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CALCULATION OF SOME TOPOLOGICAL INDICES OF GRAPHS

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ABSTRACT

In this paper, we give some theoretical results, for the index Wiener$W$, degree distance DD and the hyper-Wiener index WW of a graph$G$, according to $d_G(k)$(The number of pairs of vertices of G that are at distance), and the diameter of G. We accomplish this by firstly, giving another proof of the inequality for the planar graphs with $n$vertices:$W(En) \leq W(Cn) \leq W(Pn)$[6], with E_n is a maximal planar graphC_n is a planar graph and P_n is a path planar graph. Secondly, we will apply the theoretical results for some graphs with diameter equals two, as Fan planar graphF_n, Wheel planar graph W_n, maximal planar graph E_n and the butterfly planar graph B_n, and some particularly graphs with diameter greater than two, as the cycle planar graphC_n and the Sunflower planar graph S_n.

Keywords: *Graph, Index Hyper-Wiener; Index Wiener, Index Degree Distance, Index First Zagreb.*

1. INTRODUCTION

A graph G is a triple consisting of a vertex set $V(G)$, an edge set $E(G)$, and a relation that associates with each edge two vertices (not necessarily distinct) called its endpoints. We denoted$|V(G)| = n$ is the vertex number of G and we denoted$|E(G)| = m$ is the edges number of G. We draw a graph on paper by placing each vertex at a point and representing each edge by a curve joining the locations of its endpoints (see Fig. 1). A path is a simple graph whose vertices can be ordered so that two vertices are adjacent if and only if they are consecutive in the list. A graph G is connected if each pair of the vertices in G belongs to a path. The degree of vertex v in a graph G, written $\deg(v)$, is the number of edges incident to v, except that each loop(the edge uv withe $u = v$) at v counts twice, and we called distance between two distinct vertices of graph G, u and v, the smallest length of path between u and v in G[3]. The diameter of G, denoted by $D(G)$, is defined as the maximum distance between any two vertices of G, that is:

$D(G) = \max\{d(u,v): \forall(u,v) \in V(G)^2\}$,[2][1]

In the following we consider only the simple planar connected graphs.

The Benzenoid planar graph, is composed of exclusivelyof hexagonal rings that are face bounded by six-membered cycles in the plane. Any two rings have either one commonedge (and are then said to be adjacent) or have no common vertices[8].

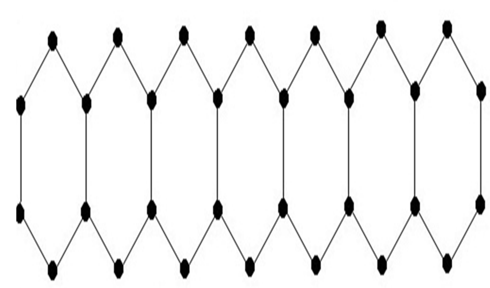

Fig.1 : The benzenoid hydrocarbons planar graph

The example of Benzenoid graphs isshown in Fig .1. The Wiener and degree distance indicesof this graph of n vertices, N hexagons and m edges isrespectively:

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$$W(G) = \frac{1}{3}(16N^3 + 132N^2 + 362N + 327)$$

And,

$$DD(G) = 5\mathrm{W(G)} - 3(2N+1)^2 \ [7].$$

Let $d_G(k)$ be the number of pairs of vertices of G that areat distance$k$,λ a real number, and :

$$\mathrm{W}_\lambda(G) = \sum_{k\geq 1} d_G(k)k^\lambda$$

$W_\lambda(G)$is called the Wiener-type invariant of G associatedto real number λ. Note that $d_G(0)$ and $d_G(1)$represent thenumber of vertices and edges, respectively[4]. The oldestand most thoroughly examined use of a topological indexin chemistry was by Wiener in the study of paraffin boilingpoints, and the topological index was called Wiener index. TheWiener index of the graph G equals to the sum of distancesbetween all pairs of vertices of the respective molecular graph,i.e:

$$\mathrm{W(G)} = \sum_{(u,v)\subseteq V(G)} \mathrm{d(u,v)}$$

(The case of$\lambda = 1$ of the$\mathrm{W}_\lambda(G)$), and we defined the index Wiener of a vertex u inthe graph G as :

$$\mathrm{w(u,G)} = \sum_{v\in V(G)} \mathrm{d(u,v)}$$

The hyper-Wienerindex WW is one of the recently conceived distance-basedgraph invariants, used as a structure descriptor for predictingphysicochemical properties of organic compounds (oftenthose significant for pharmacology, agriculture, environment protection,etc.). The hyper-Wiener index was introduced byRandic and has been extensively studied, it is defined as:

$$WW(G) = \tfrac{1}{2}(W_1(G) + W_2(G))[4].$$

In connection withcertain investigations in mathematical chemistry, Dobryninand Kochetova introduced firstly in connection with certainchemical applications, and at the same time by Gutmanwho named it the Schultz index (degree distance), definedas:

$$\mathrm{DD(G)} = \sum_{(u,v)\subseteq V(G)} \mathrm{(deg(u) + deg(v))d(u,v)}$$

Thisname was eventually accepted by most authors. The degreedistance attracted much attention after it was discovered. Ithas been demonstrated that $DD(G)$ and $W(G)$ are closelymutually related for certain classes of molecular graphs[3].The Zagreb indices have been introduced more than thirtyyears ago by Gutman and Trinajestic. They are defined as:

$$\mathrm{M}_1(G) = \sum_{u\in\{V(G)\}} \mathrm{deg(u)}^2[4][5].$$

2. THE MAIN RESULT

In this section we give some theoretic results about$W(G)$, $WW(G)$and $DD(G)$.

Theorem 1. Let Gbe a connected finite undirected graphwithout loops or multiple edges, with n vertices, $m$edges, andwith $D(G) \geq 2$, we have :

$$W(G) = n(n-1) - m + d_G(3) + 2d_G(4) + \cdots + (D-2)d_G(D)$$

Proofs:

$$W(G) = W_1(G) = d_G(1) + 2d_G(2) + 3d_G(3) + \cdots + Dd_G(D)$$

we have :

$$\frac{n(n-1)}{2} = d_G(1) + d_G(2) + \cdots + d_G(D) = m + d_G(2) + \cdots + d_G(D)$$

$$d_G(2) = m - \tfrac{n(n-1)}{2} - \cdots - d_G(D)\square$$

Corollary 1. Let Gbe a Graph with $n$vertices, $m$edges
and with $D(G) = 2$, then :

$$W(G) = n(n-1) - m$$

Proofs: We use the Theorem 1, with $D(G) = 2$.

Corollary 2.[6] Let$C_n$be a simple planar graph with n
vertices, then :

$$W(E_n) \leq W(C_n) \leq W(P_n)$$

with$E_n$is a maximal planar graph, and $P_n$is a path planar
graph.

Proofs: We have $W(C_n) \leq W(P_n)$evident.
We use the precedent theorem to proof
$W(E_n) \leq W(C_n)$as follow: We have
$W(G) = n(n-1) - m + d_G(3) + 2d_G(4) + \cdots + (D-2)d_G(D)$, for $D(G) = 2$the $m$is the maximal then $W(C_n)$is minimal for all other planar graph □.

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The Precedent result is for the wiener index and crochetedthe planar graphs, we give in the corollary 4 a result, similarlyfor an index degree distance and for the Trees.

Remark 1.[6] Let $T_n$be a Tree with $n$vertices, then

$$W(S_n) \leq W(T_n) \leq W(P_n)$$

with$S_n$is the star tree, and $P_n$is a path tree.

Theorem 2 Let Gbe a connected finite undirected graph
without loops or multiple edges, with n vertices, $m$edges,
and with $D(G) \geq 2$, we have :

$$WW(G) = \frac{1}{2}\big(3n(n-1) - 4m + (3^2-3)d_G(3) + \cdots + (D^2+D-6)d_G(D)\big)$$

Proofs: $WW(G) = \frac{1}{2}(W_1(G) + W_2(G))$
we have $W(G) = W_1(G)$, then we will needed to :

$$W_2(\mathrm{G}) = \sum_{k\geq 1} d_G(k)k^2$$

$$= d_G(1)1^2 + d_G(2)2^2 + \cdots + d_G(D)D^2$$

we apply the previous proof, with

$$d_G(2) = m - \frac{n(n-1)}{2} - \cdots - d_G(D)$$

and we put $t = 2n(n-1) - 3m$, we get to:

$$W_2(\mathrm{G}) = m + d_G(2)2^2 + d_G(3)3^2 + \cdots + d_G(D)D^2$$
$$= t + (3^2-4)d_G(3) + \cdots + (D^2-4)d_G(D) \square$$

Corollary 3. Let Gbe a Graph with $n$vertices, $m$edges
and with $D(G) = 2$, then :

$$WW(G) = \frac{3}{2}n(n-1) - 2m$$

Proofs: we use the theorem 2, with $D(G) = 2$

Theorem 3. Let Gbe a connected finite undirected graph
without loops or multiple edges, with n vertices, $m$edges,
and with $D(G) \geq 2$, we have :

$$\mathrm{DD}(G) = \sum_{u\in V(G)} \mathrm{w(u,G)\,deg(u)}$$

Proofs:

$$\mathrm{DD}(G) = \sum_{\{u,v\}\subseteq V(G)} (\deg(\mathrm{u}) + \deg(v))d(u,v)$$

$$= \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} \big(\deg(u) + \deg(v)\, d(u,v)\big)$$

$$= \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} \deg(v)\, d(u,v) + \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} \deg(u)\, d(u,v)$$

We have :

$$\sum_{u\in V(G)}\sum_{v\in V(G)} \deg(v)\, d(u,v) = \sum_{u\in V(G)}\sum_{v\in V(G)} \deg(u)\, d(u,v)$$

Then;

$$DD(G) = \sum_{u\in V(G)}\sum_{v\in V(G)} \deg(u)\, d(u,v)$$

$= \sum_{u\in V(G)} \mathrm{w(u,G)deg(u)} \square$

Corollary 4. Let Gbe a Graph with $n$vertices, $m$edges
and with $D(G) = 2$, then :

$$DD(G) = 4(n-1)m - \mathrm{M}_1(G)$$

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Proofs: we use theorem 3 we have :

$$DD(G) = \sum_{u\in V(G)} \mathrm{w}(\mathrm{u},\mathrm{G})\deg(\mathrm{u})$$

$$\mathrm{w}(\mathrm{u},\mathrm{G}) = \sum_{v\in V(G)} \mathrm{d}(\mathrm{u},\mathrm{v})$$

we have $D(G) = 2$then:

$$\mathrm{w}(\mathrm{u},\mathrm{G}) = \sum_{\substack{v\in V(G)\\ d(u,v)=1}} \mathrm{d}(\mathrm{u},\mathrm{v}) + \sum_{\substack{v\in V(G)\\ d(u,v)=2}} \mathrm{d}(\mathrm{u},\mathrm{v})$$

$$\sum_{\substack{v\in V(G)\\ d(u,v)=1}} \mathrm{d}(\mathrm{u},\mathrm{v}) = \deg(u)$$

$$n = \sum_{\substack{v\in V(G)\\ d(u,v)=1}} \mathrm{d}(\mathrm{u},\mathrm{v}) + n_2 + 1$$

with$n_2$is the number of vertex $v$with $d(u,v) = 2$then :

$$w(u,G) = \deg(u) + 2((n-1) - \deg(u))$$

$$DD(G) = \sum_{u\in V(G)} (\deg(u) + 2((n-1) - \deg(u)))\deg(u)$$

$$= 2(n-1)\sum_{v\in V(G)} \deg(u) - \sum_{u\in V(G)} \deg(u)\deg(u)$$

$$= 4(n-1)m - \mathrm{M}_1(G)\square$$

Theorem 4.[7] If $T_n$is a tree on n vertices , then:

$$DD(T_n) = 4W(T_n) - n(n-1)$$

Corollary 5. Let $T_n$be a Tree with $n$vertices, then:

$$DD(S_n) \leq DD(T_n) \leq DD(P_n)$$

with$S_n$is the star tree,and $P_n$is a path tree.

Proofs: We use the Remark 1 and the Theorem 4.

3. APPLICATION

1. Application about graphs of diameter two

In this section we will apply the Corollaries of the precedent section for some Graphs with diameter equalstwo, as Fan planar graph F_n, Wheel planar graph W_n(see the Fig. 2), maximal planar graph $E_n$and thebutterfly planar graph B_n(see the Fig. 3). We will startwith the calculation of their the first Zagreb index.

Lemma 1.$F_n$is a Fan planar graph, $W_n$is a Wheelplanar graph, $E_n$is a maximal planner graph and $B_n$isa butterfly planar graph with the number of vertices $n$and the number of edges m we have:

G_n	m	$M_1(G_n)$	n
F_n	$2n-3$	$n^2+7n-18$	$n\geq 3$
W_n	$2n-2$	n^2+7n-8	$n\geq 3$
E_n	$3n-6$	$2n^2+12n-44$	$n\geq 4$
B_n	$2n-4$	$\frac{4}{3}n^2+\frac{4}{3}-10$	$n\geq 6$

Proof: evident.

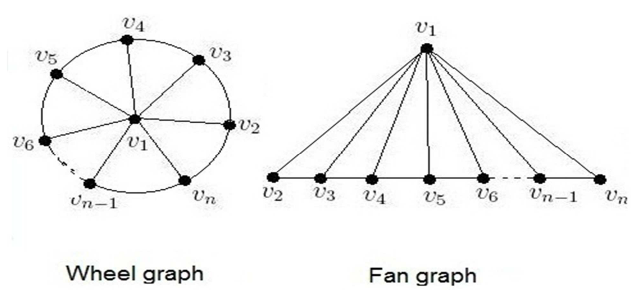

Fig.2. The Wheel planar graph $W_n$and Fan planar graph F_n

Theorem 5.$F_n$is a Fan planar graph (see the Fig. 2)with the number of vertices $n$and the number of edges$m$we have :

$W(F_n)$	n^2-3n+3	$n\geq 3$
$DD(F_n)$	$7n^2-27n+30$	$n\geq 3$
$WW(F_n)$	$\frac{3}{2}n^2-\frac{11}{2}n+6$	$n\geq 3$

Proof: We will just apply the precedent corollaries, and
using the Lemma 1.

Theorem 6.$W_n$is a Wheel planar graph (see the Fig.2) with the number of vertices $n$and the number ofedges $m$we have :

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$W(W_n)$	n^2-3n+2	$n\geq 5$
$DD(W_n)$	$7n^2-23n+16$	$n\geq 4$
$WW(W_n)$	$\frac{3}{2}n^2-\frac{7}{2}n$	$n\geq 3$

Proof: We will just apply the precedent corollaries, and
using the Lemma 1.

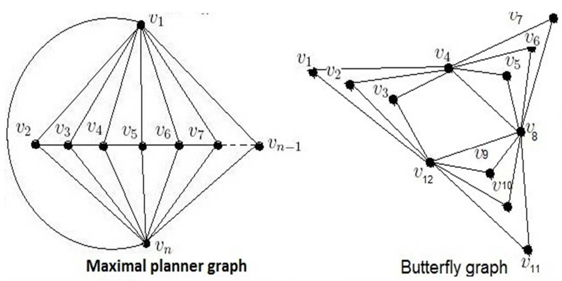

Fig.3. The Maximal planar graph E_n and Butterfly planar graph B_n

Theorem 7. E_n is a Maximal planar graph (see the Fig.3) with the number of vertices n and the number of edge ms we have :

$W(E_n)$	n^2-4n+6	$n\geq 3$
$DD(E_n)$	$10n^2-48n+68$	$n\geq 4$
$WW(E_n)$	$\frac{3}{2}n^2-\frac{15}{2}n+12$	$n\geq 4$

Proof: We will just apply the precedent corollaries, and
using the Lemma 1.

Theorem 8. B_n is a Butterfly planar graph (see the Fig. 3) of the number of vertices n and the number of edges m we have :

$W(B_n)$	n^2-3n+4	$n\geq 3$
$DD(B_n)$	$\frac{20}{3}n^2-\frac{76}{3}n+26$	$n\geq 6$
$WW(B_n)$	$\frac{3}{2}n^2-\frac{19}{2}n+16$	$n\geq 6$

Proof: We will just apply the precedent corollaries, and
using the Lemma 1.

2. Application about some particular graphs with
diameter greater than two

In the section we will see the graphs G of $D(G)\geq 2$, as the Sunflower planar graph S_n and the cycle planar graph C_n, We start with the Sunflower.

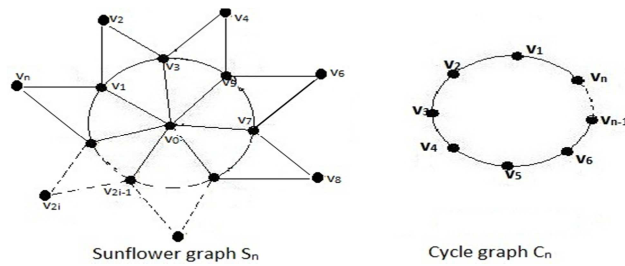

Fig.4.The Sunflower planar graph S_n and the Cycle planar graph C_n

The sunflower planar graph S_n is a graph with always has a odd number vertices n and a number of edges $m=2(n-1)$. The central vertex v_0 has a degree $\deg(v_0)=\frac{n-1}{2}$, the odd index vertices $v_1,v_3,\dots,v_{n-1}$ have a degree $\deg(v_{2i+1})=5$ and the even index vertices $v_2,v_4,\dots,v_n$ have a degree $\deg(v_{2i})=2$.

Lemma 2. S_n is a Sunflower planar graph $n\geq 11$, with the number of vertices n and the number of edges
$m\ (m=2(n-1))$ we have :

$$W(v_i, S_n)=\begin{cases}\frac{7}{2}n-\frac{35}{2} & \text{if i is even and } I\neq 0\\ \frac{3}{2}n-\frac{3}{2} & \text{if } i=0\\ \frac{5}{2}n-\frac{23}{2} & \text{if i is odd and } I\neq 0\end{cases}$$

And,

$d_{S_n}(1)$	$2n-2$
$d_{S_n}(2)$	$\frac{1}{8}n^2+n-\frac{9}{8}$
$d_{S_n}(3)$	$\frac{1}{4}n^2-2n+\frac{7}{4}$
$d_{S_n}(4)$	$\frac{1}{8}n^2-\frac{3}{2}n+\frac{11}{8}$

Proof: evident.

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Theorem 9. S_n is a Sunflower planar graph $n \geq 11$, with the number of vertices n and the number of edges m we have :

$W(S_n)$	$\frac{3}{2}n^2 - 8n + \frac{13}{2}$
$DD(S_n)$	$\frac{21}{2}n^2 - \frac{115}{2}n + 47$
$WW(S_n)$	$\frac{25}{8}n^2 - \frac{176}{8}n + \frac{151}{8}$

Proof: We have just applied the Theorems 1, 2 and 3,
and using the Lemma 2.

Lemma 3. C_n is a Cycle planar graph $n \geq 2$, with the number of vertices n and the number of edges m $(m = n)$ we have :

$$w(v_i, C_n) = \begin{cases} \frac{1}{4}n^2, if\ i\ even \\ \frac{1}{4}n^2 - \frac{1}{4}, if\ i\ odd \end{cases}$$

And,

$$d_{C_n}(i) = \begin{cases} \text{n, if n is even and } 1 \leq i < \frac{n}{2} \\ \frac{n}{2}, \text{ if n is even and } i = \frac{n}{2} \\ \text{n, if n is even and } 1 \leq i \leq \frac{n-1}{2} \end{cases}$$

Proof: evident.

Theorem 10. C_n is a Cycle planar graph $n \geq 2$, with the number of vertices n and the number of edges m, we have :

$W(C_n)$	$\frac{1}{8}n^3$	If n even
	$\frac{1}{8}n^3 - \frac{1}{8}n$	If n odd
$DD(C_n)$	$\frac{1}{2}n^3$	If n even
	$\frac{1}{2}n^3 - \frac{1}{2}n$	If n odd
$WW(C_n)$	$\frac{n^2(n+2)(n+1)}{48}$	If n even
	$\frac{n(n+3)(n^2-1)}{48}$	If n odd

Proof: We have just applied the Theorems 1, 2 and 3,and using the Lemma 3.

4. CONCLUSION

We have mentioned here some theoretical results about the Wiener index W, degree distance index DD and The hyper-Wiener index WW of a simple planar connected graphs, relating to the $d_G(k)$, and the diameter of G. We have finished our work by giving some examples of graphs with deferments diameter, as the Fan planar graph F_n, Wheel planar graph W_n, maximal planar graph E_n, the butterfly planar graph B_n, the cycle planar graph C_n and the Sunflower planar graph S_n.

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