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Research Paper

Kirchhoff, Multiplicative and Additive Degree-Kirchhoff Indices in Random Cyclodecane Chains

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Abstract

The Kirchhoff index serves as a significant measure in characterizing molecular topological structures. It quantifies atomic connectivity within molecules and facilitates the correlation and prediction of physicochemical properties and biological activities of chemical compounds, thereby holding considerable practical value. This paper derives recurrence relations for the expected values of three variants of the Kirchhoff index, the multiplicative degree-Kirchhoff index, and the additive degree-Kirchhoff index in random cyclodecane chains using a recursive approach. Based on these relations, the extremal values and average values of these indices are obtained for a cyclodecane chain composed of n regular decagons. Furthermore, it is shown that the expected Kirchhoff indices of the random cyclodecane chain equal the average of the corresponding indices over five specific structural configurations of the chain.

1 Introduction

Graph theory provides various parameters with wide applications in physics, chemistry, biology, and other disciplines. In practical applications, real-world entities are often represented as nodes, and the relationships between them as edges, thereby transforming actual problems into graph models for analysis. Distance serves as a fundamental measure for quantifying relationships between objects. In electrical network theory, the voltage required to generate a unit current between two nodes reflects their effective connectivity. Resistance distance, introduced by Klein and Randić [1], defines the effective resistance between pairs of vertices

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as a graph-theoretic distance and establishes summation rules for its computation in arbitrary graphs. Lukovits et al. further considered the sum of resistance distances over all vertex pairs as a graph invariant [2]. Chen and Zhang [3] developed a complete set of local rules that simplify and enhance the efficiency of calculating resistance distances in trees. Based on resistance distance, the Wiener index was defined as the sum of shortest path lengths between all vertex pairs [4], and the Gutman index was introduced by Ivan Gutman using vertex degrees [5]; relevant studies on these indices can be found in [6–8]. The Kirchhoff index was defined by Klein and co-authors based on resistance distances [9]. Subsequently, the multiplicative degree-Kirchhoff index was introduced by Chen and co-workers as the sum over all vertex pairs of the product of resistance distance and vertex degrees [10], and the additive degree-Kirchhoff index was defined by Gutman et al. [11].

In recent years, increasing research attention has been devoted to the study of the Kirchhoff index. Sajjad et al. investigated the resistance distance and Kirchhoff index of a class of claw-free double-triangle graphs [12]. Sun et al. determined the extremal values of the Kirchhoff index in linear triangle chains [13], while Chen et al. established the extreme values of the Gutman index and the degree-Kirchhoff index in helical and biphenyl hexagonal chains [14]. Research on the Kirchhoff index of three-dimensional graph structures has also been progressively developed. Li et al. computed the resistance distance and Kirchhoff index of the cyclic triangular bipyramid hexahedron [15], and Zhao et al. derived formulas for the Kirchhoff index and degree-Kirchhoff index of linear tetrahedron chains [16]. The study of Kirchhoff indices in random polygon chains constitutes another emerging research direction. Qin and Ma investigated the Kirchhoff index of random hexagonal-quadrilateral chains and spiral connections [17], Li et al. obtained the maximum expected values of the Kirchhoff index in random polyomino chains [18], Zhang et al. established the expected values of the multiplicative and additive degree-Kirchhoff indices in random polyphenylene chains [19], and Zhu and Geng derived expressions and extremal values for the multiplicative and additive degree-Kirchhoff indices in random polygonal chains [20]. Hechao Liu et al. obtained closed-form expressions for three types of Kirchhoff indices in random cyclooctane chains [21], and Wei et al. deduced explicit formulas for the expected values of the Wiener index and Kirchhoff index in random pentagonal chains [22]. Recent studies provide a comprehensive understanding of the Kirchhoff index and its applications [23–25].

On the basis of previous studies, this work extends the complexity and chain length of chemical structures. The recursive method is employed to compute three types of Kirchhoff indices for random cyclodecane chains. Section 2 introduces fundamental concepts of the Kirchhoff index, multiplicative degree-Kirchhoff index, and additive degree-Kirchhoff index, along with a detailed structural description of random cyclodecane chains. Section 3 presents the derivation of expected values, extremal values, and average values of these indices for random cyclodecane chains. Finally, Section 4 summarizes the obtained results and suggests directions for future research.

2 Preliminaries

Let $G = (V(G), E(G))$ be a graph, where $V(G) = \{v_1, v_2, \ldots, v_n\}$ denotes the vertex set and $E(G) = \{e_1, e_2, \ldots, e_m\}$ denotes the edge set of G. The number of edges incident to a vertex $u \in V(G)$ is called its degree, denoted by $d_G(u)$. The length of the shortest path between vertices u and v is denoted by $d_G(u, v)$. The sum of resistance distances from a vertex v_i to all other vertices in G is defined as

$$r(v_i \mid G) = \sum_{j=1}^{n} r(v_i, v_j),$$

where $r(v_i, v_j)$ denotes the resistance distance between v_i and v_j, and by convention, $r(v_i, v_i) = 0$.

The important definitions that need to be used in the paper are given below:

Definition 2.1. ([1]). The *resistance distance* between vertices u and v in graph G, denoted by $r_G(u, v)$, is defined as the effective resistance between them when G is regarded as an electrical network.

Definition 2.2. ([4]). The *Wiener index* of a graph G is defined as

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v). \tag{1}$$

Definition 2.3. ([9]). The Kirchhoff index of a graph G is defined as

$$Kf(G) = \sum_{\{u,v\}\subseteq V(G)} r_G(u, v). \tag{2}$$

An equivalent formulation of the Kirchhoff index is given by:

$$\begin{aligned} Kf(G) = \sum_{i<j} r(v_i, v_j) &= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} r(v_i, v_j) \\ &= \frac{1}{2}\sum_{i=1}^{n} r(v_i \mid G). \end{aligned} \tag{3}$$

Definition 2.4. ([10]). The multiplicative degree-Kirchhoff index of a graph G is defined as

$$Kf^*(G) = \sum_{\{u,v\}\subseteq V(G)} \big(d_G(u) \cdot d_G(v)\big) r_G(u, v). \tag{4}$$

Definition 2.5. ([11]). The additive degree-Kirchhoff index of a graph G is defined as

$$Kf^+(G) = \sum_{\{u,v\}\subseteq V(G)} \big(d_G(u) + d_G(v)\big) r_G(u, v). \tag{5}$$

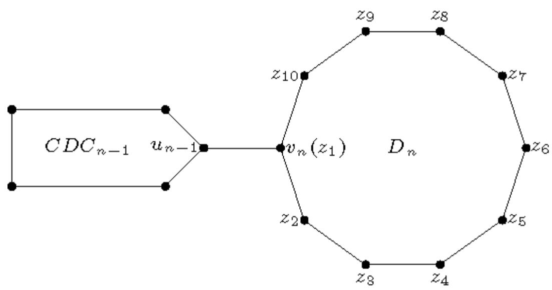


Figure 1: The cyclodecane chain CDC_n consisting of n regular decagons.

Figure 1 illustrates a cyclodecane chain CDC_n comprising n regular decagons. This structure can be recursively constructed by connecting a terminal regular decagon D_n to the preceding chain CDC_{n-1} through a cut edge.

Let $\mathrm{CDC}_n = D_1D_2\cdots D_n$ be a cyclodecane chain comprising n (where $n \geq 2$) regular decagons, where each D_t (for $t = 2, 3, \ldots, n$) denotes the t-th decagon attached to D_{t-1} via the cut edge $u_{t-1}v_t$. Within each decagon D_t, the vertices located at distances 1 through 5 from vertex v_t are labeled as o_t, m_t, s_t, w_t, and l_t, respectively. For instance, as illustrated in Figure 1, if $v_n = z_1$, then $z_2 = z_{10} = o_n$, $z_3 = z_9 = m_n$, $z_4 = z_8 = s_n$, $z_5 = z_7 = w_n$, and $z_6 = l_n$.

In the cyclodecane chain CDC_n with n regular decagons, there exist several special types of CDC_n. For example: for any $2 < t < n-1$, if $u_t = o_t$ holds true, then this cyclodecane chain CDC_n is denoted as CO_n; if $u_t = m_t$, then it is denoted as CM_n; if $u_t = s_t$, then it is denoted as CS_n; if $u_t = w_t$, then it is denoted as CW_n; if $u_t = l_t$, then it is denoted as CL_n.

When $n \geq 3$, the terminal decagon D_{n+1} of CDC_{n+1} can be connected to the o_n, m_n, s_n, w_n, and l_n points of D_n, that is, there are five random connection modes. The five different resulting graphs obtained can be denoted as CDC^1_{n+1}, CDC^2_{n+1}, CDC^3_{n+1}, CDC^4_{n+1}, and CDC^5_{n+1}, respectively, as shown in Figure 2. A random cyclodecane chain with n regular decagons, denoted by CDC_n, is constructed through $n-2$ steps following the connection method described below. At each step t, the terminal decagon is attached according to one of the following five stochastic cases:

1. The transition $\mathrm{CDC}_{t-1} \to \mathrm{CDC}^1_t$ occurs with probability p_1;
2. The transition $\mathrm{CDC}_{t-1} \to \mathrm{CDC}^2_t$ occurs with probability p_2;
3. The transition $\mathrm{CDC}_{t-1} \to \mathrm{CDC}^3_t$ occurs with probability p_3;
4. The transition $\mathrm{CDC}_{t-1} \to \mathrm{CDC}^4_t$ occurs with probability p_4;
5. The transition $\mathrm{CDC}_{t-1} \to \mathrm{CDC}^5_t$ occurs with probability $1 - p_1 - p_2 - p_3 - p_4$.

Here, p_1, p_2, p_3, and p_4 are constants independent of the step index t, satisfying

$$0 \leq p_1, p_2, p_3, p_4 \leq 1 \quad \text{and} \quad 0 \leq p_1 + p_2 + p_3 + p_4 \leq 1.$$

In particular, $\mathrm{CDC}_n(1,0,0,0)$, $\mathrm{CDC}_n(0,1,0,0)$, $\mathrm{CDC}_n(0,0,1,0)$, $\mathrm{CDC}_n(0,0,0,1)$, and $\mathrm{CDC}_n(0,0,0,0)$ correspond to the chains CO_n, CM_n, CS_n, CW_n, and CL_n, respectively.

3 Main conclusion

3.1 The Kirchhoff index of random cyclodecane chains

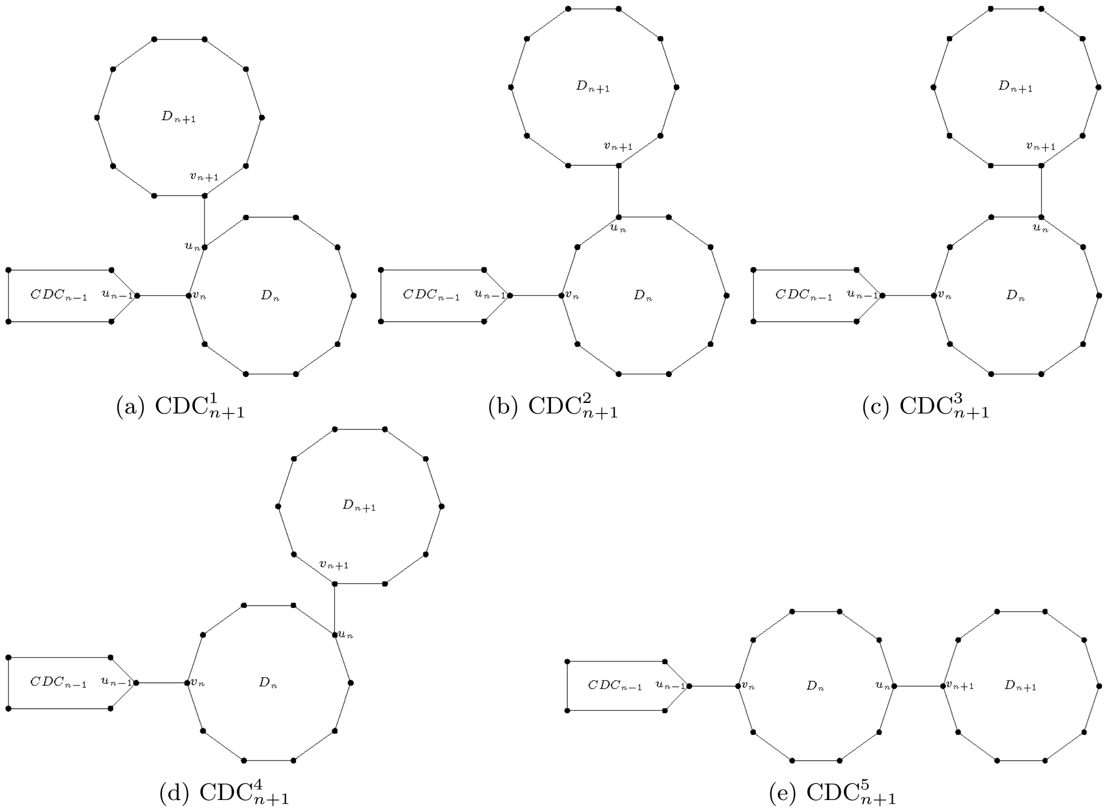
Let $E[Kf(\mathrm{CDC}(n; p_1, p_2, p_3, p_4))]$ denote the mathematical expectation of the Kirchhoff index of the random cyclodecane chain $\mathrm{CDC}(n; p_1, p_2, p_3, p_4)$, and define $r(u|G) = \sum\limits_{v \in V(G)} r(u, v)$.

Theorem 3.1. *Let* CDC_n *be a cyclodecane chain with* n *(*$n \geq 1$*) regular decagons. Then the recursive formula for the Kirchhoff index of* $\mathrm{CDC}(n; p_1, p_2, p_3, p_4)$ *is given by:*

$$Kf(\mathrm{CDC}_n) = Kf(\mathrm{CDC}_{n-1}) + 10r(u_{n-1}|\mathrm{CDC}_{n-1}) + 268(n-1) + \frac{171}{2}. \tag{6}$$

Proof. For any vertex $v \in V(\mathrm{CDC}_{n-1})$, from Figure 1, the following relation is obtained

$$r(z_i, v) = r(z_i, u_{n-1}) + r(u_{n-1}, v),$$



(a) CDC^1_{n+1} (b) CDC^2_{n+1} (c) CDC^3_{n+1} (d) CDC^4_{n+1} (e) CDC^5_{n+1}

Figure 2: Five connection modes of cyclodecane chains.

and

$$r(z_i, v) = r(u_{n-1}, v) + \begin{cases} 1, & i = 1, \\ 1 + \frac{9}{10} = \frac{19}{10}, & i = 2, 10, \\ 1 + \frac{16}{10} = \frac{26}{10}, & i = 3, 9, \\ 1 + \frac{21}{10} = \frac{31}{10}, & i = 4, 8, \\ 1 + \frac{24}{10} = \frac{34}{10}, & i = 5, 7, \\ 1 + \frac{25}{10} = \frac{35}{10}, & i = 6. \end{cases} \tag{7}$$

For any $z_k \in V(D_n)$ $(1 \leq k \leq 10)$, the following equality is obtained:

$$\sum_{j=1}^{10} r(z_k, z_j) = 2 \times \left(\frac{9}{10} + \frac{16}{10} + \frac{21}{10} + \frac{24}{10} \right) + \frac{25}{10} = \frac{33}{2}.$$

From the definition $r(u|G) = \sum_{v \in V(G)} r(u,v)$ and formula (7), it can be derived that

$$\begin{aligned} r(z_i|\mathrm{CDC}_n) &= \sum_{j=1}^{10} r(z_i, z_j) + \sum_{v \in V(\mathrm{CDC}_{n-1})} r(z_i, v) \\ &= \frac{33}{2} + 10(n-1)r(z_i, u_{n-1}) + r(u_{n-1}|\mathrm{CDC}_{n-1}). \end{aligned}$$

Thus, the resistance distance sum is given by:

$$r\left(z_i \mid \mathrm{CDC}_n\right) = r\left(u_{n-1} \mid \mathrm{CDC}_{n-1}\right) + \begin{cases} 10n + \frac{13}{2}, & i = 1, \\ 19n - \frac{5}{2}, & i = 2, 10, \\ 26n - \frac{19}{2}, & i = 3, 9, \\ 31n - \frac{29}{2}, & i = 4, 8, \\ 34n - \frac{35}{2}, & i = 5, 7, \\ 35n - \frac{37}{2}, & i = 6. \end{cases} \tag{8}$$

The following relation is obtained:

$$\begin{aligned} Kf\left(\mathrm{CDC}_n\right) &= Kf\left(\mathrm{CDC}_{n-1}\right) + \sum_{i=1}^{10} r\left(z_i|\mathrm{CDC}_n\right) - \frac{1}{2}\sum_{i=1}^{10}\sum_{j=1}^{10} r\left(z_i, z_j\right) \\ &= Kf\left(\mathrm{CDC}_{n-1}\right) + 10r\left(u_{n-1}|\mathrm{CDC}_{n-1}\right) + 268\left(n-1\right) + \frac{171}{2}. \end{aligned}$$

Thus Equation (6) holds. The proof is complete. ■

Theorem 3.2. *Let* $\mathrm{CDC}(n; p_1, p_2, p_3, p_4)$ *be a random cyclodecane chain with* n $(n \geq 1)$ *regular decagons. Denoting* $U_n^1 = E\left[r(u_n|\mathrm{CDC}_n)\right]$*, the following expression is obtained:*

$$U_n^1 = \left(\frac{35}{2} - 8p_1 - \frac{9}{2}p_2 - 2p_3 - \frac{1}{2}p_4\right)n^2 + \left(8p_1 + \frac{9}{2}p_2 + 2p_3 + \frac{1}{2}p_4 - 1\right)n. \tag{9}$$

Proof. Since u_n has five possible configurations, the analysis proceeds by considering the following five cases.

Case 1: $\mathrm{CDC}_n \to \mathrm{CDC}_{n+1}^1$. In this case, $u_n = z_2$ or z_{10}, and the probability that $r(u_n|\mathrm{CDC}_n)$ equals $r(z_2|\mathrm{CDC}_n)$ is p_1.

Case 2: $\mathrm{CDC}_n \to \mathrm{CDC}_{n+1}^2$. In this case, $u_n = z_3$ or z_9, and the probability that $r(u_n|\mathrm{CDC}_n)$ equals $r(z_3|\mathrm{CDC}_n)$ is p_2.

Case 3: $\mathrm{CDC}_n \to \mathrm{CDC}_{n+1}^3$. In this case, $u_n = z_4$ or z_8, and the probability that $r(u_n|\mathrm{CDC}_n)$ equals $r(z_4|\mathrm{CDC}_n)$ is p_3.

Case 4: $\mathrm{CDC}_n \to \mathrm{CDC}_{n+1}^4$. In this case, $u_n = z_5$ or z_7, and the probability that $r(u_n|\mathrm{CDC}_n)$ equals $r(z_5|\mathrm{CDC}_n)$ is p_4.

Case 5: $\mathrm{CDC}_n \to \mathrm{CDC}_{n+1}^5$. In this case, $u_n = z_6$, and the probability that $r(u_n|\mathrm{CDC}_n)$

equals $r(z_6|\mathrm{CDC}_n)$ is $1-p_1-p_2-p_3-p_4$.

$$\begin{aligned}
U_n^1 &= p_1 r\left(z_2|\mathrm{CDC}_n\right)+p_2 r\left(z_3|\mathrm{CDC}_n\right)+p_3 r\left(z_4|\mathrm{CDC}_n\right)+p_4 r\left(z_5|\mathrm{CDC}_n\right)\\
&\quad+(1-p_1-p_2-p_3-p_4) r\left(z_6|\mathrm{CDC}_n\right)\\
&= p_1\left[r\left(u_{n-1}|\mathrm{CDC}(n-1;p_1,p_2,p_3,p_4)\right)+19n-\frac{5}{2}\right]\\
&\quad+p_2\left[r\left(u_{n-1}|\mathrm{CDC}(n-1;p_1,p_2,p_3,p_4)\right)+26n-\frac{19}{2}\right]\\
&\quad+p_3\left[r\left(u_{n-1}|\mathrm{CDC}(n-1;p_1,p_2,p_3,p_4)\right)+31n-\frac{29}{2}\right]\\
&\quad+p_4\left[r\left(u_{n-1}|\mathrm{CDC}(n-1;p_1,p_2,p_3,p_4)\right)+34n-\frac{35}{2}\right]\\
&\quad+(1-p_1-p_2-p_3-p_4)\left[r\left(u_{n-1}|\mathrm{CDC}(n-1;p_1,p_2,p_3,p_4)\right)+35n-\frac{37}{2}\right].
\end{aligned}$$

Given that $E(U_n^1)=U_n^1$, the following recurrence relation is obtained:

$$\begin{aligned}
U_n^1 &= p_1\left[U_{n-1}^1+19n-\frac{5}{2}\right]+p_2\left[U_{n-1}^1+26n-\frac{19}{2}\right]+p_3\left[U_{n-1}^1+31n-\frac{29}{2}\right]\\
&\quad+p_4\left[U_{n-1}^1+34n-\frac{35}{2}\right]+(1-p_1-p_2-p_3-p_4)\left[U_{n-1}^1+35n-\frac{37}{2}\right]\\
&= U_{n-1}^1+(35-16p_1-9p_2-4p_3-p_4)n+\left(16p_1+9p_2+4p_3+p_4-\frac{37}{2}\right).
\end{aligned}\tag{10}$$

From the initial value

$$U_1^1=E\left[r\left(u_1|\mathrm{CDC}(1;p_1,p_2,p_3,p_4)\right)\right]=\left(\frac{9}{10}+\frac{16}{10}+\frac{21}{10}+\frac{24}{10}\right)\times 2+\frac{25}{10}=\frac{33}{2},$$

and substituting into Equation (10), Equaion (9) is obtained by recursion. The proof is completed. ■

The expected value of the Kirchhoff index of the random cyclodecane chain can be derived from Theorem 3.1 and Theorem 3.2.

Theorem 3.3. *Let* CDC_n *be a random cyclodecane chain with* n $(n\geq 1)$ *regular decagons. Then the expected value of* CDC_n *is given by:*

$$\begin{aligned}
E\left[Kf\left(\mathrm{CDC}(n;p_1,p_2,p_3,p_4)\right)\right] &= \frac{1}{3}\left(175-80p_1-45p_2-20p_3-5p_4\right)n^3\\
&\quad+(46+80p_1+45p_2+20p_3+5p_4)n^2\\
&\quad-\frac{1}{3}\left(\frac{113}{2}+160p_1+90p_2+40p_3+10p_4\right)n.
\end{aligned}\tag{11}$$

Proof. Taking the expected value on both sides of Equation (6), and using Equation (9), the following relation is obtained:

$$\begin{aligned}
E\left[Kf\left(\mathrm{CDC}(n;p_1,p_2,p_3,p_4)\right)\right] &= E\left[Kf\left(\mathrm{CDC}(n-1;p_1,p_2,p_3,p_4)\right)\right]\\
&\quad+10E\left(r(u_{n-1}|\mathrm{CDC}_{n-1})\right)+268n-\frac{365}{2}\\
&= E\left[Kf\left(\mathrm{CDC}(n-1;p_1,p_2,p_3,p_4)\right)\right]+10U_{n-1}^1+268n-\frac{365}{2}.
\end{aligned}$$

Thus,

$$\begin{aligned} E\left[Kf\left(\mathrm{CDC}(n+1;p_1,p_2,p_3,p_4)\right)\right] = {} & E\left[Kf\left(\mathrm{CDC}(n;p_1,p_2,p_3,p_4)\right)\right] \\ & + (175-80p_1-45p_2-20p_3-5p_4)n^2 \\ & + (267+80p_1+45p_2+20p_3+5p_4)n + \frac{171}{2}. \end{aligned} \tag{12}$$

Substituting the initial value $E[Kf(\mathrm{CDC}(1;p_1,p_2,p_3,p_4))] = \frac{171}{2}$ into Equation (12), Equation (11) is obtained recursively. The proof is completed. ■

Since

$$\mathrm{CDC}(n;1,0,0,0),\ \mathrm{CDC}(n;0,1,0,0),\ \mathrm{CDC}(n;0,0,1,0),\ \mathrm{CDC}(n;0,0,0,1),\ \mathrm{CDC}(n;0,0,0,0)$$

correspond to the chains CO_n, CM_n, CS_n, CW_n and CL_n, respectively, the following corollary is obtained by substituting the respective parameter values

$$(p_1,p_2,p_3,p_4) = \begin{cases} (1,0,0,0), & \text{for } \mathrm{CO}_n, \\ (0,1,0,0), & \text{for } \mathrm{CM}_n, \\ (0,0,1,0), & \text{for } \mathrm{CS}_n, \\ (0,0,0,1), & \text{for } \mathrm{CW}_n, \\ (0,0,0,0), & \text{for } \mathrm{CL}_n. \end{cases}$$

into Equation (11).

Corollary 3.4. *The Kirchhoff indices of the five special cyclodecane chains* CO_n*,* CM_n*,* CS_n*,* CW_n *and* CL_n *are given by:*

$$\begin{aligned} Kf\left(\mathrm{CO}_n\right) &= \frac{95}{3}n^3+126n^2-\frac{433}{6}n, \\ Kf\left(\mathrm{CM}_n\right) &= \frac{130}{3}n^3+91n^2-\frac{293}{6}n, \\ Kf\left(\mathrm{CS}_n\right) &= \frac{155}{3}n^3+66n^2-\frac{193}{6}n, \\ Kf\left(\mathrm{CW}_n\right) &= \frac{170}{3}n^3+51n^2-\frac{133}{6}n, \\ Kf\left(\mathrm{CL}_n\right) &= \frac{175}{3}n^3+46n^2-\frac{113}{6}n. \end{aligned}$$

The extremal graphs where the Kirchhoff index of cyclodecane chains attains its upper and lower bounds are characterized as follows:

Theorem 3.5. *Among all cyclodecane chains* $\mathrm{CDC}(n;p_1,p_2,p_3,p_4)$ *with* n *(*$n \geq 3$*) regular decagons,* CL_n *is the unique chain attaining the maximum Kirchhoff index, while* CM_n *is the unique chain attaining the minimum Kirchhoff index.*

Proof. Define the function $f(p_1,p_2,p_3,p_4) = E\left[Kf\left(\mathrm{CDC}(n;p_1,p_2,p_3,p_4)\right)\right]$. From Theorem 3.3, it follows that:

$$\begin{aligned} f(p_1,p_2,p_3,p_4) = {} & \left(-\frac{80}{3}n^3+80n^2-\frac{160}{3}n\right)p_1 + \left(-15n^3+45n^2-30n\right)p_2 \\ & + \left(-\frac{20}{3}n^3+20n^2-\frac{40}{3}n\right)p_3 + \left(-\frac{5}{3}n^3+5n^2-\frac{10}{3}n\right)p_4 \\ & + \frac{175}{3}n^3+46n^2-\frac{113}{6}n. \end{aligned}$$

For $n \geq 3$, the following inequalities hold:

$$\frac{\partial f}{\partial p_1} = -\frac{80}{3}n^3 + 80n^2 - \frac{160}{3}n < 0,$$
$$\frac{\partial f}{\partial p_2} = -15n^3 + 45n^2 - 30n < 0,$$
$$\frac{\partial f}{\partial p_3} = -\frac{20}{3}n^3 + 20n^2 - \frac{40}{3}n < 0,$$
$$\frac{\partial f}{\partial p_4} = -\frac{5}{3}n^3 + 5n^2 - \frac{10}{3}n < 0.$$

Given that $0 \leq p_1, p_2, p_3, p_4 \leq 1$ and $0 \leq p_1 + p_2 + p_3 + p_4 \leq 1$, it follows that:

$$f(p_1, p_2, p_3, p_4) \leq \frac{175}{3}n^3 + 46n^2 - \frac{113}{6}n.$$

Equality holds if and only if $p_1 = p_2 = p_3 = p_4 = 0$, which implies that CL_n is the unique cyclodecane chain attaining the maximum Kirchhoff index.

$$\begin{aligned}
f(p_1, p_2, p_3, p_4) &= \left(-\frac{80}{3}n^3 + 80n^2 - \frac{160}{3}n\right)(p_1 + p_2) + \left(\frac{35}{3}n^3 - 35n^2 + \frac{70}{3}n\right) p_2 \\
&\quad + \left(-\frac{20}{3}n^3 + 20n^2 - \frac{40}{3}n\right) p_3 + \left(-\frac{5}{3}n^3 + 5n^2 - \frac{10}{3}n\right) p_4 \\
&\quad + \frac{175}{3}n^3 + 46n^2 - \frac{113}{6}n \\
&\geq \left(-\frac{20}{3}n^3 + 20n^2 - \frac{40}{3}n\right)(p_2 + p_3) + \left(\frac{55}{3}n^3 - 55n^2 + \frac{110}{3}n\right) p_2 \\
&\quad + \left(-\frac{5}{3}n^3 + 5n^2 - \frac{10}{3}n\right) p_4 + \frac{95}{3}n^3 + 126n^2 - \frac{433}{6}n \\
&\geq \left(-\frac{5}{3}n^3 + 5n^2 - \frac{10}{3}n\right)(p_2 + p_4) + \left(20n^3 - 60n^2 + 40n\right) p_2 \\
&\quad + \frac{75}{3}n^3 + 146n^2 - \frac{513}{6}n \\
&\geq \left(20n^3 - 60n^2 + 40n\right) p_2 + \frac{70}{3}n^3 + 151n^2 - \frac{533}{6}n.
\end{aligned}$$

It is evident that

$$f(p_1, p_2, p_3, p_4) \geq \left(20n^3 - 60n^2 + 40n\right) p_2 + \frac{70}{3}n^3 + 151n^2 - \frac{533}{6}n. \tag{13}$$

Equality in Equation (13) holds if and only if $p_1 + p_2 = 1$, $p_2 + p_3 = 1$, $p_2 + p_4 = 1$, and

$$0 \leq p_1 + p_2 + p_3 + p_4 \leq 1,$$

which implies

$$(p_1, p_2, p_3, p_4) = (0, 1, 0, 0).$$

Substituting $p_2 = 1$ into Equation (13) yields

$$f(p_1, p_2, p_3, p_4) \geq \frac{130}{3}n^3 + 91n^2 - \frac{293}{6}n.$$

Equality holds if and only if $(p_1, p_2, p_3, p_4) = (0, 1, 0, 0)$, which corresponds to CM_n being the unique cyclodecane chain attaining the minimum Kirchhoff index. This completes the proof. ■

3.2 The multiplicative degree-Kirchhoff index of random cyclodecane chains

In a cyclodecane chain CDC_n with n $(n \geq 2)$ regular decagons, the first and the n-th regular decagons each contain exactly one vertex of degree 3, while the remaining 9 vertices are of degree 2. Among the other $n-2$ regular decagons, there are 2 vertices of degree 3, with the remaining vertices having degree 2. In D_n, $d(z_1) = 3$ and $d(z_i) = 2$ for $2 \leq i \leq 10$, which gives

$$\sum_{v \in V(\mathrm{CDC}_{n-1})} d_{\mathrm{CDC}_n}(v) = 2 \times 8(n-1) + 3 \times 2(n-1) - 1 = 22n - 23.$$

For D_n,

$$\begin{aligned}\sum_{j=1}^{10} d(z_j) r(z_j, z_i) &= 2 \times \sum_{j=1}^{10} r(z_j, z_i) + r(z_1, z_i) \\ &= \begin{cases} 33, & i = 1, \\ 33 + \frac{9}{10} = \frac{339}{10}, & i = 2, 10, \\ 33 + \frac{16}{10} = \frac{346}{10}, & i = 3, 9, \\ 33 + \frac{21}{10} = \frac{351}{10}, & i = 4, 8, \\ 33 + \frac{24}{10} = \frac{354}{10}, & i = 5, 7, \\ 33 + \frac{25}{10} = \frac{71}{2}, & i = 6. \end{cases}\end{aligned} \tag{14}$$

The explicit expression for the expectation of $Kf^*(\mathrm{CDC}(n; p_1, p_2, p_3, p_4))$ is derived below:

Theorem 3.6. *Let* $\mathrm{CDC}(n; p_1, p_2, p_3, p_4)$ *be a random cyclodecane chain with* n $(n \geq 1)$ *regular decagons. Denote* $V = V(\mathrm{CDC}_n)$, $V_1 = V(\mathrm{CDC}_{n-1})$, $V_2 = V(\mathrm{CDC}_{n-1}) \setminus \{u_{n-1}\}$, *then*

$$\begin{aligned} E\left[Kf^*(\mathrm{CDC}(n; p_1, p_2, p_3, p_4))\right] =& \frac{11}{15}(385 - 176p_1 - 99p_2 - 44p_3 - 11p_4)n^3 \\ &+ \frac{11}{5}(45 + 176p_1 + 99p_2 + 44p_3 + 11p_4)n^2 \\ &+ \frac{1}{15}(-755 - 3872p_1 - 2178p_2 - 968p_3 - 242p_4)n \\ &- 22. \end{aligned} \tag{15}$$

Proof. Let $Kf^*(\mathrm{CDC}_n) = A_1 + B_1 + C_1$, where

$$\begin{aligned} A_1 &= \sum_{\{u,v\} \subseteq V_1} d(u)d(v)r(u,v), \\ B_1 &= \sum_{v \in V_1} \sum_{z_i \in V(D_n)} d(v)d(z_i)r(z_i, v), \\ C_1 &= \sum_{\{z_i, z_j\} \subseteq V(D_n)} d(z_i)d(z_j)r(z_i, z_j). \end{aligned}$$

From Equations (7) and (14), the following relations are obtained:

$$
\begin{aligned}
A_1 &= \sum_{\{u,v\}\subseteq V_2} d(u)d(v)r(u,v) + \sum_{v\in V_2} d_{\mathrm{CDC}_n}(u_{n-1})d(v)r(u_{n-1},v)\\
&= Kf^*\left(\mathrm{CDC}_{n-1}\right) + \sum_{v\in V_1} d(v)r(u_{n-1},v),\\
B_1 &= \sum_{v\in V_1} d(v)\left[3\left(r(u_{n-1},v)+1\right) + 4\left(r(u_{n-1},v)+\frac{19}{10}\right) + 4\left(r(u_{n-1},v)+\frac{26}{10}\right)\right.\\
&\left. +4\left(r(u_{n-1},v)+\frac{31}{10}\right) + \left(r(u_{n-1},v)+\frac{34}{10}\right) + 2\left(r(u_{n-1},v)+\frac{7}{2}\right)\right]\\
&= 21\sum_{v\in V_1} d(v)r(u_{n-1},v) + 54(22n-23),\\
C_1 &= \frac{1}{2}\sum_{i=1}^{10} d(z_i)\left(\sum_{j=1}^{10} d(z_j)r(z_j,z_i)\right) = 363.
\end{aligned}
$$

The multiplicative degree-Kirchhoff index thus satisfies the recurrence relation:

$$
Kf^*(\mathrm{CDC}_n) = Kf^*(\mathrm{CDC}_{n-1}) + 22\sum_{v\in V_1} d(v)r(u_{n-1},v) + 1188n - 879. \tag{16}
$$

Let $U_n^2 = E\left[\sum_{v\in V(\mathrm{CDC}(n;p_1,p_2,p_3,p_4))} d(v)r(u_n,v)\right]$. Following the derivation approach for U_n^1, the expectation expands as

$$
\begin{aligned}
U_n^2 &= p_1\sum_{v\in V} d(v)r(z_2,v) + p_2\sum_{v\in V} d(v)r(z_3,v) + p_3\sum_{v\in V} d(v)r(z_4,v) + p_4\sum_{v\in V} d(v)r(z_5,v)\\
&\quad + (1-p_1-p_2-p_3-p_4)\sum_{v\in V} d(v)r(z_6,v)\\
&= p_1\left[\sum_{v\in V_1} d(v)r(u_{n-1},v) + \frac{209}{5}n - \frac{49}{5}\right] + p_2\left[\sum_{v\in V_1} d(v)r(u_{n-1},v) + \frac{286}{5}n - \frac{126}{5}\right]\\
&\quad + p_3\left[\sum_{v\in V_1} d(v)r(u_{n-1},v) + \frac{341}{5}n - \frac{181}{5}\right] + p_4\left[\sum_{v\in V_1} d(v)r(u_{n-1},v) + \frac{374}{5}n - \frac{214}{5}\right]\\
&\quad + (1-p_1-p_2-p_3-p_4)\left[\sum_{v\in V_1} d(v)r(u_{n-1},v) + 77n - 45\right]\\
&= U_{n-1}^2 + \frac{1}{5}(385-176p_1-99p_2-44p_3-11p_4)n + \frac{1}{5}(176p_1+99p_2+44p_3+11p_4-225).
\end{aligned}
$$

The initial value is given by $U_1^2 = \sum_{v\in V(\mathrm{CDC}_1)} d(v)r(u_1,v) = 33$. Solving the recurrence relation yields:

$$
U_n^2 = \frac{1}{10}(385-176p_1-99p_2-44p_3-11p_4)n^2 + \frac{1}{10}(176p_1+99p_2+44p_3+11p_4-65)n+1. \tag{17}
$$

The recurrence relation for the multiplicative degree-Kirchhoff index is therefore given by:

$$\begin{aligned}
&E\left[Kf^*\left(\mathrm{CDC}(n+1;p_1,p_2,p_3,p_4)\right)\right]\\
&=E\left[Kf^*\left(\mathrm{CDC}(n;p_1,p_2,p_3,p_4)\right)\right]\\
&\quad+\frac{11}{5}\left(385-176p_1-99p_2-44p_3-11p_4\right)n^2\\
&\quad+\frac{11}{5}\left(475+176p_1+99p_2+44p_3+11p_4\right)n+331.
\end{aligned}\tag{18}$$

Substituting the initial value $E\left[Kf^*\left(\mathrm{CDC}(1;p_1,p_2,p_3,p_4)\right)\right]=309$ into Equation (18), Equation (15) is established by mathematical induction. ■

Substituting the parameter sets $(p_1,p_2,p_3,p_4)=(1,0,0,0)$, $(0,1,0,0)$, $(0,0,1,0)$, $(0,0,0,1)$, and $(0,0,0,0)$ into Equation (15) yields the following corollary.

Corollary 3.7. *The multiplicative degree-Kirchhoff indices of the five cyclodecane chains* CO_n, CM_n, CS_n, CW_n, *and* CL_n *are given by*

$$\begin{aligned}
E\left[Kf^*(\mathrm{CO}_n)\right]&=\frac{2299}{15}n^3+\frac{2431}{5}n^2-\frac{4627}{15}n-22,\\
E\left[Kf^*(\mathrm{CM}_n)\right]&=\frac{3146}{15}n^3+\frac{1584}{5}n^2-\frac{2933}{15}n-22,\\
E\left[Kf^*(\mathrm{CS}_n)\right]&=\frac{3751}{15}n^3+\frac{979}{5}n^2-\frac{1723}{15}n-22,\\
E\left[Kf^*(\mathrm{CW}_n)\right]&=\frac{4114}{15}n^3+\frac{616}{5}n^2-\frac{997}{15}n-22,\\
E\left[Kf^*(\mathrm{CL}_n)\right]&=\frac{4235}{15}n^3+99n^2-\frac{151}{3}n-22.
\end{aligned}$$

Theorem 3.8. *Among all cyclodecane chains with n ($n\geq 3$) regular decagons,* CL_n *is the unique chain attaining the maximum multiplicative degree-Kirchhoff index, while* CM_n *is the unique chain attaining the minimum multiplicative degree-Kirchhoff index.*

Proof. Let $\mathrm{CDC}(n;p_1,p_2,p_3,p_4)$ be a random cyclodecane chain with n ($n\geq 3$) regular decagons. From Theorem 3.6, the expected multiplicative degree-Kirchhoff index is given by:

$$\begin{aligned}
g(p_1,p_2,p_3,p_4)&=E\left[Kf^*\left(\mathrm{CDC}(n;p_1,p_2,p_3,p_4)\right)\right]\\
&=\left(-\frac{1936}{15}n^3+\frac{1936}{5}n^2-\frac{3872}{15}n\right)p_1\\
&\quad+\left(-\frac{1089}{15}n^3+\frac{1089}{5}n^2-\frac{2178}{15}n\right)p_2\\
&\quad+\left(-\frac{484}{15}n^3+\frac{484}{5}n^2-\frac{968}{15}n\right)p_3\\
&\quad+\left(-\frac{121}{15}n^3+\frac{121}{5}n^2-\frac{242}{15}n\right)p_4\\
&\quad+\left(\frac{847}{3}n^3+99n^2-\frac{151}{3}n-22\right).
\end{aligned}$$

For $n\geq 3$, the partial derivatives satisfy

$$\frac{\partial g}{\partial p_1}=-\frac{1936}{15}n^3+\frac{1936}{5}n^2-\frac{3872}{15}n<0,$$

$$\frac{\partial g}{\partial p_2} = -\frac{1089}{15}n^3 + \frac{1089}{5}n^2 - \frac{2178}{15}n < 0,$$
$$\frac{\partial g}{\partial p_3} = -\frac{484}{15}n^3 + \frac{484}{5}n^2 - \frac{968}{15}n < 0,$$
$$\frac{\partial g}{\partial p_4} = -\frac{121}{15}n^3 + \frac{121}{5}n^2 - \frac{242}{15}n < 0.$$

Consequently, the function is bounded above by:

$$g(p_1, p_2, p_3, p_4) \leq \frac{847}{3}n^3 + 99n^2 - \frac{151}{3}n - 22.$$

Equality holds if and only if $p_1 = p_2 = p_3 = p_4 = 0$, which implies that CL_n is the unique cyclodecane chain attaining the maximum multiplicative degree-Kirchhoff index. The function $g(p_1, p_2, p_3, p_4)$ further satisfies the inequalities

$$\begin{aligned}
g(p_1, p_2, p_3, p_4) &= \left(-\frac{1936}{15}n^3 + \frac{1936}{5}n^2 - \frac{3872}{15}n\right)(p_1 + p_2) \\
&\quad + \left(\frac{847}{15}n^3 - \frac{847}{5}n^2 + \frac{1694}{15}n\right)p_2 \\
&\quad + \left(-\frac{484}{15}n^3 + \frac{484}{5}n^2 - \frac{968}{15}n\right)p_3 \\
&\quad + \left(-\frac{121}{15}n^3 + \frac{121}{5}n^2 - \frac{242}{15}n\right)p_4 \\
&\quad + \frac{847}{3}n^3 + 99n^2 - \frac{151}{3}n - 22 \\
&\geq \left(-\frac{484}{15}n^3 + \frac{484}{5}n^2 - \frac{968}{15}n\right)(p_2 + p_3) \\
&\quad + \left(\frac{1331}{15}n^3 - \frac{1331}{5}n^2 + \frac{2662}{15}n\right)p_2 \\
&\quad + \left(-\frac{121}{15}n^3 + \frac{121}{5}n^2 - \frac{242}{15}n\right)p_4 \\
&\quad + \left(\frac{2299}{15}n^3 + \frac{2431}{5}n^2 - \frac{4627}{15}n - 22\right) \\
&\geq \left(-\frac{121}{15}n^3 + \frac{121}{5}n^2 - \frac{242}{15}n\right)(p_2 + p_4) \\
&\quad + \left(\frac{1452}{15}n^3 - \frac{1452}{5}n^2 + \frac{2904}{15}n\right)p_2 \\
&\quad + \frac{1815}{15}n^3 + \frac{2915}{5}n^2 - \frac{5595}{15}n - 22 \\
&\geq \left(\frac{1452}{15}n^3 - \frac{1452}{5}n^2 + \frac{2904}{15}n\right)p_2 \\
&\quad + \frac{1694}{15}n^3 + \frac{3036}{5}n^2 - \frac{5837}{15}n - 22.
\end{aligned}$$

It is evident that:

$$g(p_1, p_2, p_3, p_4) \geq \left(\frac{1452}{15}n^3 - \frac{1452}{5}n^2 + \frac{2904}{15}n\right)p_2 + \frac{1694}{15}n^3 + \frac{3036}{5}n^2 - \frac{5837}{15}n - 22. \quad (19)$$

Equality holds if and only if $p_1 + p_2 = 1$, $p_2 + p_3 = 1$, $p_2 + p_4 = 1$, and

$$0 \leq p_1 + p_2 + p_3 + p_4 \leq 1,$$

which implies

$$(p_1, p_2, p_3, p_4) = (0, 1, 0, 0).$$

Substituting $p_2 = 1$ into Equation (19) yields:

$$g(p_1, p_2, p_3, p_4) \geq \frac{3146}{15}n^3 + \frac{1584}{5}n^2 - \frac{2933}{15}n - 22.$$

Equality holds if and only if $(p_1, p_2, p_3, p_4) = (0, 1, 0, 0)$, which corresponds to CM_n being the unique cyclodecane chain attaining the minimum multiplicative degree-Kirchhoff index. This completes the proof. ∎

3.3 The additive degree-Kirchhoff index of random cyclodecane chains

This section presents the calculation of the expectation for $Kf^+\left(\mathrm{CDC}(n; p_1, p_2, p_3, p_4)\right)$.

Theorem 3.9. *Let* $\mathrm{CDC}(n; p_1, p_2, p_3, p_4)$ *be a random cyclodecane chain with* n $(n \geq 1)$ *regular decagons. Denote* $V = V(\mathrm{CDC}_n)$, $V_1 = V(\mathrm{CDC}_{n-1})$, $V_2 = V(\mathrm{CDC}_{n-1}) \setminus \{u_{n-1}\}$. *The expected additive degree-Kirchhoff index is given by*

$$\begin{aligned} E\left[Kf^+\left(\mathrm{CDC}(n; p_1, p_2, p_3, p_4)\right)\right] = &\frac{22}{3}(35 - 16p_1 - 9p_2 - 4p_3 - p_4)n^3 \\ &+ (133 + 352p_1 + 198p_2 + 88p_3 + 22p_4)n^2 \\ &- \frac{1}{3}(179 + 704p_1 + 396p_2 + 176p_3 + 44p_4)n - 10. \end{aligned} \tag{20}$$

Proof. Let $Kf^+\left(\mathrm{CDC}(n; p_1, p_2, p_3, p_4)\right) = A_2 + B_2 + C_2$, where

$$\begin{aligned} A_2 &= \sum_{\{u,v\} \subseteq V_1} (d(u) + d(v))\, r(u, v), \\ B_2 &= \sum_{v \in V_1} \sum_{z_i \in V(D_n)} (d(v) + d(z_i))\, r(v, z_i), \\ C_2 &= \sum_{\{z_i, z_j\} \subseteq V(D_n)} (d(z_i) + d(z_j))\, r(z_i, z_j). \end{aligned}$$

From Equations (7) and (14), the following relations are derived:

$$\begin{aligned} A_2 &= \sum_{\{u,v\} \subseteq V_2} (d(u) + d(v))\, r(u, v) + \sum_{v \in V_2} (d_{\mathrm{CDC}_n}(u_{n-1}) + d(v))\, r(u_{n-1}, v) \\ &= Kf^+(\mathrm{CDC}_{n-1}) + r(u_{n-1}|\mathrm{CDC}_{n-1}), \end{aligned}$$

$$\begin{aligned} B_2 &= \sum_{v \in V_1} \sum_{z_i \in V(D_n)} d(v) r(v, z_i) + \sum_{v \in V_1} \sum_{z_i \in V(D_n)} d(z_i) r(v, z_i) \\ &= 10 \sum_{v \in V_1} d(v) r(u_{n-1}, v) + 21 r(u_{n-1}|\mathrm{CDC}_{n-1}) + \frac{53}{2}(22n - 23) + 540(n - 1), \end{aligned}$$

$$C_2 = \frac{1}{2}\sum_{i=1}^{10}\sum_{j=1}^{10}(d(z_i)+d(z_j))\,r(z_i,z_j) = \frac{693}{2}.$$

The additive degree-Kirchhoff index thus satisfies the recurrence relation

$$\begin{aligned} Kf^{+}(\mathrm{CDC}_n) =& Kf^{+}(\mathrm{CDC}_{n-1}) + 10\sum_{v\in V_1} d(v)r(u_{n-1},v) \\ &+ 22r(u_{n-1}|\mathrm{CDC}_{n-1}) + 1123n - 803. \end{aligned} \tag{21}$$

Let $U_n^3 = E[r(u_n|\mathrm{CDC}(n,p_1,p_2,p_3,p_4))]$. From Equations (7) and (8), the expectation expands as

$$\begin{aligned} U_n^3 &= p_1 r(z_2|\mathrm{CDC}_n) + p_2 r(z_3|\mathrm{CDC}_n) + p_3 r(z_4|\mathrm{CDC}_n) + p_4 r(z_5|\mathrm{CDC}_n) \\ &\quad + (1-p_1-p_2-p_3-p_4) r(z_6|\mathrm{CDC}_n) \\ &= U_{n-1}^3 + (35-16p_1-9p_2-4p_3-p_4)n + \left(-\frac{37}{2}+16p_1+9p_2+4p_3+p_4\right). \end{aligned}$$

Substituting the initial value $U_1^3 = \frac{33}{2}$ into the recurrence relation yields:

$$U_n^3 = \frac{1}{2}(35-16p_1-9p_2-4p_3-p_4)n^2 + \frac{1}{2}(-2+16p_1+9p_2+4p_3+p_4)n. \tag{22}$$

From Equations (21) and (22), the recurrence relation for the expected additive degree-Kirchhoff index is obtained:

$$\begin{aligned} E[Kf^{+}(\mathrm{CDC}(n+1;p_1,p_2,p_3,p_4))] = & E[Kf^{+}(\mathrm{CDC}(n;p_1,p_2,p_3,p_4))] \\ &+ 22(35-16p_1-9p_2-4p_3-p_4)n^2 \\ &+ (1036+352p_1+198p_2+88p_3+22p_4)n \\ &+ 330. \end{aligned}$$

Substituting the initial value $E[Kf^{+}(\mathrm{CDC}(1;p_1,p_2,p_3,p_4))] = 320$ into the recurrence relation, Equation (20) is established by mathematical induction. ∎

Substituting the parameter sets $(p_1,p_2,p_3,p_4) = (1,0,0,0)$, $(0,1,0,0)$, $(0,0,1,0)$, $(0,0,0,1)$, and $(0,0,0,0)$ into Equation (20) yields the following corollary.

Corollary 3.10. *The additive degree-Kirchhoff indices of the five cyclodecane chains* CO_n, CM_n, CS_n, CW_n, *and* CL_n *are given by:*

$$\begin{aligned} Kf^{+}(\mathrm{CO}_n) &= \frac{418}{3}n^3 + 485n^2 - \frac{883}{3}n - 10, \\ Kf^{+}(\mathrm{CM}_n) &= \frac{572}{3}n^3 + 331n^2 - \frac{575}{3}n - 10, \\ Kf^{+}(\mathrm{CS}_n) &= \frac{682}{3}n^3 + 221n^2 - \frac{355}{3}n - 10, \\ Kf^{+}(\mathrm{CW}_n) &= \frac{748}{3}n^3 + 155n^2 - \frac{223}{3}n - 10, \\ Kf^{+}(\mathrm{CL}_n) &= \frac{770}{3}n^3 + 133n^2 - \frac{179}{3}n - 10. \end{aligned}$$

Theorem 3.11. *Among all cyclodecane chains with* n $(n \geq 3)$ *regular decagons,* CL_n *is the unique chain attaining the maximum additive degree-Kirchhoff index, while* CM_n *is the unique chain attaining the minimum additive degree-Kirchhoff index.*

Proof. Let $\mathrm{CDC}(n; p_1, p_2, p_3, p_4)$ be a random cyclodecane chain with n ($n \geq 3$) regular decagons. From Theorem 3.9, the expected additive degree-Kirchhoff index is given by:

$$\begin{aligned} h(p_1,p_2,p_3,p_4) &= E\left[Kf^{+}\left(\mathrm{CDC}(n;p_1,p_2,p_3,p_4)\right)\right] \\ &= \left(-\frac{352}{3}n^3+352n^2-\frac{704}{3}n\right)p_1+\left(-66n^3+198n^2-132n\right)p_2 \\ &\quad+\left(-\frac{88}{3}n^3+88n^2-\frac{176}{3}n\right)p_3 \\ &\quad+\left(-\frac{22}{3}n^3+22n^2-\frac{44}{3}n\right)p_4+\frac{770}{3}n^3+133n^2-\frac{179}{3}n-10. \end{aligned}$$

For $n \geq 3$, the partial derivatives satisfy

$$\begin{aligned} \frac{\partial h}{\partial p_1} &= -\frac{352}{3}n^3+352n^2-\frac{704}{3}n<0, \\ \frac{\partial h}{\partial p_2} &= -66n^3+198n^2-132n<0, \\ \frac{\partial h}{\partial p_3} &= -\frac{88}{3}n^3+88n^2-\frac{176}{3}n<0, \\ \frac{\partial h}{\partial p_4} &= -\frac{22}{3}n^3+22n^2-\frac{44}{3}n<0. \end{aligned}$$

Given that $0 \leq p_1, p_2, p_3, p_4 \leq 1$ and $0 \leq p_1 + p_2 + p_3 + p_4 \leq 1$, it follows that:

$$h(p_1,p_2,p_3,p_4) \leq \frac{770}{3}n^3+133n^2-\frac{179}{3}n-10.$$

Equality holds if and only if $p_1 = p_2 = p_3 = p_4 = 0$, which implies that CL_n is the unique cyclodecane chain attaining the maximum additive degree-Kirchhoff index.
The function $h(p_1, p_2, p_3, p_4)$ further satisfies the inequalities

$$\begin{aligned} h(p_1,p_2,p_3,p_4) &= \left(-\frac{352}{3}n^3+352n^2-\frac{704}{3}n\right)(p_1+p_2) \\ &\quad+\left(\frac{154}{3}n^3-154n^2+\frac{308}{3}n\right)p_2+\left(-\frac{88}{3}n^3+88n^2-\frac{176}{3}n\right)p_3 \\ &\quad+\left(-\frac{22}{3}n^3+22n^2-\frac{44}{3}n\right)p_4+\frac{770}{3}n^3+133n^2-\frac{179}{3}n-10 \\ &\geq \left(-\frac{88}{3}n^3+88n^2-\frac{176}{3}n\right)(p_2+p_3) \\ &\quad+\left(\frac{242}{3}n^3-242n^2+\frac{484}{3}n\right)p_2+\left(-\frac{22}{3}n^3+22n^2-\frac{44}{3}n\right)p_4 \\ &\quad+\frac{418}{3}n^3+485n^2-\frac{883}{3}n-10 \\ &\geq \left(-\frac{22}{3}n^3+22n^2-\frac{44}{3}n\right)(p_2+p_4) \\ &\quad+\left(\frac{264}{3}n^3-264n^2+\frac{528}{3}n\right)p_2+110n^3+573n^2-\frac{1059}{3}n-10 \\ &\geq \left(\frac{264}{3}n^3-264n^2+\frac{528}{3}n\right)p_2+\frac{308}{3}n^3+595n^2-\frac{1103}{3}n-10. \end{aligned} \tag{23}$$

The equality holds if and only if $p_1+p_2=1$, $p_2+p_3=1$, $p_2+p_4=1$, and $0 \le p_1+p_2+p_3+p_4 \le 1$, that is, $(p_1,p_2,p_3,p_4)=(0,1,0,0)$. Substituting $p_2=1$ into Equation (23), one obtains

$$h(p_1,p_2,p_3,p_4) \ge \frac{572}{3}n^3 + 331n^2 - \frac{575}{3}n - 10.$$

The equality holds if and only if $(p_1,p_2,p_3,p_4)=(0,1,0,0)$, which implies that CM_n is the unique cyclodecane chain with the minimum additive degree-Kirchhoff index. This completes the proof. ■

Remark 1. In the first three sections, the Kirchhoff index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of the random cyclodecane chain are derived in detail, and the three types of Kirchhoff index expressions with five special random structures are obtained. The extreme value problem of the random cyclodecane chain about the three types of Kirchhoff index is depicted, which provides ideas for the exploration of the Kirchhoff index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of any random decagon chart.

3.4 Average values of three types of Kirchhoff indices for random cyclodecane chains

Let Θ_n denote the set of all cyclodecane chains with n regular decagons. The average values of the three types of Kirchhoff indices over all cyclodecane chains in Θ_n are defined respectively as

$$\mathrm{Kf}_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{\mathrm{CDC}_n\in\Theta_n}\mathrm{Kf}(\mathrm{CDC}_n),$$
$$\mathrm{Kf}^*_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{\mathrm{CDC}_n\in\Theta_n}\mathrm{Kf}^*(\mathrm{CDC}_n),$$
$$\mathrm{Kf}^+_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{\mathrm{CDC}_n\in\Theta_n}\mathrm{Kf}^+(\mathrm{CDC}_n).$$

Since each chain in Θ_n is generated with equal probability, the average values are obtained when

$$(p_1,p_2,p_3,p_4,1-p_1-p_2-p_3-p_4) = \left(\frac{1}{5},\frac{1}{5},\frac{1}{5},\frac{1}{5},\frac{1}{5}\right).$$

Substituting

$$(p_1,p_2,p_3,p_4) = \left(\frac{1}{5},\frac{1}{5},\frac{1}{5},\frac{1}{5}\right),$$

into the expectation expressions of Theorems 3.3, 3.6 and 3.9 yields the following result.

Theorem 3.12. *The average values of the three types of Kirchhoff indices for the family of cyclodecane chains Θ_n are given respectively by:*

$$Kf_{\mathrm{avr}}(\Theta_n) = \frac{145}{3}n^3 + 76n^2 - \frac{233}{6}n,$$
$$Kf^*_{\mathrm{avr}}(\Theta_n) = \frac{3509}{15}n^3 + \frac{1221}{5}n^2 - \frac{2207}{15}n - 22,$$
$$Kf^+_{\mathrm{avr}}(\Theta_n) = \frac{638}{3}n^3 + 265n^2 - \frac{443}{3}n - 10.$$

Moreover, the following identities hold:

$$Kf_{\text{avr}}(\Theta_n) = \frac{1}{5}\left(Kf(\text{CO}_n) + Kf(\text{CM}_n) + Kf(\text{CS}_n) + Kf(\text{CW}_n) + Kf(\text{CL}_n)\right),$$

$$Kf^*_{\text{avr}}(\Theta_n) = \frac{1}{5}\left(Kf^*(\text{CO}_n) + Kf^*(\text{CM}_n) + Kf^*(\text{CS}_n) + Kf^*(\text{CW}_n) + Kf^*(\text{CL}_n)\right),$$

$$Kf^+_{\text{avr}}(\Theta_n) = \frac{1}{5}\left(Kf^+(\text{CO}_n) + Kf^+(\text{CM}_n) + Kf^+(\text{CS}_n) + Kf^+(\text{CW}_n) + Kf^+(\text{CL}_n)\right).$$

Remark 2. Closed-form expressions are established for the average values of the Kirchhoff index, multiplicative degree-Kirchhoff index, and additive degree-Kirchhoff index of random cyclodecane chains. These results provide a methodological framework for investigating mean values in arbitrary random decagon systems.

Remark 3. The average values of the Kirchhoff indices for the five specific chains CO_n, CM_n, CS_n, CW_n and CL_n collectively determine the overall average values of the Kirchhoff indices for the entire family Θ_n of cyclodecane chains comprising n regular decagons.

4 Discussion

This work provides a comprehensive computational framework for determining three fundamental types of Kirchhoff indices in random cycloalkane chains. The methodologies and results established herein open several avenues for future research. Specifically, the expectation, extreme values, and average values of other significant topological indices such as the Hosoya index and Merrifield-Simmons index in random cyclodecane chains warrant further investigation. Additionally, extending this analysis to related topological indices, including the Somobor index, would contribute to a more complete understanding of the structure-property relationships in these chemical systems.

5 Conclusion

This study employs recurrence methods to derive closed-form expressions for the expected values of the Kirchhoff index, multiplicative degree-Kirchhoff index, and additive degree-Kirchhoff index of random cyclodecane chains. Through this approach, explicit formulas for these three types of Kirchhoff indices are obtained for five specific cyclodecane chain structures: CO_n, CM_n, CS_n, CW_n, and CL_n. Furthermore, the extreme values and average values of these indices are systematically characterized. A significant finding reveals that the mean values of the Kirchhoff indices of these five specific chains collectively determine the overall average values of the Kirchhoff indices for the entire family Θ_n of cyclodecane chains comprising n regular decagons.

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