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INVERSE SUM INDEG INDEX: BOUNDS AND EXTREMAL RESULTS

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ABSTRACT. In order to enhance quantitative-structure property-relationships investigations, Vukičević and Gašperov in 2010 proposed numerous novel vertex-degree-based graph invariants. After their examination, they found that only twenty of these are reasonably efficient predictors of physicochemical properties of chemical substances. The inverse sum indeg (ISI) index is one of these twenty invariants. The primary purpose of the present survey is to collect the known mathematical properties of ISI index, mainly bounds and extremal results. Some open problems and conjectures are also stated.

1. Prologue

As explained in detail in Section 3, a large number of "bond incident degree" (BID) graph invariants are being considered in the present-day literature. Their general formula is Eq. (2). The simplest and oldest such BID-index is the "first Zagreb index", in which $\phi(d_u,d_v) = d_u + d_v$. It was introduced as early as in the 1970s [61], and was eventually extensively studied [21, 54]. An immediate modification of this index would be to replace the degree of each vertex by its inverse ("indegree"). This would result in a "sum indeg" invariant, for which $\phi(d_u,d_v) = \frac{1}{d_u} + \frac{1}{d_v}$. It is easy to show that the respective BID index is equal to the number of vertices. Thus, such a "sum indeg" index would be fully insensitive to the structure of the underlying graph and therefore of no applicative value. A possible way out of this difficulty is the replacing of $\frac{1}{d_u} + \frac{1}{d_v}$ by its inverse, i.e., setting $\phi(d_u,d_v) = \left[\frac{1}{d_u} + \frac{1}{d_v}\right]^{-1}$. This leads to the "inverse sum indeg" index, ISI. Indeed, this modification of the original first Zagreb index showed to possess interesting mathematical properties and to be of value in (mainly chemical) applications. In what follows, we survey the main mathematical results that have accumulated since 2010, when this graph invariant was conceived [116].

2. Introduction

A graph invariant is a property of a graph that remains the same under graph isomorphism [49]. A graph invariant may be a number (for example, the number of vertices of a graph), a sequence (for example, the degree sequence of a graph), etc. In chemical graph theory, the graph invariants that take only numerical values are usually referred to as topological indices.

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$, such that $|V(G)| = n$ is the order and $|E(G)| = m$ the size of G.

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For additional (chemical-)graph-theoretical notation and terminology see Section 3 and the books [20, 22, 49, 112, 117].

In order to enhance quantitative-structure property-relationships investigations, Vukičević and Gašperov [116] proposed numerous novel vertex-degree-based topological indices. After their examination, they found that only twenty of these are efficient predictors of physicochemical properties of chemical substances. The inverse sum indeg (ISI) index is one among those twenty chemically usable graph invariants.

For a graph G, its ISI index is defined as

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}, \tag{1}$$

where d_u denotes the degree (= number of first neighbors) of the vertex u of G.

The inverse sum indeg index did not show an impressive predictive power in the seminal paper, but its nice and simple definition attracted researchers, leading to numerous publications. Among them, the papers dealing with its chemical application rarely appear. There have been some attempts to use ISI index to predict the physicochemical properties of anticancer drugs [13, 30] and antivirals used in the treatment of the COVID-19 [28, 74]. Apart from these applications of ISI index in the medicinal chemistry, we found only one paper assessing the energetic properties of monocarboxylic acids by the inverse indeg index [29]. Recently, there have been several attempts to enhance the application potential in chemical investigations of the inverse sum indeg index by slightly modifying its formula. These endeavors exhibited promising results that need to be further investigated. Since the modifications of the ISI index are beyond the scope of this review article, they will not be further elaborated. However, a reader interested in these modified versions of the ISI index should see [34, 92, 96] and the references quoted therein.

The mathematical aspects of the ISI index were extensively investigated, and a large number of papers is devoted to this topic. In particular, extensively studied are its extremal problems and bounds. It may be useful (at least for the newcomers to chemical graph theory) to have a source providing a collection of known mathematical results on the ISI index, in order to identify which mathematical aspects of this topological index have yet to be studied or which existing mathematical work on this index is incomplete. Therefore, the main goal of this review is to provide a summary of the existing bounds and extremal results on the ISI index.

This paper is organized as follows. The next section gives definitions and notations to be used in the subsequent parts of the paper. Extremal results concerning the ISI index are summarized in the Section 4. Some open problems and conjectures are also given in this section. Section 5 consists of two subsections; the first is about lower bounds, whereas the second is concerned with upper bounds.

3. Preliminaries

A graph of order at least 2 is known as a *non-trivial graph*. The path, star, cycle, and complete graphs of order n are denoted by P_n, S_n, C_n, and K_n, respectively. A degree of a vertex u equals the number of edges that are incident to this vertex, and is labeled by d_u. The smallest and the largest among vertex degrees in a graph G are the *minimum vertex degree* (δ) and the *maximum vertex degree* (Δ). A graph with the maximum vertex degree at most 4 is often referred to as a *molecular graph*. A connected graph of order n and size $n+k-1$ is a connected *k-cyclic graph*. For $k=1,2$, such graphs are referred to as *connected unicyclic, bicyclic graphs,* respectively. By an *n-order graph*, we mean a graph of order n. A graph containing no cycle of length 3 is referred to as a *triangle-free graph*.

A *bipartite graph* is a graph whose vertex set can be partitioned into two sets A_1, A_2, in such a way that no two vertices from each of these two sets are adjacent; the sets A_1 and A_2 are the partite sets of the respective bipartite graph. If, in addition, every vertex of the set A_i is adjacent to all the vertices of the other partite set for $i=1,2$, then the bipartite graph under consideration is the *complete bipartite graph*. The complete bipartite graph with p vertices in its one partite set and q vertices in its second partite set is denoted by $K_{p,q}$. A bipartite graph G is said to be (s,t)-*semiregular bipartite* (or simply *semiregular bipartite*) if every vertex in one of the partite sets of G has degree s and every vertex in the other partite set of G has degree t, where $s \neq t$.

The *complement of* G, denoted by $\overline{G}$, is the graph with the same vertices as G, provided that two vertices in $\overline{G}$ are adjacent if and only if they are not adjacent in G.

The *degree set* of G is the set consisting of all different elements of the degree sequence of G. The graph G is said to be regular if the degree set of G is a singleton set; if this singleton set is $\{t\}$ then G is said to be t-regular. If two vertices u and v of G are adjacent, then each of them is called a *neighbor* of the other. A vertex u of G is said to be a *pendent vertex* if $d_u = 1$. A vertex u of G of degree zero is an *isolated vertex*. By the *minimum non-pendent vertex degree* of G, we mean the least degree of non-pendent vertices of G. For an edge $uv \in E(G)$, the number $d_u + d_v - 2$ is the *degree of uv*. The least and largest numbers among the degrees of edges of G are the *minimum and maximum edge degrees of* G, respectively; they are denoted by δ_e and Δ_e, respectively. By an edge-regular graph, we mean a graph in which all edges have the same degree.

The *distance* $d(u,v)$ between two vertices u and v of G is the length of any shortest path in G connecting u and v. The eccentricity of a vertex u of G is defined as $\max_{x \in V(G)} d(u,x)$. The *radius* of G is the least eccentricity of all vertices of G.

A subset S of the vertex set (respectively, edge set) of a graph is said to be an *independent set* (respectively, *matching*) if the elements of S are pairwise non-adjacent. An independent set (respectively, a matching) consisting of the maximum possible vertices (respectively, edges) of a graph G is a *maximum independent set* (respectively, *maximum matching*) of G. The cardinality of a maximum independent set (respectively, maximum matching) of a graph G is the *independence number* (respectively, *matching number*) of G.

The *vertex connectivity* of a non-trivial connected graph is the minimum number of vertices whose removal results in a disconnected or trivial graph. The *edge connectivity* of a non-trivial connected graph is the minimum number of edges whose removal results in a disconnected graph.

The *chromatic number* of G is the minimum number of colors needed to color the vertices of G so that no two adjacent vertices have the same color. The *clique number* of G is the maximum order of a complete subgraph of G. A covering set C of G is a subset of $V(G)$, such that at least one end-vertex of every edge of G belongs to C. The covering number of G is the least cardinality of all covering sets of G. The least number of vertices whose deletion from G results in a bipartite graph is the *vertex bipartiteness* (or *bipartite vertex frustration* of G, [44, 120]).

Most of the topological indices defined via vertex degrees of a graph, found in the present-day literature, satisfy the following general setting [67, 116]:

$$BID_{\phi}(G) = \sum_{uv \in E(G)} \phi(d_u, d_v), \tag{2}$$

where ϕ is a real-valued symmetric function defined on the Cartesian square of the degree set of G.

For instance, the choices $\phi(d_u,d_v) = \ln(d_u + d_v)$ and $\phi(d_u,d_v) = \ln(d_u d_v)$ in Eq. (2) yield the natural logarithm of the multiplicative-sum Zagreb index Π_1^* (see [41, 55]) and the natural logarithm of the multiplicative second Zagreb index Π_2 (see [50, 55]), respectively.

The topological indices of the form (2) are referred to as *bond incident degree (BID) indices* [114]. Another frequently used name for such indices is *vertex-degree-based (VDB) topological indices* [27, 35].

Remark 3.1. *Since the higher-order connectivity indices [72, 73] are VDB topological indices but not BID indices, the class of BID indices form a proper subclass of the class of VDB topological indices. Therefore, for the sake of preciseness we prefer to call the topological indices of the form* (2) *as BID indices instead of VDB topological indices.*

In Table 1 several choices of the function ϕ for which Eq. (2) corresponds to the most popular topological indices (mentioned particularly in Section 5). Here α stands for a real number and $p \neq 0$. The topological indices ${}^0R_2$, R_1, R_{-1}, and ${}^0R_3$ are known as the first Zagreb index [21, 54, 56, 61], the second Zagreb index [21, 31, 59], the modified second Zagreb index [99], and the forgotten topological index [46], respectively.

We note here that the general zeroth-order Randić index is named in the literature also as "general first Zagreb index" [79] and "variable first Zagreb index" [93]. The general Randić index is identical to what sometimes is called "variable second Zagreb index" [93].

We also mention here that the topological indices $R_{-1/2}$, $2 \cdot \chi_{-1}$, $\chi_{-1/2}$, χ_2, and SO_{-1} are identical with the Randić index [78, 103], the harmonic index [12, 42], the sum-connectivity index [12, 122], the hyper-Zagreb index [12, 109], and the ISI index, respectively. As usual, for the sake of simplicity, we use the notions R, H, and χ for $R_{-1/2}$, $2 \cdot \chi_{-1}$ and $\chi_{-1/2}$, respectively.

Remark 3.2. *In the recent literature on BID indices, often the "reciprocal" of a particular index is considered, defined as*

$$BID_{\phi,rec}(G) = \sum_{uv \in E(G)} \frac{1}{\phi(d_u, d_v)}. \tag{3}$$

In the case of ISI, such "reciprocal ISI index" would be trivial, since bearing in mind the definition of ISI, Eq. (1), we get

$$\begin{aligned} ISI_{rec}(G) &= \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u d_v} = \sum_{uv \in E(G)} \left[\frac{1}{d_u} + \frac{1}{d_v}\right] \\ &= \sum_{u \in V(G)} d_u \frac{1}{d_u} = n \end{aligned}$$

where we applied the identity [40, 51]

$$\sum_{uv\in E(G)} \big[g(u)+g(v)\big] = \sum_{u\in V(G)} d(u)\,g(u)$$

valid for any function g of the vertices of the graph G.

TABLE 1. Some BID indices considered in the present article.

Function $\phi(d_u,d_v)$	Eq. (2) corresponds to	Symbol
$(d_u)^{\alpha-1}+(d_v)^{\alpha-1}$	general zeroth-order Randić index [7, 68]	${}^0R_\alpha$
$(d_u d_v)^\alpha$	general Randić index [19, 111]	R_α
$(d_u+d_v)^\alpha$	general sum-connectivity index [12, 123]	χ_α
$(d_u-d_v)^2$	sigma index [2, 47, 60]	σ
$\lvert d_u-d_v\rvert$	Albertson's irregularity index [1, 39]	A_{irr}
$\sqrt{(d_u)^2+(d_v)^2}$	Sombor index [52, 84]	SO
$\Big((d_u)^p+(d_v)^p\Big)^{1/p}$	p-Sombor index [84, 105]	SO_p
$2\sqrt{d_u d_v}(d_u+d_v)^{-1}$	geometric-arithmetic index [32, 101, 115]	GA
$\Big((d_u)^2+(d_v)^2\Big)(d_u d_v)^{-1}$	symmetric division deg index [8, 116]	SDD

4. Extremal Results

The mathematical study of the ISI index was initiated in the paper [107], where several extremal results were reported. We start presenting a result concerning the minimum ISI index of molecular trees.

Theorem 4.1. [107] *The path graph P_n uniquely attains the minimum ISI index over the class of n-order molecular trees, for every $n\in\{6,7,\ldots\}$.*

For most of the topological indices, the following property holds: if the path P_n graph has the maximum/minimum value of the considered topological index in the class of all n-order molecular trees, then P_n also attains the maximum/minimum value, respectively, of the considered topological index in the class of all n-order trees, provided n is sufficiently large. However, this property does not hold for the case of the ISI index; as it can be seen from the next result.

Theorem 4.2. [107] *Among n-order trees, the star graph S_n uniquely attains the minimum ISI index for every $n\in\{4,5,\ldots\}$.*

For $n-k \geq 2$, let $B_{n,k}$ be the tree obtained from the path P_{n-k} by attaching k pendent vertices to one of its pendent vertices. (In the literature, the graph $B_{n,k}$ is sometimes referred to as broom or comet.)

Theorem 4.3. [107] *Over the class of n-order trees with maximum degree Δ, the graph $B_{n,\Delta}$ uniquely attains the minimum ISI index for every $n \in \{4,5,\ldots\}$.*

The extremal graph mentioned in Theorem 4.3 is extremal also in the next result.

Theorem 4.4. [107] *Over the class of n-order trees with p pendent vertices, the graph $B_{n,p}$ attains the minimum ISI index for every $n \in \{4,5,\ldots\}$.*

Note that Theorem 4.4 does not provide all trees with minimum ISI index among the considered trees. For example, for $n \geq 7$, the tree depicted in Figure 1 has the same ISI-value as $B_{n,4}$.

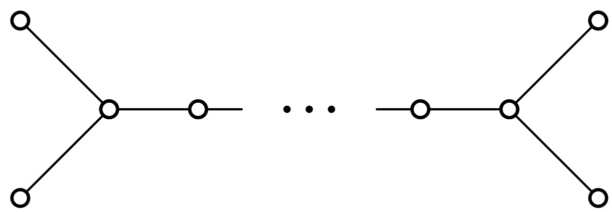

FIGURE 1. An n-order tree having the same ISI-value as the graph $B_{n,4}$, for $n \geq 7$.

In [107], it was proved that if v and w are non-adjacent vertices of a graph G, and if $G+vw$ denotes the graph obtained from G by adding the edge vw, then

$$ISI(G) < ISI(G+uv)\,. \tag{4}$$

Inequality (4) and Theorem 4.2 yield the following result.

Theorem 4.5. [107] *Among n-order connected graphs, the complete graph K_n uniquely attains the maximum ISI index, while the star graph S_n uniquely attains the minimum ISI index, for every $n \in \{4,5,\ldots\}$.*

In [107], the authors posed the next two problems and determined extremal trees of order up to 20 corresponding to each of these problems.

Problem 1. [107] *Characterize the graphs having maximum ISI index in the class of all molecular trees of fixed order.*

Problem 2. [107] *Characterize the graphs having maximum ISI index in the class of all trees of fixed order.*

Although Problem 1 has now been solved, Problem 2 is still open. In what follows, several results concerning the solutions to these problems are given.

The next result gives a solution to Problem 1 when the maximum degree is at most 3.

Theorem 4.6. [9] *Among n-order trees of maximum degree at most* 3,

(i): *trees containing no vertex of degree* 2 *are the only graphs with maximum ISI index, where n is an even integer greater than* 3*;*

(ii): *trees containing exactly one vertex of degree* 2*, which is adjacent to a pendent vertex, are the only graphs with maximum ISI index, where n is an odd integer greater than* 4*.*

Let $m_{i,j}$ be the number of the edges (of a graph) whose one end vertex has degree i and the other end vertex has degree j. Denote by $\mathscr{T}_n^*$ the class of the n-order molecular trees satisfying the following conditions:

$$\begin{aligned}
m_{4,4} &= k-1, m_{4,3} = 2k-1+\left\lfloor \frac{r}{2} \right\rfloor, \\
m_{4,1} &= 3-\left\lceil \frac{r}{2} \right\rceil, \\
m_{3,3} &= m_{3,2} \ = \ m_{2,2} = 0, \\
m_{3,1} &= 4k-2+2\left\lfloor \frac{r}{2} \right\rfloor, \\
m_{4,2} &= m_{2,1} = \begin{cases} 0 & \text{if } r \in \{0,2,4,6\}, \\ 1 & \text{if } r \in \{1,3,5\}, \end{cases}
\end{aligned}$$

where $n = 7k + r \geq 8$ provided that k is a positive integer and $0 \leq r \leq 6$. The next result gives the complete solution to Problem 1.

Theorem 4.7. [70] *The members of the class $\mathscr{T}_n^*$ are the only graphs attaining maximum ISI index among all n-order molecular trees, for every $n \in \{8, 9, \dots\}$.*

Problem 2 was attacked in [24], where not only several structural properties of the desired extremal tree were reported, but also a related problem and three conjectures were posed. (Problem 2 was also solved in [24] for $n \leq 150$.)

Before presenting the first result towards the solution of Problem 2, we specify some terminology.

Let $(d_0, d_1, \dots, d_{n-1})$ be a non-increasing degree sequence of a connected graph G with vertex set $V(G) = \{v_0, v_1, \dots, v_{n-1}\}$, where $d_i = d_{v_i}$ for $i = 0, 1, \dots, n-1$. Following Li et al. [76], we introduce an *ordering* of the vertices of G induced by *breadth-first search (BFS)*: create a sorted list of vertices beginning with v_0; append all neighbors $u_1, u_2, \dots, u_{d_0}$ of v_0 sorted by decreasing degrees; then append all neighbors of u_1 that are not already in the list, also sorted by decreasing degrees; continue recursively with $u_2, u_3, \dots$, until all vertices of G are processed. In this way, we get a rooted graph, with root v_0. The distance $d(v, v_0)$ is called the height $h(v)$ of a vertex $v \in V(G)$.

Let G be a connected rooted graph with root v_0. A well ordering $\prec$ of the vertices is called *breadth-first searching ordering* [18, 121] with non-increasing degrees (BFS ordering for short) if the following conditions hold for all vertices $u, v \in V(G)$:
(i) $u \prec v$ implies $h(u) \leq h(v)$;
(ii) $u \prec v$ implies $d(u) \geq d(v)$;
(iii) let $uv, xy \in E(G)$ and $uy, xv \notin E(G)$ with $h(u) = h(x) = h(v) - 1 = h(y) - 1$. If $u \prec x$, then $v \prec y$.

A graph having a BFS ordering of its vertices is known as a *BFS graph*.

Theorem 4.8. [24] *Among connected graphs with fixed degree sequence, there exists a BFS graph with the maximum ISI index.*

A BFS graph that is a tree is also known as a *greedy tree*. For every fixed degree sequence π, there exists a unique greedy tree with the degree sequence π. Thus, Theorem 4.8 implies the next result.

Corollary 4.9. [24] *Among trees with fixed degree sequence, the greedy tree attains the maximum ISI index.*

Before stating the next result towards the solution of Problem 2, we mention here that two results similar to Corollary 4.9 for unicyclic and bicyclic graphs of minimum degree 1 were reported in [25].

We remark here that a graph with maximum ISI index in the classes of graphs mentioned in Theorem 4.8 and Corollary 4.9 needs not to be a BFS graph, and a BFS graph in the class of connected graphs with fixed degree sequence may or may not have maximum ISI index [24]; see the two examples given in [81].

The next result provides a step closer to the solution of Problem 2.

Theorem 4.10. [24] *Let T be a tree with maximum ISI index among n-order trees and let d be a positive integer satisfying $1 \leq d \leq n-1$. Then the subgraph of T, induced by its vertices of degree greater than or equal to d is also a tree.*

Now, we state a problem and a conjecture, posed in [24], concerned with the solution of Problem 2.

Problem 3. [24] *Let T be a tree with maximum ISI index among all n-order trees. Characterize the degree sequence of T.*

Conjecture 1. [24] *Let T be a tree with maximum ISI index among all n-order trees. This tree T is unique. Also, if $n \geq 20$, then T is obtained from the star graph $S_{\Delta+1}$ by attaching pendent vertices to some vertices of $S_{\Delta+1}$.*

The next result settles Conjecture 4.2 of [24], which provides further a step closer to the solution of Problem 2.

Theorem 4.11. [80] *Let T be a tree with maximum ISI index among n-order trees, where $n \geq 20$. Then T has no vertex of degree 2.*

The next result settles Conjecture 4.4 of [24], which provides a further contribution towards the solution of Problem 2.

Theorem 4.12. [80] *Let T be a tree with maximum ISI index among non-trivial n-order trees and let Δ be the maximum degree of T. Then $ISI(T) < 2n-2-\Delta$.*

The next result is yet another contribution towards the solution of Problem 2.

Theorem 4.13. [80] *Let T be a tree with maximum ISI index among n-order trees, where $n \geq 137$. Then $ISI(T) > 3n/2$.*

Theorems 4.12 and 4.13 imply:

Corollary 4.14. [80] *Let T be a tree with maximum ISI index among n-order trees, where $n \geq 11$. Then the maximum degree of T is less than $n/2$.*

By a branching vertex in a tree, we mean a vertex of degree greater than 2. We now state another conjecture, posed in [80], concerned with Problem 2.

Conjecture 2. [80] *Let T be a tree with maximum ISI index among all n-order trees. Then the number of branching vertices of T is at most $\Delta + 1$.*

Observe that if the word "trees" is replaced with "connected graphs" in Theorems 4.1–4.4, then the resulting statements remain valid because of (4). This observation also implies:.

Theorem 4.15. [107] *Among n-order connected graphs with minimum degree 1, the star graph S_n uniquely attains the minimum ISI-value, for every $n \in \{4, 5, \dots\}$.*

A graph whose degree set consists of only two elements is a bidegreed graph.

Theorem 4.16. [96, 107] *In the class of connected n-order graphs of minimum degree $\delta \geq 2$,*

- *If δn is even, then only δ-regular graphs attain minimum ISI index.*
- *If δn is odd, then only the bidegreed graphs in which one vertex has degree $\delta + 1$ and all other vertices have degree δ, attain minimum ISI index.*

The next result may be considered as a maximal version of Theorems 4.15 and 4.16.

Theorem 4.17. [107] *Let $KD_{n,\delta}$ be the graph obtained from the complete graph K_{n-1} by adding a new vertex, adjacent to exactly δ vertices of K_{n-1}. Among n-order connected graphs with minimum degree δ, $KD_{n,\delta}$ uniquely attains the maximum ISI index, for every $n \in \{4, 5, \dots\}$.*

The problem of finding graphs with minimum and maximum values of ISI in the class of molecular graphs of fixed order and minimum degree was attacked in [63].

The next result may be considered as a variant of Theorem 4.16.

Theorem 4.18. [96, 107] *In the class of n-order graphs with maximum degree $\Delta \geq 2$,*

- *If Δn is even, then only Δ-regular graphs attain the maximum ISI index.*
- *If Δn is odd, then only the bidegreed graphs in which one vertex has degree $\Delta - 1$ and all other vertices have degree Δ, attain the maximum ISI index.*

By (4), a graph having minimum ISI index in the class of n-order connected graphs of maximum degree Δ must be a tree. Hence, by Theorem 4.3, such a tree is $B_{n,\Delta}$. The graphs having minimum ISI index among all graphs (including disconnected ones) of a given maximum degree, without isolated vertices, were reported in [96].

For $k \geq 1$ and for the sequence of non-negative integers $q_1, \dots, q_k$, the graph $H_{q_1,\dots,q_k}$ is obtained from the complete graph K_k on the vertex set $\{1, \dots, k\}$ by attaching q_i new pendent vertices to vertex i for each $i = 1, \dots, k$. Further, for given $k \geq 1$ and $p \geq 0$, let $KP_{k,p} = H_{q_1,\dots,q_k}$ where $q_1, \dots, q_k$ are chosen so that $\sum_{i=1}^{k} q_i = p$ and $q_i \in \left\{ \left\lfloor \frac{p}{k} \right\rfloor, \left\lceil \frac{p}{k} \right\rceil \right\}$ for each $i = 1, \dots, k$.

Theorem 4.19. [107] *Among n-order graphs with p pendent vertices, the graph $KP_{n-p,p}$ uniquely attains the maximum ISI index.*

Following [25], we define a special extremal BFS graph as follows. A connected k-cyclic BFS graph with vertex set $\{v_1, v_2, \dots, v_n\}$ and with non-increasing degree sequence $(d_1, d_2, \dots, d_n)$ is said to be a special extremal BFS graph if the vertices v_1, v_2, v_3, form a triangle, where $k \geq 1$, $d_i = d_{v_i}$, $d_n = 1$ and $n \geq 3$.

Theorem 4.20. [25] *Among all connected graphs with minimum degree* 1 *and with fixed degree sequence, there exists a special extremal BFS graph having maximum ISI index.*

The paper [23] examines the problems of characterizing graphs having maximum ISI index in the classes of connected graphs of fixed order and (i) vertex connectivity, (ii) edge connectivity, (iii) chromatic number, (iv) clique number, (v) independence number, (vi) covering number, and (vii) vertex bipartiteness. Similar problems concerning (I) matching number, (II) independence number, and (III) vertex connectivity, were attacked also in [14] independently.

A cactus graph is a connected graph in which every edge lies on at most one cycle. Let $\mathscr{C}_{n,k}$ be the class of n-order cactus graphs with k cycles, such that every graph in $\mathscr{C}_{n,k}$ satisfies the conditions: $m_{2,2} = n - 5k + 5$, $m_{2,3} = 6k - 6$, and $m_{i,j} = 0$ for $(i, j) \notin \{(2,2), (2,3), (3,2)\}$.

Theorem 4.21. [71] *The members of the class $\mathscr{C}_{n,k}$ are the only graphs attaining minimum ISI index among n-order cacti with k cycles, for $k \geq 1$ and $n \geq 6k - 3$.*

If "k cycles, for $k \geq 1$ and $n \geq 6k - 3$" in Theorem 4.21 is replaced by "$k = 2$ cycles", then the resulting statement remains valid; see [71]. Because of this observation and the condition $n \geq 6k - 3$ mentioned in Theorem 4.21, it is natural to pose the following problem.

Problem 4. *Characterize the graphs attaining minimum ISI index in the class of n-order cacti with k cycles, for $k \geq 3$ and $n < 6k - 3$.*

In [71], the following conjecture related to Problem 4 was also stated

Conjecture 3. [71] *The members of the class $\mathscr{C}_{n,k}$ are the only graphs attaining minimum ISI index among n-order cacti with k cycles, for $k \geq 3$ and $5k - 3 \leq n < 6k - 3$.*

Let $\mathscr{H}_{n,k}$ be the class of connected k-cyclic graphs of order n, such that every graph in $\mathscr{C}_{n,k}$ satisfies the conditions: $m_{2,2} = n - 5k + 5$, $m_{i,j} = 0$ for $(i, j) \notin \{(2,2), (2,3), (3,2)\}$ and $m_{2,3} = 6k - 6$.

Theorem 4.22. [71] *The members of the class $\mathscr{H}_{n,k}$ are the only graphs attaining minimum ISI index among connected k-cyclic graphs of order n, for $k \geq 1$ and $n \geq 6k - 3$.*

In view of Theorem 4.22, there is a problem and a conjecture corresponding to Problem 4 and Conjecture 3.

Since every tree is a bipartite graph, from (4) and Theorem 4.2, it follows that S_n uniquely attains the minimum ISI index over the class of n-order bipartite connected graphs. However, in Theorem 2 of [110] it was erroneously stated that P_n is the extremal graph. The next theorem may be considered as the maximal version of this result.

Theorem 4.23. [110] *In the class of n-order bipartite graphs, the complete bipartite graph $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ has maximum ISI-value for $n \geq 2$.*

The graphs attaining the maximum and second-maximum ISI-value in the classes of n-order bipartite graphs of fixed diameter and n-order bipartite graphs, respectively, were also determined [110].

Next, we give some extremal results regarding k-polygonal systems.

By a *k-polygonal system*, we mean a connected geometric figure obtained by concatenating congruent regular k-polygons side to side in a plane in such a way that the figure divides the plane into one infinite (external) region and several finite (internal) regions, and all internal regions are congruent regular k-polygons. In a given k-polygonal system, two polygons having a common side are said to be *adjacent polygons*. The *characteristic graph* of a k-polygonal system is a graph CG whose vertices correspond to k-polygons of the system and two vertices of CG are adjacent if and only if the corresponding k-polygons are adjacent. By a *k-polygonal chain*, we mean a k-polygonal system whose characteristic graph is a path graph. In a k-polygonal chain, a k-polygon adjacent to exactly one (respectively, two) k-polygon(s) is said to be *external* (respectively, *internal*) *k-polygon*. For $k = 3,4,5,6$, the corresponding k-polygonal chains/systems are known as triangular, polyomino, pentagonal, hexagonal chains/systems, respectively. (Hexagonal systems (also referred to as *benzenoid systems*) are of outstanding importance in chemical graph theory; for example, see [36, 53].)

Every k-polygonal system can be represented by a graph, in which the edges correspond to the sides of a k-polygon and the vertices represent the points where two sides of a k-polygon meet. In what follows, by a k-polygonal chain/system we mean the graph corresponding to the k-polygonal chain/system.

In a polyomino chain, an internal square having a vertex of degree 2 is known as a *kink*. In a pentagonal chain, a kink is an internal pentagon containing an edge connecting the vertices of degrees 2. A polyomino/pentagonal chain having at least 3 squares is said to be a *zigzag polyomino/pentagonal chain* if it consists of only kinks and external squares.

A *segment* in a polyomino/pentagonal chain is a maximal linear sub-chain, including the kinks and/or external squares/pentagons at its ends. The number of squares/pentagons in a segment is called its *length*. A segment is said to be *internal* if it contains no external square/pentagon.

Theorems 2.10 and 2.12 of [10] give the next result.

Theorem 4.24. *Among all polyomino chains with n squares, the linear chain uniquely attains the minimum ISI index for $n \geq 3$. For $n \geq 3$, the zigzag chain uniquely achieves the maximum ISI index in the class of polyomino chains with n squares in which no internal segment of length three has an edge connecting the vertices of degree three.*

For $n \geq 3$, let Ω_n be the class of all those pentagonal chains with n pentagons in which every internal segment of length 3 (if it exists) contains no edge with end-vertices of degrees 3. Theorems 3.6 of [11] implies the next result.

Theorem 4.25. *In the class Ω_n, The linear and zigzag chains uniquely attain the minimum and maximum values, respectively, of the ISI index.*

None of the general results reported in [3] imply any extremal result concerning triangular chains. Thus, we pose:.

Problem 5. *Characterize the graphs having the minimum and maximum values of ISI index in the class of all triangular chains with a given number of triangles.*

A *fluoranthene system* F is a molecular graph constructed from two hexagonal systems, say H_1 and H_2, in the following way. Let u and v be degree 2 vertices of H_1 having a common neighbor of degree 3. Let x and y be adjacent degree 2 vertices of H_2. Then F is obtained from H_1 and H_2 by adding two edges ux and vy. Fluoranthene systems have also been extensively studied in chemical graph theory; for details see [55].

The problem of characterizing systems having maximum and minimum values of the ISI index in the class of all fluoranthene systems with a given number of hexagons, under certain conditions, was attacked in [65]; see also [114].

It is important to note that there are numerous articles in the literature presenting general results on BID indices (or VDB indices) of hexagonal systems (and other analogous systems) and general graphs, with specific restrictions. For example, see the recent survey paper [77] (and its references related to the mentioned topic) for general graphs, and the references related to the indicated topic in the survey papers [4, 6, 12]. We leave it to the interested readers to check which such general results yield extremal results (as special cases) for ISI.

5. Bounds

Observe that every result given in Section 4 gives either a lower bound or an upper bound on the ISI index in terms of certain graph invariants (for example, order, maximum degree, etc.). For every such extremal graph invariant, there exists at least one graph attaining it. In this section, we list those bounds that do not satisfy this property. That is, for every bound given in the present section, there exist some values of the graph invariants for which no graph attains the considered bound. For instance, for the bounds stated in Theorem 5.1, there exists no graph with $n = 10$ and $m = 11$; generally, if $m \neq n$, then the mentioned bound is not attained.

5.1. *Lower Bounds.*

The very first lower bound on the ISI index was reported in [107].

Theorem 5.1. [107] *If G is an n-order graph of size m, then*

$$ISI(G) \geq 2m - n$$

with equality if and only if G is a 2-regular graph.

Since

$$\frac{m^2}{n} - (2m - n) = \frac{(n-m)^2}{n} \geq 0,$$

the next result is better than Theorem 5.1.

Theorem 5.2. [43] *If G is an n-order graph of size m, then*

$$ISI(G) \geq \frac{m^2}{n}$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.

Theorem 5.3. [43] *Let G be a graph with m edges and p pendent vertices, and with the minimum non-pendent vertex of degree δ_1. Then*

$$ISI(G) \geq \frac{\delta_1(m-p)}{2} + \frac{\delta_1 p}{\delta_1 + 1},$$

with equality if and only if either G is regular or the degree set of G is $\{1,\Delta\}$.

The next result is the corrected version of Theorem 2.6 of [100].

Theorem 5.4. [16] *Let G be a non-trivial connected graph of size m, with p pendent vertices, maximum degree Δ, and minimum non-pendant vertex degree δ_1. Then*

$$ISI(G) \geq \frac{p\,\delta_1}{\Delta+1} + (m-p)\sqrt{\frac{2\Delta\,\delta_1^6}{\Delta^6+2\delta_1^5+4\delta_1^2\,\Delta^3}}$$

with equality if and only if $G \in \{C_n, P_n, S_n\}$.

Theorem 5.5. [98] *Let G be a non-trivial graph of size m, maximum degree Δ and minimum degree δ. Then*

$$ISI(G) \geq m\left[1+\ln\left(\frac{\delta^2}{2\Delta}\right)\right]$$

with equality if and only if G is 2-regular.

Next, we present a few lower bounds on the ISI index involving the topological indices given in Table 1.

Theorem 5.6. [89] *If G is a non-trivial connected graph with m edges, then*

$$ISI(G) \geq \frac{H(G)\cdot R_1(G)}{2m} \tag{5}$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.

The next result is the corrected version of Theorem 2.7 of [100].

Theorem 5.7. [16, 87, 102] *Let G be a non-trivial connected graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$ISI(G) \geq \frac{\sqrt{\Delta^3\,\delta^3}}{m\,(\Delta^3+\delta^3)}H(G)\cdot R_1(G) \tag{6}$$

with equality if and only if G is regular.

The right-hand side of (6) depends on five parameters, including all the three parameters of the right-hand side of (5). Also, it holds that

$$\frac{H(G)\cdot R_1(G)}{2m} \geq \frac{\sqrt{\Delta^3\,\delta^3}}{m\,(\Delta^3+\delta^3)}H(G)\cdot R_1(G)\,.$$

Moreover, the class of graphs attaining the equality in (6) is a subclass of the class of the graphs attaining the equality in (5). Thus, the inequality (5) is better than (6).

Theorem 5.8. [43] *The inequalities*

$$ISI(G) \geq \frac{\delta^2}{m}\chi(G)^2 \quad \text{and} \quad ISI(G) \geq \frac{m^2\,\delta^2}{{}^0R_2(G)}$$

hold for every connected graph G of size m and minimum degree δ. Also, the inequality

$$ISI(G) \geq \frac{R_1(G)}{2\Delta}$$

holds for every connected graph G with the maximum degree Δ. Furthermore, the inequalities

$$ISI(G) \geq \frac{\delta^2 H(G)}{2} \quad \text{and} \quad ISI(G) \geq \frac{{}^0R_2(G)}{2} - \frac{{}^0R_3(G)}{4\delta}$$

holds for connected graph G the minimum degree δ. Equality in any of the inequalities given in the present theorem holds if and only if G is a regular graph.

All inequalities of Theorem 5.8, except the last one, follow from the inequality given in Theorem 5.2; see [57]. Also, the last inequality of Theorem 5.8 follows from the one given in the next theorem (see [89]).

Theorem 5.9. [89] *If G is a non-trivial connected graph with minimum edge degree δ_e, then*

$$ISI(G) \geq \frac{{}^0R_2(G)}{2} - \frac{{}^0R_3(G)}{2(\delta_e+2)}$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.

Theorem 5.10. [57] *Let G be a connected graph with minimum edge degree δ_e and maximum edge degree Δ_e. Then*

$$ISI(G) \geq \frac{4R_{-1}(G) \cdot R_1(G) + (\Delta_e+2)(\delta_e+2)H(G)^2}{4\,(\Delta_e+\delta_e+4)\,R_{-1}(G)}$$

with equality if and only if G is regular or semiregular bipartite.

Theorem 5.11. [57] *Let G be a connected graph of size m, minimum edge degree δ_e and maximum edge degree Δ_e. Then*

$$ISI(G) \geq \frac{R_1(G)[SDD(G)+2m] + m^2(\Delta_e+2)(\delta_e+2)}{[SDD(G)+2m]\,(\Delta_e+\delta_e+4)}$$

and

$$ISI(G) \geq \frac{4mR_1(G) + (\Delta_e+2)(\delta_e+2)\,GA(G)^2}{4m\,(\Delta_e+\delta_e+4)}$$

where the equality in either of these two inequalities holds if and only if for every pair of edges $st, uv \in E(G)$, the following condition holds:

$$\frac{d_s}{d_t} + \frac{d_t}{d_s} = \frac{d_u}{d_v} + \frac{d_v}{d_u}.$$

The inequality given in the next result follows from the first inequality of Theorem 5.11.

Corollary 5.12. [33] *Let G be a connected graph of size $m \geq 2$ and minimum edge degree δ_e. Then*

$$ISI(G) \geq \frac{m^2(\delta_e+2)}{SDD(G)+2m}$$

with equality if and only if G is either regular or semiregular bipartite.

Theorem 5.13. [33] *Let G be a connected graph of size $m \geq 2$ and maximum edge degree Δ_e. Then*

$$ISI(G) \geq \frac{\left[{}^0R_2(G)\right]^2}{(\Delta_e + 2)[SDD(G) + 2m]}$$

with equality if and only if G is either regular or semiregular bipartite.

Theorem 5.14. [43] *If G is an n-order tree, then*

$$ISI(G) \geq \frac{R_1(G)}{n}$$

with equality if and only if $G \cong S_n$.

In Theorem 5.14, if G is any triangle-free connected graph of order $n \geq 2$, then the inequality given there still holds [106], where the equality (in that case) holds if and only if G is a complete bipartite graph.

Theorem 5.15. [43] *The inequality*

$$ISI(G) \geq \frac{\chi(G)^2}{R_{-1}(G)}$$

holds for every connected graph G. If the graph G has m edges then

$$ISI(G) \geq m \sqrt[m]{\frac{\Pi_2(G)}{\Pi_1^*(G)}}.$$

In addition, if the graph G has minimum degree δ and maximum degree Δ, then

$$ISI(G) \geq \frac{m^2\sqrt{\delta\Delta}}{(\delta + \Delta)R(G)}.$$

Equality in any of these inequalities holds if and only if G is either a regular graph or a semiregular bipartite graph.

The last inequality of Theorem 5.15 follows from the one given in Theorem 5.2; see [57].

Theorem 5.16. [43] *For any connected graph G with at least 3 vertices,*

$$ISI(G) \geq H(G)$$

holds with equality if and only if G is the path graph with 3 vertices.

If the size of the graph G is not less than its order, then the inequality of Theorem 5.16 follows from the one given in Theorem 5.2 (see [57]).

Theorem 5.17. [95] *If G is any non-trivial connected graph, then*

$$ISI(G) \geq \frac{GA(G)^2}{2H(G)}$$

with equality if and only if G is an edge-regular graph.

Theorem 5.18. [95] *If G is a connected graph of size $m \geq 2$, minimum edge degree δ_e, and maximum edge degree Δ_e, then*

$$ISI(G) \geq \frac{R_{1/2}(G)}{2(m-1)}\left[GA(G) - \frac{2m\,\Pi_2(G)^{1/m}}{R_{1/2}(G)\,\Pi_1^*(G)^{1/m}} - \frac{\left(\sqrt{\Delta_e+2}-\sqrt{\delta_e+2}\right)^2 R_{1/2}(G)}{2(\Delta_e+2)(\delta_e+2)}\right]$$

with equality if and only if G is an edge-regular graph.

Theorem 5.19. [58] *If G is a graph with minimum degree at least 1 and if $0 < \alpha < 1$, then*

$$ISI(G) \geq \frac{R_\alpha(G)^{1/\alpha}}{[\chi_{\alpha/(1-\alpha)}(G)]^{(1-\alpha)/\alpha}}$$

with equality if and only if

$$(d_i+d_j)\,(d_i d_j)^{\alpha-1} = (d_u+d_v)\,(d_u d_v)^{\alpha-1}$$

for every pair of edges $ij, uv \in E(G)$.

The inequality given in Theorem 5.19 was independently derived in [57] for $\alpha = 1/2$.

Theorem 5.20. [58] *If $\alpha > 1$ and if G is a graph with maximum degree Δ and minimum degree $\delta \geq 1$, then*

$$ISI(G) \geq \frac{[R_\alpha(G)]^{1/\alpha}[\chi_{-\alpha/(\alpha-1)}(G)]^{(\alpha-1)/\alpha}}{c_\alpha\left(\delta^{(2\alpha^2-\alpha)/(\alpha-1)}, \Delta^{(2\alpha^2-\alpha)/(\alpha-1)}\right)}$$

with equality if and only if G is regular, where

$$c_p(\omega,\Omega) = \max\left\{\frac{1}{p}\left(\frac{\omega}{\Omega}\right)^{1/q} + \frac{1}{q}\left(\frac{\Omega}{\omega}\right)^{1/p}, \frac{1}{p}\left(\frac{\Omega}{\omega}\right)^{1/q} + \frac{1}{q}\left(\frac{\omega}{\Omega}\right)^{1/p}\right\},$$

with $q = p/(p-1)$. In addition,

$$ISI(G) \geq \frac{R_2(G) + 4\Delta^3\delta^3\,\chi_{-2}(G)}{2\,(\Delta^3+\delta^3)}$$

with equality if and only if every component of G is either δ-regular or Δ-regular.

Theorem 5.21. [58] *If G is a graph of size m, maximum degree Δ, and minimum degree $\delta \geq 1$, then*

$$ISI(G) \geq \left(\frac{2\Delta^3\delta^3}{\Delta^6+\delta^6}\sqrt{R_4(G)\,\chi_{-4}(G)} + m(m-1)\frac{\Pi_2(G)^{2/m}}{\Pi_1^*(G)^{2/m}}\right)^{1/2}$$

with equality if and only if G is regular. Also, if $\alpha > 0$, then it holds that

$$ISI(G) \geq \frac{\sqrt{\Delta\delta}}{\Delta+\delta}\,m\left(\frac{m}{R_{-\alpha}(G)}\right)^{1/(2\alpha)}$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.

Theorem 5.22. [45] *Let G be a connected graph with minimum degree at least 8. If the condition $d_u \leq d_v \leq \sqrt{2} d_u$ holds for every edge $uv \in (G)$, then $ISI(G) > SDD(G)$.*

Theorem 5.23. [34] *If G is a graph with maximum degree $\Delta \geq 1$, then*

$$ISI(G) \geq \frac{NI(G)}{\Delta}, \tag{7}$$

where

$$NI(G) = \sum_{uv \in E(G)} \frac{S(u)\,S(v)}{S(u)+S(v)} \quad \text{and} \quad S(w) = \sum_{xw \in E(G)} d_x .$$

If G is connected, then equality in (7) holds if and only if G is regular.

Theorem 5.24. [66] *If G is any graph, then*

$$ISI(G) > \frac{1}{2}\left({}^{0}R_2(G) - SO(G)\right).$$

Additional lower bounds on the ISI index can be found in [17, 62, 75, 88, 97, 100]. Also, lower bounds on the ISI index concerning graph operations can be found in [38, 86, 100, 104, 118].

5.2. *Upper Bounds.* The mathematical study of the ISI index was initiated in [107], where, among other results, the following upper bound on the ISI index has been obtained.

Theorem 5.25. [107] *If G is a graph of size m and maximum degree Δ, then $ISI(G) \leq \Delta m/2$ with equality if and only if G is Δ-regular.*

Corollary 5.26. [107] *If G is an n-order molecular graph, then*

$$ISI(G) \leq 4n$$

with equality if and only if G is 4-regular.

Theorem 5.27. [43] *Let G be a graph with m edges and p pendent vertices, and with maximum degree Δ. Then*

$$ISI(G) \leq \frac{\Delta(m-p)}{2} + \frac{p\Delta}{\Delta+1},$$

with equality if and only if either G is a regular graph or the degree set of G is $\{1, \Delta\}$.

Theorem 5.28. [58] *If G is an n-order graph with size m, maximum degree Δ, and minimum degree $\delta \geq 1$, then*

$$ISI(G) \leq \frac{(\Delta+\delta)^2}{4\Delta\delta}\frac{m^2}{n},$$

with equality if and only if G is regular. Also, it holds that

$$ISI(G) \leq \left[1 + \frac{1}{4}\left(1 - \frac{1+(-1)^{m+1}}{2m^2}\right)\frac{(\Delta-\delta)^2}{\Delta\delta}\right]\frac{m^2}{n}.$$

Theorem 5.29. [43] *If G is a connected n-order graph of size m, then*

$$ISI(G) \leq \frac{2nm - \xi(G)}{4} \quad \text{and} \quad ISI(G) \leq \frac{m(n - \mathrm{rad}(G))}{2},$$

with equality if and only if either $G \cong K_n$ or G is the graph obtained from K_n by removing a perfect matching, where $\mathrm{rad}(G)$ is the radius of G and $\xi(G)$ is the eccentric connectivity index [108], defined as

$$\xi(G) = \sum_{u \in V(G)} d_u \varepsilon_u .$$

Theorem 5.30. [34] *If G is a graph with minimum degree $\delta \geq 1$, then*

$$ISI(G) \leq \frac{NI(G)}{\delta}, \tag{8}$$

where $NI(G)$ is defined in Theorem 5.23. If G is connected, then equality in (8) holds if and only if G is regular.

In the remaining part of this section, we provide upper bounds on the ISI index involving topological indices defined in Table 1.

Theorem 5.31. [107] *For any graph G, the inequality*

$$ISI(G) \leq \frac{{}^0R_2(G)}{4}$$

holds, where equality holds if and only if every component of G is regular.

The inequality given in the next theorem was obtained also in [91] from a more general inequality.

Theorem 5.32. [43] *For every connected graph G, it holds that*

$$ISI(G) \leq \frac{1}{2} R_{1/2}(G),$$

with equality if and only if G is regular.

Theorem 5.33. [43] *The inequality*

$$ISI(G) \leq \frac{\sqrt{m \cdot R_1(G)}}{2}$$

holds for every connected graph G with m edges. Also, the inequalities

$$ISI(G) \leq \frac{R_1(G)}{2\delta} \quad \text{and} \quad ISI(G) \leq \frac{{}^0R_3(G)}{4\delta}$$

hold for every connected graph G with minimum degree δ. Moreover, the inequalities

$$ISI(G) \leq \frac{\Delta^2}{2} R(G), \quad ISI(G) \leq \sqrt{\frac{\Delta^3}{2}} \chi(G),$$

and

$$ISI(G) \leq \frac{\Delta^2 H(G)}{2} \quad \text{and} \quad ISI(G) \leq \frac{{}^0R_2(G)}{2} - \frac{{}^0R_3(G)}{4\Delta}$$

hold for every connected graph G with maximum degree Δ. Equality in any of the inequalities given in the present theorem holds if and only if G is regular.

The last inequality of Theorem 5.33 follows also from the one given in the next theorem (see [89]).

Theorem 5.34. [89] *If G is a non-trivial connected graph with maximum edge degree Δ_e, then*

$$ISI(G) \le \frac{{}^0R_2(G)}{2} - \frac{{}^0R_3(G)}{2(\Delta_e+2)}$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.

Theorem 5.35. [85] *For any graph G, it holds that*

$$ISI(G) \le 2^{-\left(\frac{1}{p}+1\right)} SO_p(G),$$

with equality if and only if G is regular.

Theorem 5.36. [58] *Let G be a graph with minimum degree $\delta \ge 1$. Then*

$$ISI(G) \le \frac{{}^0R_3(G)}{4\delta} - \frac{A_{irr}(G)^2}{2\,{}^0R_2(G)},$$

$$ISI(G) \le 2^{-\alpha-1}\delta^{1-\alpha}\chi_\alpha(G), \quad \text{if} \quad \alpha \ge 1, \tag{9}$$

$$ISI(G) \le \frac{1}{2\delta^{2\alpha-1}} R_\alpha(G), \quad \text{if} \quad \alpha > 1/2, \tag{10}$$

$$ISI(G) \le \frac{{}^0R_\alpha(G)}{4\delta^{\alpha-2}}, \quad \text{if} \quad \alpha \ge 2, \tag{11}$$

where equality in any of the above inequalities is attained if and only if G is regular.

We remark here that (9) is a generalized version of the inequality given in Theorem 5.31. Also, (10) and (11) are generalized versions of the second and third inequalities of Theorem 5.33, respectively.

Theorem 5.37. [90] *If G is a non-trivial connected graph, then*

$$ISI(G) \le \frac{1}{4}\left({}^0R_2(G) - \frac{A_{irr}(G)^2}{{}^0R_2(G)}\right)$$

with equality if and only if there exists a real number ε such that the condition $\frac{|d_u-d_v|}{d_u+d_v} = \varepsilon$ holds for every edge $uv \in E(G)$.

Theorem 5.38. [94] *If G is any non-trivial connected graph, then*

$$ISI(G) \le \frac{1}{2}\left({}^0R_2(G) - \frac{SO(G)^2}{{}^0R_2(G)}\right).$$

Also, if the graph G has size m, then

$$ISI(G) \le \frac{1}{2}\left({}^0R_2(G) - \frac{SO_{red}(G)^2}{{}^0R_2(G)} + H(G) - 2m\right),$$

where SO_{red} is the reduced Sombor index [52] defined as

$$SO_{red}(G) = \sum_{uv\in E(G)} \sqrt{(d_u-1)^2+(d_v-1)^2}.$$

In addition, if the graph G has order n, then

$$ISI(G) \leq \frac{1}{2}\left({}^{0}R_2(G) - \frac{SO_{avr}(G)^2}{{}^{0}R_2(G)} + \frac{4m^2}{n^2}H(G) - \frac{4m^2}{n^2}\right)$$

and

$$ISI(G) \leq \frac{1}{2}\left({}^{0}R_2(G) - \frac{SO\left(\overline{G}\right)^2}{{}^{0}R_2(G)} + \frac{(n-1)^2}{2}H(G) - m(n-1)\right),$$

where SO_{avr} is the reduced Sombor index [52] defined as

$$SO_{avr}(G) = \sum_{uv\in E(G)} \sqrt{\left(d_u - \frac{2m}{n}\right)^2 + \left(d_v - \frac{2m}{n}\right)^2}.$$

Equality in any of the above four inequalities holds if and only if G is an edge-regular graph.

Theorem 5.39. [106] *If G is a non-trivial triangle-free connected graph of order n, then*

$$ISI(G) \leq \frac{1}{4}\left({}^{0}R_2(G) - \frac{\sigma(G)}{n}\right)$$

with equality if and only if G is a complete bipartite graph.

Theorem 5.40. [66] *If G is any graph, then*

$$ISI(G) \leq \frac{1}{2\sqrt{2}}\left(\sqrt{2}\,{}^{0}R_2(G) - SO(G)\right)$$

with equality if and only if every component of G is regular.

Theorem 5.41. [58] *Let G be a graph of minimum degree at least* 1 *and maximum degree* Δ. *Then*

$$ISI(G) \leq \frac{\Delta\cdot GA(G)}{2},$$

$$ISI(G) \leq 2^{-\alpha-1}\Delta^{1-\alpha}\chi_\alpha(G), \quad \text{if} \quad 0 \leq \alpha < 1, \tag{12}$$

$$ISI(G) \leq \frac{R_\alpha(G)}{2\Delta^{2\alpha-1}}, \quad \text{if} \quad 0 \leq \alpha \leq 1/2, \tag{13}$$

$$ISI(G) \leq \frac{{}^{0}R_\alpha(G)}{4\Delta^{\alpha-2}}, \quad \text{if} \quad 1 \leq \alpha < 2, \tag{14}$$

where equality in any of the above inequalities is attained if and only if G is regular.

Note that (12) and (14) are generalized versions of the inequality given in Theorem 5.25. Also, (13) is a generalized version of the inequality given in Theorem 5.32.

Theorem 5.42. [100] *If G is any connected graph of size m, the*

$$ISI(G) \leq \frac{\sqrt{m\cdot\chi_2(G)}}{4}$$

with equality if and only if G is a regular graph.

It was proved in [89] that all the inequalities given in Theorems 5.33 and 5.42 follow directly from the one given in Theorem 5.32.

Theorem 5.43. [89] *If G is a connected graph of size $m \geq 2$, minimum edge degree δ_e, and maximum edge degree Δ_e, then*

$$ISI(G) \leq \frac{(\delta_e + \Delta_e + 4)^2 R_1(G)^2}{4m(\Delta_e+2)(\delta_e+2)\left(\Pi_2(G)\right)^{1/m}\left(\Pi_1^*(G)\right)^{1/m}}$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.

Corollary 5.44. [89] *If G is a non-trivial connected graph of order n, size m, minimum degree δ, maximum degree Δ, minimum edge degree δ_e, and maximum edge degree Δ_e, then*

$$ISI(G) \leq \frac{n\left(\delta_e + \Delta_e + 4\right)^2 R_1(G)^2}{4m^2(\Delta_e+2)(\delta_e+2)\left(\Pi_1^*(G)\right)^{2/m}} \leq \frac{n(\Delta+\delta)^2 R_1(G)^2}{4m^2\Delta\delta\left(\Pi_1^*(G)\right)^{2/m}}$$

where the equality in the first inequality holds if and only if G is either a regular graph or a semiregular bipartite graph, whereas in the second inequality if G is regular.

Theorem 5.45. [89] *If G is a non-trivial connected graph of size m, minimum edge degree δ_e, and maximum edge degree Δ_e, then*

$$ISI(G) \leq \frac{1}{2(\delta_e+2)}\left(m\left(\Pi_1^*(G)\right)^{2/m} - {}^0R_3(G) + m^2\left(\Delta_e - \delta_e\right)^2 \cdot \alpha(m)\right)$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph, where

$$\alpha(m) = \frac{1}{m}\left\lfloor\frac{m}{2}\right\rfloor\left(1 - \frac{1}{m}\left\lfloor\frac{m}{2}\right\rfloor\right) = \frac{1}{4}\left(1 - \frac{(-1)^{m+1}+1}{2m^2}\right).$$

Corollary 5.46. [89]

$$ISI(G) \leq \frac{1}{2(\delta_e+2)}\left(\frac{n^2}{m}\left(\Pi_2(G)\right)^{2/m} - {}^0R_3(G) + m^2\left(\Delta_e - \delta_e\right)^2 \cdot \alpha(m)\right)$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.

Theorem 5.47. [89] *If G is a non-trivial connected graph of size m, minimum edge degree δ_e and maximum edge degree Δ_e, then*

$$ISI(G) \leq \frac{{}^0R_2(G)^2 - m \cdot {}^0R_3(G) + m^2\left(\Delta_e - \delta_e\right)^2 \cdot \alpha(m)}{2m(\delta_e+2)}$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph, where $\alpha(m)$ is defined in Theorem 5.45.

Theorem 5.48. [89] *If G is a non-trivial connected graph of size m, minimum degree δ, maximum degree Δ, minimum edge degree δ_e, and maximum edge degree Δ_e, then*

$$ISI(G) \leq \frac{H(G) \cdot R_1(G)}{2m} + \frac{m\left(\Delta_e - \delta_e\right)\left(\Delta^2 - \delta^2\right) \cdot \alpha(m)}{(\delta_e+2)(\Delta_e+2)}$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph, where $\alpha(m)$ is defined in Theorem 5.45.

The next result (similar to Theorem 5.48) is the corrected version of Theorem 2.2 of [100].

Theorem 5.49. [16, 102] *Let G be a non-trivial connected graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$ISI(G) \leq \frac{H(G)\cdot R_1(G)}{2m} + \frac{(\Delta-\delta)^2\,(\Delta+\delta)\alpha_m}{2m\Delta\delta}$$

with equality if and only if G is regular, where

$$\alpha_m = m\left[\frac{m}{2}\right]\left(1-\frac{1}{m}\left[\frac{m}{2}\right]\right).$$

Theorem 5.50. [9] *If G is a non-trivial connected graph of order n, minimum edge degree δ_e, and maximum edge degree Δ_e, then*

$$ISI(G) \leq \frac{n\,(\Delta_e+\delta_e+4)\,R_1(G) - {}^0R_2(G)^2}{n(\Delta_e+2)(\delta_e+2)} \tag{15}$$

and

$$ISI(G) \leq \frac{n\,(\Delta_e+\delta_e+4)^2\,R_1(G)^2}{4(\Delta_e+2)(\delta_e+2)\,{}^0R_2(G)^2}, \tag{16}$$

where equality in both inequalities holds if and only if G is regular or semiregular bipartite. Also, if G is a non-trivial connected graph with order n, minimum degree δ, and maximum degree Δ, then

$$ISI(G) \leq \frac{n(\Delta+\delta)^2 R_1(G)^2}{4\Delta\,\delta\,{}^0R_2(G)^2}. \tag{17}$$

We remark here that both (16) and (17) follow from (15); see [9].

Theorem 5.51. [9] *If G is a non-trivial connected graph of size m, minimum edge degree δ_e, and maximum edge degree Δ_e, then*

$$ISI(G) \leq \frac{(\Delta_e+\delta_e+4)\,R(G)^2\,H(G)\,R_1(G) - 2m^4}{(\Delta_e+2)(\delta_e+2)R(G)^2\,H(G)}, \tag{18}$$

$$ISI(G) \leq \frac{(\Delta_e+\delta_e+4)^2\;H(G)\,R(G)^2\,R_1(G)^2}{8(\Delta_e+2)(\delta_e+2)m^4}, \tag{19}$$

$$ISI(G) \leq \frac{(\Delta_e+\delta_e+4)\,\chi(G)^2\,R_{-1}(G)\,R_1(G) - m^4}{(\Delta_e+2)(\delta_e+2)\chi(G)^2\,R_{-1}(G)}, \tag{20}$$

$$ISI(G) \leq \frac{(\Delta_e+\delta_e+4)^2\;\chi(G)^2\,R_{-1}(G)\,R_1(G)^2}{4(\Delta_e+2)(\delta_e+2)m^4}, \tag{21}$$

$$ISI(G) \leq \frac{(\Delta_e+\delta_e+4)\,R_1(G) - m\,(\Pi_1^*(G))^{1/m}\,(\Pi_2(G))^{\frac{1}{m}}}{(\Delta_e+2)(\delta_e+2)} \tag{22}$$

and

$$ISI(G) \leq \frac{n(\Delta_e+\delta_e+4)R_1(G) - m^2(\Pi_1^*(G))^{2/m}}{n(\Delta_e+2)(\delta_e+2)}, \tag{23}$$

where the equality in any of these inequalities holds if and only if G is regular or semiregular bipartite. Also, if G is a non-trivial connected graph of size m, minimum degree δ, and maximum degree Δ, then

$$ISI \leq \frac{(\Delta+\delta)^2 H(G) R(G)^2 R_1(G)^2}{8\Delta\delta m^4}.$$

Note that both (19) and (20) follow from (18). Also, (21) follows from (20), whereas (23) follows from (22); for details, see [9].

Theorem 5.52. [58] *If $\alpha > 1$ and G is a graph with minimum degree at least 1, then*

$$ISI(G) \leq R_\alpha(G)^{1/\alpha}[\chi_{-\alpha/(\alpha-1)}(G)]^{(\alpha-1)/\alpha}.$$

If G is connected, then equality is attained if and only if G is either a regular graph or a semiregular bipartite graph.

Theorem 5.53. [58] *If G is a graph of size m and minimum degree at least 1, then*

$$ISI(G) \leq \frac{1}{2}R_1(G)\cdot H(G) - m(m-1)\left(\frac{\Pi_2(G)}{\Pi_1^*(G)}\right)^{1/m}$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph. In addition,

$$ISI(G) \leq \frac{m}{2}\left(\frac{R_\alpha(G)}{m}\right)^{1/(2\alpha)} \quad \text{for } \alpha \geq 1/2.$$

with equality if and only if

- *G is regular, when $\alpha > 1/2$;*
- *each connected component of G is regular, when $\alpha = 1/2$.*

The next result provides an inequality similar to the first inequality of Theorem 5.53.

Theorem 5.54. [48] *If G is a graph of size m, maximum degree Δ, and minimum degree at least 1, then*

$$ISI(G) \leq \frac{\Delta}{2}GA(G)^2 - m(m-1)\left(\frac{\Pi_2(G)}{\Pi_1^*(G)}\right)^{1/m}$$

with equality if and only if G is regular.

Theorem 5.55. [33] *Let G be a graph of size $m \geq 1$, maximum degree Δ, and minimum degree δ. Then*

$$ISI(G) \leq \frac{(a_1+a_2)\sqrt{(m-1)\,{}^0R_2(G) + m\Pi_1^*(G)^{1/m}} - 2m - SDD(G)}{a_1 a_2}$$

with equality if and only if G is regular, where

$$a_1 = \sqrt{\frac{8}{\Delta}} \quad \text{and} \quad a_2 = \sqrt{\frac{\Delta}{\delta^2} + \frac{1}{\Delta} + \frac{6}{\delta}}.$$

Additional upper bounds on ISI can be found in [15, 17, 62, 75, 88, 97, 100]. In addition, upper bounds on ISI related to graph operations can be found in [37, 38, 64, 86, 98, 100, 104, 118].

6. Epilogue

In this review we presented most of the mathematical results that until now have been established for the ISI-index. As made clear in Section 3, ISI is just one among the multitude of presently investigated BID-type graph invariants, Eq. (2). In a number of studies, the general properties of BID-indices were studied, either for any real-valued symmetric function ϕ, or by assuming that ϕ possesses some additional properties; see the most recent works along these lines [26, 69, 82, 83, 113, 119] and the references cited therein. Needles to say, all such results imply, as a special case, a corresponding result for the ISI-index.

By the present review we hope to make the ISI-index familiar to colleagues interested in graph invariants, and to help them to do their own research in this area. More research is not only welcome, but is necessary since the theory of the ISI-index is far from being completed.

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