Bol. Soc. Paran. Mat.
©SPM – E-ISSN-2175-1188
SPM: www.spm.uem.br/bspm

(3s.) **v. 2025 (43)** : 1–10.
ISSN-0037-8712
doi:10.5269/bspm.72273

Taekyun Kim Stress Power α-Index

H. M. Gowramma, P. Siva Kota Reddy, Taekyun Kim and R. Rajendra

ABSTRACT: In this study, we introduce the Taekyun Kim α-index, a novel topological index for graphs, where $\alpha \in \mathbb{R}$, which involves stresses and degrees of nodes. We calculate this index for a few common graphs and prove a few results. Further, a QSPR analysis is carried for Taekyun Kim 2-index and physical properties of lower alkanes and linear regression models have been provided.

Key Words: Graph, Neighborhood of a node, Stress of a node, Path, Geodesic, Topological index.

Contents

1. Introduction

For common terms and concepts in graph theory, we refer to Harary [2]'s textbook. The unconventional ideas will be provided when needed.

Let $G = (V, E)$ be a undirected graph that is finite and connected. If v is an internal node of a shortest path (also called geodesic) P in G, then we say that P passes through v. The symbol $\deg(v)$ indicates a node v's degree in G.

In 1953, Shimbel presented the idea of a node's stress in a network (graph) as a centrality metric [27]. Numerous fields, including psychology, sociology, and biology, have used this centrality metric (see, for example, [4,25]). The number of geodesics that travel through a node v in a graph G is its stress, and it is represented as $\mathrm{str}_G(v)$ or, in short, by $\mathrm{str}(v)$ if there is no chance of misunderstanding. We designate Θ_G as the highest stress among all of the nodes in G and θ_G as the smallest stress among all of the nodes in G.

K. Bhargava et al. have examined the ideas of total stress of a graph and stress regular graphs in [1]. A graph G is said to be k-stress regular if $\mathrm{str}(v) = k$, $\forall v \in V(G)$. The total stress of a graph G, denoted by $N_{\mathrm{str}}(G)$, is defined as

$$N_{\mathrm{str}}(G) = \sum_{v \in V} \mathrm{str}(v).$$

Raksha Poojary et al. [9,10] have studied the concept of total stress of G but by calling it as the stress of G.

A topological index (or connectivity index) of a chemical structure (molecular graph) is nothing but a (real) number that correlates given chemical structure with a physical property or chemical reactivity. Several topological indices have been explored for graphs with numerous applications in Chemistry [29,30], for instance, Wiener index, Harary index, Zagreb index etc.

Submitted May 20, 2024. Published June 25, 2024
2010 *Mathematics Subject Classification:* 05C05, 05C07, 05C30

R. Rajendra et al. [14] introduced the first and second stress indices of graphs which are stress based topological indices. These indices of a graph G are defined as follows:

$$\text{First stress index}: \mathcal{S}_1(G) = \sum_{v \in V(G)} \text{str}(v)^2, \tag{1.1}$$

$$\text{Second stress index}: \mathcal{S}_2(G) = \sum_{uv \in E(G)} \text{str}(u) \cdot \text{str}(v). \tag{1.2}$$

R. Rajendra et al. [21] have carried a QSPR analysis for first stress index and demonstrated that first stress index can be used as predictive measure for physical properties of low alkanes. R. Rajendra et al. [24] have carried a QSPR analysis for total stress index and shown that the total stress index is also an useful topological index for predicting the physical properties of low alkanes. We recommend that the reader to study the publications [3,5,6,8,11-20,22-24,26,28] 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 $\mathcal{N}$ denotes the number of geodesics of length ≥ 2 in G. In section 2, we introduce a novel topological index namely, Taekyun Kim stress power α-index, which involves powers of stresses of nodes, where α is a positive real number. We observe that for $\alpha = 0, 1, 2$, the Taekyun Kims stress power α-index reduces to the order of graphs, total stress index and first stress index, respectively. In section 3, some inequalities are established, some results are obtained and for some standard graphs Taekyun Kims stress power α-index is computed. In section 4, we analyze the correlation between Taekyun Kim stress power α-index of chemical structures (molecular graphs) and physical properties of lower alkanes.

2. Taekyun Kim Stress Power α-Index

Definition 2.1 *The Taekyun Kim stress power α-index (or simply, TKSP α-index) $\mathcal{TKSP}_\alpha(G)$ of a graph (simple, connected) G is defined by*

$$\mathcal{TKSP}_\alpha(G) = \sum_{v \in V(G)} str(v)^\alpha \tag{2.1}$$

where α is a non-negative real number.

Observation. For any graph $G = (V, E)$, we have

$$\mathcal{TKSP}_0(G) = \sum_{v \in V(G)} \text{str}(v)^0 = |V|, \text{ the order of of } G,$$

$$\mathcal{TKSP}_1(G) = \sum_{v \in V(G)} \text{str}(v) = N_{\text{str}}(G), \text{ the total stress of } G \text{ (See [1])},$$

and

$$\mathcal{TKSP}_2(G) = \sum_{v \in V(G)} \text{str}(v)^2 = \mathcal{S}_1(G), \text{ the first stress index of } G \text{ (See [21])}.$$

3. Some Results

Proposition 3.1 *For any graph G,*

$$0 \leq \mathcal{TKSP}_\alpha(G) \leq |V|\mathcal{N}^\alpha \tag{3.1}$$

and

$$|V|\theta_G^\alpha \leq \mathcal{TKSP}_\alpha(G) \leq |V|\Theta_G^\alpha. \tag{3.2}$$

Proof: For any node v in G, we have $0 \leq \mathrm{str}(v) \leq \mathcal{N}$. Hence we have $0 \leq \mathrm{str}(v)^{\alpha} \leq \mathcal{N}^{\alpha}$ and so by Definition 2.1, the inequality (3.1) follows.

For any node v in G, $\theta_G \leq \mathrm{str}(v) \leq \Theta_G$. Using this inequality in Definition 2.1, we establish (3.2). □

Corollary 3.1 *Let G be a graph. If $\mathcal{N} = 0$ in G, then $\mathcal{TKSP}_{\alpha}(G) = 0$. In particular, for the complete graph K_n, $\mathcal{TKSP}_{\alpha}(K_n) = 0$.*

Proof: By Proposition 3.1, it follows that, if $\mathcal{N} = 0$, then $\mathcal{TKSP}_{\alpha}(G) = 0$. For K_n, $N = 0$ as there is no shortest path of length ≥ 2, and consequently, $\mathcal{TKSP}_{\alpha}(K_n) = 0$. □

Theorem 3.1 *Let G be a graph. Then, $\mathcal{TKSP}_{\alpha}(G) = 0$ iff G is a complete graph.*

Proof: Suppose that $\mathcal{TKSP}_{\alpha}(G) = 0$. Then it is evident from Definition 2.1 that $\mathrm{str}(x)^{\alpha} = 0, \forall x \in V(G)$ and hence $\mathrm{str}(x) = 0$, for all $x \in V(G)$. 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 is a contradiction. Hence, u, v are adjacent in G. Therefore, G is complete.

Conversely, suppose that the graph G is complete. Then by Corollary 3.1, $\mathcal{TKSP}_{\alpha}(G) = 0$. □

Proposition 3.2 *For the complete bipartite graph $K_{m,n}$,*

$$\mathcal{TKSP}_{\alpha}(K_{m,n}) = m\left[\frac{n(n-1)}{2}\right]^{\alpha} + n\left[\frac{m(m-1)}{2}\right]^{\alpha}.$$

Proof:

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

$$\mathrm{str}(v_i) = \frac{1}{2}n(n-1), \quad 1 \leq i \leq m \tag{3.3}$$

and

$$\mathrm{str}(u_j) = \frac{1}{2}m(m-1), \quad 1 \leq j \leq n. \tag{3.4}$$

Employing (3.3) and (3.4) in Definition 2.1, we have

$$\begin{aligned} \mathcal{TKSP}_{\alpha}(K_{m,n}) &= \sum_{i=1}^{m} \mathrm{str}(v_i)^{\alpha} + \sum_{j=1}^{n} \mathrm{str}(u_j)^{\alpha} \\ &= \sum_{j=1}^{m}\left[\frac{n(n-1)}{2}\right]^{\alpha} + \sum_{i=1}^{n}\left[\frac{m(m-1)}{2}\right]^{\alpha} \\ &= m\left[\frac{n(n-1)}{2}\right]^{\alpha} + n\left[\frac{m(m-1)}{2}\right]^{\alpha}. \end{aligned}$$

□

Proposition 3.3 *If G is a r-stress regular graph, then*

$$\mathcal{TKSP}_{\alpha}(G) = |V|r^{\alpha}.$$

Proof: Suppose that G is an r-stress regular graph. Then for any vertex x in G, $\text{str}(x) = r$. Using this fact in Definition 2.1, we have

$$\mathcal{TKSP}_\alpha(G) = \sum_{x \in V(G)} r^\alpha = |V| r^\alpha. \qquad \square$$

Corollary 3.2 *For a cycle C_n,*

$$\mathcal{TKSP}_\alpha(C_n) = \begin{cases} n\left[\dfrac{(n-1)(n-3)}{8}\right]^\alpha, & \text{when } n \text{ is odd;} \\ n\left[\dfrac{n(n-2)}{8}\right]^\alpha, & \text{when } n \text{ is even,} \end{cases}$$

Proof: In the cycle C_n, for any node v, we have

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

Therefore, the cycle C_n is

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

and so by Proposition 3.3, the result follows. $\square$

Proposition 3.4 *Let T be a tree on n nodes. Then*

$$\mathcal{TKSP}_\alpha(T) = \sum_{v \in I} \left[\sum_{1 \le i < j \le m} |C_i^v||C_j^v|\right]^\alpha,$$

where I is the collection of all internal (non-pendant) nodes in T and the collections $C_1^v, \ldots, C_m^v$ denote the node sets of the components of $T - v$ for an internal node v of degree $m = m(v)$.

Proof: Since a pendant node in T has 0 stress, we concentrate on internal nodes and to compute the TKSP α-index. Let v be an internal node of T of degree $m = m(v)$. Let $C_1^v, \ldots, C_m^v$ be the node sets of the components of $T - v$. As there is only one path between any two nodes in a tree, it is clear that

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

Hence by the Definition 2.1, we have

$$\mathcal{TKSP}_\alpha(T) = \sum_{v \in I} \left[\sum_{1 \le i < j \le m} |C_i^v||C_j^v|\right]^\alpha.$$

where I is the collection of all internal (non-pendant) nodes in T. $\square$

Corollary 3.3 *For path graph P_n on n nodes*

$$\mathcal{TKSP}_\alpha(P_n) = \sum_{i=2}^{n-1} [(i-1)(n-i)]^\alpha.$$

Proof:

Let P_n be the path graph on n nodes (shown in Figure 1) with node set $\{v_1, v_2, \ldots, v_n\}$.

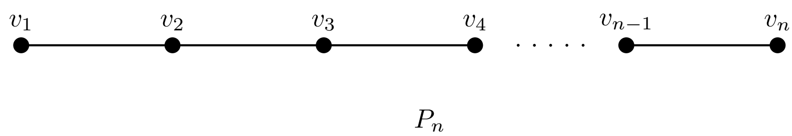

Figure 1: The path P_n on n nodes

We have, $\deg(v_i) = 2$, for $2 \leq i \leq n-1$ and

$$\text{str}(v_i) = \sum_{1 \leq i < j \leq 2} |C_i^{v_i}||C_j^{v_i}| = (i-1)(n-i), \text{ for } 2 \leq i \leq n-1.$$

Therefore, by Proposition 3.4, the result follows.

□

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 common node v.

Proposition 3.5 *For the windmill graph $Wd(n,m)$,*

$$\mathcal{TKSP}_\alpha(Wd(n,m)) = \left[\frac{m(m-1)(n-1)^2}{2}\right]^\alpha.$$

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

$$\mathcal{TKSP}_\alpha(F_k) = [2k(k-1)]^\alpha.$$

Proof: Any node other than the universal node has 0 stress in $Wd(n,m)$. The only shortest paths passing through universal node v are of length 2. So, $\text{str}(v) = \dfrac{m(m-1)(n-1)^2}{2}$ and by Definition 2.1, we have

$$\mathcal{TKSP}_\alpha(Wd(n,m)) = \left[\frac{m(m-1)(n-1)^2}{2}\right]^\alpha$$

As the friendship graph F_k on $2k+1$ nodes is the windmill $Wd(3,k)$, we have

$$\mathcal{TKSP}_\alpha(F_k) = \left[\frac{k(k-1)(3-1)^2}{2}\right]^\alpha = [2k(k-1)]^\alpha.$$

□

Proposition 3.6 *Let W_n denote the wheel graph on $n \geq 4$ nodes. Then*

$$\mathcal{TKSP}_\alpha(W_n) = \left[\frac{(n-1)(n-4)}{2}\right]^\alpha + (n-1) \times \begin{cases} \left[\dfrac{(n-2)(n-4)}{8}\right]^\alpha, & \text{if } n \text{ is even;} \\ \left[\dfrac{(n-1)(n-3)}{8}\right]^\alpha, & \text{if } n \text{ is odd.} \end{cases}$$

Proof: In W_n with $n \geq 4$, there are $n-1$ peripheral nodes and one central node, say v. Then

$$\text{str}(v) = \frac{(n-1)(n-4)}{2}. \tag{3.5}$$

Let q be a peripheral node. Note that v is adjacent to all the peripheral nodes in W_n. So, there is no shortest path passing through q containing v. Hence contributing nodes for str(q) are the remaining peripheral nodes. Let us denote the cycle $W_n - v$ (on $n-1$ nodes) by C_{n-1}. Then

$$\begin{aligned}
\mathrm{str}_{W_n}(q) &= \mathrm{str}_{W_n-v}(q) \\
&= \mathrm{str}_{C_{n-1}}(q) \\
&= \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n-1 \text{ is odd;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n-1 \text{ is even,} \end{cases} \\
&= \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.} \end{cases}
\end{aligned} \tag{3.6}$$

Let us denote the set of all the peripheral nodes in W_n by P. Then, using (3.5) and (3.6) in Definition 2.1, we have

$$\begin{aligned}
\mathcal{TKSP}_\alpha(W_n) &= \mathrm{str}(v)^\alpha + \sum_{q\in P} \mathrm{str}(q)^\alpha \\
&= \left[\frac{(n-1)(n-4)}{2}\right]^\alpha + (n-1) \times \begin{cases} \left[\dfrac{(n-2)(n-4)}{8}\right]^\alpha, & \text{if } n \text{ is even;} \\ \left[\dfrac{(n-1)(n-3)}{8}\right]^\alpha, & \text{if } n \text{ is odd.} \end{cases}
\end{aligned}$$

□

4. Correlation between TKSP α-index and physical properties of lower alkanes

As we observed in section 2, TKSP 0-index, TKSP 1-index and TKSP 2-index are respectively, order of the (molecular) graphs, total stress index and first stress index. In [30], it is discussed that the order of the (molecular) graphs i.e. the number of carbon atoms is a valuable descriptor for the structure–property modeling of lower alkanes. R. Rajendra et al. [24] have carried a QSPR analysis for total stress index and have shown that the total stress index is an useful topological index for predicting the physical properties of low alkanes. R. Rajendra et al. [21] have carried a QSPR analysis for first stress index and have shown that the total stress index is also an useful topological index for predicting the physical properties of low alkanes. In this section, we analyze the correlation between TKSP α-index of molecular graphs and physical properties of lower alkanes.

The TKSP 3-index of chemical structures (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 are given in Table 1. The numerical values in columns 3 to 9 of the Table 1 are obtained from Needham et al. [7] (the same data can be found in [30]). For the values of TKSP 1-index and TKSP 2-index of molecular graphs of lower alkanes one can refer [24] and [21], respectively.

Table 1: TKSP 3-index, boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes

Alkane	$\mathcal{TKSP}_3$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	118	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	152	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	216	9.5	122.1	25.72	21.8	160.6	31.6	

Hexane	560	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	623	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	640	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	793	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	686	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	2003	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	2095	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	2093	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	2103	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	2365	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	2185	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	2187	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	2447	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	2457	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	5888	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	6003	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	5904	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	5807	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	5744	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	6379	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	5922	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	6019	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	6118	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	6345	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	5920	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	5859	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	6480	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	1672	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	6434	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	10808	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	6037	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	14988	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	15114	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	14798	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	14376	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	14132	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	8581	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	15374	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	14502	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	14502	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	19494	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	15240	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	15050	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	14188	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	14608	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	14790	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	13872	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	14258	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	14924	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	13942	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	14762	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	15184	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	15500	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	14916	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	14312	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	14628	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	15176	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	14860	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	15196	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	14518	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	15050	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	13998	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	15436	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	11404	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	15760	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	15042	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Table 2: Correlation coefficient r between the physical properties (P) of lower alkanes and TKSP α-index for $\alpha = 0, 1, 2, 3$

P	$\mathcal{TKSP}_0$	$\mathcal{TKSP}_1$	$\mathcal{TKSP}_2$	$\mathcal{TKSP}_3$
bp	0.9493	0.9087	0.9025	0.8567
mv	0.9660	0.9340	0.9507	0.9013
mr	0.9979	0.9160	0.9442	0.9074
hv	0.9107	0.9435	0.9114	0.8504
ct	0.9053	0.8377	0.8625	0.8402
cp	−0.7429	−0.9349	−0.8841	−0.7939
st	0.7464	0.7117	0.7361	0.7613

We have computed the correlation coefficient between the physical properties of lower alkanes and TKSP α-index for $\alpha = 0, 1, 2, 3$ and are presented in Table 2. The numerical values in columns 2 and 3 of the Table 2 can be found in [21] and [24], respectively. The values of the correlation coefficient r in Table 2 reveals that TKSP α-index ($\alpha = 0, 1, 2, 3$) can be used for QSPR analysis and to propose regression models to make predictions of physical properties of lower alkanes.

Conclusion

We have introduced a novel topological index for graphs namely, Taekyun Kim stress power α-index (or simply, TKSP α-index) which involves stresses of nodes, where $\alpha \geq 0$. For $\alpha = 0, 1, 2$, it is respectively, order of graphs, total stress index and first stress index. TKSP α-index ($\alpha = 0, 1, 2, 3$) can be used as a predictive measure for physical properties of low alkanes. It will be interesting to explore the properties of TKSP α-index for various real values of α.

Acknowledgments

The constructive comments on this manuscript by anonymous reviewers are appreciated.

References

1. Bhargava, K., Dattatreya, N. N. and Rajendra, R., *On stress of a vertex in a graph*, Palest. J. Math., 12(3), 15–25, (2023).

2. Harary, F. , *Graph Theory*, Addison Wesley, Reading, Mass, (1972).

3. 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), 66-77, (2020).

4. Indhumathy, M., Arumugam, S., Baths, Veeky and Singh, Tarkeshwar, *Graph theoretic concepts in the study of biological networks*, Applied Analysis in Biological and Physical Sciences, Springer Proceedings in Mathematics & Statistics, 186, 187-200, (2016).

5. Lavanya, E., Sriraj, M. A. and Siva Kota Reddy, P., *Entropy Measures of $g - C_3N_5$ using Topological Indices*, Bol. Soc. Parana. Mat. (3), accepted for publication.

6. Mahesh, K. B., Rajendra, R. and Siva Kota Reddy, P., *Square Root Stress Sum Index for Graphs*, Proyecciones, 40(4), 927-937, (2021).

7. 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, 4186–4194, (1988).

8. 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), 81–85, (2022).

9. Poojary, R., Arathi Bhat, K., Arumugam, S. and Manjunatha Prasad, K., *The stress of a graph*, Commun. Comb. Optim., 8(1), 53-65, (2023).

10. Poojary, R., Arathi Bhat, K., Arumugam, S. and Manjunatha Prasad, K., *Stress of a graph and its computation*, AKCE Int. J. Graphs Comb., 20(2), 200-208, (2023).

11. 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), 400-408, (2023).

12. Rajendra, R, Mahesh, K. B., and Siva Kota Reddy, P., *Mahesh Inverse Tension Index for Graphs*, Adv. Math., Sci. J., 9(12), 10163-10170, (2020).

13. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Stress-Sum Index for Graphs*, Sci. Magna, 15(1), 94-103, (2020).

14. Rajendra, R., Siva Kota Reddy, P. and Cangul, I. N., *Stress indices of graphs*, Adv. Stud. Contemp. Math. (Kyungshang), 31(2), 163-173, (2021).

15. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Tosha Index for Graphs*, Proc. Jangjeon Math. Soc., 24(1), 141-147, (2021).

16. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Rest of a vertex in a graph*, Adv. Math., Sci. J., 10(2), 697-704, (2021).

17. 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), 149-160, (2022).

18. Rajendra, R., Bhargava, K., Shubhalakshmi, D. and Siva Kota Reddy, P., *Peripheral Harary Index of Graphs*, Palest. J. Math., 11(3), 323-336, (2022).

19. 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), 275-282, (2022).

20. 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), 175-188, (2023).

21. Rajendra, R., Siva Kota Reddy, P., Cangul, I. N. and Alloush, K. A. A, *A QSPR Analysis for Physical Properties of Lower Alkanes using First Stress Index*, European Chemical Bulletin, 12(10), 5810-5814, (2023).

22. Rajendra, R., Siva Kota Reddy, P., Harshavardhana, C. N. and Alloush, K. A. A, *Squares Stress Sum Index for Graphs*, Proc. Jangjeon Math. Soc., 26(4), 483-493, (2023).

23. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Stress-Difference Index for Graphs*, Bol. Soc. Parana. Mat. (3), 42 (2024), 1-10.

24. Rajendra, R., Siva Kota Reddy, P., Cangul, I. N. and Gowramma, H. M., *Total Stress as a Topological Index*, Submitted for publication.

25. Shannon, P., Markiel, A., Ozier, O., Baliga, N. S., Wang, J. T., Ramage, D., Amin, N., Schwikowski, B., and Idekar, T., *Cytoscape: a software environment for integrated models of biomolecular interaction networks*, Genome Res., 13(11), 2498–2504, (2003).

26. 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), 145-156, (2020).

27. Shimbel, A., *Structural Parameters of Communication Networks*, *Bull. Math. Biol.*, 15, 501-507, (1953).

28. 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), 175-181, (2020).

29. Wiener, H., *Structural determination of paraffin boiling points*, J. Amer. Chem. Soc., 69(1), 17-20, (1947).

30. Xu, K., Das, K. C., and Trinajstic, N., *The Harary Index of a Graph*, Springer-Verlag, Berlin, Heidelberg, (2015).

H. Mangala Gowramma (Corresponding author)
Department of Mathematics
Siddaganga Institute of Technology
Tumakuru-572103, India
Affiliated to Visvesvaraya Technological University
Belagavi-590 018, India.
E-mail address: rgowrir@yahoo.com

and

P. Siva Kota Reddy
Department of Mathematics
JSS Science and Technology University
Mysuru–570 006, India.
E-mail address: pskreddy@jssstuniv.in

and

Taekyun Kim
Department of Mathematics
Kwangwoon University

Seoul-139-701, Republic of Korea.
E-mail address: tkkim@kw.ac.kr

and

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