Proceedings of the Jangjeon Mathematical Society
26 (2023), No. 4, pp. 483 - 493
www.jangjeon.or.kr
http://dx.doi.org/10.17777/pjms2023.26.4.483

SQUARES STRESS SUM INDEX FOR GRAPHS

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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. In this paper, we introduce a new topological index for graphs called squares stress sum index using stresses of vertices. We establish some inequalities, prove some results and compute squares stress sum index for some standard graphs. Further, a QSPR analysis is carried for squares stress sum index of molecular graphs and physical properties of lower alkanes and linear regression models are presented for some physical properties.

2020 MATHEMATICS SUBJECT CLASSIFICATION. 05C09.

KEYWORDS AND PHRASES: Graph, Neighborhood of a vertex, Stress of a vertex, Geodesic, Stress, Topological index.

1. INTRODUCTION

For standard terminology and notion in graph theory, we follow the textbook 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 [15]. This centrality measure has applications in biology, sociology, psychology, etc., (See [3,14]). The stress of a vertex v in a graph G, denoted by $\text{str}_G(v)$ $\text{str}(v)$, 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 $\text{str}(v) = k$ for all $v \in V(G)$. For new topological indices, we suggest the reader to refer the papers [4, 6–13].

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[2]Date of Manuscript Submission: February 02, 2023

Rajendra *et al.* [8] have introduced two topological indices of for graphs called first stress index and second stress index, using stresses of vertices. 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

$$\mathcal{S}_1(G) = \sum_{v \in V(G)} \mathrm{str}(v)^2 \tag{1}$$

$$\mathcal{S}_2(G) = \sum_{uv \in E(G)} \mathrm{str}(u)\,\mathrm{str}(v). \tag{2}$$

In this paper, we introduce such topological index for graphs using stress on vertices called squares stress sum index. Further, we establish some inequalities and compute squares stress sum index for some standard graphs. Also, a QSPR analysis is carried for squares stress sum index of molecular graphs and physical properties of lower alkanes and linear regression models are presented for boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions.

2. Squares Stress Sum Index for Graphs

Definition 2.1. *The squares stress sum index $\mathcal{SSS}(G)$ of a simple graph G is defined as*

$$\mathcal{SSS}(G) = \sum_{uv \in E(G)} str(u)^2 + str(v)^2 \tag{3}$$

Observation: From the Definition 2.1, it follows that, for any graph G,

$$2m\theta_G^2 \le \mathcal{SSS}(G) \le 2m\Theta_G^2$$

where m is the number of edges in G.

Example 2.1. *Consider the graph G given in Figure 1.*

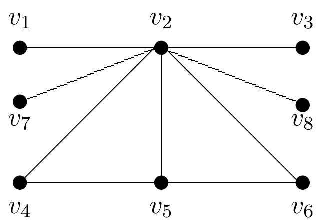

Figure 1. A graph G

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 squares stress sum index of G is:

$\mathcal{SSS}(G) = (str(v_2)^2 + str(v_1)^2) + (str(v_2)^2 + str(v_3)^2) + (str(v_2)^2 + str(v_7)^2)$

$$
\begin{aligned}
&+ (str(v_2)^2 + str(v_8)^2) + (str(v_2)^2 + str(v_4)^2) + (str(v_2)^2 + str(v_5)^2)\\
&+ (str(v_2)^2 + str(v_6)^2) + (str(v_4)^2 + str(v_5)^2) + (str(v_5)^2 + str(v_6))^2\\
=&(19^2 + 0^2) + (19^2 + 0^2) + (19^2 + 0^2) + (19^2 + 0^2) + (19^2 + 0^2)\\
&+ (19^2 + 1^2) + (19^2 + 0^2) + (0^2 + 1^2) + (1^2 + 0^2)\\
=&136.
\end{aligned}
$$

Proposition 2.2. *Let N be the number of geodesics of length ≥ 2 in a graph G. Then*

$$0 \leq \mathcal{SSS}(G) \leq 2N^2(|E| - t), \tag{4}$$

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, $0 \leq \text{str}(v) \leq N$. Hence by the Definition 2.1, we have

$$0 \leq \mathcal{SSS}(G) \leq 2N^2(|E| - t), \tag{5}$$

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

Corollary 2.3. *If there is no geodesic of length ≥ 2 in a graph G, then $\mathcal{SSS}(G) = 0$. Moreover, for a complete graph K_n, $\mathcal{SSS}(K_n) = 0$.*

Proof. If there is no geodesic of length ≥ 2 in a graph G, then $N = 0$. Hence, by the Proposition 2.2, we have $\mathcal{SSS}(G) = 0$.

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

Theorem 2.4. *For a graph G, $\mathcal{SSS}(G) = 0$ if and only if neighbours of every vertex induce a complete subgraph of G.*

Proof. Suppose that $\mathcal{SSS}(G) = 0$. Then by the Definition 2.1, $\text{str}(u)^2 + \text{str}(v)^2 = 0$, $\forall uv \in E(G)$. Hence $\text{str}(v) = 0$, $\forall v \in V(G)$. Let $v \in V(G)$. We need to show that neighbors of v induce a complete subgraph of G. If v is a pendant vertex, then there is nothing to prove. Suppose that v is not a pendant vertex. We claim that any two neighbouring vertices are adjacent in G. If there are two neighbours u and w of v that are not adjacent in G, then uvw is a graph geodesic passing through v, which implies $\text{str}(v) \geq 1$, a contradiction. Hence our claim holds. Thus neighbours of v induce a complete subgraph of G. Since v is arbitrary in $V(G)$, the neighbours of every vertex induce a complete subgraph of G.

Conversely, suppose that neighbours of every vertex in G induce a complete subgraph of G. Let $v \in V(G)$. Since neighbors of v induce a complete subgraph of G, any two neighbouring vertices are adjacent and so there is no geodesic of length ≥ 2 passing through v. Since v is an arbitrary vertex in G, by the Corollary 2.3, it follows that $\mathcal{SSS}(G) = 0$. □

Proposition 2.5. *For the complete bipartite $K_{m,n}$,*

$$\mathcal{SSS}(K_{m,n}) = \frac{mn}{4}\left[n^2(n-1)^2 + m^2(m-1)^2\right].$$

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,

$$\text{str}(v_i) = \frac{n(n-1)}{2} \text{ for } 1 \leq i \leq m \tag{6}$$

and

$$\text{str}(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \leq j \leq n. \tag{7}$$

Using (6) and (7) in the Definition 2.1, we have

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

□

Proposition 2.6. *If $G = (V, E)$ is a k-stress regular graph, then*

$$\mathcal{SSS}(G) = 2k^2|E|.$$

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

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

By the Definition 2.1, we have

$$\begin{aligned}
\mathcal{SSS}(G) &= \sum_{uv \in E(G)} \text{str}(u)^2 + \text{str}(v)^2 \\
&= \sum_{uv \in E(G)} k^2 + k^2 \\
&= 2k^2|E|.
\end{aligned}$$

□

Corollary 2.7. *For a cycle C_n,*

$$\mathcal{SSS}(C_n) == \begin{cases} \dfrac{n(n-1)^2(n-3)^2}{32}, & \text{if } n \text{ is odd} \\[2mm] \dfrac{n^3(n-2)}{32}, & \text{if } n \text{ is even.} \end{cases}$$

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

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

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 vertices and n edges, by the Proposition 2.6, we have

$$\begin{aligned} \mathcal{SSS}(C_n) &= 2n \times \begin{cases} \left(\dfrac{(n-1)(n-3)}{8}\right)^2, & \text{if } n \text{ is odd} \\ \left(\dfrac{n(n-2)}{8}\right)^2, & \text{if } n \text{ is even.} \end{cases} \\ &= \begin{cases} \dfrac{n(n-1)^2(n-3)^2}{32}, & \text{if } n \text{ is odd} \\ \dfrac{n^3(n-2)}{32}, & \text{if } n \text{ is even.} \end{cases} \end{aligned}$$

□

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

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

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,

$$\text{str}(v) = \sum_{1\le i<j\le m}|C_i^v||C_j^v| \tag{8}$$

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 (8) in the Definition 2.1 ((3)), we have

$$\begin{aligned} \mathcal{SSS}(T) &= \sum_{uv\in J}\text{str}(u)^2+\text{str}(v)^2 + \sum_{uv\in P}\text{str}(u)^2+\text{str}(v)^2 \\ &= \sum_{uv\in J}\text{str}(u)^2+\text{str}(v)^2 + \sum_{w\in Q}\text{str}(w)^2 \\ &= \sum_{uv\in J}\left[\left(\sum_{1\le i<j\le m(u)}|C_i^u||C_j^u|\right)^2 + \left(\sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\right)^2\right] \end{aligned}$$

$$+\sum_{w\in Q}\left(\sum_{1\le i<j\le m(w)}|C_i^w||C_j^w|\right)^2.$$

□

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

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

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).

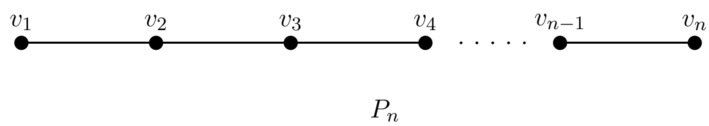

FIGURE 2. The path P_n on n vertices.

We have,

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

Then

$$\begin{aligned}\mathcal{SSS}(P_n)&=\sum_{uv\in E(P_n)}\mathrm{str}(u)^2+\mathrm{str}(v)^2\\&=\sum_{i=1}^{n-1}\mathrm{str}(v_i)^2+\mathrm{str}(v_{i+1})^2\\&=\sum_{i=1}^{n-1}[(i-1)^2(n-i)^2+i^2(n-i-1)^2].\end{aligned}$$

□

Proposition 2.10. *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 vertex v. Then*

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

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

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

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, $\mathrm{str}(v)=\dfrac{m(m-1)(n-1)^2}{2}$. Note that there are

$m(n-1)$ edges incident on v and the edges that are not incident on v have end vertices of stress zero. Hence by the Definition 2.1, we have

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

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

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

□

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

$$\mathcal{SSS}(W_n) = \begin{cases}\dfrac{(n-1)\,(n-4)^2\,(n(19n-44)+28)}{64}, & \textit{if } n \textit{ is even;}\\ \dfrac{(n-1)^3\,(n(19n-146)+283)}{64}, & \textit{if } n \textit{ is odd.}\end{cases}$$

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

$$\mathrm{str}(v) = \frac{(n-1)(n-4)}{2} \tag{9}$$

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 $\mathrm{str}(p)$ are the rest peripheral vertices. So, by denoting the cycle $W_n - p$ (on $n-1$ vertices) by C_{n-1}, we have

$$\begin{aligned}\mathrm{str}_{W_n}(p) &= \mathrm{str}_{W_n - v}(p)\\ &= \mathrm{str}_{C_{n-1}}(p)\\ &= \begin{cases}\dfrac{(n-2)(n-4)}{8}, & \text{if } n-1 \text{ is odd;}\\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n-1 \text{ is even,}\end{cases}\\ &= \begin{cases}\dfrac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;}\\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.}\end{cases} \qquad (10)\end{aligned}$$

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 (9) and (10) in the Definition 2.1, we have

$$\begin{aligned}\mathcal{SSS}(W_n) &= \sum_{xy\in R}[\mathrm{str}(x)^2 + \mathrm{str}(y)^2] + \sum_{xy\in Q}[\mathrm{str}(x)^2 + \mathrm{str}(y)^2]\\ &= (n-1)[\mathrm{str}(v)^2 + \mathrm{str}(p)^2] + (n-1)\cdot 2\cdot \mathrm{str}(p)^2\end{aligned}$$

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

$$+2(n-1)\times\begin{cases}\left(\frac{(n-2)(n-4)}{8}\right)^2, & \text{if } n \text{ is even;}\\ \left(\frac{(n-1)(n-3)}{8}\right)^2, & \text{if } n \text{ is odd.}\end{cases}$$

$$=\begin{cases}\frac{(n-1)\,(n-4)^2\,(n(19n-44)+28)}{64}, & \text{if } n \text{ is even;}\\ \frac{(n-1)^3\,(n(19n-146)+283)}{64}, & \text{if } n \text{ is odd.}\end{cases}$$

□

3. A QSPR Analysis

We carry a QSPR analysis for some physical properties of lower alkanes with squares stress sum index of molecular graphs. Table 1 gives the squares stress sum index $\mathcal{SSS}(G)$ 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. [5] (the same values can be found in [16]).

Table 1. Squares stress sum index, boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes

Alkane	$\mathcal{SSS}(G)$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dy\ cm^{-1}}$
Pentane	68	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	93	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	208	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	251	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	256	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	356	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	294	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	518	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	583	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	591	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	1184	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	754	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	656	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	648	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	607	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	819	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	1120	125.7	162.6	39.19	41.5	296.2	24.64	21.76

2-Methylheptane	1211	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	1220	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	1219	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	1184	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	1460	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	1310	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	1311	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	1302	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	1500	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	1320	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	1275	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	1512	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	1335	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	1551	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	2199	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	1401	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	2184	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	2305	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	2313	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	2305	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	2232	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	1638	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	2644	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	2426	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	2426	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	2434	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	2426	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	2698	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	2434	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	2442	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	2708	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	2314	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	2353	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	2698	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	2361	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	2765	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	2773	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	2765	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	2829	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	2555	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	2683	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	2819	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	2827	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	2696	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	2692	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	2819	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	2435	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	3158	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	2478	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	3104	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	2950	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Regression Models. Using Table 1, a study was carried out with a linear regression model

$$P = A + B \cdot \mathcal{SSS}(G)$$

where P = Physical property and $\mathcal{SSS}(G)$ = squares stress sum index. The correlation coefficient r, its square r^2, standard error (se), t-value and p-value are computed and tabulated in Table 2 followed by linear regression models.

TABLE 2. r,r^2, se, t and p for the physical properties (P) and squares stress sum index

P	r	r^2	se	t	p
bp	0.8685	0.7543	(4.04) (0.0020)	(15.63) (14.34)	$(4.892E-24)$ $(4.192E-22)$
mv	0.9041	0.8174	(1.92) (0.0009)	(69.12) (17.31)	$(5.068E-64)$ $(1.944E-26)$
mr	0.9238	0.8535	(0.52) (0.0002)	(57.75) (19.76)	$(7.084E-59)$ $(1.172E-29)$
hv	0.8348	0.6970	(0.77) (0.0003)	(39.37) (12.41)	$(4.700E-48)$ $(4.888E-19)$
ct	0.8771	0.7693	(4.76) (0.0024)	(47.89) (14.94)	$(1.473E-53)$ $(5.049E-23)$
cp	-0.7504	0.5631	(0.45) (0.0002)	(66.44) (-9.29)	$(6.903E-63)$ $(1.143E-13)$
st	0.7649	0.5851	(0.31) (0.0001)	(58.07) (9.501)	$(4.395E-57)$ $(7.592E-14)$

The linear regression models for boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes are as follows:

$$bp = 63.22737617 + 0.029266201 \cdot \mathcal{SSS}(G) \tag{11}$$

$$mv = 133.1062639 + 0.016821169 \cdot \mathcal{SSS}(G) \tag{12}$$

$$mr = 30.30250151 + 0.005230315 \cdot \mathcal{SSS}(G) \tag{13}$$

$$hv = 30.32609248 + 0.004822983 \cdot \mathcal{SSS}(G) \tag{14}$$

$$ct = 228.1905044 + 0.035922337 \cdot \mathcal{SSS}(G) \tag{15}$$

$$cp = 30.01654316 - 0.002117652 \cdot \mathcal{SSS}(G) \tag{16}$$

$$st = 18.38372560 + 0.001483931 \cdot \mathcal{SSS}(G) \tag{17}$$

The values of r,r^2, se, t and p in Table 2 for the physical properties are good except for surface tensions which has $r^2 = 0.5851$ and critical pressures which has $r = -0.7504$ (with $r^2 = 0.5631$). Hence the linear regression models (11)-(15) can be used as predictive tools.

4. Conclusion

Table 2, reveals that the linear regression models (11)-(15) are useful tools in predicting the physical properties - boiling points, molar volumes, molar refractions, heats of vaporization and critical temperatures of low alkanes. It shows that squares stress sum index can be used as predictive means in QSPR researches.

Acknowledgments

The authors thank the anonymous reviewers for their careful reading of our manuscript and their many insightful comments and suggestions.

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