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CANGUL STRESS INDEX FOR GRAPHS

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Abstract. We introduce a new topological index for graphs called Cangul stress index using stresses of nodes. Also, we establish some inequalities, prove some results and compute Cangul stress index for some standard graphs. Further, a correlation analysis is carried to measure the strength of the linear relationship between Cangul stress index of chemical structures (molecular graphs) and physical properties of lower alkanes.

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1. Introduction

We refer to the textbook of Harary [5] 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 [24]. This centrality measure has applications in biology, sociology, psychology, etc., (See [7,22]). The stress of a node v in a graph G, denoted by $\mathrm{str}_G(v)$ or $\mathrm{str}(v)$, 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

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k-stress regular if $\mathrm{str}(v) = k$ for all $v \in V(G)$. We recommend that the reader to study the publications [2,3,6,8,10–21,23,25,26] 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 Cangul Stress Index. Further, we establish some inequalities and compute Cangul stress index for some standard graphs.

2. Cangul Stress Index

Definition 2.1. The Cangul stress index $CS(G)$ of a graph G is defined as

$$CS(G) = \sum_{uv \in E(G)} [\mathrm{str}(u) + \mathrm{str}(v)]\, \mathrm{str}(u)\, \mathrm{str}(v). \tag{1}$$

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

$$2m\theta_G^3 \leq CS(G) \leq 2m\Theta_G^3,$$

where m is the number of edges in G.

Proposition 2.2. *For a graph G,*

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

where t is the number of edges with at least one end node of 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 node, for any node v in G, $0 \leq \mathrm{str}(v) \leq N$. Hence by the Definition 2.1, the result follows. □

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

Proof. If there is no geodesic of length ≥ 2 in a graph G, then $N = 0$. Hence, by the Proposition 2.2, we have $CS(G) = 0$.
In K_n, there is no geodesic of length ≥ 2 and so $CS(K_n) = 0$. □

Theorem 2.4. *For a graph G, $CS(G) = 0$ iff G is complete.*

Proof. Suppose that $CS(G) = 0$. Then by the Definition 2.1, $[\mathrm{str}(u) + \mathrm{str}(v)]\, \mathrm{str}(u)\, \mathrm{str}(v) = 0$, $\forall uv \in E(G)$. Hence $\mathrm{str}(v) = 0$, $\forall v \in V(G)$. 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 2.3, it follows that $CS(G) = 0$. □

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

$$CS(K_{m,n}) = \frac{1}{8}m^2n^2(m-1)(n-1)\left[n(n-1)+m(m-1)\right].$$

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,

$$\mathrm{str}(v_i) = \frac{n(n-1)}{2} \text{ for } 1 \leq i \leq m \tag{3}$$

and

$$\mathrm{str}(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \leq j \leq n. \tag{4}$$

Using (3) and (4) in the Definition 2.1, we have

$$\begin{aligned}
CS(K_{m,n}) &= \sum_{uv\in E(G)} [\mathrm{str}(u)+\mathrm{str}(v)]\,\mathrm{str}(u)\,\mathrm{str}(v)\\
&= \sum_{1\leq i\leq m,\ 1\leq j\leq n} [\mathrm{str}(v_i)+\mathrm{str}(u_j)]\,\mathrm{str}(v_i)\mathrm{str}(u_j)\\
&= \sum_{1\leq i\leq m,\ 1\leq j\leq n} \left[\frac{n(n-1)}{2}+\frac{m(m-1)}{2}\right]\frac{n(n-1)}{2}\cdot\frac{m(m-1)}{2}\\
&= \frac{1}{8}m^2n^2(m-1)(n-1)\left[n(n-1)+m(m-1)\right].
\end{aligned}$$

□

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

$$CS(G) = 2k^3|E|.$$

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 2.1, we have

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

□

Corollary 2.7. *For a cycle* C_n,

$$CS(C_n) = \begin{cases} \dfrac{n(n-1)^3(n-3)^3}{256}, & \text{if } n \text{ is odd}\\[2mm] \dfrac{n^4(n-2)^3}{256}, & \text{if } n \text{ is even.} \end{cases}$$

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

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

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 2.6, we have

$$\begin{aligned} CS(C_n) &= 2n \times \begin{cases} \left[\dfrac{(n-1)(n-3)}{8}\right]^3, & \text{if } n \text{ is odd} \\ \left[\dfrac{n(n-2)}{8}\right]^3, & \text{if } n \text{ is even.} \end{cases} \\ &= \begin{cases} \dfrac{n(n-1)^3(n-3)^3}{256}, & \text{if } n \text{ is odd} \\ \dfrac{n^4(n-2)^3}{256}, & \text{if } n \text{ is even.} \end{cases} \end{aligned}$$

□

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

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

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,

$$\text{str}(v) = \sum_{1 \le i < j \le m} |C_i^v||C_j^v|. \tag{5}$$

Let J denotes the set of internal(non-pendant) edges, and P denotes pendant edges in T. Then using (5) in the Definition 2.1, we have

$$\begin{aligned}
CS(T) &= \sum_{uv\in J} [\{\mathrm{str}(u)+\mathrm{str}(v)\}\,\mathrm{str}(u)\,\mathrm{str}(v)] + \sum_{uv\in P} [\{\mathrm{str}(u)+\mathrm{str}(v)\}\,\mathrm{str}(u)\,\mathrm{str}(v)]\\
&= \sum_{uv\in J} [\mathrm{str}(u)+\mathrm{str}(v)]\,\mathrm{str}(u)\,\mathrm{str}(v)\\
&= \sum_{uv\in J} \left[\left\{\sum_{1\le i<j\le m(u)} |C_i^u||C_j^u| + \sum_{1\le i<j\le m(v)} |C_i^v||C_j^v|\right\}\right.\\
&\qquad \left.\left(\sum_{1\le i<j\le m(u)} |C_i^u||C_j^u|\right)\left(\sum_{1\le i<j\le m(v)} |C_i^v||C_j^v|\right)\right].
\end{aligned}$$

□

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

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

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 node sequence $v_1, v_2, \ldots, v_n$ (shown in Figure 1).

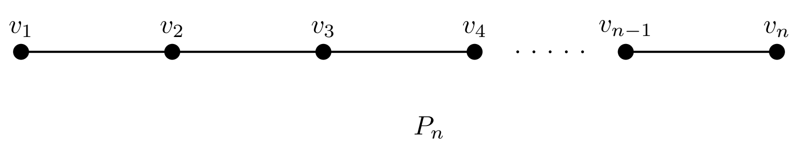

FIGURE 1. The path P_n on n nodes.

We have,

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

Then

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

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

□

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 node v. Then*

$$CS(Wd(n,m)) = 0.$$

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

$$CS(F_k) = 0.$$

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 $Wd(n,m)$. Hence by the Definition 2.1, we have

$$CS(Wd(n,m)) = 0.$$

Since the friendship graph F_k on $2k+1$ nodes is nothing but $Wd(3,k)$, it follows that $CS(F_k) = 0$.

□

3. A Correlation Analysis

In this section, a correlation analysis is carried to measure the strength of the linear relationship between Cangul stress index of chemical structures (molecular graphs) and physical properties of lower alkanes.

The experimental values for the physical properties-Boiling points (*bp*) $°C$, molar volumes (*mv*) cm^3, molar refractions (*mr*) cm^3, heats of vaporization (*hv*) kJ, critical temperatures (*ct*) $°C$, critical pressures (*cp*) atm, and surface tensions(*st*) $dyne\ cm^{-1}$ of considered alkanes are given in Table 1 along with the Cangul 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 [9]).

TABLE 1. Cangul stress index and values of the physical properties of considered low alkanes

Alkane	CS	$\frac{bp}{°C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{°C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	168	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	120	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	0	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	912	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	786	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	768	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	468	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	3488	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	3202	90.1	147.7	34.59	34.8	257.9	27.2	19.29

3-Methylhexane	3072	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylpentane	3060	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	2440	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	2860	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	2916	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	2340	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	2268	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	10656	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	10092	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	9648	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	9420	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	7232	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	8460	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	9000	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	7356	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	9528	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	7896	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	8848	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	8976	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	8856	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	5412	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	7896	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	7194	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	8580	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	27792	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	26796	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	25728	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	24810	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	24516	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	14924	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	23688	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	24050	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	24732	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	24732	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	25800	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	21912	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	23148	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	23664	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	21144	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	23310	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	23520	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	20916	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	22996	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	21318	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	21624	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	22692	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	20582	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	22388	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	23054	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	20916	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	20538	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	20832	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	11480	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	21240	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	22680	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	18850	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	14370	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	19584	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	20020	141.6	169.9	43.2	41.8	334.5	26.85	23.31

The correlation coefficient (r) and the coefficient of determination (r^2) are computed to measure the strength of the linear relationship between Cangul stress index of chemical structures (molecular graphs) and physical properties of lower alkanes using the Table 1. The computed values of r and r^2 are presented in Table 2.

Table 2. r and r^2 for the physical properties (P) and Cangul stress index

P	r	r^2
bp	0.8571	0.7346
mv	0.8998	0.8097
mr	0.8946	0.8004
hv	0.8778	0.7705
ct	0.8096	0.6554
cp	−0.8401	0.7058
st	0.7504	0.5630

From Table 2, it follows that there is a very strong positive correlation between Cangul stress index and the physical properties-boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures and surface tensions of low alkanes. There is a very strong negative correlation between Cangul stress index and critical pressures of low alkanes. Hence Cangul stress index can be used as a predictive measure for physical properties of low alkanes.

4. Conclusion

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

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Data availability : Not applicable

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