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ON THE MODIFIED WIENER INDEX AND ITS CHEMICAL APPLICABILITY

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ABSTRACT. The sum of distances between all the pairs of vertices in a connected graph is known as Wiener index of the graph. In this paper, we initiate a novel distance based topological index namely the modified Wiener index $MW(G)$ of a graph G. First, we prove the chemical application of $MW(G)$. Further, we obtain some mathematical properties as well.

1. INTRODUCTION

Let $G = (V, E)$ be a graph. The number of vertices of G we denote by n and the number of edges we denote by m, thus $|V(G)| = n$ and $|E(G)| = m$. By the open neighborhood of a vertex v of G, we mean the set $N_G(v) = \{u \in V(G)\colon uv \in E(G)\}$. The degree of a vertex v, denoted by $deg(v)$, is the cardinality of its open neighborhood. The neighborhood degree of a pendant vertex v, $deg_G(N(v))$ is the cardinality of $deg_G(u)$, where $uv \in E(G)$. The distance between the vertices $v_i, v_j \in V(G)$, is equal to the length of the shortest path starting at v_i and ending at v_j, and will be denoted by $d(v_i, v_j|G)$. For undefined terminologies we refer the reader to [7].

The oldest molecular structure is the one put forward in 1947 by H. Wiener [13], nowadays referred to as the Wiener index and denoted by W. It is defined

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as the sum of distance between all pairs of vertices of a graph.

$$W(G) = \sum_{\{u,v \subseteq V(G)\}} d(u,v \setminus G) = \sum_{1 \leq i < j \leq n} d(u,v \setminus G).$$

For details on its chemical applications and mathematical properties one may refer to [2–4, 8–10, 12–15] and the references cited therein.

The terminal Wiener index $TW(G)$ [5] of a connected graph G is defined as the sum of the distances between all pairs of its pendant vertices.
Thus if $V_T = \{v_1, v_2, \cdots, v_k\}$ is the set of all pendent vertices of G, then

$$TW(G) = \sum_{\{u,v \subseteq V_T(G)\}} d(u,v \setminus G) = \sum_{1 \leq i < j \leq k} d(u,v \setminus G)$$

The degree-distance [1] and the Gutman index [6] are defined as :

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)[deg_G(u) + deg_G(v)].$$

$$GI(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)[deg_G(u) deg_G(v)].$$

Motivated by the Wiener index, we compute the modified Wiener index which is defined as follows:

$$MW(G) = \frac{1}{2} \sum_{j=1}^{n} \sum_{i=1}^{n} d(v_i, v_j)^2.$$

2. Applicability of $MW(G)$

In this section, we compare the predicting power of $MW(G)$ with other distance based topological indices, like the Wiener index $W(G)$, terminal Wiener index $TW(G)$, hyper-Wiener index $WW(G)$, degree-distance index $DD(G)$ and the Gutman index $GI(G)$. For this study, we have framed the following regression model:

$$P = a(TI) + b$$

$$P = a(TI)^2 + b(TI) + c$$

$$P = a + b \ln(TI)$$

where P denote the physical property, TI denote the topological index and a, b, c are the regression coefficients.

Here we have examined the chemical applicability of the MW, W, TW, DD and GI indices for the set of octane isomers. We consider the physical like properties [boiling points(BP), molar volumes (mv) at $20°$C, molar refractions (mr) at $20°$C, heats of vaporization (hv) at $25°$C, surface tensions (st) $20°$C and melting points (mp), acentric factor (AcentFac) and DHVAP]. The values are compiled in Table A [9].

In the following Tables 1 to 5 the statistical parameters for the linear, quadratic and logarithmic QSPR models are given.

Table 1. **Model Summary and Parameter Estimates**

Dependent Variable radius

Equation	Model Summary					Parameter Estimates		
	R Square	F	df1	df2	Sig	Constant	b1	b2
Linear	719	40 906	1	16	000	1 150	002	
Logarithmic	437	12 443	1	16	003	437	227	
Quadratic	811	32 235	2	15	000	1 368	000	7 325E-006

The independent variable is Modified_Wiener

Table 2. **Model Summary and Parameter Estimates**

Dependent Variable radius

Equation	Model Summary					Parameter Estimates		
	R Square	F	df1	df2	Sig	Constant	b1	b2
Linear	053	903	1	16	356	1 839	- 003	
Logarithmic	148	2 782	1	16	115	2 519	- 214	
Quadratic	819	33 970	2	15	000	2 986	- 063	001

The independent variable is W

Table 3. **Model Summary and Parameter Estimates**

Dependent Variable: radius

Equation	Model Summary					Parameter Estimates		
	R Square	F	df1	df2	Sig.	Constant	b1	b2
Linear	.794	61.773	1	16	.000	2.086	-.021	
Logarithmic	.853	92.655	1	16	.000	2.886	-.415	
Quadratic	.871	50.702	2	15	.000	2.376	-.049	.001

The independent variable is TW.

Table 4. **Model Summary and Parameter Estimates**

Dependent Variable: radius

Equation	Model Summary					Parameter Estimates		
	R Square	F	df1	df2	Sig.	Constant	b1	b2
Linear	.481	14.843	1	16	.001	.647	.004	
Logarithmic	.492	15.518	1	16	.001	-3.820	1.004	
Quadratic	.502	7.568	2	15	.005	-.748	.016	-2.558E-005

The independent variable is DD.

Table 5. **Model Summary and Parameter Estimates**

Dependent Variable: radius

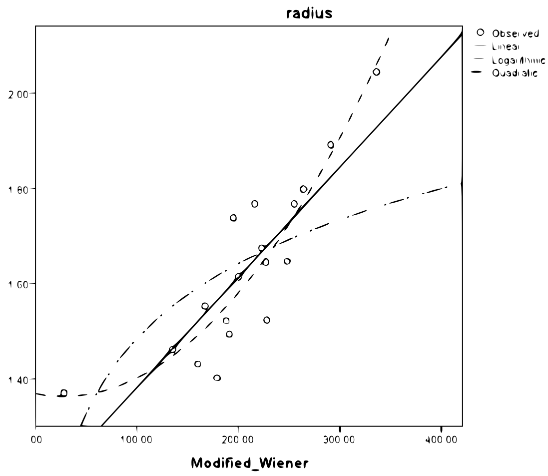
Equation	Model Summary					Parameter Estimates		
	R Square	F	df1	df2	Sig.	Constant	b1	b2
Linear	.399	10.622	1	16	.005	1.060	.003	
Logarithmic	.436	12.347	1	16	.003	-1.554	.614	
Quadratic	.503	7.588	2	15	.005	-.125	.016	-3.228E-005

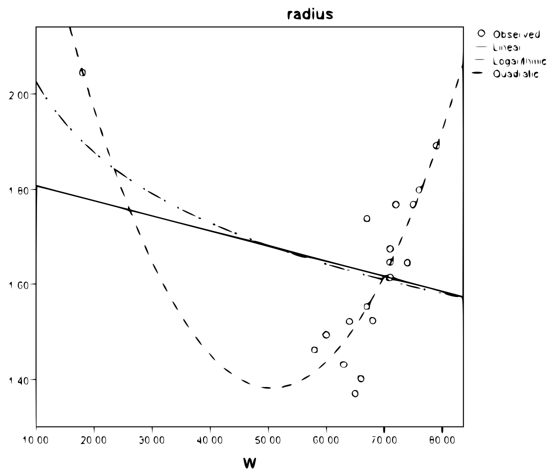
The independent variable is GI.

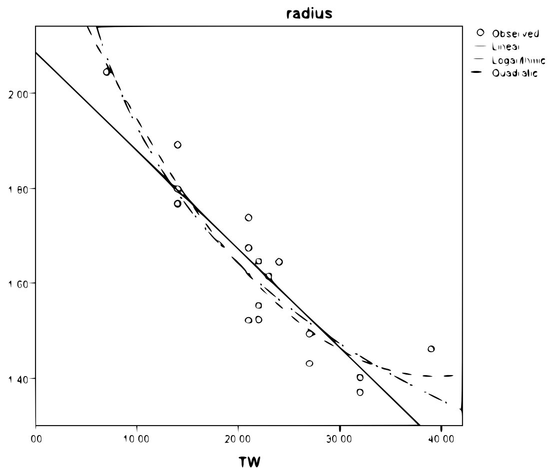
From the statistical results we learn:

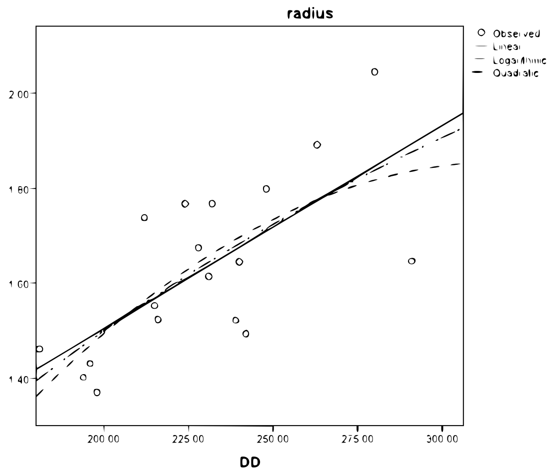
- The quadratic model is found to be the most accurate in all cases.
- The most accurate QSPR model for predicting the radius of curvature amongst considered models is the quadratic model with the terminal Wiener index.
- The modified Wiener index is better than W, TW, DD and GI in the case of linear model in predicting the radius of curvature.
- For quadratic model the predicting power of MW is better than DD and GI.

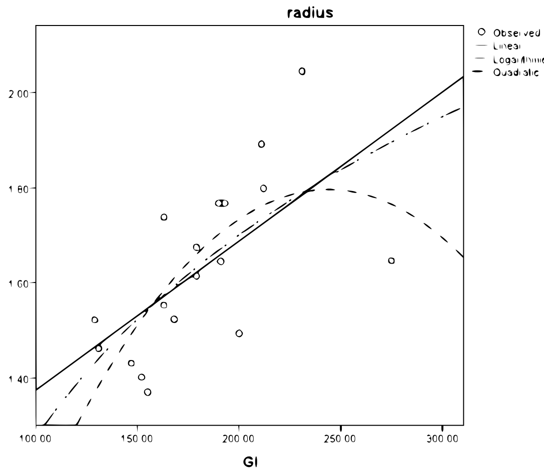
The correlation coefficient of MW, W, TW, DD and GI with the radius of curvature are depicted in the following figures.











Thus, the QSPR results revealed that the modified Wiener index is a better candidate to predict the radius of curvature of octane isomers.

3. Mathematical Properties of $MW(G)$

In this section we shall obtain the mathematical properties of the modified Wiener index.

Theorem 3.1. *Let G be any connected graph having a full degree vertex. Then*

$$MW(G) \;=\; 2n(n-1) - 3m\,.$$

Proof. Let $V(G) = v_1, v_2, v_3, \cdots, v_n$ be the vertex set of G containing a full degree vertex v_i. i.e $deg(v_i) = n-1$. Let v_j be a vertex of G such that $d(v_i, v_j) = 2$. Then clearly there exists $n-1$ vertices at distance 1 and $n-1-deg(v_j)$ vertices at distance 2. Therefore,

$$\begin{aligned}
MW(G) &= \frac{1}{2}\sum_{j=1}^{n}\sum_{i=1}^{n} d(v_i, v_j)^2. \\
&= \frac{1}{2}\left\{\sum\sum d(v_1, v_j)^2 + \sum\sum d(v_2, v_j)^2 + \ldots \sum\sum d(v_n, v_j)^2\right\} \\
&= \frac{1}{2} \sum\sum d(v_1, v_j)^2 + \frac{1}{2}\sum\sum d(v_2, v_j)^2 + \ \ldots + \frac{1}{2}\sum\sum d(v_n, v_j)^2 \\
&= \frac{1}{2}\ \left[1^2 \deg(v_1) + 2^2(n-1-\deg(v_1))\right] + \frac{1}{2}\ \left[1^2 \deg(v_2) + 2^2(n-1-\deg(v_2))\right] \\
&+ \ + \ldots + \frac{1}{2}\ \left[1^2 \deg(v_n) + 2^2(n-1-\deg(v_n))\right] \\
&= 2n(n-1) - 3m
\end{aligned}$$

as asserted. □

Since the modified Wiener index of any graph having a full degree vertex can be calculated in terms of order and size of a given graph G. Therefore, we have the following corollaries.

Corollary 3.1. *For complete graph K_n, $MW(K_n) = m$.*

Proof. Since by Theorem 1, $MW(G) = 2n(n-1) - 3m$. Therefore,

$$\begin{aligned}
MW(K_n) &= 2n(n-1) - 3\left[\frac{n(n-1)}{2}\right] \\
&= \frac{n(n-1)}{2} \\
&= m.
\end{aligned}$$

□

Corollary 3.2. *For wheel graph W_n, $MW(W_n) = 2(n-1)(n-3)$.*

Corollary 3.3. *For star graph $K_{1,n-1}$, $MW(K_{1,n-1}) = (n-1)(2n-3)$.*

Theorem 3.2. *Let $G+x$ be any connected graph obtained from G, then modified Wiener index of $G+x$ is given by*

$$MW(G+x) = n(2n-1) - 3m.$$

Proof. Let G be any connected graph with vertex set $V = \{v_1, v_2, v_3, \cdots, v_n\}$. Then the graph $G+x$ is obtained by attaching a new vertex x by joining all the vertices of to the vertex x. In this case the order and size of $G+x$ is $n+1$ and $m+n$ respectively. Further, $deg(x) = n$. Using Theorem 1, we get

$$\begin{aligned} MW(G+x) &= 2(n+1)(n+1-1) - 3(m+n) \\ &= 2n^2 + 2n - 3m - 3n \\ &= n(2n-1) - 3m, \end{aligned}$$

as desired. □

Theorem 3.3. *Let $G_1 = (n_1, m_1)$ and $G_2 = (n_2, m_2)$ be any two connected graphs. Then*

$$MW(G_1 + G_2) = 2n_1^2 + 2n_2^2 - 2(n_1 + n_2) - 3(m_1 + m_2) + 2n_1 n_2.$$

Proof. Let $V(G_1) = \{v_1, v_2, v_3, \cdots, v_{n_1}\}$ and $V(G_2) = \{u_1, u_2, u_3, \cdots, u_{n_2}\}$ be the vertices of G_1 and G_2 respectively. Let $(d_1, d_2, d_3, \cdots, d_{n_1})$ and $(d'_1, d'_2, d'_3, \cdots, d'_{n_2})$ be the degree sequence of G_1 and G_2 respectively. Now the modified Wiener-index of $G_1 + G_2$ can be divided into four cases:

$MW(G_1 + G_2) = \frac{1}{2}$ [square of distance between the vertices n_1 and n_1 are the number of vertices in G_1] $+\frac{1}{2}$ [square of distance between the vertices n_1 and n_2 are the number of vertices in G_1 and G_2] $+\frac{1}{2}$ [square of distance between the vertices n_2 and n_1 are the number of vertices in G_2 and G_1] $+\frac{1}{2}$ [square of distance between the vertices n_2 and n_2 are the number of vertices in G_2].
Thus,

$$\begin{aligned}
MW(G_1+G_2) &= \frac{1}{2}[(d_1+d_2+\cdots+d_{n_1})(1)^2[(n_1-d_1-1)+(n_1-d_2-1)\\
&+ \cdots+(n_1-d_n-1)]2^2+n_1n_2\\
&+ (d'_1+d'_2+\cdots+d'_{n_1})(1)^2\{(n_1-d'_1-1)+(n_1-d'_2-1)\\
&+ \cdots+(n_1-d'_n-1)\}2^2]\\
&= \frac{1}{2}[(d_1+d_2+\cdots+d_{n_1})+4n_1(n_1-1)\\
&- 4(d_1+d_2+\cdots+d_{n_1})+n_1n_2+4n_2(n_2-1)+n_1n_2\\
&- 4(d'_1+d'_2+\cdots+d'_{n_2})]\\
&= \frac{1}{2}[4n_1(n_1-1)-3\sum_{i=1}^{n} d_i+n_1n_2+4n_2(n_2-1)\\
&- 3\sum_{j=1}^{n} d_j]\\
&= 2n_1^2+2n_2^2-2(n_1+n_2)-3(m_1+m_2)+2n_1n_2.
\end{aligned}$$

□

Corollary 3.4. *Suppose $G_1 = C_n$ and $G_2 = K_n$ of same order $n \geq 3$. Then*

$$MW(C_n+K_n) = \frac{n(9n-11)}{2}.$$

Corollary 3.5. *Suppose $G_1 = C_n$ and $G_2 = P_n$ of same order $n \geq 3$. Then*

$$MW(C_n+P_n) = 6n^2-10n+3.$$

Corollary 3.6. *Suppose $G_1 = C_n$ and $G_2 = W_n$ of same order $n \geq 4$. Then*

$$MW(C_n+P_n) = 6n^2-13n+6.$$

Corollary 3.7. *Suppose $G_1 = P_n$ and $G_2 = K_n$ of same order $n \geq 2$. Then*

$$MW(C_n+P_n) = \frac{9n^2-11n+6}{2}.$$

Corollary 3.8. *Suppose $G_1 = P_n$ and $G_2 = W_n$ of same order $n \geq 4$. Then*

$$MW(P_n+W_n) = 6n^2-13n+9.$$

Corollary 3.9. *Suppose $G_1 = K_n$ and $G_2 = W_n$ of same order $n \geq 4$. Then*

$$MW(K_n+W_n) = \frac{9n^2-17n+12}{2}.$$

4. CONCLUSION

In this paper, we have initiated a study of modified Wiener index and further it is shown that the modified Wiener index has better predicating power in QSPR studies of octane isomers, compared to the degree distance and Gutman indices. For further, research one can study the extremal graphs for the modified Wiener index.

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