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Total Tension as a Topological Index

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ABSTRACT: In this article, we see the total tension of a graph as a topological index and establish a relation between total tension index and total stress of a graph. We deduce that a graph is complete if and only if its total tension and the number of geodesics in it are equal. We also deduce that the total tension of an n-vertex connected proper subgraph of a complete graph K_n with $n \geq 3$ vertices is greater than the total tension of K_n. We obtain a formula for computing total tension of a tree. Further, a QSPR analysis has been carried to demonstrate that total tension index can be used as a predictive measure for physical properties of lower alkanes. Linear regression models involving total tension index have been presented for some physical properties of lower alkanes.

Key Words: Geodesic, topological index, total stress, total tension.

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1. Introduction

For standard terms and concepts in graphs, refer to Harary's book [3]. This article will provide non-standard terms when needed. Let $G = (V, E)$ denote an undirected graph that is finite, simple and connected. A shortest path in G between two nodes x and y, is called a geodesic between x and y. The number of geodesics in a graph G is denoted by $f(G)$ or simply f, and f_i denotes the number of geodesics of length i in G. The molecular graph of a chemical molecule is a simple connected graph in which the chemical bonds that bind its atoms together are represented as edges and the atoms themselves as nodes.

In essence, topological indices are theoretical molecular descriptors. In chemistry, these graph invariants are essential (see [7, 10, 11]). For graphs having significant applications in Chemistry, a variety of topological indices have been investigated, such as the Wiener index, Zagreb index, Harary index, etc. (see [10, 11]).

Alfonso Shimbel [9] introduced the concept 'stress of a node' in a network in 1953 as a centrality measure. The stress of a node u in a graph G, denoted by $\mathrm{str}_G(u)$ (or simply $\mathrm{str}(u)$), is the number of geodesics passing through u. The notion of total stress (stress number) of a graph has been introduced and studied by K. Bhargava et al. [1]. The total stress of a graph G, denoted by $N_{\mathrm{str}}(G)$, is given by

$$N_{\mathrm{str}}(G) = \sum_{u \in V} \mathrm{str}(u) \tag{1.1}$$

Inspired by the ideas of stress on a vertex and total stress of a graph, K. Bhargava et al. [2] have introduced and investigated the notion of tension on edge in a graph and total tension of a graph. The tension on an

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edge e in a graph G, denoted by $\tau_G(e)$ or simply $\tau(e)$, is defined as the number of geodesics in G passing through e. Tension on an edge is always ≥ 1. The total tension of G, denoted by $N_\tau(G)$, is defined as

$$N_\tau(G) = \sum_{e \in E} \tau(e) \tag{1.2}$$

In [4,5], Madhumitha et. al have obtained formulae for the evaluation of total tension of certain graphs, generalized complements of some standard graphs and graph operations with diameter less than or equal to two.

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 lower alkanes are presented in the following Table 1. For QSPR analysis for TTI of molecular graphs with the physical properties of lower alkanes we use this data. For the experimental data of numerical values in columns 2 to 8 of the Table 1 one can refer [7] or [11].

Table 1: Experimental values of the physical properties of low alkanes

Alkane	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	114.8	157.3	38.76	37.2	303	29	21.56

2,3,4-Trimethylpentane	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Throughout this study, we refer to a graph as a simple connected graph. In section 2, we see total tension as a topological index and obtain some results. Mainly, we establish a relation between total tension index and total stress of a graph. We deduce that a graph is complete if and only if its total tension and the number of geodesics in it are equal. We also deduce that the total tension of an n-vertex connected proper subgraph of a complete graph K_n with $n \geq 3$ vertices is greater than the total tension of K_n. We obtain a formula for computing total tension of a tree. Section 3 presents the results of a QSPR investigation of the physical properties of lower alkanes using the total tension index of molecular graphs, along with some excellent linear regression models for some physical properties.

2. Total tension as a molecular descriptor

A topological index, often referred to as a molecular descriptor, is a mathematical formula that may be applied to any graph that represents any molecular structure. One can evaluate mathematical values and look into some other physicochemical aspects of molecules using such a topological index. It is therefore a useful strategy for avoiding costly and time-consuming laboratory experiments.

The physical properties of chemical compounds are converted into numerical data via quantitative structure-property relationship (QSPR) investigations, which are then used to build regression models and investigate correlations between the physical attributes and the structure of the compounds. With QSPR, a number of topological indices have been examined.

Since isomorphic graphs have same total tension, the total tension is a graph invariant i.e., the total tension is a molecular descriptor(i.e., a topological index). We call total tension $N_\tau(G)$ of a graph G as total tension index (TTI) of G. The following proposition gives bounds for the TTI.

Proposition 2.1 *For any graph G,*

$$|E(G)| \leq N_\tau(G) \leq |E(G)|f(G) \tag{2.1}$$

Proof: For an edge e in G, we have

$$1 \leq \tau(e) \leq f(G).$$

Using this in the definition of total tension (1.2), we have the inequality (2.1). □

Proposition 2.2 *If G is a t-tension regular graph, then*

$$N_\tau(G) = |E(G)|t \tag{2.2}$$

Proof: If G is t-tension regular, then $\tau(e) = t$, $\forall e \in E(G)$ and so from (1.2), we have

$$N_\tau(G) = \sum_{e\in E(G)} t = |E(G)|t.$$

□

Theorem 2.1 *For any graph G,*

$$N_\tau(G) = N_{str}(G) + f(G). \tag{2.3}$$

Proof: By counting the number of geodesics and the internal edges in geodesics, we see that, for any graph G of diameter d, the Total stress of G is given by

$$N_{\mathrm{str}}(G) = \sum_{i=1}^{d} f_i(i-1), \tag{2.4}$$

where f_i denotes the number of geodesics of length i in G (see [1, Proposition 2.6]). Also, the TTI of G is given by

$$N_\tau(G) = \sum_{i=1}^{d} if_i \tag{2.5}$$

(see [2, Proposition 3.3]). Also,

$$f(G) = \sum_{i=1}^{d} f_i \tag{2.6}$$

Now, from the equations (2.4), (2.5) and (2.6), we have

$$N_{\mathrm{str}}(G) = N_\tau(G) - f(G).$$

Re-arranging terms, we get the result (2.3). □

Corollary 2.1 *For the complete graph K_n, $N_\tau(K_n) = \binom{n}{2}$.*

Proof: For K_n, we have $N_{\text{str}}(K_n) = 0$ and $f(G) = \binom{n}{2}$. Therefore from Eq.(2.3), we have $N_\tau(K_n) = \binom{n}{2}$. □

Corollary 2.2 *A graph G is a complete graph if and only if $N_\tau(G) = f(G)$.*

Proof: In [6], it is proved that $N_{\text{str}}(G) = 0$ if and only if G is complete. Using this fact in Eq.(2.3) of Theorem 2.1, it follows that, G is complete if and only if $N_\tau(G) = f(G)$. □

Corollary 2.3 *An n-vertex connected graph G is complete if and only if $N_\tau(G) = \binom{n}{2}$.*

Proof: Let G be an n-vertex connected graph. Suppose that G is complete. Then by the Corollary 2.1, $N_\tau(G) = \binom{n}{2}$.

Conversely, suppose that $N_\tau(G) = \binom{n}{2}$. Then from Eq.(2.3),

$$N_{\text{str}}(G) + f(G) = \binom{n}{2} \tag{2.7}$$

Since G is connected, there is a path between any two vertices in G and hence there is at least one geodesic between any pair of vertices in G. Therefore there are at least $\binom{n}{2}$ geodesics in G i.e.,

$$f(G) \geq \binom{n}{2} \tag{2.8}$$

Using (2.8) in (2.7), we have

$$\begin{aligned} \binom{n}{2} &= N_{\text{str}}(G) + f(G) \geq N_{\text{str}}(G) + \binom{n}{2} \\ \Longrightarrow \quad 0 &\geq N_{\text{str}}(G) \end{aligned} \tag{2.9}$$

But

$$N_{\text{str}}(G) \geq 0 \tag{2.10}$$

Now from (2.9) in (2.10), we have $N_{\text{str}}(G) = 0$. Then, G is complete (because $N_{\text{str}}(G) = 0$ if and only if G is complete [6]). □

Corollary 2.4 *For a tree T on n nodes, from [1, Proposition 3.2], we have*

$$N_\tau(T) = \sum_{v \in I} \left[\sum_{1 \leq i < j \leq m} |C_i^v||C_j^v| \right] + \binom{n}{2}, \tag{2.11}$$

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

Proof: For a tree T on n nodes, we have

$$N_{\text{str}}(T) = \sum_{v \in I} \left[\sum_{1 \leq i < j \leq m} |C_i^v||C_j^v| \right], \tag{2.12}$$

where I is the set of all non-pendant internal nodes in T and the sets $C_1^v, \ldots, C_m^v$ denote the node sets in the components of $T - v$ for an internal node v of degree $m = m(v)$. Also, since there is only one path between every pair of vertices in a tree, we have

$$f(T) = \binom{n}{2} \tag{2.13}$$

Now, using (2.12) and (2.13) in (2.3), we get (2.11). □

Corollary 2.5 *For a tree T on $n \geq 2$ vertices,*

(i) $N_\tau(T) = 1$, *for* $n = 2$*;*

(ii) $N_\tau(T) > \binom{n}{2}$, *for* $n > 2$.

(iii) $N_\tau(T) > N_\tau(K_n)$

Proof:

(i) For $n = 2$, $T = P_2$ and so $N_\tau(T) = 1$.

(ii) For $n > 2$, T is not a complete graph and hence $N_{\text{str}}(T) > 0$ (because $N_{\text{str}}(G) = 0$ if and only if G is complete [6]). Then by Eq.(2.3) of Theorem 2.1, it follows that,

$$N_\tau(T) = N_{\text{str}}(T) + f(T) > f(T) = \binom{n}{2}.$$

(iii) For the complete graph, we have $N_\tau(K_n) = f(K_n) = \binom{n}{2}$. Hence from (ii), we have $N_\tau(T) > N_\tau(K_n)$. □

Corollary 2.6 *If G is an n-vertex connected proper subgraph of K_n with $n \geq 3$, then $N_\tau(G) > N_\tau(K_n)$.*

Proof: Suppose that G is an n-vertex connected proper subgraph of K_n with $n \geq 3$. Since G is connected, there is a path between any two vertices in G and hence there is at least one geodesic between any pair of vertices in G. Therefore there are at least $\binom{n}{2}$ geodesics in G i.e.,

$$f(G) \geq \binom{n}{2} \tag{2.14}$$

Since G is a proper subgraph of K_n, we have

$$N_{\text{str}}(G) > 0, \tag{2.15}$$

because $N_{\text{str}}(G) \geq 0$ and $N_{\text{str}}(G) = 0$ if and only if G is complete [6]. Then using (2.14) and (2.15) in Eq.(2.3) of Theorem 2.1, we get

$$N_\tau(G) = N_{\text{str}}(G) + f(G) > 0 + \binom{n}{2} = \binom{n}{2} = N_\tau(K_n).$$ □

The following theorem give a formula for computing TTI of tress.

Theorem 2.2 *For a tree T,*

$$N_\tau(T) = \sum_{e \in E(T)} |V(C_1^e)||V(C_2^e)|, \tag{2.16}$$

where C_1^e and C_2^e are the components of $T - e$ corresponding to $e \in E(T)$.

Proof: Let T be a tree. From [2, Proposition 2.3], for an edge $e \in E(T)$, the tension on e is

$$\tau_T(e) = |V(C_1^e)||V(C_2^e)|,$$

where C_1^e and C_2^e are the components of $T - e$. Therefore

$$N_\tau(T) = \sum_{e \in E} \tau_T(e) = \sum_{e \in E(T)} |V(C_1^e)||V(C_2^e)|.$$ □

Proposition 2.3 *If G is a subgraph of a tree T, then*

$$N_\tau(G) \leq N_\tau(T). \tag{2.17}$$

The inequality will be strict if G is a proper subgraph of T.

Proof: Let G be a subgraph of a tree T. Since there is one and only one path between any two vertices in a tree, we have

$$\tau_G(e) \leq \tau_T(e)$$

for any edge e in G. Therefore, from (1.2),

$$N_\tau(G) = \sum_{e\in E(G)} \tau_G(e) \leq \sum_{e\in E(G)} \tau_T(e) \leq \sum_{e\in E(T)} \tau_T(e) = N_\tau(T).$$

When G is a proper sub graph of T, the size of G is less than the size of T and hence there is at least one edge in T that is not in G. Also, tension of any edge in T is ≥ 1. Therefore the inequality is strict (2.17). □

Remark 2.1 *If G is a subgraph of a graph G', then the inequality $N_\tau(G) \leq N_\tau(G')$ need not be true, if G' is not a tree. For example, consider the complete graph K_n and any spanning tree T of K_n. From the Corollary 2.5, we have $N_\tau(T) > N_\tau(K_n)$.*

3. A QSPR Analysis for TTI

We perform a QSPR study for TTI of molecular graphs of lower alkanes with their physical characteristics in this part. The TTIs of molecular graphs were calculated using Eq.(2.16). Table 2 lists the calculated TTI N_τ values of molecular graphs. QSPR analysis is performed using the experimental values of the physical properties of the considered lower alkanes listed in Table 1, such as boiling points (bp) $^\circ C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporisation (hv) kJ, critical temperatures (ct) $^\circ C$, critical pressures (cp) atm, and surface tensions (st) $dyne\ cm^{-1}$.

Table 2: TTI N_τ of low alkanes

Alkane	N_τ
Pentane	20
2-Methylbutane	18
2,2-Dithylpropane	16
Hexane	35
2-Methylpentane	32
3-Methylpentane	31
2,3-Dimethylbutane	29
2,2-Dimethylbutane	28
Heptane	56
2-Methylhexane	52
3-Methylhexane	50
3-Ethylpentane	48
2,3-Dimethylpentane	46
2,4-Dimethylpentane	48
2,2-Dimethylpentane	46
3,3-Dimethylpentane	44
2,3,3-Trimethylbutane	42
Octane	84

Alkane	N_τ
2-Methylheptane	79
3-Methylheptane	76
4-Methylheptane	75
4-Ethylhexane	72
2,2-Dimethylhexane	71
2,3-Dimethylhexane	70
2,4-Dimethylhexane	71
2,5-Dimethylhexane	74
3,3-Dimethylhexane	67
3,4-Dimethylhexane	68
3-Ethyl-3-methylpentane	64
3-Ethyl-2-methylpentane	67
2,3,3-Trimethylpentane	62
2,3,4-Trimethylpentane	65
2,2,3-Trimethylpentane	63
2,2,4-Trimethylpentane	66
Nonane	120
3-Ethylheptane	104

Alkane	N_τ
4-Ethylheptane	102
2-Methyloctane	114
3-Methyloctane	110
4-Methyloctane	108
2,2-Dimethylheptane	104
2,3-Dimethylheptane	102
2,4-Dimethylheptane	102
2,5-Dimethylheptane	104
2,6-Dimethylheptane	108
3,3-Dimethylheptane	98
3,4-Dimethylheptane	98
3,5-Dimethylheptane	100
4,4-Dimethylheptane	96
3-Ethyl-2-methylhexane	96
4-Ethyl-2-methylhexane	98
3-Ethyl-3-methylhexane	92
3-Ethyl-4-methylhexane	94

Alkane	N_τ
2,3,3-Trimethylhexane	90
2,3,4-Trimethylhexane	92
2,3,5-Trimethylpentane	96
2,4,4-Trimethylhexane	92
3,3,4-Trimethylhexane	88
2,2,3-Trimethylhexane	92
2,2,4-Trimethylhexane	94
2,2,5-Trimethylhexane	98
3,3-Diethylpentane	88
2,2-Diethyl-3-ethylpentane	88
2,3-Diethyl-3-ethylpentane	86
2,4-Diethyl-3-ethylpentane	90
2,2,3,3-Tetramethylpentane	82
2,2,3,4-Tetramethylpentane	86
2,2,4,4-Tetramethylpentane	88
2,3,3,4-Tetramethylpentane	84

Regression Models:

An investigation was conducted using the following linear regression model

$$Y = A + B \cdot N_\tau$$

where Y = Physical property and N_τ = TTI of molecular graphs of low alkanes. We have calculated and tabulated the correlation coefficient r, its square r^2, standard error (se), t-value, and p-value in Table 3 using Tables 1 and 2.

Table 3: r,r^2, se, t and p for the physical properties (Y) and TTI N_τ

Y	r	r^2	se	t	p
bp	0.9436	0.8904	0.049	23.33	$7.1E-34$
mv	0.9720	0.9447	0.045	33.84	$7.4E-44$
mr	0.9616	0.9247	0.014	28.68	$2.4E-39$
hv	0.9648	0.9308	0.007	30.03	$1.4E-40$
ct	0.8889	0.7902	0.082	15.88	$2.1E-24$
cp	-0.9366	0.8772	0.004	-21.87	$3.2E-32$
st	0.8110	0.6577	0.006	11.26	$5.2E-17$

For the physical properties - bp, mv, mr, hv, ct, cp and st of low alkanes, the linear regression models are displayed below:

$$bp = 29.0394 + 1.1314 \cdot N_\tau \tag{3.1}$$

$$mv = 113.9705 + 0.6435 \cdot N_\tau \tag{3.2}$$

$$mr = 24.8343 + 0.1937 \cdot N_\tau \tag{3.3}$$

$$hv = 23.7939 + 0.1983 \cdot N_\tau \tag{3.4}$$

$$ct = 193.2791 + 1.2954 \cdot N_\tau \tag{3.5}$$

$$cp = 33.4115 - 0.0940 \cdot N_\tau \tag{3.6}$$

$$st = 16.1893 + 0.0620 \cdot N_\tau \tag{3.7}$$

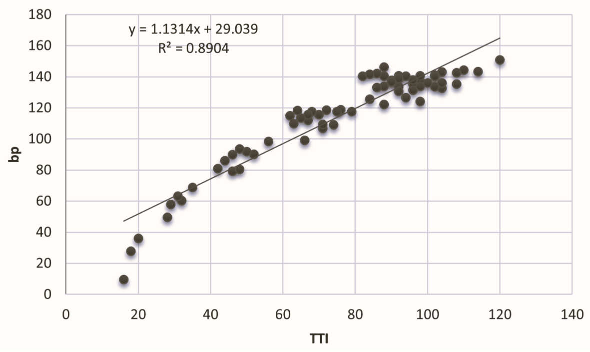

Figure 1: Model for *bp*

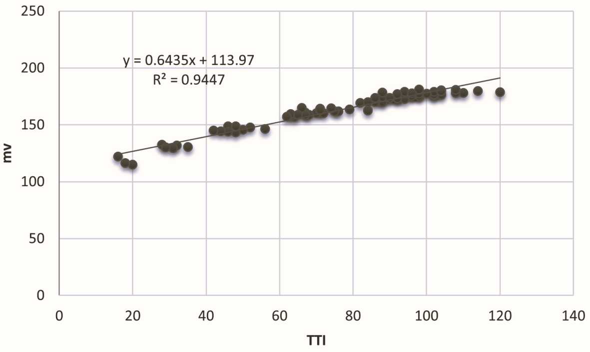

Figure 2: Model for *mv*

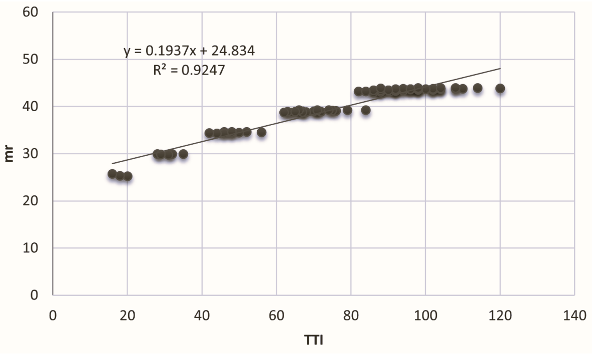

Figure 3: Model for *mr*

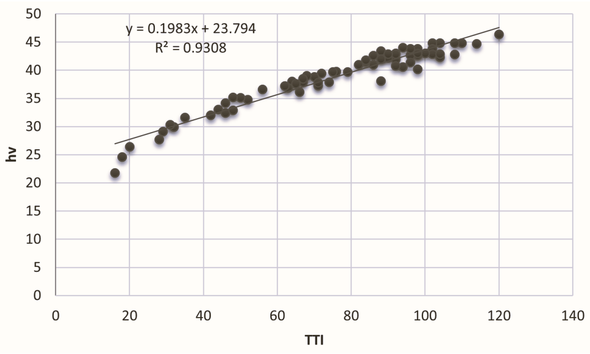

Figure 4: Model for *hv*

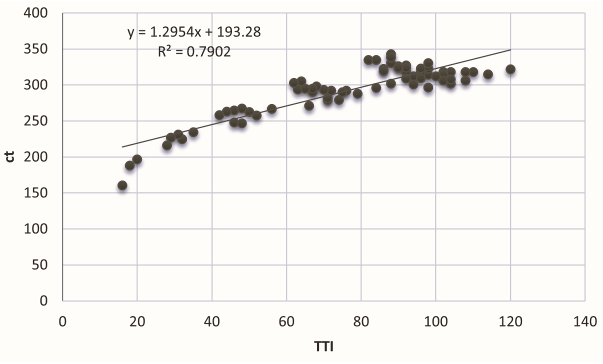

Figure 5: Model for *ct*

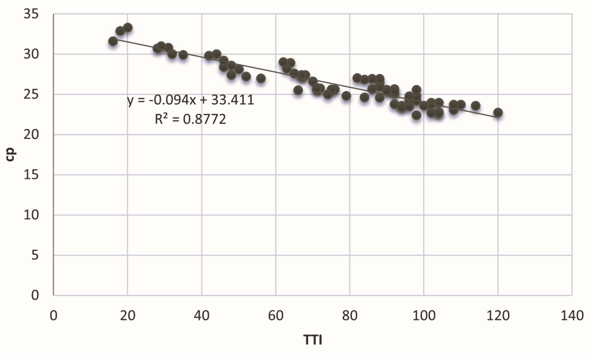

Figure 6: Model for *cp*

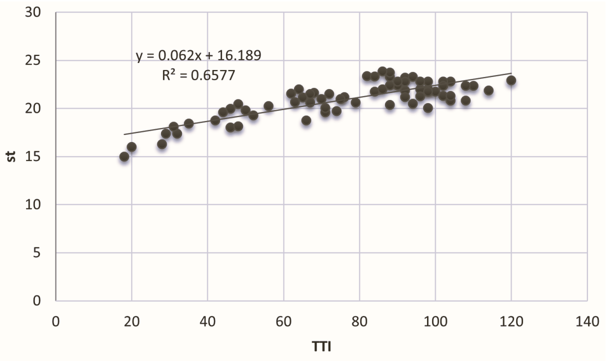

Figure 7: Model for *st*

Except for surface tensions, the numerical values of r, r^2, se, t, and p (found in Table 3) for the physical properties are excellent. According to the regression study, low alkanes' physical characteristics show strong linear correlations with TTI, as seen by high r^2 values. This implies that TTI can accurately anticipate the molecular characteristics of low alkanes. Predictions can therefore be made using the linear regression models (3.1)-(3.6).

4. Conclusion

From the Table 3, it follows that the linear regression models (3.1)-(3.6) are useful for predicting the physical properties of low alkanes. This demonstrates that in QSPR investigations, the total tension index may be employed as a predictive indicator.

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