An analysis on the Wiener number and the spectrum of detour matrix of the molecular graph of benzenoid hydrocarbons

P. Gayathri$^1$* and T. Ragavan$^2$

Abstract
The detour matrix of a molecular graph is obtained and the procedure to find the detour matrix and detour spectrum is explained. The relation among the detour matrix and distance matrix are given. The detour polynomial is computed. The Wiener number is calculated and also it is compared with the DS value of the molecular graphs considered. The correlation coefficient reveals that there is a close relationship among the Wiener number and DS value of the molecular graphs.

Keywords
Wiener number, Detour matrix, Detour polynomial, Detour spectrum, Detour index, Benzenoid hydrocarbon.

AMS Subject Classification:
92E10, 11CXX, 05CXX

1. Introduction
Chemical graph theory is an interdisciplinary science that applies Graph Theory to the study of molecular structures. The molecules or chemical compounds are modeled by an undirected graph. Chemistry produces the objects of its own study and chemical composition is a unify concept for all the investigational sciences. There are no restrictions on the design of structural invariants; the limiting factor is one’s own imagination [1]. Molecular structure is one of the most fruitful scientific concepts of this century. In the molecular graph the vertices represent atoms or group of atoms and edges represent chemical bonds between atoms or group of atoms [2]. The molecular descriptor is the final result of a logic and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment [3–5]. The basic assumptions are that different molecular structures have different chemical properties and similar molecular structures have similar molecular properties. Each molecular representation represents a different way to look at the molecular structure and its chemical meaning is strongly immersed in the framework of the chemical theories [6]. The detour matrix can be used to compute a novel topological index called the detour index in the same way as the distance matrix can be used to generate the Wiener index. The detour index which is a Wiener-like, index and also in earlier studies the term-the detour index is introduced and the properties of this index and its uses in structure-property relationships are given. The usefulness of the detour index is deflated by the fact that to date no method is available to compute the index.
Let G be a connected graph with vertex set $V(G) = v_1, v_2, \ldots, v_n$. The ordinary graph spectrum is formed by the eigen values of the adjacency matrix. In what follows we denote the ordinary eigen values of the graph G by $\lambda_i, i = 1, 2, \ldots, n$ and the respective spectrum by spec(G). The detour matrix $\Delta = \Delta(G)$ of G is defined so that its $(i,j)$- entry is equal to the length of longest path between vertices i and j. The eigen values of the $\Delta(G)$ are said to be the $\Delta$-eigen values of G and form the $\Delta$-spectrum of $\Delta(G)$, denoted by spec $\Delta(G)$. Since the detour matrix is symmetric, all its eigen values $\lambda_i, i = 1, 2, \ldots, n$ are real and can be labeled so that $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_n$.

### 2. Preliminaries

#### 2.1 Wiener number of a graph G:

H. Wiener defined Wiener index $W(G)$ as the sum of smallest distance between all vertices of the graph G,

$$W(G) = \sum_{i<j} d(v_i, v_j)$$

The Wiener index $W(G)$ of a graph G is defined as the sum of the half of the distances between every pair of vertices of G.

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

#### 2.2 Detour matrix:

The detour matrix $\Delta$, sometimes also called the maximum path matrix or maximal topological distances matrix, of a graph is a symmetric matrix whose $(i,j)^{th}$ entry is the length of the longest path from vertex i to vertex j, or $\infty$ if there is no such path.

#### 2.3 Detour polynomial:

The characteristic polynomial $P_D(G,x)$ of the Detour matrix of a graph G is called the Detour polynomial is defined as

$$P_D(G,x) = det(xI - \Delta)$$

Where I is the $N \times N$ unit matrix.

The coefficient form of the detour polynomial is obtained by expanding the above determinant

$$P_D(G,x) = x^N - C_1 x^{N-1} - \ldots - C_{N-1} x - C_N$$

#### 2.4 Detour spectrum:

The roots of the detour polynomial $\lambda_i; i = 1, 2, \ldots, N$ are referred to as the detour spectrum $\lambda$. Sum of squares of the elements in the detour spectrum is equal to the trace of $\Delta^2$.

$$DS: \sum_i \lambda_i^2 = tr\Delta^2$$

#### 2.5 Detour index:

The detour index $\omega$ is defined in the same way as the Wiener index W, (i.e.) the detour index is equal to the half sum of the elements of the detour matrix.

$$\omega = \frac{1}{2} \sum_i \sum_j (\Delta)_{ij}$$

### 3. Calculation of Wiener number, Detour matrix, Detour polynomial and Detour spectrum of benzenoid hydrocarbon molecular graph:

For the following molecular graph G, its Wiener number, Detour matrix, Detour polynomial and Detour spectrum of G are determined and given below:

**Figure 1. G: The benzenoid hydrocarbons molecular graph**

**Figure 2. Benzene**

**Figure 3. Naphthalene**

**Table:**

<table>
<thead>
<tr>
<th>$W(G)$</th>
<th>$\Delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 2 &amp; 3 &amp; 2 &amp; 1 \ 1 &amp; 0 &amp; 1 &amp; 2 &amp; 3 &amp; 2 \ 2 &amp; 1 &amp; 0 &amp; 1 &amp; 2 &amp; 3 \ 3 &amp; 2 &amp; 1 &amp; 0 &amp; 1 &amp; 2 \ 2 &amp; 3 &amp; 2 &amp; 1 &amp; 0 &amp; 1 \ 1 &amp; 2 &amp; 3 &amp; 2 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; 5 &amp; 4 &amp; 3 &amp; 4 &amp; 5 \ 5 &amp; 0 &amp; 5 &amp; 4 &amp; 3 &amp; 4 \ 4 &amp; 5 &amp; 0 &amp; 5 &amp; 4 &amp; 3 \ 3 &amp; 4 &amp; 5 &amp; 0 &amp; 5 &amp; 4 \ 4 &amp; 3 &amp; 4 &amp; 5 &amp; 0 &amp; 5 \ 5 &amp; 4 &amp; 3 &amp; 4 &amp; 5 &amp; 0 \end{pmatrix}$</td>
</tr>
</tbody>
</table>

$$P_D(G,x) = det(xI - \Delta)$$

$$W = 27$$

$$DS : \sum_i \lambda_i^2 = 546$$

An analysis on the Wiener number and the spectrum of detour matrix of the molecular graph of benzenoid hydrocarbons — 550/553
An analysis on the Wiener number and the spectrum of detour matrix of the molecular graph of benzenoid hydrocarbons — 551/553

\[ W(G) = \begin{pmatrix}
0 & 1 & 2 & 3 & 2 & 3 & 4 & 3 & 2 & 1 \\
0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 \\
2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 \\
3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 \\
2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 \\
3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 \\
4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\
3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 \\
2 & 3 & 4 & 3 & 2 & 3 & 2 & 1 & 0 & 1 \\
1 & 2 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0
\end{pmatrix} \]

\[ \Delta = \begin{pmatrix}
0 & 9 & 8 & 7 & 6 & 9 & 8 & 7 & 8 & 9 \\
9 & 0 & 9 & 8 & 7 & 8 & 7 & 6 & 7 & 8 \\
8 & 9 & 0 & 9 & 8 & 7 & 6 & 5 & 6 & 7 \\
7 & 8 & 9 & 0 & 9 & 8 & 7 & 8 & 9 & 6 \\
6 & 7 & 8 & 9 & 0 & 9 & 8 & 7 & 6 & 5 \\
9 & 8 & 7 & 8 & 9 & 0 & 9 & 8 & 7 & 6 \\
8 & 7 & 6 & 7 & 8 & 9 & 0 & 9 & 8 & 7 \\
7 & 6 & 5 & 8 & 7 & 8 & 9 & 0 & 9 & 8 \\
8 & 7 & 6 & 9 & 6 & 7 & 8 & 9 & 0 & 9 \\
9 & 8 & 7 & 6 & 5 & 6 & 7 & 8 & 9 & 0
\end{pmatrix} \]

\[ P_D(G,x) = \det (xI - \Delta) \]

\[ \lambda = 67.51, -1.87, -1.87, -5.38, -11.07, -10.59, -9.22, -9.22, -8.99, -9.29 \]

\[ DS: \sum \lambda_i^2 = 5165.37 \]

\[ W = 109 \]

Figure 4. Anthracene
An analysis on the Wiener number and the spectrum of detour matrix of the molecular graph of benzenoid hydrocarbons — 552/553

$DS: \sum \lambda_i^2 = 22717.56$

$W = 279$

$\Delta =$

$P_D(G, x) = \text{det}(xl - \Delta)$

$=x^{18} + 0.021x^{17} - 33272.5x^{16} - 5.11155 \times 10^6x^{15} - 4.06501 \times 10^8x^{14} - 2.10039 \times 10^{10}x^{13} - 7.67878 \times 10^{11}x^{12} - 2.068 \times 97 \times 10^{13}x^{11} - 4.18626 \times 10^{14}x^{10} - 6380439412770080x^9 - 72274380792934272x^8 - 583952677851577088x^7 - 299.532095179539968x^6 - 50076094689925726720x^5 + 54659836674132189184x^4 + 49848954580209696780x^3 + 19583850907975992379392x^2 + 3871425474105464x^{24610816} + 300428369019077496860$

$\lambda = 250.60, 3.262, -2.428, -4.777, -23.790, -23.121,$


$DS: \sum \lambda_i^2 = 67369.47$

$W = 569$

Table I:

<table>
<thead>
<tr>
<th>Molecular graph</th>
<th>w</th>
<th>DS</th>
<th>W(DS)</th>
<th>W^2</th>
<th>(DS)^2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>27</td>
<td>546</td>
<td>14742</td>
<td>729</td>
<td>298116</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>109</td>
<td>5165.47</td>
<td>563036.23</td>
<td>11881</td>
<td>26682060.32</td>
</tr>
<tr>
<td>Anthracene</td>
<td>279</td>
<td>22717.56</td>
<td>6338199.24</td>
<td>77841</td>
<td>516087532.4</td>
</tr>
<tr>
<td>Tetracene</td>
<td>569</td>
<td>67369.47</td>
<td>38333228.43</td>
<td>323761</td>
<td>4533645488.08</td>
</tr>
<tr>
<td>Total</td>
<td>984</td>
<td>95798.5</td>
<td>45249205.0</td>
<td>414212</td>
<td>5081713216.8</td>
</tr>
</tbody>
</table>

Figure 5. Tetracene
we conclude that the topological invariants depict the real connection among atoms. Hence, distance, eccentricity and connectivity have been constructed construction oriented and also indices based upon their degree, topological index $W$ was proposed by Wiener and more and molecular graphs is very appealing and easier way. The first obtained using the molecular structures by the corresponding is a critical procedure, but the graph theoretical descriptor is observed that the coefficient of correlation between $W$ graph, the Wiener and detour spectrum are computed and it is 0.98. In QSPR development and studies for the compounds for all four of the benzenoid hydrocarbons molecular graphs $r = \frac{N \sum WDS - (\sum W)(\sum DS)}{\sqrt{N \sum W^2 - (\sum W)^2} \sqrt{N \sum DS^2 - (\sum DS)^2}}$ $= \frac{[4 \times 414212] - (984)^2 \sqrt{[4 \times 5081713216.8] - (95798.5)^2}}{\sqrt{[4 \times 414212] - (984)^2} \sqrt{[4 \times 5081713216.8] - (95798.5)^2}} = 0.98$

4. Conclusion:

For all four of the benzenoid hydrocarbons molecular graph, the Wiener and detour spectrum are computed and it is observed that the coefficient of correlation between $W$ and DS of the benzenoid hydrocarbons molecular graph is 0.98. In QSPR development and studies for the compounds is a critical procedure, but the graph theoretical descriptor is a very appealing and easier way. The first index $W$ was proposed by Wiener and more, construction oriented and also indices based upon their degree, distance, eccentricity and connectivity have been constructed because of their simple, speediness, and accuracy. Hence, we conclude that the topological invariants depict the real connection among atoms.

References