Global and Stochastic Analysis
Vol. 12 No. 1 (January, 2025)

Received: 19th June 2024 **Revised: 29th July 2024** **Accepted: 12th August 2024**

MODIFIED KASHVI-TOSHA STRESS INDEX FOR GRAPHS

HOWIDA ADEL ALFRAN, P. SOMASHEKAR, AND P. SIVA KOTA REDDY*

Abstract. We introduce a new topological index for graphs called Modified Kashvi-Tosha stress index using stresses of nodes. Also, we establish some inequalities, prove some results and compute Modified Kashvi-Tosha stress index for some standard graphs. Further, a QSPR analysis is carried for Modified Kashvi-Tosha stress index and physical properties of lower alkanes and linear regression models have been provided.

1. Introduction

We refer to the textbook of Harary [4] for standard terminology and concepts in graph theory. This article will provide non-standard information when needed.

Let $G = (V, E)$ be a graph (finite, simple, connected and undirected). The distance between two nodes 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 node v in G if v is an internal node of P.

The concept of stress of a node in a network (graph) has been introduced by Shimbel as centrality measure in 1953 [23]. This centrality measure has applications in biology, sociology, psychology, etc., (See [6, 21]). The stress of a node v in a graph G, denoted by $\text{str}_G(v)$ or $\text{str}(v)$, is the number of geodesics passing through it. We denote the maximum stress among all the nodes of G by Θ_G and minimum stress among all the nodes 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 $\text{str}(v) = k$ for all $v \in V(G)$. We recommend that the reader to study the publications [2, 3, 5, 7, 9–20, 22, 24, 25] for novel stress/degree based topological indices.

In this work, a finite simple connected graph is referred to as a graph, G denotes a graph and N denotes the number of geodesics of length ≥ 2 in G. In this paper we introduce a novel topological index for graphs using stress on nodes called Modified Kashvi-Tosha Stress Index. Further, we establish some inequalities and compute Modified Kashvi-Tosha stress index for some standard graphs.

2000 *Mathematics Subject Classification.* 05C05, 05C07, 05C09, 05C38, 05C92.
Key words and phrases. Graph, Geodesic, Stress of a node, Topological index.
*Corresponding author.

2. Modified K-T Stress Index for Graphs

In [26], a novel topological index for graphs has been introduced, namely, Kashvi-Tosha stress index. Further, the authors established some inequalities, proved some results and computed the Kashvi-Tosha stress index for some standard graphs. Kashvi-Tosha stress index can be used as a predictive measure for physical properties of low alkanes. It will be interesting to explore further properties of Kashvi-Tosha stress index.

Definition 2.1. The Kashvi-Tosha stress index $KT(G)$ of a graph G is defined as

$$KT(G) = \sum_{uv \in E(G)} [\operatorname{str}(u) + \operatorname{str}(v) + \operatorname{str}(u)\operatorname{str}(v)]. \tag{2.1}$$

By the motivation of the above work, in this paper we have defined the Modified Kashvi-Tosha stress index of a graph as follows:

Definition 2.2. The Modified Kashvi-Tosha stress index $\mathbb{M}(G)$ of a graph G is defined as

$$\mathbb{M}(G) = \sum_{uv \in E(G)} \left[\operatorname{str}(u)^2 + \operatorname{str}(v)^2 + \operatorname{str}(u)\operatorname{str}(v)\right]. \tag{2.2}$$

Observation: From the Definition 2.2, it follows that, for any graph G,

$$3m\theta_G^2 \leq \mathbb{M}(G) \leq 3m\Theta_G^2,$$

where m is the number of edges in G.

Proposition 2.3. *For any graph G,*

$$0 \leq \mathbb{M}(G) \leq N^2(3|E| - t), \tag{2.3}$$

where t is the number of edges with at least one end node of zero stress in G.

Proof. By the definition of stress of a node, for any node v in G, $0 \leq \operatorname{str}(v) \leq N$. Hence by the Definition 2.2, we have

$$0 \leq \mathbb{M}(G) \leq 2N^2|E| + N^2(|E| - t) = N^2(3|E| - t), \tag{2.4}$$

where t is the number of edges with at least one end node of zero stress in G. □

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

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

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

Theorem 2.5. *For a graph G, $\mathbb{M}(G) = 0$ iff G is complete.*

Proof. Suppose that $\mathbb{M}(G) = 0$. Then by the Definition 2.2, $\operatorname{str}(u)^2 + \operatorname{str}(v)^2 + \operatorname{str}(u)\operatorname{str}(v) = 0$, $\forall uv \in E(G)$. Hence $\operatorname{str}(v) = 0$, $\forall v \in V(G)$. If $|V(G)| = 1$ or 2, then G is a complete graph as $G \cong K_1$ or K_2. Assume that $|V(G)| > 2$. Let u, v be any two distinct nodes in G. We claim that u, v are adjacent in G. For, if u, v are not adjacent in G, then there is a geodesic in G between u and v passing through at least one node, say w making $\mathrm{str}(w) \geq 1$, which a contradiction. Hence, u, v are adjacent in G. Therefore, G is complete.

Conversely, suppose that the graph G is complete. Then by Corollary 2.4, it follows that $\mathbb{M}(G) = 0$. □

Proposition 2.6. *For the complete bipartite $K_{m,n}$,*

$$\mathbb{M}(K_{m,n}) = \frac{mn}{4}[n^2(n-1)^2 + m^2(m-1)^2 + mn(n-1)(m-1)].$$

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,

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

and

$$\mathrm{str}(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \leq j \leq n. \tag{2.6}$$

Using (2.5) and (2.6) in the Definition 2.2, we have

$$\begin{aligned}
\mathbb{M}(K_{m,n}) &= \sum_{uv \in E(G)} [\mathrm{str}(u)^2 + \mathrm{str}(v)^2 + \mathrm{str}(u)\,\mathrm{str}(v)] \\
&= \sum_{1 \leq i \leq m,\ 1 \leq j \leq n} [\mathrm{str}(v_i)^2 + \mathrm{str}(u_j)^2 + \mathrm{str}(v_i)\,\mathrm{str}(u_j)] \\
&= \sum_{1 \leq i \leq m,\ 1 \leq j \leq n} \left[\frac{n^2(n-1)^2}{4} + \frac{m^2(m-1)^2}{4} + \frac{n(n-1)}{2} \cdot \frac{m(m-1)}{2}\right] \\
&= \frac{mn}{4}[n^2(n-1)^2 + m^2(m-1)^2 + mn(n-1)(m-1)].
\end{aligned}$$

□

Proposition 2.7. *If $G = (V, E)$ is a k-stress regular graph, then*

$$\mathbb{M}(G) = 3k^2|E|.$$

Proof. Suppose that G is a k-stress regular graph. Then

$$\mathrm{str}(v) = k \text{ for all } v \in V(G).$$

By the Definition 2.2, we have

$$\begin{aligned}
\mathbb{M}(G) &= \sum_{uv \in E(G)} \mathrm{str}(u)^2 + \mathrm{str}(v)^2 + \mathrm{str}(u)\,\mathrm{str}(v) \\
&= \sum_{uv \in E(G)} k^2 + k^2 + k \cdot k \\
&= 3k^2|E|.
\end{aligned}$$

□

Corollary 2.8. *For a cycle C_n,*

$$\mathbb{M}(C_n) = \begin{cases} \dfrac{3n(n-1)^2(n-3)^2}{64}, & \text{if } n \text{ is odd} \\ \dfrac{3n^3(n-2)^2}{64}, & \text{if } n \text{ is even.} \end{cases}$$

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

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

Hence C_n is

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

Since C_n has n nodes and n edges, by the Proposition 2.7, we have

$$\mathbb{M}(C_n) = 3n \times \begin{cases} \dfrac{(n-1)^2(n-3)^2}{64}, & \text{if } n \text{ is odd} \\ \dfrac{n^2(n-2)^2}{64}, & \text{if } n \text{ is even.} \end{cases}$$

$$= \begin{cases} \dfrac{3n(n-1)^2(n-3)^2}{64}, & \text{if } n \text{ is odd} \\ \dfrac{3n^3(n-2)^2}{64}, & \text{if } n \text{ is even.} \end{cases}$$

□

Proposition 2.9. *Let T be a tree on n nodes. Then*

$$\mathbb{M}(T) = \sum_{uv \in J} \left[\left(\sum_{1 \le i < j \le m(u)} |C_i^u||C_j^u| \right)^2 + \left(\sum_{1 \le i < j \le m(v)} |C_i^v||C_j^v| \right)^2 + \sum_{1 \le i < j \le m(u)} |C_i^u||C_j^u| \sum_{1 \le i < j \le m(v)} |C_i^v||C_j^v| \right] + \sum_{w \in Q} \sum_{1 \le i < j \le m(w)} |C_i^w||C_j^w|,$$

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

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

$$\operatorname{str}(v) = \sum_{1 \le i < j \le m} |C_i^v||C_j^v| \tag{2.7}$$

Let J denotes the set of internal(non-pendant) edges, and P denotes pendant edges and Q denotes the set of all nodes adjacent to pendent nodes in T. Then using (2.7) in the Definition 2.2, we have

$$\mathbb{M}(T) = \sum_{uv \in J} [\operatorname{str}(u)^2 + \operatorname{str}(v)^2 + \operatorname{str}(u)\operatorname{str}(v)]$$

$$+\sum_{uv\in P}[\operatorname{str}(u)^2+\operatorname{str}(v)^2+\operatorname{str}(u)\operatorname{str}(v)]$$

$$=\sum_{uv\in J}[\operatorname{str}(u)^2+\operatorname{str}(v)^2+\operatorname{str}(u)\operatorname{str}(v)]+\sum_{w\in Q}\operatorname{str}(w)$$

$$=\sum_{uv\in J}\Bigg[\Bigg(\sum_{1\le i<j\le m(u)}|C_i^u||C_j^u|\Bigg)^2+\Bigg(\sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\Bigg)^2 + \sum_{1\le i<j\le m(u)}|C_i^u||C_j^u|\sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\Bigg] + \sum_{w\in Q}\sum_{1\le i<j\le m(w)}|C_i^w||C_j^w|.$$

□

Corollary 2.10. *For the path P_n on n nodes*

$$\mathbb{M}(P_n)=\sum_{i=1}^{n-1}[(i-1)^2(n-i)^2+i^2(n-i-1)^2+i(i-1)(n-i)(n-i-1)].$$

Proof. The proof of this corollary follows by above Proposition 2.9. We follow the proof of the Proposition 2.9 to compute the index. Let P_n be the path with node sequence $v_1, v_2, \ldots, v_n$ (shown in Figure 1).

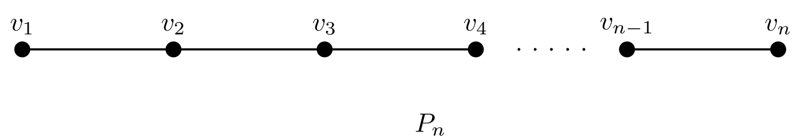

FIGURE 1. The path P_n on n nodes.

We have,

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

Then

$$\mathbb{M}(P_n)=\sum_{uv\in E(P_n)}[\operatorname{str}(u)^2+\operatorname{str}(v)^2+\operatorname{str}(u)\operatorname{str}(v)]$$

$$=\sum_{i=1}^{n-1}\operatorname{str}(v_i)^2+\operatorname{str}(v_{i+1})^2+\operatorname{str}(v_i)\operatorname{str}(v_{i+1})$$

$$=\sum_{i=1}^{n-1}[(i-1)^2(n-i)^2+i^2(n-i-1)^2+i(i-1)(n-i)(n-i-1)].$$

□

Proposition 2.11. *Let $Wd(n,m)$ denotes the windmill graph constructed for $n\ge 2$ and $m\ge 2$ by joining m copies of the complete graph K_n at a shared universal node v. Then*

$$\mathbb{M}(Wd(n,m))=\frac{m^3(m-1)^2(n-1)^5}{4}.$$

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

$$\mathbb{M}(F_k) = 8k^3(k-1)^2.$$

Proof. Clearly the stress of any node other than universal node is zero in $Wd(n,m)$, because neighbors of that node induces a complete subgraph of $Wd(n,m)$. Also, since there are m copies of K_n in $Wd(n,m)$ and their nodes are adjacent to v, it follows that, the only geodesics passing through v are of length 2 only. So, $\mathrm{str}(v) = \dfrac{m(m-1)(n-1)^2}{2}$. Note that there are $m(n-1)$ edges incident on v and the edges that are not incident on v have end nodes of stress zero. Hence by the Definition 2.2, we have

$$\begin{aligned}\mathbb{M}(Wd(n,m)) &= m(n-1)\,\mathrm{str}(v)^2 \\ &= m(n-1)\left[\frac{m(m-1)(n-1)^2}{2}\right]^2 \\ &= \frac{m^3(m-1)^2(n-1)^5}{4}\end{aligned}$$

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

$$\mathbb{M}(F_k) = \frac{k^3(k-1)^2(3-1)^5}{4} = 8k^3(k-1)^2.$$

□

3. A QSPR Analysis for Modified K-T Stress Index

In this section, a QSPR analysis is carried for Modified K-T stress index of chemical structures (molecular graphs) and physical properties of lower alkanes and linear regression models are presented.

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 are given in Table 1 along with the Modified K-T stress index of chemical structures (molecular graphs). The numerical values in columns 3 to 9 of the Table 1 are obtained from [27] (the same can be referred in [8]).

Table 1. Modified K-T stress index and values of the physical properties of considered low alkanes

Alkane	$\mathbb{M}$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	92	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	108	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	144	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	292	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	317	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	320	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	392	49.7	132.7	29.93	27.7	216.2	30.7	16.3

2,3-Dimethylbutane	343	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	742	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	776	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	774	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylpentane	762	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	890	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	810	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	810	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	906	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	926	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	1624	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	1667	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	1652	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	1639	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	1596	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	1865	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	1460	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	1695	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	1710	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	1832	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	1684	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	1643	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	1836	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	1566	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	1863	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	2556	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	1731	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	3192	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	3244	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	3208	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	3166	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	3076	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	2302	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	3436	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	3222	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	3218	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	3211	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	3296	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	3424	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	3188	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	3224	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	3404	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	3070	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	3128	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	3380	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	3100	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	3419	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	3452	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	3488	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	3463	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	3244	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	3274	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	3476	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	3450	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	3368	146.2	170.2	43.11	43.4	342.8	26.94	23.75

2,2-Dimethyl-3-ethylpentane	3440	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	3332	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	3128	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	3683	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	2943	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	3680	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	5022	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Regression Models. An investigation was conducted with a linear regression model

$$P = A + B \cdot \mathbb{M}$$

where P = Physical property and $\mathbb{M}$ =Modified K-T Stress Index, using Table 1.

The computed values of correlation coefficient r, its square r^2, standard error (se), t-value and p-value are presented in Table 2 followed by the linear regression models.

TABLE 2. r,r^2, se, t and p for the physical properties (P) and Modified K-T stress index

P	r	r^2	se	t	p
bp	0.881	0.776	(3.7876) (0.0015)	(16.828) (15.248)	($9.359E-26$) ($1.799E-23$)
mv	0.911	0.831	(1.8195) (0.0007)	(73.417) (18.129)	($9.443E-66$) ($1.548E-27$)
mr	0.928	0.862	(0.5010) (0.0002)	(60.839) (20.398)	($2.309E-60$) ($1.895E-30$)
hv	0.857	0.735	(0.7065) (0.0003)	(42.898) (13.638)	($1.883E-50$) ($5.258E-21$)
ct	0.881	0.776	(4.6071) (0.0018)	(49.802) (15.233)	($1.156E-54$) ($1.894E-23$)
cp	−0.773	0.597	(0.4258) (0.0002)	(70.545) (−9.962)	($1.324E-64$) ($7.492E-15$)
st	0.798	0.637	(0.3020) (0.0001)	(60.956) (9.912)	($2.090E-58$) ($1.495E-14$)

For boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes, the linear regression models are given below:

$$bp = 63.7387 + 0.0226 \cdot \mathbb{M} \quad (3.1)$$

$$mv = 133.5839 + 0.0129 \cdot \mathbb{M} \quad (3.2)$$

$$mr = 30.4828 + 0.0040 \cdot \mathbb{M} \quad (3.3)$$

$$hv = 30.3067 + 0.0038 \cdot \mathbb{M} \quad (3.4)$$

$$ct = 229.4426 + 0.0275 \cdot \mathbb{M} \quad (3.5)$$

$$cp = 30.0344 - 0.0017 \cdot \mathbb{M} \quad (3.6)$$

$$st = 18.4103 + 0.0011 \cdot \mathbb{M} \quad (3.7)$$

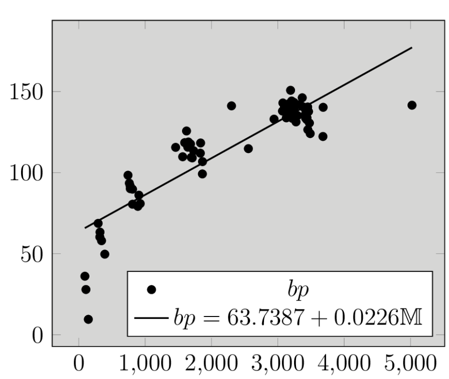

FIGURE 1. Model for bp

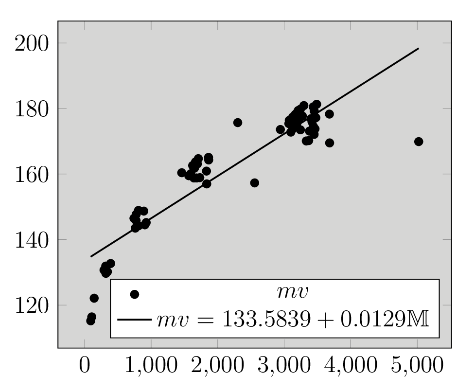

FIGURE 2. Model for mv

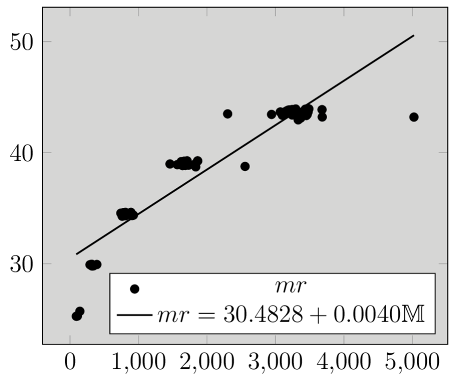

FIGURE 3. Model for *mr*

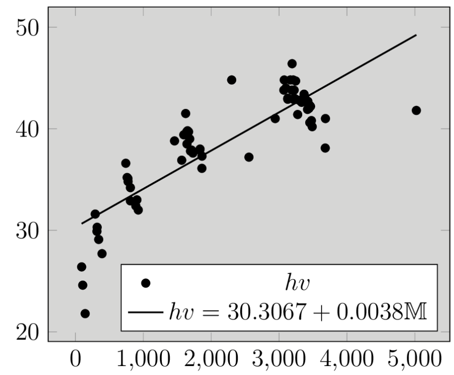

FIGURE 4. Model for *hv*

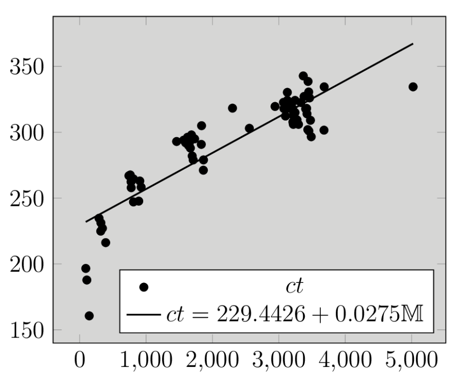

FIGURE 5. Model for *ct*

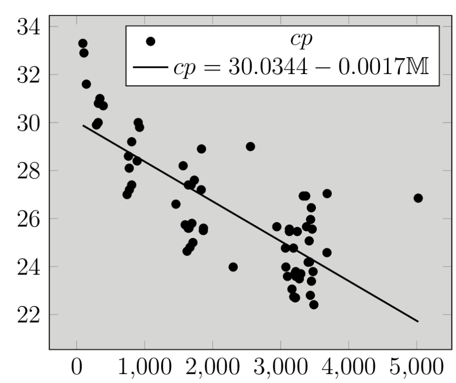

FIGURE 6. Model for *cp*

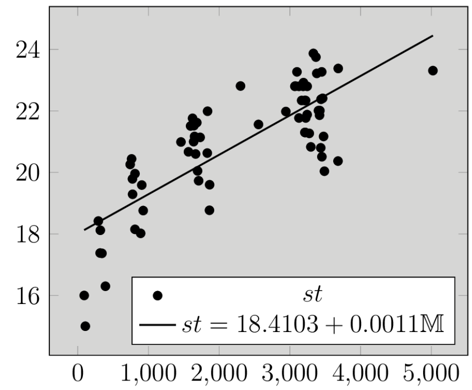

FIGURE 7. Model for st

From the Table 2, it follows that the linear regression models (3.1)-(3.5) can be used to make predictions.

Conclusion. In this paper, a novel topological index for graphs has been introduced, namely, Modified K-T stress index. Further, we established some inequalities, proved some results and computed the Modified K-T stress index for some standard graphs. Modified K-T stress index can be used as a predictive measure for physical properties of low alkanes. It will be interesting to explore further properties of Modified K-T stress index.

Acknowledgement. The authors would like to thank the anonymous reviewers for their comments and suggestions.

References

1. Bhargava, K., Dattatreya, N. N. and Rajendra, R.: On stress of a vertex in a graph, *Palest. J. Math.*, **12**(3) (2023), 15—25.
2. Gowramma, H. M., Siva Kota Reddy, P., Kim, T. and Rajendra, R.: Taekyun Kim α-Index of Graphs, *Bol. Soc. Parana. Mat. (3)*, accepted for publication.
3. Gowramma, H. M., Siva Kota Reddy, P., Kim, T. and Rajendra, R.: Taekyun Kim Stress Power α-Index, *Bol. Soc. Parana. Mat. (3)*, accepted for publication.
4. Harary, F.: *Graph Theory*, Addison Wesley, Reading, Mass, 1972.
5. Hemavathi, P. S., Lokesha, V., Manjunath, M., Siva Kota Reddy, P. and Shruti, R.: Topological Aspects of Boron Triangular Nanotube And Boron-α Nanotube, *Vladikavkaz Math. J*, **22**(1) (2020), 66–77.
6. Indhumathy, M., Arumugam, S., Baths, V. and Singh, T.: Graph theoretic concepts in the study of biological networks, *Springer Proc. Math. Stat.*, **186** (2016), 187–200.
7. Mahesh, K. B., Rajendra, R. and Siva Kota Reddy, P.: Square Root Stress Sum Index for Graphs, *Proyecciones*, **40**(4) (2021), 927–937.
8. Needham, D. E., Wei, I. C. and Seybold, P. G.: Molecular modeling of the physical properties of alkanes, *Journal of the American Chemical Society*, **110**(13) (1988), 4186—4194.
9. Pinto, R. M., Rajendra, R., Siva Kota Reddy, P. and Cangul, I. N.: A QSPR Analysis for Physical Properties of Lower Alkanes Involving Peripheral Wiener Index, *Montes Taurus J. Pure Appl. Math.*, **4**(2) (2022), 81—85.
10. Prakasha, K. N., Siva Kota Reddy, P. and Cangul, I. N.: Atom-Bond-Connectivity Index of Certain Graphs, *TWMS J. App. Eng. Math.*, **13**(2) (2023), 400–408.

11. Rajendra, R., Mahesh, K. B. and Siva Kota Reddy, P.: Mahesh Inverse Tension Index for Graphs, *Adv. Math., Sci. J.*, 9(12) (2020), 10163–10170.
12. Rajendra, R., Siva Kota Reddy, P. and Cangul, I. N.: Stress indices of graphs, *Adv. Stud. Contemp. Math. (Kyungshang)*, **31**(2) (2021), 163–173.
13. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N.: Tosha Index for Graphs, *Proc. Jangjeon Math. Soc.*, **24**(1) (2021), 141–147.
14. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N.: Rest of a vertex in a graph, *Adv. Math., Sci. J.*, **10**(2) (2021), 697–704.
15. Rajendra, R., Siva Kota Reddy, P., Mahesh, K.B. and Harshavardhana, C. N.: Richness of a Vertex in a Graph, *South East Asian J. Math. Math. Sci.*, **18**(2) (2022), 149–160.
16. Rajendra, R., Bhargava, K., Shubhalakshmi, D. and Siva Kota Reddy, P.: Peripheral Harary Index of Graphs, *Palest. J. Math.*, **11**(3) (2022), 323–336.
17. Rajendra, R., Siva Kota Reddy, P. and Prabhavathi, M.: Computation of Wiener Index, Reciprocal Wiener index and Peripheral Wiener Index Using Adjacency Matrix, *South East Asian J. Math. Math. Sci.*, **18**(3) (2022), 275–282.
18. Rajendra, R., Siva Kota Reddy, P., Harshavardhana, C. N., Aishwarya, S. V. and Chandrashekara, B. M.: Chelo Index for graphs, *South East Asian J. Math. Math. Sci.*, **19**(1) (2023), 175–188.
19. Rajendra, R., Siva Kota Reddy, P., Harshavardhana, C. N., and Alloush, Khaled A. A.: Squares Stress Sum Index for Graphs, *Proc. Jangjeon Math. Soc.*, **26**(4) (2023), 483–493.
20. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N.: Stress-Difference Index for Graphs, *Bol. Soc. Parana. Mat. (3)*, **42** (2024), 1–10.
21. Shannon, P., Markiel, A., Ozier, O., Baliga, N. S., Wang, J. T., Ramage, D., Amin, N., Schwikowski, B. and Ideker, T.: Cytoscape: A Software Environment for Integrated Models of Biomolecular Interaction Networks, *Genome Research*, **13**(11) (2003), 2498-–2504.
22. Shanthakumari, Y., Siva Kota Reddy, P., Lokesha, V. and Hemavathi, P. S.: Topological Aspects of Boron Triangular Nanotube and Boron-Nanotube-II, *South East Asian J. Math. Math. Sci.*, **16**(3) (2020), 145–156.
23. Shimbel, A.: Structural Parameters of Communication Networks, *Bulletin of Mathematical Biophysics*, **15** (1953), 501–507.
24. Siva Kota Reddy, P., Prakasha, K. N. and Cangul, I. N.: Randić Type Hadi Index of Graphs, *Trans. Natl. Acad. Sci. Azerb. Ser. Phys.-Tech. Math. Sci. Mathematics*, **40**(4) (2020), 175–181.
25. Siva Kota Reddy, P. and Somashekar, P.: Sombor Stress Index for Graphs, *Proc. Jangjeon Math. Soc.*, **28**(1) (2025), to appear.
26. Somashekar, P. and Siva Kota Reddy, P.: Kashvi-Tosha Stress Index for Graphs, Communicated for Publication.
27. Xu, K., Das, K. C. and Trinajstic, N.: *The Harary Index of a Graph*, Heidelberg, Springer, 2015.

Howida Adel AlFran: Department of Mathematics, AL-Leith University College, Umm Al-Qura University, Kingdom of Saudi Arabia.
Email address: hafran@uqu.edu.sa

P. Somashekar: Department of Mathematics, FMaharani's Science College for Women (Autonomous), Mysuru-570 005, India.
Email address: somashekar2224@gmail.com

P. Siva Kota Reddy: Department of Mathematics, JSS Science and Technology University, Mysuru-570 006, India
Email address: pskreddy@jssstuniv.in; pskreddy@sjce.ac.in