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A Study on Face Index of Chemical Graph Structures and their Derivatives

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ABSTRACT: A topological index is a numeric parameter that may describe the biological, physical and chemical properties which are contingent on the structural behaviour of different chemical compounds. In the vast class of topological indices: one of the index is, the face index which has been recently introduced and it assists in predicting the bond energies, the intermolecular forces, the boiling points and densities of different chemical compounds. This paper derives the formulae for the face index of the tadpole, the ladder and the wheel graphs, their subdivision graphs and the line graphs of their subdivision graphs. And briefly analysis their face indices trends.

Key Words: Subdivision graph, line graph, face index, tadpole graph, ladder graph, wheel graph.

Contents

1. Introduction and Preliminaries

The exploration and study of the newly formed nano-materials, crystalline substances and even pharmaceutical compounds have received wide attention in the previous years since they have potential application in a number of scientific and industrial sectors. Qualifying such materials by some standard test procedures can be time-consuming and costly. To overcome these difficulties, researchers have progressively turned to computer-based methods of dealing with them, including Quantitative Structure-Activity Relationship (QSAR) models, and Quantitative Structure -Property Relationship (QSPR) models. The approaches enable the scientists to calculate the physical, chemical and biological properties of molecules, merely on the basis of structural aspects, without the use of large scale laboratory testing [1,2,3]. A central component in the development of QSPR and QSAR models is the use of *topological indices* (TIs), which are numerical descriptors derived from the molecular graph representations of chemical structures. These indices are invariant under graph isomorphism and encapsulate critical information about the connectivity and branching of molecular frameworks. Topological indices have played a pivotal role in theoretical chemistry by enabling the correlation of molecular structure with various properties such as boiling points, stability, toxicity, and reactivity. For instance, indices like the Wiener index, Zagreb indices, Randić connectivity index, and the Estrada index have been widely used for the prediction of thermodynamic properties, biological activity, and pharmacokinetics of chemical compounds [4,5,6].

In addition, the TIs play an important role in rational designing of new materials and medicinals. They are especially useful in isomer separation, structure-based drug design and the optimization of molecular libraries to serve high-throughput screening. As well, topological descriptors have also found significant application in chemical documentation systems and in clustering and similarity analysis of molecular data sets. Mathematical basis of these indices and its applicability in different fields such as nanotechnology, environmental chemistry, medicinal chemistry etc has been discussed largely in literature

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[7,8,9]. Several recent studies have further expanded the scope of TIs by incorporating concepts from algebraic graph theory, spectral graph analysis, and fuzzy logic, thereby enhancing their discriminatory power and predictive capabilities in modeling complex molecular behaviors. These interdisciplinary advances have not only enriched the theoretical understanding of molecular graphs but have also led to more accurate and generalizable QSPR/QSAR models that can accommodate larger and more diverse chemical datasets [1,2,26].

Graph theory has been found to be a very useful mathematical tool to describe and analyze the properties of chemical compounds that involves aliasing the molecular structures of these chemical materials as graphs. Atoms are in this representation represented by the vertices of the graph, and the chemical bonds between the atoms are modeled through the edges. Such an abstraction makes it possible to analyze more in detail the geometry of molecules, bonding schemes, and structural periodicities using a range of graph-theoretic methods. A molecular graph may formally be demonstrated as: $G = G(V, E)$, where V is the collection of nodes (atoms) and E is the collection of edges (bonds). These structural models have allowed development of numerical descriptors referred to as topological indices (TIs) to correlate the structure of molecules with their physical, chemical, or biological properties [3,1,8]. Over the last few decades, numerous topological indices have been developed and widely applied in theoretical chemistry and QSPR/QSAR studies. These indices include the Wiener index, Randić index, Zagreb indices, molecular connectivity index, edge connectivity index, vertex connectivity index, and more recently, the face index. Each index captures specific aspects of the molecular structure such as branching, path lengths, or connectivity. The Wiener index, for instance, is based on the sum of distances between all pairs of vertices and has found extensive applications in predicting boiling points and other thermodynamic properties [4,5,9]. The Randić index is another important topological index used to measure molecular branching and has been associated with various pharmacokinetic and bioactivity parameters. Collectively, these indices provide valuable insights into molecular behavior without requiring experimental data [6,2,7].

The Face Index ($\mathcal{FI}$) stands out among them, as recently proposed by Jamil et al., and proved to be a highly effective manner of characterising some classes of compounds with polymeric and planar structures [24,12,13,27]. In particular, $\mathcal{FI}$ shows a good correlation with physio-chemical characteristics (including boiling points, densities, octane numbers, melting points, bond energy, and the intermolecular forces). That usefulness of the index is particularly evident when applied to chemical compounds that show polymerization structures, e.g., silicon carbides, benzenoid hydrocarbons, and carbon nanotubes, in which standard indices are unlikely to be effective in describing the complexity of ring and surface structures [24,25,15,28]. For a planar chemical graph G, the face index is defined as:

$$\mathcal{FI} = \sum_{F \in \mathcal{F}(G)} d(F) = \sum_{\mu \backsim F \in \mathcal{F}(G)} d(\mu)$$

where $\mathcal{F}(G)$ denotes the set of faces of the graph G, $d(\mu)$ is the degree of vertex μ, and $\mu \backsim F$ denotes that vertex μ is incident to the face F. This formulation allows $\mathcal{FI}$ to encode both face-vertex interactions and structural complexity of planar chemical graphs, offering a novel angle to model reactivity and interaction potential in extended molecular frameworks [10,9,8].

Here we shall discuss again some of the most basic types of graph transformation and graph that we use very commonly in chemical graph theory and also in the description of networks, and these are the line graph, subdivision graph, tadpole graph and the ladder graph. They are the fundamental tools in mathematical chemistry, nanotechnology and information science of analyzing the molecular and extended structures involving these graph constructions. Other special cases of graphs are covered in more detail e.g. the wheel graph W_n and the rim that is its boundary component that can be found in [16,17]. Given a simple graph G, the following derived graphs are defined as:

(i) The *line graph* $L(G)$ is constructed by representing each edge of G as a vertex in $L(G)$. Two vertices in $L(G)$ are adjacent if and only if their corresponding edges in G share a common vertex. Line graphs find applications in modeling communication links and molecular bonding interactions [18,19].

(ii) The *subdivision graph* $S(G)$ is obtained by replacing each edge of G with a path of length 2, effectively inserting a new vertex into every edge. This operation results in a bipartite graph structure and is particularly useful in representing molecular graphs with intermediate bonding states [3,8].

(iii) A *tadpole graph* $T_{n,k}$ consists of a cycle C_n connected to a path of length k. These graphs are often used to represent substituted cyclic compounds in organic chemistry, such as alkyl-benzenes or other mono-substituted aromatics [20,21].

(iv) The *ladder graph* is the Cartesian product of two paths $P_n \square P_2$. Visually resembling a ladder with n rungs, it is frequently encountered in the modeling of nanoribbon structures and also finds applications in electrical grid design, circuit analysis, and wireless communication networks [2,22, 23].

The tadpole graph structure is useful in chemical graph theory: many substituted cyclic molecules e.g. n-alkylbenzenes: with a combination of the cyclic and the linear chain motifs can be topologically modelled using the tadpole graph. Conversely, the ladder graph and its rigid regularity, symmetry are perfect to describe the parallel chain or ladder-shaped molecules present in conducting materials and in sensor arrays. In addition, properties related to graphs like bipartiteness, even degree sequence and planar embedding, make it applicable when modeling signal paths in electronics and energy distribution networks. The main purpose of the present paper is to examine the face index corresponding to the following graph structures- wheel, ladder and tadpole graphs and their line graph and subdivision graph variants. We seek to obtain analytic expressions of face index in both cases and do a comparative analysis of values of face index in lower-order cases. This kind of exploration is useful in understanding how face-vertex interactions develop, in how various graph transformations, and in developing a more profound understanding of structural complexity in applied graph models [10,24,25].

2. Results

The main results of the paper have been divided in the following three subsections. We partitioned the face set of a graph G depending upon the degree of each face to prove results.

2.1. Face index for tadpole, wheel and the ladder graphs

In this sub-section, we derive the formulae for the face index of the tadpole, wheel and the ladder graphs. We begin our results with the following theorem.

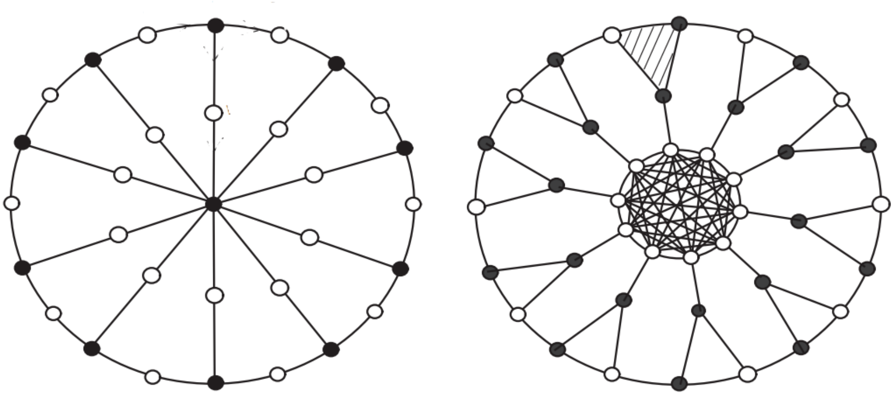

Figure 1: Visual representation of transformations applied to the wheel graph W_n:
(a) The subdivision graph $S(W_n)$, illustrating vertex insertion along edges;
(b) The corresponding line graph $L(S(W_n))$, emphasizing edge adjacency after subdivision.

Theorem 2.1 *For any tadpole graph $T_{n,k}$, where $n \geq 3$ and $k \geq 1$, the face incidence index is given by:*

$$\mathcal{FI}(T_{n,k}) = 4n + 2k + 1.$$

Proof: We begin by understanding the structure of the tadpole graph $T_{n,k}$. This graph is formed by attaching a path of length k to a single vertex of a cycle C_n. In terms of planar embedding, such a graph consists of exactly two faces:

- One **internal face**, which is bounded by edges forming the cycle and some from the path,
- One **external face**, which encompasses all the outer region including the remaining part of the path.

Let us denote a face of degree j by $\digamma_j$, where the degree is defined as the sum of degrees of all vertices incident with that face:

$$\sum_{\mu \backsim \digamma} d(\mu) = j,$$

and let $|\digamma_j|$ represent the number of faces having degree j.

According to the planar representation of $T_{n,k}$, the degrees of the faces depend on the number of vertices in the cycle and the length of the attached path. Table 1 gives the degrees for the internal and external faces based on the size of the cycle.

Number of vertices in cycle	3	4	5	-	-	-	n
Degree of internal face	7	9	11	-	-	-	$2n+1$
Degree of external face	$2k+6$	$2k+8$	$2k+10$	-	-	-	$2(k+n)$

Table 1: The degrees of internal and external faces of $T_{n,k}$.

From Table 1, we observe that:

- The **internal face** has degree $2n+1$. This comes from the cycle C_n, which contributes n edges, and the connection to the path contributes $n+1$ additional connections (due to how the cycle and path are connected in a plane).
- The **external face** has degree $2(k+n)$, accounting for all the outer edges and the path connected back to the cycle.

By the definition of the *face incidence index* $\mathcal{FI}$, which is the sum of the degrees of all the faces in the planar embedding of the graph, we have:

$$\mathcal{FI}(T_{n,k}) = \sum_{\mu \backsim \digamma \in \mathcal{F}(G)} d(\mu).$$

Breaking this into contributions from the internal and external faces:

$$\mathcal{FI}(T_{n,k}) = \sum_{\mu \backsim \digamma_j} d(\mu) + \sum_{\mu \backsim \digamma_\infty} d(\mu),$$

where $\digamma_j$ denotes the internal face and $\digamma_\infty$ denotes the external face.

Since there is only **one** internal face and **one** external face:

$$\mathcal{FI}(T_{n,k}) = (\text{degree of } \digamma_j) \cdot |\digamma_j| + (\text{degree of } \digamma_\infty) \cdot |\digamma_\infty|.$$

Substituting the values:

$$\mathcal{FI}(T_{n,k}) = (2n+1) \cdot 1 + 2(k+n) \cdot 1 = (2n+1) + 2k + 2n.$$

Combining like terms:

$$\mathcal{FI}(T_{n,k}) = 4n + 2k + 1.$$

Hence, the face incidence index of the tadpole graph $T_{n,k}$ is:

$$\mathcal{FI}(T_{n,k}) = 4n + 2k + 1.$$

This completes the proof.
Now, we derive the formula of the face index for the wheel graph W_n.

Theorem 2.2 *Let W_n be the wheel graph formed by connecting a central vertex to all vertices of a cycle C_n. Then, for $n \geq 3$, the face incidence index of W_n is given by:*

$$\mathcal{FI}(W_n) = n^2 + 9n.$$

Proof: The wheel graph W_n consists of:

- A central vertex connected to all n vertices of the cycle C_n,
- n triangular regions formed between consecutive vertices of the cycle and the central vertex,
- An outer region bounded by the cycle, forming the external face.

In the planar embedding of W_n, there are two types of faces:

1. n internal faces (denoted by F_j), each being a triangle with an increasing degree as n increases,
2. One external face (denoted by F_∞), surrounding the outer boundary of the wheel.

The degrees of the internal and external faces are shown in Table 2 below.

Number of vertices n	3	4	5	6	-	-	-	n
Degree of internal face j	9	10	11	12	-	-	-	$n+6$
Number of internal faces $\|j\|$	3	4	5	6	-	-	-	n
Degree of external face	9	12	15	18	-	-	-	$3n$

Table 2: The degrees of the internal and external faces of W_n.

From Table 2, we generalize:

- Each of the n internal faces has degree $n + 6$,
- The single external face has degree $3n$.

By definition, the face incidence index $\mathcal{FI}(W_n)$ is the sum of degrees of all the faces in the planar embedding of the graph:

$$\mathcal{FI}(W_n) = \sum_{\mu \backsim F \in \mathcal{F}(G)} d(\mu).$$

This can be split into the sum of degrees of internal and external faces:

$$\mathcal{FI}(W_n) = \sum_{\mu \backsim F_j} d(\mu) + \sum_{\mu \backsim F_\infty} d(\mu).$$

Substituting the known values:

$$\mathcal{FI}(W_n) = (\text{degree of } F_j) \cdot |F_j| + (\text{degree of } F_\infty) \cdot |F_\infty|.$$

Using the expressions from Table 2:

$$\mathcal{FI}(W_n) = (n+6) \cdot n + 3n = n^2 + 6n + 3n = n^2 + 9n.$$

Thus, for $n \geq 3$, the face incidence index of the wheel graph W_n is:

$$\mathcal{FI}(W_n) = n^2 + 9n,$$

which completes the proof.

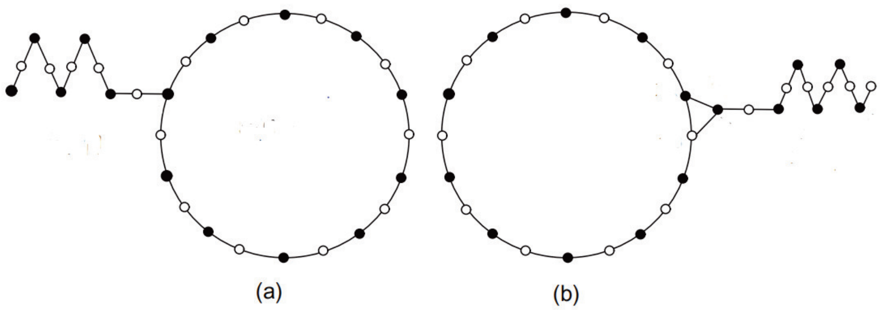

Figure 2: (a) Subdivision graph of the tadpole graph $T_{n,k}$, denoted by $S(T_{n,k})$; (b) Line graph of the subdivision graph, denoted by $L_s(T_{n,k})$.

In the next theorem, the formula of the $\mathcal{FI}$ has been presented for the ladder graph.

Theorem 2.3 *For a ladder graph L_n, the face index of L_n is given by:*

$$\mathcal{FI}(L_n) = 18n - 20, \qquad for \;\; n > 2.$$

Proof: The ladder graph L_n consists of two categories of faces, the internal faces $\digamma_{10}$, $\digamma_{12}$ and an external face $\digamma_{\infty}$. Where $|\digamma_{10}|$ is always 2 and $|\digamma_{12}| = (n-3)$, while sum of degree of vertices of external face is $6n-4$. Now, by the definition of the face index,

$$\begin{aligned}
\mathcal{FI}(L_n) &= \sum_{\mu \backsim \digamma \in \mathcal{F}(G)} d(\mu) \\
&= \sum_{\mu \backsim \digamma_{10}} d(\mu) + \sum_{\mu \backsim \digamma_{12}} d(\mu) + \sum_{\mu \backsim \digamma_{\infty}} d(\mu) \\
&= 10.|\digamma_{10}| + 12.|\digamma_{12}| + 6n - 4 \\
&= 10(2) + 12(n-3) + 6n - 4 \\
&= 18n - 20,
\end{aligned}$$

which completes the proof.

2.2. Face index for subdivision graphs of the tadpole, wheel and the ladder graphs

By keeping in view the importance of the subdivision graphs, we devote this subsection to derive the formulae of the face index for the subdivision graphs $S(G)$ of the tadpole, ladder and wheel graphs.

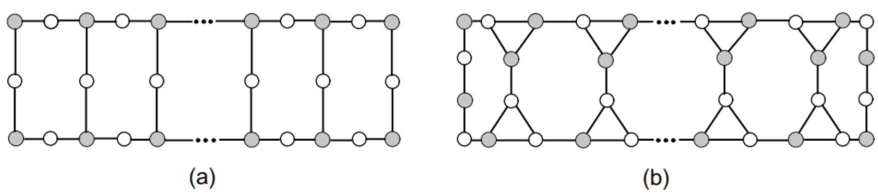

Figure 3: (a) Subdivision graph of the ladder graph L_n, denoted by $S(L_n)$; (b) Line graph of the subdivision graph, denoted by $L(S(L_n))$.

Theorem 2.4 *Consider the subdivision graph $S(T_{n,k})$ of the tadpole graph, where n denotes the number of vertices in the cycle and k is the number of vertices in the path attached to the cycle. Then, for $n \geq 3$ and $k \geq 1$, the face incidence index of $S(T_{n,k})$ is given by:*

$$\mathcal{FI}(S(T_{n,k})) = 8n + 4k + 1.$$

Proof: The subdivision graph $S(T_{n,k})$ is constructed by inserting a new vertex into each edge of the tadpole graph $T_{n,k}$, effectively transforming each edge into a path of length two. This operation increases the number of vertices and edges in the graph, and also alters the structure of the faces in its planar embedding.

The planar embedding of $S(T_{n,k})$ contains exactly two categories of faces. The first is the internal face, denoted by F_j, where j represents the degree of the face. The second is the external face, denoted by F_∞, which surrounds the graph from the outside. For each face F, we define its degree as the sum of degrees of the vertices incident to it, that is,

$$\sum_{\mu \backsim F} d(\mu) = j.$$

Let $|F_j|$ denote the number of internal faces of degree j. The values of degrees for both internal and external faces, corresponding to different values of n, are summarized in Table 3.

Number of vertices in cycle	3	4	5	-	-	-	n
Degree of internal face	13	17	21	-	-	-	$4n+1$
Degree of external face	$4(k+3)$	$4(k+4)$	$4(k+5)$	-	-	-	$4(k+n)$

Table 3: The degrees of the internal and external faces of $S(T_{n,k})$.

From the pattern observed in the table, the degree of the internal face is given by $4n+1$, and there is exactly one such face. The degree of the external face is $4(k+n)$, and it also appears only once in the embedding.

According to the definition of the face incidence index $\mathcal{FI}$, which is the total sum of degrees of all faces in the planar embedding of the graph, we have:

$$\mathcal{FI}(S(T_{n,k})) = \sum_{\mu \backsim F \in \mathcal{F}(G)} d(\mu).$$

This sum can be separated into contributions from the internal and external faces:

$$\mathcal{FI}(S(T_{n,k})) = \sum_{\mu \backsim F_j} d(\mu) + \sum_{\mu \backsim F_\infty} d(\mu).$$

Substituting the values from Table 3, we obtain:

$$\mathcal{FI}(S(T_{n,k})) = (4n+1) \cdot 1 + 4(k+n) \cdot 1.$$

Simplifying this expression:

$$\mathcal{FI}(S(T_{n,k})) = 4n + 1 + 4k + 4n = 8n + 4k + 1.$$

This gives the required result, and thus the proof is complete.

Theorem 2.5 *Let $S(W_n)$ be the subdivision graph of the wheel graph. Then, the face index of $S(W_n)$ is given by:*

$$\mathcal{FI}(S(W_n)) = n^2 + 17n, \quad for \ n \geq 3.$$

Number of vertices (n)	3	4	5	6	-	-	-	n
Degree of internal face (j)	15	16	17	18	-	-	-	n+12
Number of internal face $\|j\|$	3	4	5	6	-	-	-	n
Degree of external face	15	20	25	30	-	-	-	5n

Table 4: The degree of internal and external faces of $S(W_n)$

Proof: The subdivision graph of the wheel graph $S(W_n)$, as shown in Fig. 1 (a) contains two categories of faces, F_j the internal face (where j changes with n) and F_∞ the external face. The degrees of the external and the internal faces are mentioned in Table 4. Now, by the definition of the $\mathcal{FI}$ and Table 4, for $n \geq 3$, we have

$$\begin{aligned}\mathcal{FI}(S((W_n)) &= \sum_{\mu \backsim F \in \mathcal{F}(G)} d(\mu) \\ &= \sum_{\mu \backsim F_j} d(\mu) + \sum_{\mu \backsim F_\infty} d(\mu) \\ &= (degree\ of\ F_j).|F_j| + (degree\ of\ F_\infty) \\ &= (n+12)(n) + 5n \\ &= n^2 + 17n,\end{aligned}$$

which is required result and completes our proof.

Theorem 2.6 *Let $S(L_n)$ be the subdivision graph of the ladder graph. Then, the face index of $S(L_n)$ is given by*

$$\mathcal{FI}(S(L_n)) = 30n - 28, \qquad for\ \ n > 1$$

Proof: The subdivision graph of the ladder graph $S(L_n)$, as shown in Fig. 3(a) consists of two types of faces, the internal faces F_{18}, F_{20} with $|F_{18}| = 2$ and $|F_{20}| = n - 3$ and the external face F_∞. While sum of degree of vertices of the external face is $10n - 4$. Now by these results and definition of the $\mathcal{FI}$

$$\begin{aligned}\mathcal{FI}(S((L_n)) &= \sum_{\mu \backsim F \in \mathcal{F}(G)} d(\mu) \\ &= \sum_{\mu \backsim F_{18}} d(\mu) + \sum_{\mu \backsim F_{20}} d(\mu) + \sum_{\mu \backsim F_\infty} d(\mu) \\ &= 18.|F_{18}| + 20.|F_{20}| + 10n - 4 \\ &= 18(2) + 20(n-3) + 10n - 4 \\ &= 30n - 28,\end{aligned}$$

which completes the proof.

2.3. Face Index for line graphs of Subdivision graphs of the Tadpole, Wheel and Ladder Graphs

This subsection is devoted to the computation of the line graphs of the subdivision graphs of the tadpole and ladder graphs.

Theorem 2.7 *Let $L_s(T_{n,k})$ be the line graph of the subdivision of the tadpole graph $T_{n,k}$. Then, for $n \geq 3$ and $k \geq 1$, the face incidence index of $L_s(T_{n,k})$ is given by:*

$$\mathcal{FI}(L_s(T_{n,k})) = 8n + 4k + 13.$$

Proof: The graph $L_s(T_{n,k})$ is obtained by first subdividing the tadpole graph $T_{n,k}$, and then taking the line graph of the resulting subdivision. In a planar embedding, this graph contains three categories of faces: an internal face of fixed degree 9 (denoted by F_9), internal faces of degree $j = 4n + 2$ (denoted by F_j), and a single external face F_∞ with degree depending on both n and k.

The number and degrees of these faces for small values of n follow a pattern which generalizes as shown in Table 5.

No. of vertices in cycle	3	4	5	-	-	-	n
Degree of internal face	14	18	22	-	-	-	$4n+2$
Degree of external face	$4k+14$	$4k+18$	$4k+22$	-	-	-	$4(k+n)+2$

Table 5: The degrees of the internal and external faces of $L_s(T_{n,k})$.

From this table, it is clear that the graph contains exactly one internal face of degree 9, denoted by F_9, and one internal face of degree $4n+2$, denoted by F_j, as well as one external face of degree $4(k+n)+2$.

By definition, the face incidence index $\mathcal{FI}$ of a planar graph is the total sum of the degrees of all its faces:

$$\mathcal{FI}(L_s(T_{n,k})) = \sum_{\mu \backsim F \in \mathcal{F}(G)} d(\mu).$$

This expression can be expanded by separating the contributions of each type of face as follows:

$$\mathcal{FI}(L_s(T_{n,k})) = \sum_{\mu \backsim F_9} d(\mu) + \sum_{\mu \backsim F_j} d(\mu) + \sum_{\mu \backsim F_\infty} d(\mu).$$

Since there is only one face of each kind, we substitute the degrees directly:

$$\mathcal{FI}(L_s(T_{n,k})) = 9 \cdot 1 + (4n+2) \cdot 1 + (4(k+n)+2) \cdot 1.$$

Simplifying the expression step-by-step:

$$\mathcal{FI}(L_s(T_{n,k})) = 9 + 4n + 2 + 4k + 4n + 2.$$

Combining like terms:

$$\mathcal{FI}(L_s(T_{n,k})) = (4n + 4n) + 4k + (9 + 2 + 2) = 8n + 4k + 13.$$

This confirms the required result and completes the proof.

Theorem 2.8 *Let $L(S(L_n))$ be the line graph of the subdivision graph of the ladder graph. Then, the face index of $L(S(L_n))$ is given by:*

$$\mathcal{FI}(L(S(L_n))) = 54n - 76, \quad for \;\; n > 1.$$

Proof: The line graph of the subdivision graph of the ladder graph $L(S(L_n))$ as shown in Fig. 3(b) consists of three internal faces F_9,F_{20}, F_{24} and an external face F_∞. The degrees of the internal and the external faces are mentioned in Table 6.

Now, by the definition of $\mathcal{FI}$ and Table 6:

$$\begin{aligned}
\mathcal{FI}(L(S(L_n))) &= \sum_{\mu \backsim F \in \mathcal{F}(G)} d(\mu) \\
&= \sum_{\mu \backsim F_9} d(\mu) + \sum_{\mu \backsim F_{20}} d(\mu) + \sum_{\mu \backsim F_{24}} d(\mu) + \sum_{\mu \backsim F_\infty} d(\mu) \\
&= 9.|F_9| + 20.|F_{20}| + 24.|F_{24}| + 12n - 8 \\
&= 9(2n-4) + 20(2) + 24(n-3) + 12n - 8 \\
&= 54n - 76,
\end{aligned}$$

n for $L[S(L_n)]$	3	4	5	6	-	-	-	n
Number of f_9	2	4	6	8	-	-	-	2n-4
Number of f_{20}	2	2	2	2	-	-	-	2
Number of f_{24}	0	1	2	3	-	-	-	n-3
Degree of f_∞	28	40	52	64	-	-	-	12n-8

Table 6: Number of F_9, F_{20}, F_{24} of $L(S(L_n))$.

which completes our proof.

Remark: The face index of the line graph of the subdivision of the wheel graph cannot be evaluated because $L_S(W_n)$ contains some edges which cannot be avoided to cross each other as shown in Fig. 1(b). So, the graph is not a planner graph, while the formula for the face index is applicable only for the planar graphs.

3. Graphical Analysis

In this section, we conclude the paper by illustrating the obtained results through graphical representations (see Fig. 4–5). In Fig. 4, the independent variable n is taken along the x-axis. Subfigure (i) displays the trends of the computed formulae for the face index $\mathcal{FI}$ of W_n and $S(W_n)$, represented by the blue and red curves, respectively. Subfigure (ii) depicts the behavior of the face index for L_n, $S(L_n)$, and $L[S(L_n)]$, each shown with distinct color patterns to highlight their variations with respect to n.

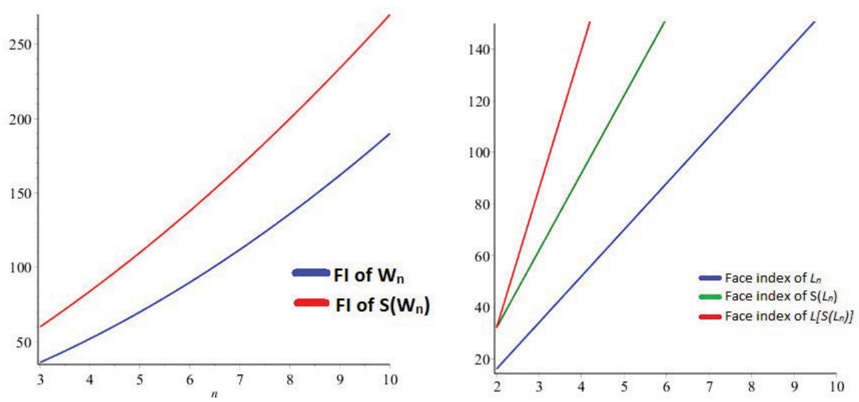

Figure 4: (i) Face index of W_n and $S(W_n)$. (ii) Face index of L_n, $S(L_n)$, and $L[S(L_n)]$.

Figure 5 presents two additional cases. Subfigure (i) shows the variation of the face index for $T_{n,k}$, while subfigure (ii) corresponds to the face index of $S(T_{n,k})$. In both cases, the horizontal axis corresponds to the parameter n, while k is fixed, allowing a clear observation of how $\mathcal{FI}$ changes with n.

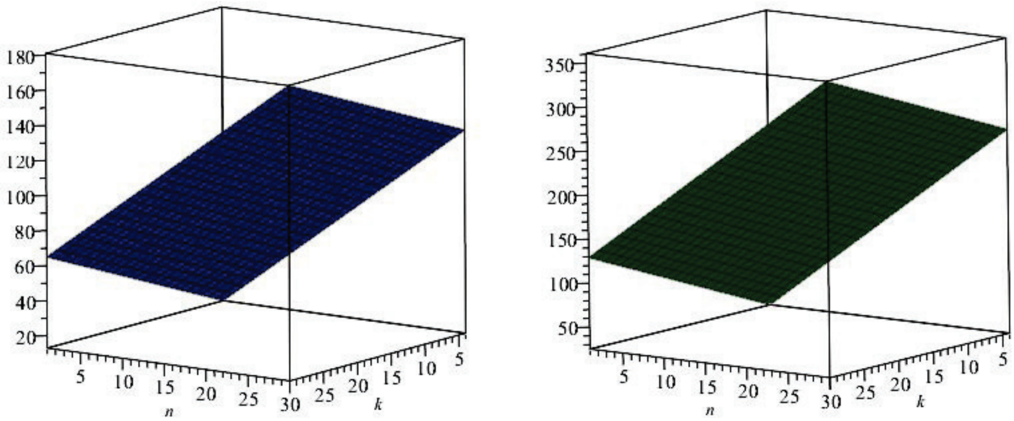

Figure 5: (i) Face index of $T_{n,k}$. (ii) Face index of $S(T_{n,k})$.

Finally, the corresponding 3D graphs (Fig. 5–??) display the dependence of the face indices for $T_{n,k}$, $S(T_{n,k})$, and $L(S(T_{n,k}))$ on both parameters n and k. These surfaces provide a comprehensive visualization of the simultaneous effect of the two variables, making it easier to identify trends and comparative growth patterns.

4. Conclusion

This study derives explicit formulae for the face index of tadpole, ladder, and wheel graphs, as well as their subdivision graphs and the line graphs of their subdivision graphs. The results provide a deeper understanding of how structural modifications influence the face index, which is useful in predicting various physicochemical properties of chemical compounds. The computed values reveal distinct trends in the face index for different graph classes, highlighting the impact of edge and vertex subdivisions. These findings contribute to the broader study of topological indices and their applications in chemical graph theory. Future research can extend this work by exploring the face index for other graph families or investigating its correlation with experimental molecular properties.

Declaration

- **Availabilty of data and materials:** The data is provided on request to the authors.
- **Authors Contribution:** All authors contributed equally in writing of this article.
- **Conflicts of interest:** The authors declare that they have no conflicts of interest and all agree to publish this paper under academic ethics.
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