics passing through it. We denote the maximum stress among all the vertices of G by Θ_G and minimum stress among all the vertices of G by θ_G. Further, the concepts of stress number of a graph and stress regular graphs have been studied by K. Bhargava, N. N. Dattatreya, and R. Rajendra in their paper [1]. A graph G is k-stress regular if $\mathrm{str}(v) = k$ for all $v \in V(G)$.

Rajendra et al. [7] have introduced two topological indices of for graphs called first stress index and second stress index, using stresses of vertices. For new topological indices, we suggest the reader to refer the papers [5-10]. The first stress index $\mathcal{S}_1(G)$ and the second stress index $\mathcal{S}_2(G)$ of a simple graph G are defined as

$$\mathcal{S}_1(G) = \sum_{v \in V(G)} \mathrm{str}(v)^2 \tag{1.1}$$

$$\mathcal{S}_2(G) = \sum_{uv \in E(G)} \mathrm{str}(u)\mathrm{str}(v). \tag{1.2}$$

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In this paper we introduce a new topological index for graphs using stress on vertices called stress-difference index. Further, we establish some inequalities and compute stress-difference index for some standard graphs. Also, we found that there is a positive correlation between the stress-difference index and some physical properties of lower alkanes.

2. Stress-Difference Index for Graphs

Definition 2.1. *The stress-difference index $\mathcal{SD}(G)$ of a simple graph G is defined as*

$$\mathcal{SD}(G) = \sum_{uv \in E(G)} |str(u) - str(v)|. \tag{2.1}$$

Observation: For any two vertices u and v in a graph $G = (V, E)$,

$$0 \leq |\mathrm{str}(u) - \mathrm{str}(v)| \leq \Theta_G - \theta_G.$$

Therefore, from the Definition 2.1, it follows that, for any graph G,

$$0 \leq \mathcal{SD}(G) \leq m(\Theta_G - \theta_G)$$

where m is the number of edges in G.

Example 2.2. *Consider the graph G given in Figure 1.*

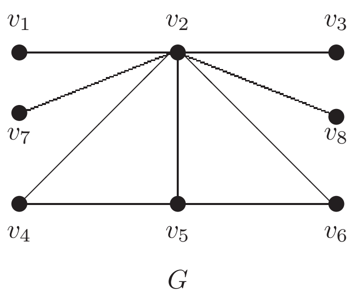

Figure 1: A graph G

The stresses of the vertices of G are as follows:
$str(v_1) = str(v_3) = str(v_7) = str(v_8) = 0,$
$str(v_2) = 19,$
$str(v_5) = 1,$
$str(v_4) = str(v_6) = 0.$
The stress-difference index of G is:

$$\begin{aligned}\mathcal{SD}(G) =& |str(v_2) - str(v_1)| + |str(v_2) - str(v_3)| + |str(v_2) - str(v_7)| \\ & + |str(v_2) - str(v_8)| + |str(v_2) - str(v_4)| + |str(v_2) - str(v_5)| \\ & + |str(v_2) - str(v_6)| + |str(v_4) - str(v_5)| + |str(v_5) - str(v_6)| \\ =& |19 - 0| + |19 - 0| + |19 - 0| + |19 - 0| + |19 - 0| + |19 - 1| \\ & + |19 - 0| + |0 - 1| + |1 - 0| \\ =& 135.\end{aligned}$$

Proposition 2.3. *Let N be the number of geodesics of length ≥ 2 in a graph G. Then*

$$0 \leq \mathcal{SD}(G) \leq N(|E| - t), \tag{2.2}$$

where t is the number of edges with end vertices having zero stress in G.

Proof. If N is the number of all geodesics of length ≥ 2 in a graph G, then by the definition of stress of a vertex, for any vertex v in G, $0 \leq \mathrm{str}(v) \leq N$. Hence by the Definition 2.1, we have

$$0 \leq \mathcal{SD}(G) \leq N(|E| - t), \tag{2.3}$$

where t is the number of edges with end vertices having zero stress in G. □

Corollary 2.4. *If there is no geodesic of length ≥ 2 in a graph G, then $\mathcal{SD}(G) = 0$. Moreover, for a complete graph K_n, $\mathcal{SD}(K_n) = 0$.*

Proof. If there is no geodesic of length ≥ 2 in a graph G, then $N = 0$. Hence, by the Proposition 2.3, we have $\mathcal{SD}(G) = 0$.

In K_n, there is no geodesic of length ≥ 2 and so $\mathcal{SD}(K_n) = 0$. □

Theorem 2.5. *For a graph G, $\mathcal{SD}(G) = 0$ if and only if $str(u) = str(v)$, $\forall uv \in E(G)$. Moreover, For a connected graph G, $\mathcal{SD}(G) = 0$ if and only if G is stress regular.*

Proof. Suppose that $\mathcal{SD}(G) = 0$. Then by the Definition 2.1, $|\mathrm{str}(u) - \mathrm{str}(v)| = 0$, $\forall uv \in E(G)$. So $\mathrm{str}(u) - \mathrm{str}(v) = 0$, $\forall uv \in E(G)$ and hence $\mathrm{str}(u) = \mathrm{str}(v)$, $\forall uv \in E(G)$. Converse part is obvious.

If G is connected, then $\mathrm{str}(u) = \mathrm{str}(v)$, $\forall uv \in E(G)$ implies that all the vertices in G have same stress. Hence for a connected graph G, $\mathcal{SD}(G) = 0$ if and only if G is stress regular. □

Corollary 2.6. *For a cycle C_n, $\mathcal{SD}(C_n) = 0$.*

Proof. For any vertex v in C_n, we have,

$$\mathrm{str}(v) = \begin{cases} \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd} \\ \dfrac{n(n-2)}{8}, & \text{if } n \text{ is even.} \end{cases}$$

Hence C_n is

$$\begin{cases} \dfrac{(n-1)(n-3)}{8}\text{-stress regular}, & \text{if } n \text{ is odd} \\ \dfrac{n(n-2)}{8}\text{-stress regular}, & \text{if } n \text{ is even.} \end{cases}$$

Therefore, by Theorem 2.5. $\mathcal{SD}(C_n) = 0$. □

Proposition 2.7. *For the complete bipartite $K_{m,n}$,*

$$\mathcal{SD}(K_{m,n}) = \frac{mn}{2} \left| n(n-1) - m(m-1) \right|.$$

Proof. Let $V_1 = \{v_1, \ldots, v_m\}$ and $V_2 = \{u_1, \ldots, u_n\}$ be the partite sets of $K_{m,n}$. We have,

$$\mathrm{str}(v_i) = \frac{n(n-1)}{2} \text{ for } 1 \leq i \leq m \tag{2.4}$$

and

$$\mathrm{str}(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \leq j \leq n. \tag{2.5}$$

Using (2.4) and (2.5) in the Definition 2.1, we have

$$\begin{aligned}
\mathcal{SD}(K_{m,n}) &= \sum_{uv\in E(G)} |\mathrm{str}(u) - \mathrm{str}(v)| \\
&= \sum_{1\le i\le m,\ 1\le j\le m} |\mathrm{str}(v_i) - \mathrm{str}(u_j)| \\
&= \sum_{1\le i\le m,\ 1\le j\le n} \left| \frac{n(n-1)}{2} - \frac{m(m-1)}{2} \right| \\
&= mn \left| \frac{n(n-1)}{2} - \frac{m(m-1)}{2} \right| \\
&= \frac{mn}{2} \left| n(n-1) - m(m-1) \right|.
\end{aligned}$$

□

Proposition 2.8. *Let T be a tree on n vertices. Then*

$$\begin{aligned}
\mathcal{SS}(T) = \sum_{uv\in J} &\left| \sum_{1\le i<j\le m(u)} |C_i^u||C_j^u| - \sum_{1\le i<j\le m(v)} |C_i^v||C_j^v| \right| \\
&+ \sum_{w\in Q} \sum_{1\le i<j\le m(w)} |C_i^w||C_j^w|.
\end{aligned}$$

where J is the set of internal(non-pendant) edges in T, Q denotes the set of all vertices adjacent to pendent vertices in T, and the sets $C_1^v, \dots, C_m^v$ denotes the vertex sets of the components of $T - v$ for an internal vertex v of degree $m = m(v)$.

Proof. We know that a pendant vertex in T has zero stress. Let v be an internal vertex of T of degree $m = m(v)$. Let $C_1^v, \dots, C_m^v$ be the components of $T - v$. Since there is only one path between any two vertices in a tree, it follows that,

$$\mathrm{str}(v) = \sum_{1\le i<j\le m} |C_i^v||C_j^v| \tag{2.6}$$

Let J denotes the set of internal(non-pendant) edges, and P denotes pendant edges and Q denotes the set of all vertices adjacent to pendent vertices in T. Then using (2.6) in the Definition 2.1, we have

$$\begin{aligned}
\mathcal{SD}(T) &= \sum_{uv\in J} |\mathrm{str}(u) - \mathrm{str}(v)| + \sum_{uv\in P} |\mathrm{str}(u) - \mathrm{str}(v)| \\
&= \sum_{uv\in J} |\mathrm{str}(u) - \mathrm{str}(v)| + \sum_{w\in Q} \mathrm{str}(w) \\
&= \sum_{uv\in J} \left| \sum_{1\le i<j\le m(u)} |C_i^u||C_j^u| - \sum_{1\le i<j\le m(v)} |C_i^v||C_j^v| \right| \\
&\quad + \sum_{w\in Q} \sum_{1\le i<j\le m(w)} |C_i^w||C_j^w|.
\end{aligned}$$

□

Corollary 2.9. *For the path P_n on n vertices*

$$\mathcal{SD}(P_n) = 2\left(n - \left\lceil \frac{n}{2} \right\rceil\right)\left(\left\lceil \frac{n}{2} \right\rceil - 1\right).$$

P_n

Figure 2: The path P_n on n vertices.

Proof. The proof of this corollary follows by above Proposition 2.8. We follow the proof of the Proposition 2.8 to compute the index. Let P_n be the path with vertex sequence $v_1, v_2, \ldots, v_n$ (shown in Figure 2).

We have,

$$\operatorname{str}(v_i) = (i-1)(n-i),\ 1 \leq i \leq n.$$

Then

$$\begin{aligned}
\mathcal{SD}(P_n) &= \sum_{uv \in E(P_n)} |\operatorname{str}(u) - \operatorname{str}(v)| \\
&= \sum_{i=1}^{n-1} |\operatorname{str}(v_i) - \operatorname{str}(v_{i+1})| \\
&= \sum_{i=1}^{n-1} |(i-1)(n-i) - (i)(n-i-1)| \\
&= \sum_{i=1}^{n-1} |2i - n| \\
&= 2\left(n - \left\lceil \frac{n}{2} \right\rceil\right)\left(\left\lceil \frac{n}{2} \right\rceil - 1\right).
\end{aligned}$$

□

Proposition 2.10. *Let $Wd(n,m)$ denotes the windmill graph constructed for $n \geq 2$ and $m \geq 2$ by joining m copies of the complete graph K_n at a shared universal vertex v. Then*

$$\mathcal{SD}(Wd(n,m)) = \frac{m^2(m-1)(n-1)^3}{2}.$$

Hence, for the friendship graph F_k on $2k+1$ vertices,

$$\mathcal{SD}(F_k) = 4k^2(k-1).$$

Proof. Clearly the stress of any vertex other than universal vertex is zero in $Wd(n,m)$,

because neighbors of that vertex induces a complete subgraph of $Wd(n,m)$. Also, since there are m copies of K_n in $Wd(n,m)$ and their vertices are adjacent to v, it follows that, the only geodesics passing through v are of length 2 only. So, $\operatorname{str}(v) = \dfrac{m(m-1)(n-1)^2}{2}$. Note that there are $m(n-1)$ edges incident on v and the edges that are not incident on v have end vertices of stress zero. Hence by the Definition 2.1, we have

$$\begin{aligned}
\mathcal{SD}(Wd(n,m)) &= m(n-1)\operatorname{str}(v) \\
&= m(n-1)\frac{m(m-1)(n-1)^2}{2} \\
&= \frac{m^2(m-1)(n-1)^3}{2}.
\end{aligned}$$

Since the friendship graph F_k on $2k+1$ vertices is nothing but $Wd(3,k)$, it follows that

$$\mathcal{SD}(F_k) = \frac{k^2(k-1)(3-1)^3}{2} = 4k^2(k-1).$$

□

Proposition 2.11. *Let W_n denotes the wheel graph constructed on $n \geq 4$ vertices. Then*

$$\mathcal{SD}(W_n) = \begin{cases} \left|\dfrac{(n-1)(3n-2)(n-4)}{8}\right|, & \textit{if } n \textit{ is even;} \\ \left|\dfrac{(n-1)^2(3n-13)}{8}\right|, & \textit{if } n \textit{ is odd.} \end{cases}.$$

Proof. In W_n with $n \geq 4$, there are $(n-1)$ peripheral vertices and one central vertex, say v. It is easy to see that

$$\text{str}(v) = \frac{(n-1)(n-4)}{2} \tag{2.7}$$

Let p be a peripheral vertex. Since v is adjacent to all the peripheral vertices in W_n, there is no geodesic passing through p and containing v. Hence contributing vertices for str(p) are the rest peripheral vertices. So, by denoting the cycle $W_n - p$ (on $n-1$ vertices) by C_{n-1}, we have

$$\begin{aligned} \text{str}_{W_n}(p) &= \text{str}_{W_n - v}(p) \\ &= \text{str}_{C_{n-1}}(p) \\ &= \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n-1 \text{ is odd;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n-1 \text{ is even,} \end{cases} \\ &= \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.} \end{cases} \end{aligned} \tag{2.8}$$

Let us denote the set of all radial edges in W_n by R, and the set of all peripheral edges by Q. Note that there are $(n-1)$ radial edges and $(n-1)$ peripheral edges in W_n. Using (2.7) and (2.8) in the Definition 2.1, we have

$$\begin{aligned} \mathcal{SD}(W_n) &= \sum_{xy \in R} [\text{str}(x) - \text{str}(y)] + \sum_{xy \in Q} [\text{str}(x) - \text{str}(y)] \\ &= (n-1)[\text{str}(v) - \text{str}(p)] + 0 \\ &= (n-1) \left| \frac{(n-1)(n-4)}{2} - \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.} \end{cases} \right| \\ &= \begin{cases} \left|\dfrac{(n-1)(3n-2)(n-4)}{8}\right|, & \text{if } n \text{ is even;} \\ \left|\dfrac{(n-1)^2(3n-13)}{8}\right|, & \text{if } n \text{ is odd.} \end{cases} \end{aligned}$$

□

3. Statistical correlation between physical properties of lower alkanes and stress-difference index

We wish to measure the strength of a linear relationship between some physical properties of lower alkanes with stress-difference index of molecular graphs. Table 1 gives the stress-difference index $\mathcal{SD}(G)$ of molecular graphs and the experimental values for the physical properties - Boiling points (bp) $^\circ C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporization (hv) kJ, critical temperatures (ct) $^\circ C$, critical pressures (cp) atm, and surface tensions(st) $dyne\ cm^{-1}$ of considered alkanes. The values given in the columns 3 to 9 in the Table 1 are taken from Needham et al. [4] (the same values can be found in [13]).

Table 1: Stress-difference index, boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes

Alkane	$\mathcal{SD}(G)$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	8	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	15	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	24	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	12	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	21	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	24	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	36	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	28	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	18	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	27	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	33	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	48	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	48	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	42	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	36	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	52	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	57	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	24	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	35	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	42	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	45	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	48	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	60	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	56	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	53	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	46	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	84	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	56	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	59	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	72	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	71	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	71	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	95	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	67	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	32	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	45	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	51	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	57	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	60	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	48	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	72	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	70	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	70	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	64	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	58	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	84	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	74	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	70	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	88	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	76	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	73	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	92	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	77	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	93	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	91	126.5	179.2	43.76	40.6	301	23.39	20.51

2,2,5-Trimethylhexane	85	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	101	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	87	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	83	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	97	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	111	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	96	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	96	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	105	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	89	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	120	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	100	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	112	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	114	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Table 2: The correlation coefficient r for Stress-difference index ($\mathcal{SD}(G)$) with physical properties (P)

P	r
bp	0.675602525
mv	0.692881016
mr	0.743091172
hv	0.586693078
ct	0.750339353
cp	-0.439540458
st	0.663642381

Table 3: The correlation coefficient r for the sum of Stress-difference index ($\mathcal{SD}(G)$) and the cube of number vertices (N^3) in molecular graphs with the physical properties (P)

P	r
bp	0.944110644
mv	0.966934244
mr	0.983160048
hv	0.923972955
ct	0.939477309
cp	-0.834169392
st	0.858254987

From the Table 2, it follows that, there is a positive correlation between the stress-difference index and the physical properties - Boiling points (bp) $^\circ C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporization (hv) kJ, critical temperatures (ct) $^\circ C$ and surface tensions(st) $dyne\ cm^{-1}$ of considered alkanes, but the degree of the association is moderate as the range of the correlation coefficient is $0.58 - 0.74$). There is a negligible inverse correlation between stress-difference index and critical pressures (cp) atm.

We have computed the correlation coefficient r for the sum of Stress-difference index and the cube of number vertices in molecular graphs ($\mathcal{SD}(G) + N^3$) with the physical properties (P). From the Table 3, it follows that, there is a strong positive correlation between the stress-difference index and the physical properties - Boiling points (bp) $^\circ C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporization (hv) kJ, critical temperatures (ct) $^\circ C$ and surface tensions(st) $dyne\ cm^{-1}$ of considered alkanes. Here the degree of the association is strong enough as the range of the correlation coefficient is $0.85 - 0.98$). Also, there is a notable inverse correlation ($r = -0.834169392$) between ($\mathcal{SD}(G) + N^3$) and critical pressures (cp) atm.

Conclusion

A large number of molecular-graph-based structure descriptors (topological indices) have been defined, depending on vertex degrees. But in this paper, we have defined a new topological index for graphs, namely, stress-difference index, without using the degrees of vertices. We have established some inequalities, proved some results and computed the stress-difference index for some standard graphs. By the statistical analysis carried in the paper, it follows that, the stress-difference index can be used together with cube of number vertices in molecular graphs to predict the physical properties of lower alkanes.

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R. Rajendra,
Department of Mathematics
Field Marshal K.M. Cariappa College
(A Constituent College of Mangalore University)
Madikeri-571 201, INDIA.
E-mail address: `rrajendrar@gmail.com`

and

P. Siva Kota Reddy (Corresponding author),
Department of Mathematics
Sri Jayachamarajendra College of Engineering
JSS Science and Technology University
Mysuru–570 006, INDIA.
E-mail address: `pskreddy@jssstuniv.in`

and

C. N. Harshavardhana,
Department of Mathematics
Government First Grade College for Women
Holenarasipur-573 211, INDIA.
E-mail address: `cnhmaths@gmail.com`