Extremal Polygonal Cacti for Wiener Index and Kirchhoff Index

MINGYAO ZENG, QIQI XIAO, ZIKAI TANG, HANYUAN DENG*

Key Laboratory of Computing and Stochastic Mathematics (Ministry of Education), College of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan 410081, P. R. China

ARTICLE INFO

Article History:
Received: 2 April 2020
Accepted: 20 August 2020
Published online 30 September 2020
Academic Editor: Akbar Ali

Keywords:
Wiener index
Kirchhoff index
Cactus
Extremal graph

ABSTRACT

For a connected graph \( G \), the Wiener index \( W(G) \) of \( G \) is the sum of the distances of all pairs of vertices, the Kirchhoff index \( Kf(G) \) of \( G \) is the sum of the resistance distances of all pairs of vertices. A \( k \)-polygonal cactus is a connected graph in which the length of every cycle is \( k \) and any two cycles have at most one common vertex. In this paper, we give the maximum and minimum values of the Wiener index and the Kirchhoff index for all \( k \)-polygonal cacti with \( n \) cycles and determine the corresponding extremal graphs, generalize results of spiro hexagonal chains with \( n \) hexagons.

© 2020 University of Kashan Press. All rights reserved

1. INTRODUCTION

In this paper, we only consider the simple undirected and connected graphs. Let \( G = (V, E) \) be a graph with vertex set \( V(G) \) and edge set \( E(G) \). For \( u \in V(G) \), \( N_G(u) \) and \( d_G(u) \) denote the neighbor set and the degree of vertex \( u \) in \( G \), respectively, where \( d_G(u) = |N_G(u)| \). For convenience, we usually simplify as \( N_u \) and \( d_u \). The distance between any two vertices of \( u \) and \( v \) is the length of a shortest path from \( u \) to \( v \) in the graph \( G \), denoted by \( d_G(u, v) \) or \( d(u, v) \). If \( u \in V(G) \) and \( G - u \) is not connected, then \( u \) is said to be a cut-vertex of \( G \).

A cactus graph is a connected graph in which no edge lies in more than one cycle, for short, a cactus graph is also called a cactus. In fact, a graph \( G \) is a cactus if and only if

*Corresponding Author (Email address: hydeng@hunnu.edu.cn)
DOI: 10.22052/ijmc.2020.225271.1497
each block of $G$ is either an edge or a cycle. A cycle of length $k$ is usually called a $k$-polygon. If each block of a cactus $G$ is a $k$-polygon, then $G$ is called a $k$-polygonal cactus. For convenience, a $k$-polygon is usually referred to as a polygon.

Let $G_{n,k}$ denote the set of all $k$-polygonal cacti with $n \geq 3$ blocks. Let $G \in G_{n,k}$ and $C$ a $k$-polygon of $G$. If $C$ contains exactly one cut-vertex, then $C$ is called a terminal polygon; otherwise, $C$ is called a non-terminal polygon, i.e., a non-terminal polygon is a polygon contains at least two cut vertices.

A cactus chain is a special $k$-polygonal cactus such that each polygon has at most two cut-vertices, and each cut-vertex is shared by exactly two polygons. In fact, a $k$-polygonal cactus is a cactus chain if and only if the smallest connected subgraph which contains all cut-vertices is a path. If $G$ is a cactus chain, then the number of polygons is called the length of $G$. Furthermore, if $G$ is a cactus chain and the distance between two cut-vertices of each non-terminal polygon is $\left\lceil \frac{k}{2} \right\rceil$, then $G$ is called a linear cactus chain. By the definition, the linear cactus chain with $n$ polygons is unique and denoted by $L_{n,k}$.

A star-like cactus is the special $k$-polygonal cactus with $n$ polygons such that all polygons have a common vertex, i.e., all polygons are terminal polygons. By the definition, it is unique and denoted by $W_{n,k}$, and $W_{n,k}$ contains exactly one cut-vertex with degree $2n$, and the degree of all the other vertices is 2.

In [17], Wang et al. gave the first three smallest Kirchhoff indices among all cacti possessing $n$ vertices and $t$ cycles. In [21], Ye et al. determined the minimum value and maximum values of general sum-connectivity index, general Platt index and second Zagreb index, respectively, among the class of $k$-polygonal cacti with $n$ polygons. In this paper, we will give the maximum and minimum values of the Wiener index and the Kirchhoff index among all $k$-polygon cacti with $n \geq 3$ blocks and characterize the corresponding extremal graphs as well.

The Wiener index $W(G)$ of a graph $G$ is based on the distances between vertex pairs, first proposed by H. Wiener [18] in 1947, and defined as the sum of the distances of all vertex pairs, i.e., $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)$. The Wiener index is used to describe the molecular structure, which was originally applied in the field of chemistry, and now is also widely used in social relationship measurement and social network, see [5, 6, 8, 14, 15, 16].

In 1993, Klein and Randić [11] introduced another distance function, the resistance distance, on the basis of electrical network theory. Inserting a unit resistance between each edge in $G$, the resistance distance between vertices $u$ and $v$ of $G$ is the effective resistance between vertices $u$ and $v$, denoted by $r_G(u,v)$ or $r_{uv}$. Based on the resistance distance, the Kirchhoff index $Kf(G)$ of a graph $G$ is defined as the sum of the resistance distances of all vertex pairs, i.e., $Kf(G) = \sum_{\{u,v\} \subseteq V(G)} r_G(u,v)$. For a vertex $u \in V(G)$, let $Kf_u(G) =$
\[ \Sigma_{u \in V(G)} r_G(u,v), \text{ then } Kf(G) = \frac{1}{2} \Sigma_{u \in V(G)} Kf_u(G). \] As a useful structure-descriptor, the Kirchhoff index was well studied in [11, 13]. Much work has been done to compute the Kirchhoff index of some classes of graphs, such as complete graphs, cycles, distance transitive graphs, circulant graphs, linear hexagonal chains, unicyclic graphs and so on, see [1, 2, 3, 4, 7, 9, 10, 12, 17, 19, 20, 22, 23].

**2. THE EXTREMAL GRAPH WITH THE MAXIMUM INDEX**

In this section, we will determine the \( k \)-polygonal cactus with the maximum Wiener index and the maximum Kirchhoff index among all \( k \)-polygon cacti with \( n \) blocks for \( k \geq 3 \) and \( n \geq 3 \).

Firstly, we introduce some lemmas.

**Lemma 1.** [11] Let \( x \) be a cut vertex of a connected graph \( G \) and \( a, b \) be vertices occurring in different components of \( G - x \). Then \( r_G(a,b) = r_G(a,x) + r_G(x,b) \).

**Lemma 2.** [7, 17] Let \( G_1 \) and \( G_2 \) be connected graphs. \( x_1 \in V(G_1) \) and \( x_2 \in V(G_2) \). If \( G \) is obtained by identifying \( x_1 \) with \( x_2 \), then \( Kf(G) = Kf(G_1) + Kf(G_2) + n_1Kf_{x_1}(G_2) + n_2Kf_{x_1}(G_1) \), where \( Kf_{x_i}(G_i) = \Sigma_{y \in V(G_i)} r_{G_i}(x_i,y) \), and \( n_i = |V(G_i)| - 1 \) for \( i = 1, 2 \).

**Lemma 3.** If \( G \in G_{n,k} \) with the maximum Wiener index or the maximum Kirchhoff index, where \( k \geq 3, n \geq 3 \), and \( C \) is a \( k \)-polygon in \( G \) with exactly two cut-vertices, then the distance between two cut-vertices of \( C \) is \( \left\lfloor \frac{k}{2} \right\rfloor \).

**Figure 1:** The graphs \( G \) and \( G' \).

**Proof.** Let \( C = w_1w_2...w_i...w_kw_1 \) be a non-terminal polygon of \( G \in G_{n,k} \), \( w_1 \) and \( w_i \) its two cut-vertices. \( G_1 \) and \( G_2 \) are the components of \( G - E(C) \) containing \( w_1 \) and \( w_i \),
respectively. If \(2 \leq i \leq \left \lfloor \frac{k}{2} \right \rfloor\), then we only need to show that \(W(G') > W(G)\) and \(Kf(G') > Kf(G)\), where \(G' = G - w_i u - w_i v + w_i^k_{(k-1)} + u + w_i^k_{(k-1)} + v\), see Figure 1.

Let \(V_1 = V(G_1), V_2 = V(G_2) \cup V(C), V'_1 = V_1 - \{w_1\}, V'_2 = V_2 - \{w_1\}\). We have

\[
W(G') - W(G) = \sum_{x,y \in V(G)} [d_{G'}(x,y) - d_G(x,y)]
= \sum_{x,y \in V_1} [d_{G'}(x,y) - d_G(x,y)] + \sum_{x,y \in V_2} [d_{G'}(x,y) - d_G(x,y)]
+ \sum_{y \in V'_1} \sum_{x \in V_2} [d_{G'}(x,y) - d_G(x,y)]
= \sum_{y \in V'_1} \sum_{x \in V_2} [d_{G'}(x,y) - d_G(x,y)]
= \sum_{y \in V'_1} \sum_{x \in V(G_2)} [d_{G'}(x,y) - d_G(x,y)]
= \sum_{y \in V'_1} \sum_{x \in V(G_2)} \sum_{i=0}^{k-1} w_{i+1}(w_i, w_{i+1})
> 0,
\]

i.e., \(W(G') > W(G)\).

Next, we consider the Kirchhoff index. Let \(H_2'\) be the induced subgraphs by \(V(C) \cup V(G_2)\) in \(G\) and \(G'\), respectively, \(n_1 = |V_1| - 1\) and \(n_2 = |V_2| - 1\). By Lemma 2 and Lemma 1, we have

\[
Kf(G') - Kf(G) = [Kf(G_1) + Kf(H_2') + n_1Kf_{w_1}(H_2') + n_2Kf_{w_1}(G_1)]
- [Kf(G_1) + Kf(H_2) + n_1Kf_{w_1}(H_2) + n_2Kf_{w_1}(G_1)]
= n_1[Kf_{w_1}(H_2') - Kf_{w_1}(H_2)]
= n_1 \sum_{x \in V_2} [r_{G'}(x, w_{i+1})] + r_{G'}(w_{i+1}, w_{i+1})]
- [r_G(x, w_i) + (w_i, w_{i+1})]
= n_1 \sum_{x \in V_2} [r_{G'}(w_{i+1}, w_i)]
= n_1 \sum_{x \in V_2} r_{G'}(w_{i+1}, w_i) > 0,
\]

i.e., \(Kf(G') > Kf(G)\). \(\square\)

Let \(G \in G_n^k, k \geq 3\) and \(n \geq 3\), and let \(C_1, C_2, \ldots, C_s\) be \(s (s \geq 1)\) cycles of length \(k\) in \(G\), \(V_1 = V(C_1) \cup V(C_2) \cup \cdots \cup V(C_s), u \in C_1\) is a cut vertex of \(G\) but not a cut vertex of \(G[V_1]\). If \(G[V_1]\) is a cactus chain and each \(k\)-polygon of \(\{C_1, C_2, \ldots, C_s\}\) has at most two cut-vertices in \(G\), \(C_s\) is a terminal polygon of \(G\), the degree of each vertex of \(V_1 - \{u\}\) is at most four in \(G\), then \(G[V_1]\) is called a pendent cactus chain of length \(s\) of \(G\), and \(C_{s-1}\) is called a neighbor polygon of the pendent cactus chain [21].
From the definition, if $G[V_i]$ is a pendent cactus chain of length $s \geq 2$, then for $1 \leq i \leq s - 1$ and $2 \leq j \leq s - 1$, each $C_i$ contains exactly two cut-vertices in $G$, and the degree of every cut-vertex of $C_j$ is equal to four in $G$.

Let $G \in G_{n,k}$, $k \geq 3$ and $n \geq 3$ and let $C_1, C_2, \ldots, C_{s+t}$ be $s + t$ ($s \geq 1, t \geq 1$) cycles in $G$ such that the induced subgraphs $G[V(C_1) \cup V(C_2) \cup \ldots \cup V(C_s)]$ and $G[V(C_{s+1}) \cup V(C_{s+2}) \cup \ldots \cup V(C_{s+t})]$ are two pendent linear cactus chains of length $s$ and $t$ respectively, i.e., the distance between two cut-vertices in the each cycle $C_i$ is $\lceil \frac{k}{2} \rceil$.

(i) If $u_0 \in V(C_1) \cap V(C_{s+1})$ and $d_G(u_0) \geq 6$, then $u_0$ is called a special vertex of $G$; (ii) If $C_0$ is a $k$-polygon of $G$ with at least three cut-vertices in $G$ such that $V(C_1) \cap V(C_0) = v_0$ and $V(C_{s+1}) \cap V(C_0) = w_0$ with $d_G(w_0) = d_G(v_0) = 4$, then $C_0$ is called a special polygon of $G$.

The following result shows that the $k$-polygon cactus with the maximum Wiener index or the maximum Kirchhoff index has no special vertices.

**Lemma 4.** If $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index, then $G$ has no special vertices.

![Figure 2: The graph $G$ in Lemma 4.](image)

**Proof.** Let $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index. By Lemma 3, all pendent chains in $G$ are linear. If $G$ has a special vertex $u_0$, then there are $s + t$ ($s \geq 1, t \geq 1$) cycles $C_1, C_2, \ldots, C_{s+t}$ in $G$ such that the induced subgraphs $G[V(C_1) \cup V(C_2) \cup \ldots \cup V(C_s)]$ and $G[V(C_{s+1}) \cup V(C_{s+2}) \cup \ldots \cup V(C_{s+t})]$ are two pendent linear cactus chains of length $s$ and $t$, respectively, and $u_0 \in V(C_1) \cap V(C_{s+1})$ and $d_G(u_0) \geq 6$, see Figure 2, i.e., $G$ is obtained from $G_1$ and $G_2$ by identifying $u_0 \in V(G_1)$ with $w_1 \in V(C_{s+1})$, where $G_2 = G[V(C_{s+1}) \cup V(C_{s+2}) \cup \ldots \cup V(C_{s+t})]$ is the linear chain $L_{n,s+t}$. 
Let $G = G_0 = G - u_0w_2 - u_0w_k + u_{\lfloor \frac{k}{2} \rfloor + 1}w_1 + u_{\frac{k}{2} + 1}w_k$, then $G' \in G_{n,k}$. Note that $W(G) = W(G_1) + W(G_2) + \sum_{x \in V_1, y \in V_2} d_G(x, y)$, where $V_1 = V(G_1) - \{u_0\}$ and $V_1 = V(G) - V(G_1)$, we have $W(G') - W(G) = \sum_{x \in V_1, y \in V_2} [d_G'(x, y) - d_G(x, y)] > 0$. Similarly,

$$Kf(G') - Kf(G) = \sum_{x \in V_1, y \in V_2} [r_G'(x, y) - r_G(x, y)] > 0.$$ 

So, $W(G') > W(G)$ and $Kf(G') > Kf(G)$, a contradiction to $G$ with the maximum Wiener index or the maximum Kirchhoff index. \qed

Now, we will show that the $k$-polygon cactus with the maximum Wiener index or the maximum Kirchhoff index also has no special polygons.

**Lemma 5.** If $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index, then $G$ has no special polygon.

**Proof.** Let $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index. By Lemmas 3 and 4, all pendant chains in $G$ are linear and $G$ has no special vertices.

If $G$ has a special polygon $C_0$, then there are $s + t(s \geq 1, t \geq 1)$ cycles $C_1, C_2, \ldots, C_{s+t}$ in $G$ such that the induced subgraphs $L_{n,s} = G[V(C_1) \cup V(C_2) \cup \cdots \cup V(C_s)]$ and $L_{n,t} = G[V(C_{s+1}) \cup V(C_{s+2}) \cup \cdots \cup V(C_{s+t})]$ are two pendant linear cactus chains of length $s$ and $t$, respectively, $v_0 \in V(C_1) \cap V(C_0)$, $w_0 \in V(C_{s+1}) \cap V(C_0)$ and $d_G(v_0) = d_G(w_0) = 4$, i.e., $G$ is obtained from $C_0 \cup G_1 \cup \cdots \cup G_r$, $L_{n,s}$ and $L_{n,t}$ by identifying $v_0 \in V(C_0)$ with $v_1 \in V(C_1)$ and identifying $w_0 \in V(C_0)$ with $w_1 \in V(C_{s+1})$, where $C_1 = v_1v_2 \cdots v_kv_1$ with two cut-vertices $v_1$ and $v_k$ and $C_{s+1} = w_1w_2 \cdots w_kw_1$ with two cut-vertices $w_1$ and $w_{\frac{k}{2} + 1}$ and $C_0 \cup G_1 \cup \cdots \cup G_r$ is obtained by attaching $k$-polygons $G_i$ ($1 \leq i \leq r$) to cut-vertices $v_i$ of $C_0$, see Figure 3. Let $G' = G - w_0w_1 - w_0w_k + u_{\lfloor \frac{k}{2} \rfloor + 1}w_2 + u_{\frac{k}{2} + 1}w_k$ where $u_1$ and $u_{\lfloor \frac{k}{2} \rfloor + 1}$ are two cut-vertices of $C_s = u_1u_2 \cdots u_ku_1$ in $G_0$. Then $G_0 \in G_{n,k}$, and $W(G) = \sum_{i=1}^r W(G_i) + W(H) + \sum_{x \in V_1, y \in V_2} d_G(x, y)$, $W(G') = \sum_{i=1}^r W(G_i) + W(L_{n,s+t+1}) + \sum_{x \in V_1, y \in V_2} d_G'(x, y)$, where $H$ is the induced subgraph of $G$ by $V(C_1) \cup V(C_2) \cup \cdots \cup V(C_{s+t})$, $L_{n,s+t+1}$ is the linear chain consisted of $C_0 \cup C_1 \cup \cdots \cup C_{s+t}$ in $G_0$, $V_1 = V(H) - R$ and $V_2 = V(G) - V(H)$ and $R = \{w_0, v_0, v_1, \ldots, v_t\}$ is the set of cut-vertices of $C_0$ in $G$. Note that $W(H) \leq W(L_{n,s+t+1})$ since $d_G(v_0, w_0) \leq \frac{k}{2}$, and $\sum_{x \in V_1, y \in V_2} d_G(x, y) - \sum_{x \in V_1, y \in V_2} d_G'(x, y) = \sum_{x \in V_1, y \in V_2} [d_G(x, y) - d_G'(x, y)]$, where $V'_2 = V(C_{s+1} \cup \cdots \cup C_{s+t}) - \{w_1\}$. Therefore,
$$\sum_{x \in V_1, y \in V'_2} [d_G(x, y) - d_G'(x, y)]$$

$$= \sum_{x \in V_1, y \in V'_2} [(d_G(x, w_0) + d_G(w_0, y)) - (d_G'(x, u_{[2]k+1}) + d_G'(u_{[2]k+1}, y))]$$

$$= \sum_{x \in V_1, y \in V'_2} [d_G(x, w_0) - d_G'(x, u_{[2]k+1})] > 0.$$ 

So, $W(G) < W(G')$. Similarly, by Lemmas 1 and 2, we can get $Kf(G) < Kf(G')$, a contradiction to $G$ with the maximum Wiener index or the maximum Kirchhoff index. 

**Theorem 6.** Let $G \in G_{n,k}$, $k \geq 3$ and $n \geq 3$. Then

$$W(G) \leq \binom{n}{3}(k - 1)^2 \left[ \frac{k}{2} \right] + \left( \frac{1}{2} nk + (k - 1)(n^2 - n) \right)\left[ \frac{k^2}{4} \right],$$

$$Kf(G) \leq \binom{n}{3} \frac{(k - 1)^2}{k} \left[ \frac{k}{2} \right]^2 + \frac{1}{12} (nk + 2(k - 1)(n^2 - n))(k^2 - 1),$$

with equality if and only if $G = L_{n,k}$ is a linear chain with $n$ $k$-polygons.

**Proof.** Let $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index. By Lemmas 3, 4 and 5, we know that $G$ is the linear chain $L_{n,k}$. So, we only need to compute $W(L_{n,k})$ and $Kf(L_{n,k})$. Let $D_u(G) = \sum_{u \in V(G)} d_G(x, u)$. If $C$ is a $k$-polygon and $u \in V(C)$, then $a = D_u(G) = \left[ \frac{k^2}{4} \right]$ and $W(C) = \frac{1}{2} ka$.

Let $L_{n,k} = C_1 \cup C_2 \cdots \cup C_n$ consist of $n$ $k$-polygons $C_1, C_2, \ldots, C_n$, $u_i$ is the common cut-vertex of $C_i$ and $C_{i+1}$, the distance $b = d(u_i, u_{i+1}) = \left[ \frac{k}{2} \right], 1 \leq i < n$.

$$W(L_{n+1,k}) = W(L_{n,k}) + W(C_{n+1}) + (k - 1)D_{u_n}(L_{n,k}) + (k - 1)na$$

$$= W(L_{n,k}) + \frac{1}{2} ka + (k - 1)nD_{u_n}(L_{n,k}) + (k - 1)na$$

$$= W(L_{n,k}) + (k - 1)nD_{u_n}(L_{n,k}) + \left[ \frac{1}{2} k + (k - 1)n \right]a.$$ 

Now, $D_{u_1}(L_{1,k}) = a$, $D_{u_2}(L_{2,k}) = a + a + (k - 1)b = 2a + (k - 1)b$, $D_{u_3}(L_{3,k}) = 2a + (k - 1)b + a + 2(k - 1)b = 3a + 3(k - 1)b$, and we have by induction that $D_{u_n}(L_{n,k}) = na + \binom{n}{2}(k - 1)b$. So,
\[ W(L_{n+1,k}) = W(L_{n,k}) + \binom{n}{2}(k-1)^2b + \left[ \frac{1}{2}k + 2(k-1)n \right]a \]
\[ = W(L_{n-1,k}) + \left[ \binom{n-1}{2} + \binom{n}{2} \right](k-1)^2b + \frac{1}{2}k + 2(k-1)n \]
\[ = W(L_{1,k}) + \sum_{i=1}^{n} \binom{i}{2}(k-1)^2b + \sum_{i=1}^{n} \left[ \frac{1}{2}k + 2(k-1)i \right]a \]
\[ = \frac{1}{2}ka + \binom{n+1}{3}(k-1)^2b + \sum_{i=1}^{n} \left[ \frac{1}{2}k + 2(k-1)i \right]a \]
\[ = \binom{n+1}{3}(k-1)^2 + \left( \frac{1}{2}k(n+1) + (k-1)n(n+1) \right) \frac{k^2}{4} \]

Similarly, let \( Kf_u(G) = \sum_{x \in V(G)} r_G(x,u) \). If \( C \) is a \( k \)-polygon and \( u \in V(C) \), then \( a' = Kf_u(C) = \frac{k^2-1}{6} \) and \( Kf(C) = \frac{1}{2}ka' = \frac{k^2-k}{12} \). Let \( b' = r_{c_i+1}(u_i,u_{i+1}) = \frac{1}{k} \left[ \frac{k}{2} \right] \left[ \frac{k}{2} \right] \). Then, \( Kf(L_{n+1,k}) = Kf(L_{n,k}) + Kf(C_{n+1}) + (k-1)Kf_{u_n}(L_{n,k}) + (k-1)n Kf_{u_n}(C_{n+1}) = Kf(L_{n,k}) + (k-1)Kf_{u_n}(L_{n,k}) + \binom{n+1}{3}(k-1)^2b' + \left( \frac{1}{2}k(n+1) + (k-1)n(n+1) \right) \frac{k^2}{4} \),

Hence the result.

Theorem 6 gives the maximum values of Wiener index and Kirchhoff index for all \( k \)-polygonal cacti with \( n \) cycles and characterizes the extremal graphs. For \( k = 6 \), we can get the maximum values of Wiener index and Kirchhoff index for all spiro hexagonal chains with \( n \) hexagons.

**Corollary 7.** [3, 4, 9] Among all spiro hexagonal chains with \( n \) hexagons, we have

(i) the unique spiro hexagonal chain with the maximum Wiener index is the spiro para-chain \( P_n \), and \( W(P_n) = \frac{25}{2} n^3 + \frac{15}{2} n^2 + 7n \);

(ii) the unique spiro hexagonal chain with the maximum Kirchhoff index is the spiro para-chain \( P_n \), and \( Kf(P_n) = \frac{25}{2} n^3 + \frac{125}{12} n^2 + \frac{5}{6} n \).

**3. The Extremal Graph with the Minimum Index**

In this section, we determine the minimum values of Wiener index and Kirchhoff index for all \( k \)-polygonal cacti with \( n \) cycles and characterizes the extremal graphs and the corresponding extremal graphs.
Theorem 8. Let $G \in G_{n,k}$, $k \geq 3$ and $n \geq 3$. Then
\[
W(G) \geq \frac{1}{2} n(k + 2(n-1)(k-1)) \left\lceil \frac{k^2}{4} \right\rceil,
\]
\[
Kf(G) \geq \frac{1}{12} n(k + 2(n-1)(k-1))(k^2-1),
\]
with equality if and only if $G = W_{n,k}$ is a star-like cactus with $n \, k$-polygons.

Proof. Let $G \in G_{n,k}$ be a cactus with the minimum Wiener index or the minimum Kirchhoff index. We first show that $G$ is a star-like cactus, i.e., each polygon in $G$ has only one cut-vertex. If there is a $k$-polygon $C_0$ in $G$ such that $C_0$ has at least two cut-vertices, then we only need to show that there is $C_0 \in G_{n,k}$ such that $W(C_0) < W(G)$ and $Kf(G_0) < Kf(G)$. Let $v_1, v_2, \ldots, v_t$ be all cut-vertices in $C_0$, $t \geq 2$, and $G_i$ the components of $G - E(C_0)$ containing $v_i$, $i = 1, 2, \ldots, t$, i.e., $G$ is obtained by attaching $G_i$ to the cut-vertex $v_i$ of $G_0$. Now, we take $G_0$ to be the cactus obtained by attaching all $G_i(i = 1, 2, \ldots, t)$ to the same vertex $v_1$ of $C_0$, see Figure 4, then $W(G) = \sum_{i=1}^{t} W(G_i) + W(C_0) + \sum_{1 \leq i < j \leq t} \sum_{x \in E_i, y \in E_j} d_G(x, y) + \sum_{i=1}^{t} \sum_{x \in E_i, y \in E_0} d_G(x, y)$, where $V_0 = V(C_0) - \{v_1, \ldots, v_t\}$.

$V_i = V(G_i) - \{v_i\}$, $1 \leq i \leq t$, and $W(G') = \sum_{i=1}^{t} W(G_i) + W(C_0) + \sum_{1 \leq i < j \leq t} \sum_{x \in E_i, y \in E_j} d_{G'}(x, y) + \sum_{i=1}^{t} \sum_{x \in E_i, y \in E_0} d_{G'}(x, y)$. Note that $\sum_{i=1}^{t} \sum_{x \in E_i, y \in E_0} d_{G'}(x, y)$ is obtained by attaching all $G_i(i = 1, 2, \ldots, t)$ to the same vertex $v_1$ of $C_0$.

So, we have $W(G') < W(G)$. Similarly, by Lemmas 1 and 2, we can get $Kf(G') < Kf(G)$.

Next, we compute $W(W_{n,k})$ and $Kf(W_{n,k})$. Let $W_{n,k} = C_1 \cup C_2 \cdots \cup C_n$ consist of $n \, k$-polygons $C_1, C_2, \cdots, C_n$, $v_0$ is the common cut-vertex of all $C_i(1 \leq i \leq t)$. Then
\[
W(W_{n+1,k}) = W(W_{n,k}) + W(C_{n+1}) + (k-1)D_{v_0}(W_{n,k}) + (k-1)nD_{v_0}(C_{n+1})
\]
\[
= W(W_{n,k}) + \frac{1}{2} ka + (k-1)D_{v_0}(W_{n,k}) + (k-1)na
\]
\[
= W(W_{1,k}) + \sum_{i=1}^{n} \left[ \frac{1}{2} k + 2(k-1)i \right] a
\]
\[
= \frac{1}{2} ka + \sum_{i=1}^{n} \left[ \frac{1}{2} k + 2(k-1)i \right] a
\]
\[
= \frac{1}{2} (n+1) (k + 2nk - 2n) \left\lceil \frac{k^2}{4} \right\rceil,
\]
and
\[
Kf(W_{n+1,k}) = Kf(W_{n,k}) + Kf(C_{n+1}) + (k-1)Kf_{v_0}(W_{n,k}) + (k-1)nKf_{v_0}(C_{n+1})
\]
\[
= Kf(W_{n,k}) + \frac{1}{2} ka' + (k-1)na' + (k-1)na'
\]
\[
= Kf(W_{1,k}) + \sum_{i=1}^{n} \left[ \frac{1}{2} k + 2(k-1)i \right] a'
\]
\[
= \frac{1}{2} ka' + \sum_{i=1}^{n} \left[ \frac{1}{2} k + 2(k-1)i \right] a'.
\]
\[ \frac{1}{12} (n + 1) (k + 2nk - 2n) (k^2 - 1). \]

Theorem 8 gives the minimum values of Wiener index and Kirchhoff index for all \( k \)-polygonal cacti with \( n \) cycles and characterizes the extremal graphs.

Figure 4: The graphs \( G \) and \( G' \) in Theorem 8.

ACKNOWLEDGEMENT. This work is supported by the National Natural Science Foundation of China (11971164) and the Department of Education of Hunan Province (19A318).

REFERENCES