COMPUTING F-REVERSE INDEX AND F-REVERSE POLYNOMIAL OF CERTAIN NETWORKS

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ABSTRACT

In this paper, we introduce the F-reverse index of a molecular graph. Considering the F-reverse index, we define the F-reverse polynomial of a molecular graph. We compute the F-reverse index and F-reverse polynomial of silicate, chain silicate, hexagonal, oxide and honeycomb networks.

Keywords: F-reverse index, F-reverse polynomial, silicate, hexagonal, oxide, honeycomb networks

Mathematics Subject Classification: 05C05, 05C07, 05C12.

1. INTRODUCTION

A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. A topological index is a numerical parameter mathematically derived from the graph structure. These indices are useful for establishing correlation between the structure of a molecular compound and its physico-chemical properties. Also these indices have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR study, see [1].

Throughout this paper, we consider finite simple connected graphs. Let $G$ be a graph with a vertex set $V(G)$ and edge set $E(G)$. Let $d_G(v)$ denote the degree of a vertex $v$ in $G$, which is the number of vertices adjacent to $v$. Let $\Delta(G)$ denote the largest of all degrees of $G$. The reverse vertex degree of a vertex $v$ in $G$ is defined as $c_v = \Delta(G) - d_G(v) + 1$. The reverse edge connecting the reverse vertices $u$ and $v$ will be denoted by $uv$. We refer to [2] for undefined term and notation.

The first reverse Zagreb beta index and the second reverse Zagreb index of a graph $G$ are defined as

$$CM_1(G) = \sum_{uv \in E(G)} (c_u + c_v),$$

$$CM_2(G) = \sum_{uv \in E(G)} c_u c_v.$$  

These indices were introduced by Ediz in [3]. For more information and recent results about reverse Zagreb indices, see [4, 5, 6, 7, 8, 9].

The forgotten topological index or F-index of a graph $G$ is defined as

$$F(G) = \sum_{uv \in E(G)} \left[ d_G(u)^2 + d_G(v)^2 \right] = \sum_{uv \in V(G)} d_G(u)^3.$$  

The F-index was studied by Furtula and Gutman in [10] and also it was studied, for example, in [11, 12, 13, 14, 15, 16, 17, 18].

Motivated by the definition of the F-index and its applications, we introduce the F-reverse index and F$_1$-reverse index of a molecular graph as follows:

The F-reverse index of a molecular graph $G$ is defined as

$$FC(G) = \sum_{uv \in E(G)} (c_u^2 + c_v^2).$$

(1)

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The \( F_1 \)-reverse index of a molecular graph \( G \) is defined as
\[
F_1C(G) = \sum_{u \in V(G)} c_u^3.
\]

Considering the \( F \)-reverse index, we introduce the \( F \)-reverse polynomial of a graph \( G \) as
\[
FC(G, x) = \sum_{u \in V(G)} x^{c_u} c_v.
\]

Silicates are very important elements of Earth’s crust. Sand and several minerals are constituted by silicates. The tetrahedron is a basic unit of silicates, in which the central vertex is silicon vertex and the corner vertices are oxygen vertices. For networks see [19]. In this paper, the \( F \)-reverse index and \( R \)-reverse polynomial of silicate, chain silicate, hexagonal, oxide and honeycomb networks are computed.

2. RESULTS FOR SILICATE NETWORKS

Silicates are obtained by fusing metal oxide or metal carbonates with sand. A silicate network is symbolized by \( SL_n \), where \( n \) is the number of hexagons between the center and boundary of \( SL_n \). A 2-dimensional silicate network is presented in Figure 1.

![Figure-1: A 2-dimensional silicated network](image)

Let \( G \) be the graph of a silicate network \( SL_n \). From Figure 1, it is easy to see that the vertices of \( SL_n \) are either of degree 3 or 6. Therefore \( \Delta(G) = 6 \). Clearly we have \( c_u = \Delta(G) - d_G(u) + 1 = 7 - d_G(u) \). The graph \( G \) has \( 15n^2 + 3n \) vertices and \( 36n^2 \) edges. In \( G \), by algebraic method, there are three types of edges based on the degree of end vertices of each edge as follows:
\[
\begin{align*}
E_{33} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, \quad |E_{33}| = 6n. \\
E_{36} &= \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 6\}, \quad |E_{36}| = 18n^2 + 6n. \\
E_{66} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}, \quad |E_{66}| = 18n^2 - 12n.
\end{align*}
\]

Thus there are three types of reverse edges as given in Table 1.

<table>
<thead>
<tr>
<th>( c_{uv} )</th>
<th>( c_v )</th>
<th>( uv \in E(G) )</th>
<th>Number of edges</th>
<th>( (4, 4) )</th>
<th>( (4, 1) )</th>
<th>( (1, 1) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_{uv} )</td>
<td>( c_v )</td>
<td>( uv \in E(G) )</td>
<td>( 6n )</td>
<td>( 18n^2 + 6n )</td>
<td>( 18n^2 - 12n )</td>
<td></td>
</tr>
</tbody>
</table>

Table-1: Reverse edge partition of \( SL_n \)

In the following theorem, we compute the \( F \)-reverse index of \( SL_n \).

**Theorem 1:** The \( F \)-reverse index of a silicate network \( SL_n \) is
\[
 FC(SL_n) = 342n^2 + 270n. \]

**Proof:** Let \( G \) be the graph of a silicate network \( SL_n \). By using equation (1) and Table 1, we obtain
\[
FC(SL_n) = \sum_{uv \in E(G)} (c_u^2 + c_v^2) \\
= (4^2 + 4^2)6n + (4^2 + 1^2) (18n^2 + 6n) + (1^2 + 1^2) (18n^2 - 12n) \\
= 342n^2 + 270n.
\]

In the following theorem, we calculate the \( F \)-reverse polynomial of \( SL_n \).
Theorem 2: The $F$ reverse polynomial of a silicate network $SL_n$ is
\[ FC(SL_n, x) = 6nx^2 + (18n^2 + 6n)x^{17} + (18n^2 - 12n)x^2. \]

Proof: Let $G$ be the graph of a silicate network $SL_n$. By using equation (2) and Table 1, we derive
\[
FC(SL_n, x) = \sum_{uv \in E(G)} x^{(c_u + c_v)}
= 6n x^{(4^2 + 4^2)} + (18n^2 + 6n)x^{(4^2 + 4^2)} + (18n^2 - 12n)x^{(4^2 + 4^2)}
= 6nx^2 + (18n^2 + 6n)x^{17} + (18n^2 - 12n)x^2.
\]

3. RESULTS FOR CHAIN SILICATE NETWORKS

We now consider a family of chain silicate networks. This network is symbolized by $CS_n$ and is obtained by arranging $n \geq 2$ tetrahedral linearly, see Figure 2.

![Figure-2: Chain silicate network](image)

Let $G$ be the graph of a chain silicate network $CS_n$ with $3n+1$ vertices and $6n$ edges. From Figure 2, it is easy to see that the vertices of $CS_n$ are either of degree 3 or 6. Therefore $\Delta(G) = 6$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 7 - d_G(u)$. In $G$, by algebraic method, there are three types of edges based on the degree of end vertices of each edge as follows:

- $E_{44} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 4\}$, $|E_{44}| = n + 4$.
- $E_{46} = \{uv \in E(G) \mid d_G(u) = 4, d_G(v) = 6\}$, $|E_{46}| = 4n - 2$.
- $E_{66} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}$, $|E_{66}| = n - 2$.

Thus there are three types of reverse edges as given in Table 2.

<table>
<thead>
<tr>
<th>$c_u, c_v \setminus uv \in E(G)$</th>
<th>(4, 4)</th>
<th>(4, 1)</th>
<th>(1, 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>$n + 4$</td>
<td>$4n - 2$</td>
<td>$n - 2$</td>
</tr>
</tbody>
</table>

Table-2: Reverse edge partition of $CS_n$

In the following theorem, we determine the $F$ reverse index of $CS_n$.

Theorem 3: The $F$ reverse index of a chain silicate network $CS_n$ is
\[ FC(CS_n) = 102n + 90. \]

Proof: Let $G$ be the graph of a silicate network $CS_n$. By using equation (1) and Table 2, we deduce
\[
FC(CS_n) = \sum_{uv \in E(G)} (c_u^2 + c_v^2)
= (4^2 + 4^2)(n + 4) + (4^2 + 1^2)(4n - 2) + (1^2 + 1^2)(n - 2)
= 102n + 90.
\]

In the following theorem, we compute the $F$ reverse polynomial of $CS_n$.

Theorem 4: The $F$ reverse polynomial of a chain silicate network $CS_n$ is
\[ FC(CS_n, x) = (n + 4)x^{17} + (4n - 2)x^{17} + (n - 2)x^2. \]

Proof: Let $G$ be the graph of a chain silicate network $CS_n$. By using equation (2) and Table 2, we derive
\[
FC(CS_n, x) = \sum_{uv \in E(G)} x^{(c_u^2 + c_v^2)}
= (n + 4)x^{(4^2 + 4^2)} + (4n - 2)x^{(4^2 + 4^2)} + (n - 2)x^{(4^2 + 4^2)}
= (n + 4)x^{32} + (4n - 2)x^{17} + (n - 2)x^2.
\]
4. RESULTS FOR HEXAGONAL NETWORKS

It is known that there exist three regular plane tilings with composition of same kind of regular polygons such as triangular, hexagonal and square. Triangular tiling is used in the construction of hexagonal networks. This network is symbolized by $H_{Xn}$, where $n$ is the number of vertices in each side of hexagon. A hexagonal network of dimension six is shown in Figure 3.

![Figure-3: Hexagonal network of dimension six](image)

Let $G$ be the graph of a hexagonal network $H_{Xn}$. The graph $G$ has $3n^2-3n+1$ vertices and $9n^2-15n+6$ edges. From Figure 3, it is easy to see that the vertices of $H_{Xn}$ are either of degree 3, 4 or 6. Therefore $\Delta(G)=6$ and $\delta(G)=3$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 7 - d_G(u)$. In $G$, by algebraic method, there are five types of edges based on the degree of end vertices of each edge as follows:

- $E_{34} = \{uv \in E(G) | d_G(u) = 3, d_G(v) = 4\}$, $|E_{34}| = 12$.
- $E_{36} = \{uv \in E(G) | d_G(u) = 3, d_G(v) = 6\}$, $|E_{36}| = 6$.
- $E_{44} = \{uv \in E(G) | d_G(u) = d_G(v) = 4\}$, $|E_{44}| = 6n-18$.
- $E_{46} = \{uv \in E(G) | d_G(u) = 4, d_G(v) = 6\}$, $|E_{46}| = 12n-24$.
- $E_{66} = \{uv \in E(G) | d_G(u) = d_G(v) = 6\}$, $|E_{66}| = 9n^2-33n+30$.

Thus there are five types of reverse edges as given in Table 3.

<table>
<thead>
<tr>
<th>c_u, c_v \ uv \in E(G)</th>
<th>(4, 3)</th>
<th>(4, 1)</th>
<th>(3, 3)</th>
<th>(3, 1)</th>
<th>(1, 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>12</td>
<td>6</td>
<td>$6n-18$</td>
<td>$12n-24$</td>
<td>$9n^2-33n+30$</td>
</tr>
</tbody>
</table>

Table-3: Reverse edge partition of $H_{Xn}$

In the following theorem, we compute the F reverse index of $H_{Xn}$.

**Theorem 5:** The F reverse index of a hexagonal network $H_{Xn}$ is $FC(H_{Xn}) = 18n^2 + 162n - 102$.

**Proof:** Let $G$ be the graph of a hexagonal network $H_{Xn}$. By using equation (1) and Table 3, we deduce

$$FC(H_{Xn}) = \sum_{uv \in E(G)} (c_u^2 + c_v^2)$$

$$= (4^2+3^2)12 + (4^2+1^2)6 + (3^2+3^2)(6n-18) + (3^2+1^2)(12n-24) + (1^2+1^2)(9n^2 - 33n + 30)$$

$$= 18n^2 + 162n - 102.$$  

In the following theorem, we calculate the F reverse polynomial of $H_{Xn}$.

**Theorem 6:** The F reverse polynomial of a hexagonal network $H_{Xn}$ is $FC(H_{Xn}, x) = 12x^5 + 6x^7 + (6x - 18)x^{10} + (12x - 24)x^{10} + (9n^2 - 33n + 30)x^2$.

**Proof:** Let $G$ be the graph of a hexagonal network $H_{Xn}$. By using equation (2) and Table 3, we derive

$$FC(H_{Xn}, x) = \sum_{uv \in E(G)} x^{c_u^2 + c_v^2}$$

$$= 12x^{(4^2+3^2)} + 6x^{(4^2+1^2)} + (6n-18)x^{(3^2+3^2)} + (12n-24)x^{(3^2+1^2)} + (9n^2 - 33n + 30)x^{(1^2+1^2)}$$

$$= 12x^{25} + 6x^{17} + (6x - 18)x^{10} + (12x - 24)x^{10} + (9n^2 - 33n + 30)x^2.$$
5. RESULTS FOR OXIDE NETWORKS

The oxide networks are of vital importance in the study of silicate networks. An oxide network of dimension \( n \) is denoted by \( \text{OX}_n \). A 5-dimensional oxide network is shown in Figure-4.

![Figure-4: Oxide network of dimension 5](image)

Let \( G \) be the graph of an oxide network \( \text{OX}_n \). From Figure 4, it is easy to see that the vertices of \( \text{OX}_n \) are either of degree 2 or 4. Therefore \( \Delta(G)=4 \). Thus \( c_u = \Delta(G) - d_G(u) + 1 = 5 - d_G(u) \). By calculation, we obtain that \( G \) has \( 9n^2 + 3n \) vertices and \( 18n^2 \) edges. In \( G \), by algebraic method, there are two types of edges based on the degree of end vertices of each edge as follows:

\[
\begin{align*}
E_{24} &= \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}, \quad |E_{24}| = 12n, \\
E_{44} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 4\}, \quad |E_{44}| = 18n^2 - 12n.
\end{align*}
\]

Thus there are two types of reverse edges as given in Table 4.

<table>
<thead>
<tr>
<th>Type</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_u, c_v )</td>
<td>( (3, 1) )</td>
</tr>
<tr>
<td>( )</td>
<td>( (1, 1) )</td>
</tr>
<tr>
<td>( )</td>
<td>( 12n )</td>
</tr>
<tr>
<td>( )</td>
<td>( 18n^2 - 12n )</td>
</tr>
</tbody>
</table>

Thus there are two types of reverse edges as given in Table 4.

In the following theorem, we compute the \( F \) reverse index of \( \text{OX}_n \).

**Theorem 7:** The \( F \) reverse index of an oxide network \( \text{OX}_n \) is

\[
FC(\text{OX}_n) = 36n^2 + 96n.
\]

**Proof:** Let \( G \) be the graph of an oxide network \( \text{OX}_n \). By using equation (1) and Table 4, we obtain

\[
FC(\text{OX}_n) = \sum_{uv \in E(G)} (c_u^2 + c_v^2)
= (3^2 + 1^2)12n + (1^2 + 1^2)(18n^2 - 12n)
= 36n^2 + 96n.
\]

In the following theorem, we determine the \( F \) reverse polynomial of \( \text{OX}_n \).

**Theorem 8:** The \( F \) reverse polynomial of an oxide network \( \text{OX}_n \) is

\[
FC(\text{OX}_n, x) = 12nx^{10} + (18n^2 - 12n)x^2.
\]

**Proof:** Let \( G \) be the graph of an oxide network \( \text{OX}_n \). By using equation (2) and Table 4, we deduce

\[
FC(\text{OX}_n, x) = \sum_{uv \in E(G)} nx^{c_u + c_v^2}
= 12nx^{(3^2 + 1^2)} + (18n^2 - 12n)x^{(1^2 + 1^2)}
= 12nx^{10} + (18n^2 - 12n)x^2.
\]

6. RESULTS FOR HONEYCOMB NETWORKS

Honeycomb networks are useful in Computer Graphics and Chemistry. A honeycomb network of dimension \( n \) is denoted by \( \text{HC}_n \), where \( n \) is the number of hexagons between central and boundary hexagon. A 4-dimensional honeycomb network is shown in Figure 5.
Let $G$ be the graph of a honeycomb network $HC_n$. From Figure 5, it is easy to see that the vertices of $HC_n$ are either of degree 2 or 3. Thus $\Delta(G) = 3$. Therefore $c_u = \Delta(G) - d_u(u) + 1 = 4 - d_u(u)$. By calculation, we obtain that $G$ has $6n^2$ vertices and $9n^2 - 3n$ edges. In $G$, by algebraic method, there are three types of edges based on the degree of end vertices of each edge as follows:

- $E_{22} = \{uv \in E(G) | d_u(u) = d_v(v) = 2\}$, $|E_{22}| = 6$.
- $E_{23} = \{uv \in E(G) | d_u(u) = 2, d_v(v) = 3\}$, $|E_{23}| = 12n - 12$.
- $E_{33} = \{uv \in E(G) | d_u(u) = d_v(v) = 3\}$, $|E_{33}| = 9n^2 - 15n + 6$.

Thus there are three types of reverse edges as given in Table 5.

<table>
<thead>
<tr>
<th>Number of edges</th>
<th>$6$</th>
<th>$12n - 12$</th>
<th>$9n^2 - 15n + 6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_u$, $c_v$</td>
<td>$(2, 2)$</td>
<td>$(2, 1)$</td>
<td>$(1, 1)$</td>
</tr>
</tbody>
</table>

Table 5: Reverse edge partition of $HC_n$.

In the following theorem, we compute the F reverse index of $HC_n$.

**Theorem 9:** The F reverse index of a honeycomb network $HC_n$ is

$$FC(HC_n) = 18n^2 + 30n.$$  

**Proof:** Let $G$ be the graph of a honeycomb network $HC_n$. By using equation (1) and Table 5, we derive

$$FC(HC_n) = \sum_{uv \in E(G)} (c_u^2 + c_v^2)$$

$$= (2^2 + 2^2)6 + (2^2 + 1^2) (12n - 12) + (1^2 + 1^2) (9n^2 - 12n + 6)$$

$$= 18n^2 + 30n.$$  

In the following theorem, we calculate the F reverse polynomial of $HC_n$.

**Theorem 10:** The F reverse polynomial of a honeycomb network $HC_n$ is

$$FC(HC_n, x) = 6x^8 + (12n - 12)x^5 + (9n^2 - 15n + 6)x^2.$$  

**Proof:** Let $G$ be the graph of a honeycomb network $HC_n$. By using equation (2) and Table 5, we deduce

$$FC(HC_n, x) = \sum_{uv \in E(G)} x^{c_u + c_v}$$

$$= 6x^8(2^2 + 2^2) + (12n - 12)x^{(2^2 + 1^2)} + (9n^2 - 15n + 6)x^{(1^2 + 1^2)}$$

$$= 6x^8 + (18n^2 - 12n)x^5 + (9n^2 - 15n + 6)x^2.$$  

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