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Symmetric Division Deg Index: Extremal Results and Bounds

Akbar Ali[a,*], Ivan Gutman[b], Izudin Redžepović[c], Abeer M. Albalahi[a], Zahid Raza[d], Amjad E. Hamza[a]

[a]*Department of Mathematics, College of Science, University of Ha'il, Ha'il, Saudi Arabia*

[b]*Faculty of Science, University of Kragujevac, Kragujevac, Serbia*

[c]*Department of Natural Sciences and Mathematics, State University of Novi Pazar, Novi Pazar, Serbia*

[d]*Department of Mathematics, College of Sciences, University of Sharjah, Sharjah, UAE*

akbarali.maths@gmail.com, gutman@kg.ac.rs, iredzepovic@np.ac.rs, a.albalahi@uoh.edu.sa, zraza@sharjah.ac.ae, boaljod2@hotmail.com

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Abstract

Existing studies show that the symmetric division deg (SDD) index deserves to be treated as a useful and practicable molecular descriptor, preferable to some of the more widely used ones. The primary purpose of this review is to summarize the existing extremal results and bounds for the SDD index. Several open problems regarding the aforementioned index, arising from the known results, are also proposed.

*Corresponding author

1 Introduction

Molecular descriptors play a significant role in the quantitative studies on structure-property and structure-activity relationships [22,34,49]. According to Todeschini and Consonni [77], a *molecular descriptor* is "the final result of a logical and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into an useful number or the result of some standardized experiment".

In order to improve the existing quantitative studies on the particular types of molecular descriptors, Vukičević and Gašperov [82] proposed and investigated a novel class of molecular descriptors, and they discovered that only a few descriptors from this class are useful for QSPR (quantitative structure-property relationship) applications. The so-called symmetric division deg (SDD) index is among such chemically useful descriptors. The SDD index of a graph G is defined as

$$SDD(G) = \sum_{uv \in E(G)} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u} \right),$$

where d_u denotes the degree of the vertex u of G and $E(G)$ is the set of edges of G. (Throughout this paper, we consider only finite graphs. The (chemical) graph-theoretical terminology and notion that are used in this article, but not defined here, can be found in relevant standard textbooks like [14, 16, 78, 83].)

Furtula et al. [28] conducted a thorough comparative analysis of the SDD index with regard to several other molecular descriptors of this kind and discovered that the SDD index is a feasible and practicable molecular descriptor that outperforms a number of other descriptors of a similar kind, and hence they concluded that it deserves to be treated as a useful and applicable molecular descriptor, preferable to some of the more widely used ones.

The mathematical properties, particularly the extremal problems and bounds, of the SDD index have been studied in detail in many publications. In order to see which mathematical aspects of this descriptor have not yet been investigated or which mathematical study on this descriptor is incomplete, it may be desirable (at least for the newcomers to chemical graph theory) to have a source of a collection consisting of known mathematical results concerning the SDD index. Thereby, the primary purpose of this review article is to summarize the existing bounds and extremal results for the SDD index. Several open problems related to this molecular descriptor are also given.

The rest of this paper is organized as follows. The next section gives definitions and notations to be used in the upcoming sections. Extremal results concerning the SDD index are summarized in Section 3; some open problems are also proposed in this section. Section 4 consists of two subsections; the first one is about lower bounds for the SDD index, while the second one is concerned with upper bounds. Section 5, the final section, gives some open problems (regarding the SDD index) arising from the known results.

2 Preliminaries

A graph of order at least 2 is known as a *non-trivial graph*. A graph with maximum degree at most 4 is known as a *molecular graph*. By a *connected r-cyclic graph*, we mean a connected graph of order n and size $n+r-1$; for $r = 1, 2, 3, 4, 5$, such graphs are referred to as *connected unicyclic, bicyclic, tricyclic, tetracyclic, pentacyclic graphs,* respectively. The path, star, cycle and complete graphs of order n are denoted by P_n, S_n, C_n and K_n, respectively. The *complete bipartite graph* with p vertices in its one partite set and q vertices in its second partite set is denoted by $K_{p,q}$. By an *n-order graph*, we mean a graph of order n. A non-regular, connected and bipartite graph G is said to be a *semiregular bipartite graph* if the vertices in each partite set of G have the same degree.

In the following, we define some graph-theoretical terms by considering a graph G. The *complement of* G is denoted by $\overline{G}$ and is defined as the graph with the same vertices as G has, 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 called 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 $d_u = 1$. By the *minimum non-pendent vertex degree* of G, we mean the least number among the degrees of all non-pendent vertices of G. For an edge $uv \in E(G)$, the number $d_u + d_v - 2$ is known as the *degree of* uv. The least and largest numbers among the degrees of all edges of G are known as the *minimum and maximum edge degrees of* G, respectively; and they are denoted by δ_e and Δ_e, respectively.

Most of the existing molecular descriptors that are defined via vertex degrees of a graph, can be obtained from the following general setting [45,82]:

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

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. (1) yield the natural logarithm of the multiplicative-sum Zagreb index Π_1^* (see [25,48]) and the natural logarithm of the multiplicative second Zagreb index Π_2 (see [37,48]), respectively.

The descriptors of the form (1) are referred to as *bond incident degree (BID) indices* [80]; another often used name for such descriptors is *vertex-degree-based (VDB) indices* [17,21].

Table 1 gives some choices of the function ϕ for which Eq. (1) corresponds to most of the descriptors used in the upcoming sections; where α is any real number. The descriptors ${}^0R_2$, R_1, R_{-1}, ${}^0R_{-1}$ and ${}^0R_3$ are known as the first Zagreb index [15,39,40,44], the second Zagreb index [15,18,42], the modified second Zagreb index [64], the inverse degree index [27] (or the modified total adjacency index [64]) and the forgotten topological index [29], respectively. We remark here that the general zeroth-order Randić index is also known as the general first Zagreb index [51] and the variable first Zagreb index [57]. Also, the general Randić index is identical to the variable second Zagreb index [57].

Table 1. Some molecular descriptors used in the present article.

Function $\phi(d_u, d_v)$	Eq. (1) corresponds to	Symbol
$(d_u)^{\alpha-1} + (d_v)^{\alpha-1}$	general zeroth-order Randić index [47]	${}^0R_\alpha$
$(d_u\, d_v)^\alpha$	general Randić index [13,76]	R_α
$(d_u + d_v)^2$	hyper-Zagreb index [7,74]	H_Z
$(d_u - d_v)^2$	sigma index [4,30,43]	σ
$\|d_u - d_v\|$	Albertson's irregularity index [3]	irr
$(d_u d_v)(d_u^2 + d_v^2)^{-1}$	inverse symmetric division deg index [64]	$ISSD$
$\sqrt{d_u + d_v - 2}(d_u\, d_v)^{-1/2}$	atom-bond connectivity index [26]	ABC
$2\sqrt{d_u\, d_v}(d_u + d_v)^{-1}$	geometric-arithmetic index [81]	GA
$(d_u d_v)(d_u + d_v)^{-1}$	inverse sum indeg index [82]	ISI

3 Extremal Results

By an extremal result concerning the SDD index, we mean a result dealing with the characterization of graphs having either the minimum value or the maximum value of the SDD index over a given class of graphs. Certainly, every result stated in the present section gives either a lower bound or an upper bound on the SDD index in terms of some particular graph invariants (for example, order, size, minimum degree, etc.); these bounds have the following notable property: for every choice of possible values of such bounds' graph invariants, there exists at least one graph attaining the corresponding bound.

The thorough study of mathematical properties regarding the SDD index seems to be initiated by Vasilyev in [79]. We first present results concerning trees.

Theorem 3.1. [79] *In the class of all n-order trees, the path graph P_n and star graph $K_{n-1,1}$ uniquely attain the minimum and maximum values, respectively, of the SDD index for every integer n greater than* 3.

The graphs with the second to fourth minimum values (and fifth to ninth minimum values) of the SDD index among all trees of a fixed, sufficiently large, order were reported in [67] (in [8], respectively).

A subset D of the vertex set of a graph is said to be a dominating set if every vertex of $V(G)\setminus D$ has at least one neighbor in D. The cardinality of a smallest possible dominating set of a graph G is known as the domination number of G.

Theorem 3.2. [23] *The graph obtained from the star graph $S_{n-\gamma+1}$ by attaching one pendent vertex to each of $\gamma - 1$ pendent vertices of $S_{n-\gamma+1}$, is the only tree attaining the maximum SDD index among all n-order trees with domination number γ, where $2 \le \gamma \le n/2$.*

A segment of a tree T is a non-trivial path P in T with the property that neither of the end vertices of P has degree 2 (in T) and that every other vertex (if exists) of P has degree 2 (in T).

Theorem 3.3. [23] *The graph $P_{n-s+1,s-1}$ obtained from the path graph P_{n-s+1} by attaching $s-1$ pendent vertices to exactly one pendent vertex of P_{n-s+1}, is the unique tree attaining the maximum SDD index among all n-order trees with s segments, where $3 \le s \le n-2$.*

If the word “segments” is replaced with the text “pendent vertices” in the statement of Theorem 3.3, then the resulting statement remains true (according to [23]). Consequently, the problem of characterizing graphs attaining the maximum SDD index among all n-order molecular trees with p pendent vertices was also solved in [23] for $p \le 4$; the next result gives a solution to this problem for two additional cases concerning p.

Theorem 3.4. [24] *Let $\mathcal{T}(n,p)$ be the class of all n-order molecular trees with p pendent vertices.*

(a). *If p is even such that it satisfies the inequality $6 \le p \le \lfloor (n+3)/2 \rfloor$, then members of the class $\mathcal{T}^{\star}(n,p)$ are the only trees attaining the maximum SDD index in $\mathcal{T}(n,p)$, where $\mathcal{T}^{\star}(n,p) \subseteq \mathcal{T}(n,p)$ and each tree in $\mathcal{T}^{\star}(n,p)$ satisfies the following three properties (i) there is no vertex of degree 3, (ii) no two vertices of degree 4 are adjacent, and (iii) every pendent vertex is adjacent with a vertex of degree 4; an example of such a tree is shown in Figure 1.*

(b). *If p is odd such that it satisfies the inequality $9 \le p \le \lfloor (n+2)/2 \rfloor$, then members of the class $\mathcal{T}'(n,p)$ are the only trees attaining the* *maximum SDD index in $\mathcal{T}(n,p)$, where $\mathcal{T}' \subseteq \mathcal{T}(n,p)$ and each tree in $\mathcal{T}'(n,p)$ satisfies the following three properties (i) there is exactly one vertex of degree 3 and it has neighbors of degree 2 only, (ii) no two vertices of degree 4 are adjacent, and (iii) every pendent vertex is adjacent with a vertex of degree 4; an example of such a tree is shown in Figure 2.*

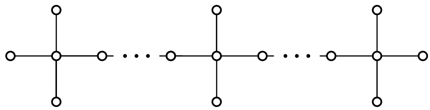

Figure 1. A tree in the class $\mathcal{T}^{\star}(n,p)$.

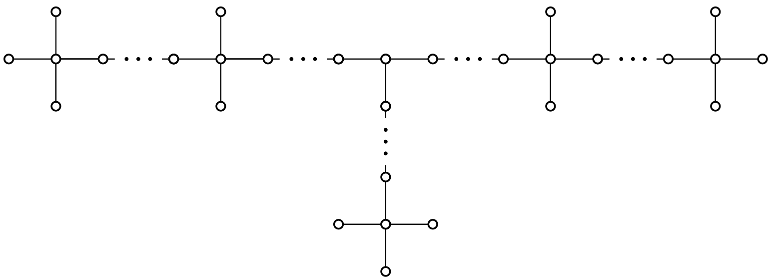

Figure 2. A tree in the class $\mathcal{T}'(n,p)$.

A vertex-induced subgraph (or simply, an induced subgraph) H of a graph G is a subgraph of G with the following property: if u and v are vertices of H such that $uv \in E(G)$ then $uv \in E(H)$.

Theorem 3.5. [24] *Over the class $\mathcal{T}(n,p)$ of all n-order molecular trees having p pendent vertices with $3 \le p \le \lfloor (n+2)/3 \rfloor$, members of the class $\mathcal{T}''(n,p)$ are the only trees attaining the minimum SDD index, where $\mathcal{T}''(n,p) \subseteq \mathcal{T}(n,p)$ and each tree in $\mathcal{T}''(n,p)$ satisfies the following three properties (i) the maximum degree is 3, (ii) there are exactly $p-2$ vertices of degree 3 and the induced subgraph consisting of these vertices is a tree, and (iii) no vertex of degree 3 has a neighbor of degree 1.*

Here, we remark that the problem of finding graphs attaining the minimum SDD index in the class of all n-order connected (molecular) non-tree graphs with m edges and p pendent vertices was also addressed in [24]. Next, we state an extremal result concerning the maximum value of n-order trees with a given diameter.

Theorem 3.6. [23] *Over the class of all n-order trees with diameter d, the graph $P_{d,n-d}$ (see Theorem 3.3) uniquely attains the maximum SDD index, where* $3 \leq d \leq n-1$.

Since the diameter of a tree with radius r is either $2r$ or $2r-1$, from Theorem 3.6 the next result follows.

Theorem 3.7. [23] *The tree $P_{2r-1,n-2r+1}$ (see Theorem 3.3) uniquely attains the maximum SDD index over the class of all n-order trees with radius r, where* $2 \leq r \leq (n-1)/2$.

We are not aware of any result concerning the minimal versions of Theorems 3.2, 3.3 and 3.6 (or 3.7), thus we propose the following problem.

Problem 1. *Characterize the graphs attaining the minimum SDD index among all n-order trees with a given*
(i) domination number,
(ii) number of segments, or
(iii) diameter (and hence radius).

Next, we summarize extremal results concerning cyclic graphs.

Theorem 3.8. [79] *In the class of all n-order (connected) unicyclic graphs, the cycle graph C_n and S_n^+, respectively, uniquely attain the minimum and maximum values of the SDD index for every integer n greater than* 3*, where S_n^+ is the graph deduced from the star graph S_n by inserting one edge.*

The graphs having the second maximum value of the SDD index in the class of unicyclic graphs mentioned in Theorem 3.8 were reported in [35]. The graphs attaining the second, third and fourth minimum values of the SDD index over the aforementioned class of unicyclic graphs (for sufficiently large n) were determined in [67]. Here, it is remarked that Theorems 3.1 and 3.8 were also obtained in [84] independently.

Theorem 3.9. [35] *The graph obtained from the cycle graph C_{n-p} by attaching p pendent vertices to exactly one vertex of C_{n-p} attains the maximum SDD index among all n-order (connected) unicyclic graphs with p pendent vertices, where $0 \leq p \leq n-3$.*

Theorem 3.10. [67] *The graphs obtained from the cycle graph C_n by adding an edge between any two non-adjacent vertices and the graphs obtained by joining two cycle graphs C_k, C_{n-k}, through an edge, are the only graphs with the minimum SDD index in the class of all n-order connected bicyclic graphs, where $n \geq 6$.*

The graphs attaining the second and third minimum values of the SDD index over the class of all connected bicyclic graphs of a fixed (sufficiently large) order were also found in [67].

Theorem 3.11. [84] *In the class of all n-order connected bicyclic graphs, the graph deduced from the $K_4 - e$ by attaching $n-4$ pendent vertices to one of the vertices of degree 3 of $K_4 - e$, uniquely attains the maximum SDD index for every integer n greater than 4, where $K_4 - e$ is the graph obtained from the complete graph K_4 by removing an edge.*

Theorem 3.12. [35] *The graph formed by identifying one vertex of the two cycles C_r, C_t and attaching p pendent vertices to the common vertex, attains the maximum SDD index among all n-order connected bicyclic graphs with p pendent vertices, where $t = n+1-r-p$ and $0 \leq p \leq n-5$.*

Theorem 3.13. [35] *In the class of all n-order connected bicyclic graphs with $n-4$ pendent vertices, the graph deduced from the $K_4 - e$ by attaching $n-4$ pendent vertices to one of the vertices of degree 3 of $K_4 - e$, uniquely attains the maximum SDD index for every integer n greater than 4, where $K_4 - e$ is the graph obtained from the complete graph K_4 by removing an edge.*

There is no result regarding the minimal versions of Theorems 3.9, 3.12 and 3.13 in the literature. Thereby, an open problem related to these theorems can be stated as follows.

Problem 2. *Characterize the graph(s) having the minimum SDD index among all n-order connected*
(i) unicyclic graphs, or
(ii) bicyclic graphs,
with a fixed number of pendent vertices.

Theorem 3.14. [53] *The graph obtained from the complete graph K_4 by replacing one of its edges with a path of length $n-3$ is the only graph attaining the minimum SDD index among all n-order connected tricyclic graphs for every integer n greater than 5.*

The graphs that attain the second minimum SDD index among all n-order connected tricyclic graphs of a given order were also reported in [53].

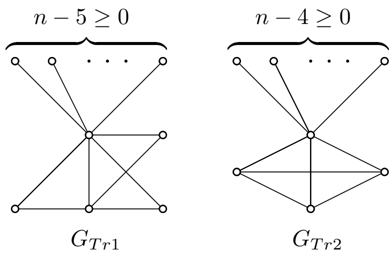

Figure 3. The graphs G_{Tr1} and G_{Tr2} mentioned in Theorem 3.15.

Theorem 3.15. [1] *The graph G_{Tr1} (G_{Tr2}, respectively), shown in Figure 3, attains uniquely the maximum SDD index over the class of all n-order connected tricyclic graphs for each $n \in \{5, 6\}$ (for every $n \in \{8, 9, \ldots\}$, respectively). For $n = 7$, both the graphs G_{Tr1} and G_{Tr2} have the maximum SDD index in the mentioned class.*

As pointed out in [54], it is not hard to determine graphs having the first two minimum values of the SDD index over the class of all tetracyclic graphs of a given order, by using an existing technique; the next result gives the unique graph with the maximum SDD index over this class.

Theorem 3.16. [1] *The graph G_{Tet1} (G_{Tet2}, respectively), shown in Figure 4, attains uniquely the maximum SDD index over the class of all n-order connected tetracyclic graphs for every $n \in \{6, 7, \ldots, 14\}$ (for every $n \in \{15, 16, \ldots\}$, respectively).*

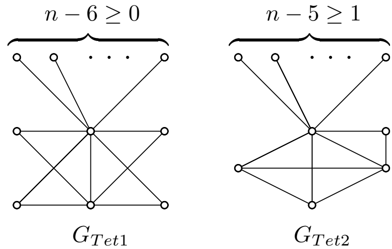

Figure 4. The graphs G_{Tet1} and G_{Tet2} mentioned in Theorem 3.16.

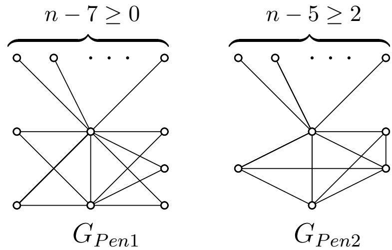

Figure 5. The graphs G_{Pen1} and G_{Pen2} mentioned in Theorem 3.17.

Theorem 3.17. [1] *The graph G_{Pen1} (G_{Pen2}, respectively), shown in Figure* 5, *attains uniquely the maximum SDD index over the class of all n-order connected pentacyclic graphs for every $n \in \{7, 8, \ldots, 13\}$ (for every $n \in \{14, 16, \ldots\}$, respectively).*

The following conjecture is due to Palacios [65].

Conjecture 1. [65] *In the class of all k-cyclic connected graphs of a given order n, the sets of extremal graphs with respect to the indices ${}^0R_{-1}$ and SDD are the same for $3 \leq k \leq 6$.*

By Theorems 3.15–3.17 and Theorem 2 of [68] (see also [46]), although Conjecture 1 is not true for small values of n but it is valid for $k = 3, 4, 5$, provided that n is sufficiently large. In [1], the following modified version of Conjecture 1 was posed.

Conjecture 2. [1] *In the class of all k-cyclic connected graphs of a given order n, the sets of extremal graphs with respect to the indices ${}^0R_{-1}$ and SDD are the same for $k \geq 6$ provided that n is sufficiently large.*

By the definition of connected r-cyclic graphs, the next result contributes towards the solution to the problem of characterizing graphs attaining the maximum SDD index over the class of all connected r-cyclic molecular graphs of a given order.

Theorem 3.18. [8] *Among all n-order molecular connected graphs of size m, with $n-1 \leq m \leq 2n$, and n being sufficiently large,*

(a). *the graphs having no vertices of degrees 2 and 3 are the only graphs attaining the maximum SDD index whenever $m+n \equiv 0 \pmod 3$;*

(b). *the members of the class $\mathcal{M}_{\mathcal{G}}$ are the only graphs attaining the maximum SDD index whenever $m+n \equiv 1$ or $2 \pmod 3$, where $\mathcal{M}_{\mathcal{G}}$ consists of the following two types of graphs G: (i) G contains no vertex of degree 2 and it contains exactly one vertex of degree 3, which is adjacent to three vertices of degree 4; (ii) G contains no vertex of degree 3 and it contains exactly one vertex of degree 2, which is adjacent to two vertices of degree 4.*

Here we remark that Theorem 3.18 follows also from a more general result reported recently in [2].

Theorem 3.19. [79] *The graph obtained from the complete graph K_{n-1} by adding a new vertex v and δ new edges between v and δ vertices of K_{n-1}, uniquely attains the maximum SDD index among all n-order graphs of minimum degree δ.*

There is no result regarding the minimal version of Theorem 3.19 in the literature. However, Vasilyev [79] proved that for every n-order graph of minimum degree δ, the inequality $SDD(G) \geq n\,\delta$ holds with equality if and only if G is δ-regular. This result implies the following corollary.

Corollary 3.20. *The 2-regular graphs are the only graphs attaining the minimum SDD index over the class of all n-order graphs of minimum degree at least 2 for $n \geq 4$. (In the case of connected graphs, C_n is the unique such extremal graph.)*

As there may or may not exist a δ-regular graph of order n for given values of n and δ, Theorem 3.19 and the comments made right after it, suggest the next problem.

Problem 3. *Characterize graphs attaining the minimum SDD index over the class of all those n-order connected graphs of minimum degree δ that are not δ-regular.*

The next result can be considered as a variant of Theorem 3.19 in which no restriction on the minimum degree of graphs is given.

Theorem 3.21. [79] *In the class of all n-order connected graphs, the complete graph K_n uniquely attains the maximum SDD index for every integer n greater than 2.*

Next, we give some extremal results regarding k-polygonal system. 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 must be congruent regular k-polygons. In a given k-polygonal system, two polygons having a common side are known as *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 the path graph. In a k-polygonal chain, a k-polygon adjacent to exactly one (respectively, two) k-polygon(s) is called *external* (respectively, *internal*) *k-polygon*. For $k = 3, 4, 5$, the corresponding k-polygonal chains/systems are known as triangular, polyomino, pentagonal chains/systems, respectively. 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.

A triangular chain of maximum degree at most 4 is known as a *linear triangular chain*. An induced subgraph of a triangular chain T_n is said to be a *segment* if it is a maximal linear triangular sub-chain of T_n. A segment containing external triangle(s) is called *external segment*. Suppose that a triangular chain T_n has s segments $S_1, S_2, S_3, ..., S_s$. The number of triangles in a segment S_i (where $1 \le i \le s$) is its *length*. The s-tuple $(a_1, a_2, \ldots, a_s)$ is said to be the *length vector* of T_n if and only if a_i is the length of S_i for $i = 1, 2, \ldots, s$. If $(a_1, a_2, \ldots, a_s)$ is a length vector of T_n and $s \ge 3$, then we assume that a_1, a_s are the lengths of the external segments. By a zigzag triangular chain, we mean a chain with $n \ge 4$ triangles and length vector

$$(a, \underbrace{4, 4, 4, \quad \cdots \quad, 4}_{\left(\lfloor \frac{n}{2} \rfloor - 2\right)-\text{times}}, b)$$

where $a, b \le 4$ and at least one of a, b is 3.

The second parts of Corollaries 3.2 and 3.3 of [5] imply the next result.

Theorem 3.22. *In the class of all those triangular chains with n triangles in which every vertex has degree at most five, the linear chain and the zigzag chain uniquely attain the minimum and maximum values of the SDD index, respectively, for $n \ge 4$.*

In a polyomino chain, an internal square having a vertex of degree 2 is known as a *kink*. A *linear polyomino chain* is the one, without kinks. A polyomino chain having at least 3 squares is said to be a *zigzag polyomino chain* if it consists of only kinks and external squares. A *segment* in a polyomino chain is a maximal linear sub-chain, including the kinks and/or external squares at its ends. The number of squares in a segment is known as its *length*. A segment is said to be *internal* if it does not contain any external square of the chain.

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

Theorem 3.23. *Among all polyomino chains with n squares, the linear chain uniquely attains the minimum SDD index for $n \ge 3$. The zigzag chain uniquely achieves the maximum SDD index over the class of all those polyomino chains with n squares in which no internal segment of length three has an edge connecting the vertices of degree three, for $n \ge 3$.*

None of the general results reported in [11] implies an extremal result concerning pentagonal chains. Thus, we pose the next problem.

Problem 4. *Characterize the graphs having the minimum and maximum values of the SDD index among all pentagonal chains with a given number of pentagons.*

It needs to be mentioned here that there exist various publications in the literature covering general results about BID indices (or VDB indices) of 6-polygonal (hexagonal) systems (and other systems) and general graphs, with certain constraints; for example, see the recent survey paper [50] (and its references related to the mentioned topic) for general graphs, and the references related to the indicated topic in the survey papers [6, 9]. We leave it to the readers to check which such general results yield extremal results concerning the SDD index.

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 known as a maximum independent set (respectively, maximum matching) of G. The cardinality of a maximum independent set (respectively, maximum matching) of a graph G is known as the independence number (respectively, matching number) of G. A perfect matching in a graph G is a matching M such that every vertex of G is incident with exactly one edge of M. The problems of finding graphs attaining the minimum (respectively, maximum) values of the SDD index over the classes of trees (respectively, molecular trees) and connected unicyclic graphs (respectively, connected molecular unicyclic graphs) possessing perfect matching were attacked in the article [70]. Du and Sun [23] characterized the graphs attaining the maximum SDD index among all trees possessing perfect matching. The graphs attaining the maximum SDD index among all n-order trees with a fixed matching number (and hence with a fixed independence number; because the addition of the matching number and the independence number of every n-order bipartite graph is n) were also found in [23]. Also, in [75], the graphs having the maximum SDD index were characterized over the classes of all (i) connected unicyclic graphs possessing perfect matching (ii) connected bicyclic graphs possessing perfect matching (iii) n-order connected unicyclic graphs with a fixed matching number (iv) n-

order connected bicyclic graphs with a fixed matching number. Recently, the problem of finding the graphs attaining the first five minimum values of the SDD index among all connected bicyclic graphs possessing perfect matching was attacked in [71]. The problem of characterizing the graphs having the maximum SDD index in the class of all connected molecular bicyclic graphs possessing perfect matching was also addressed in [71].

4 Bounds

Recall that every result given in Section 3 gives either a lower bound or an upper bound on the SDD index in terms of some certain graph invariants (for example, order, size, minimum degree, etc.); for every choice of possible values of such bounds' graph invariants, there exists at least one graph attaining the corresponding bound. 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 bound's graph invariants for which no graph attains the considered bound. For instance, the bound's graph invariants in Theorem 4.3 are n and m, but if one takes $n = 100$ and $m = 101$ then no 100-order molecular (connected) graph of size 101 exists attaining the mentioned bound.

4.1 Lower Bounds

We start this section by listing two very simple but notable lower bounds on the SDD index derived in [79].

Theorem 4.1. [79] *If G is a connected graph of size m, then the inequality $SDD(G) \geq 2m$ holds with equality if and only if G is regular.*

Theorem 4.2. [79] *If G is an n-order graph of minimum degree δ, then the inequality $SDD(G) \geq n\,\delta$ holds with equality if and only if G is δ-regular.*

The next result gives a solution to the minimal version of Theorem 3.18 for the case when $m \in \{n-1, n\}$.

Theorem 4.3. [8] *If G is an n-order molecular (connected) graph of size m such that $n-1 \leq m \leq 2n$ and $n \geq 3$, then $SDD(G) \geq n+m$ with equality if and only if G is either the path graph P_n or the cycle graph C_n.*

A path $P : v_1 v_2 \cdots v_t$ in a graph G is said to be a pendent path if one of the two vertices v_1, v_t, is pendent (in G) and the other one has degree at least 3 (in G), and every remaining vertex (if exists) of P has degree 2 (in G).

Theorem 4.4. [67] *If G is a graph with m edges and k pendent paths, then*

$$SDD(G) \geq \frac{2}{3}k + 2m.$$

In [8], it was proved that either if G is a regular graph or if the maximum degree of G is 3 such that $m_{1,2} = k = m_{2,3}$ and $m_{1,3} = 0$, then the inequality given in Theorem 4.4 becomes equality, where $m_{i,j}$ denotes the number of those edges of G whose one end-vertex has the degree i and the other end-vertex has the degree j.

Theorem 4.5. [35] *If G is a connected graph with size m, number of pendent vertices p and minimum non-pendent vertex degree δ_1, then*

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

with equality if and only if G is either a regular graph or a graph having the degree set $\{1, \Delta\}$ such that at least one end-vertex of every edge of G has degree Δ, where $\Delta \geq 2$.

We remark here that the graphs attaining the bound given in Theorem 4.5 were not fully characterized in [35]; the same case is with the next two results, however we are stating the next two results without any changes and leaving to readers the exercise of characterizing graphs (in the next two results).

Theorem 4.6. [35] *If G is a connected graph with order n, size m, number of pendent vertices p, maximum degree Δ, hyper Zagreb index H_Z and* *minimum non-pendent vertex degree* δ_1*, then*

$$SDD(G) \geq \sqrt{\frac{\left(n - p\left(\Delta + \frac{1}{\Delta}\right)\right)^2 (H_Z - p(\Delta+1)^2)}{m-p}} \\ - 4(m-p)^2\left(\frac{\Delta}{\delta_1} - \frac{\delta_1}{\Delta}\right) + p\left(\delta_1 + \frac{1}{\delta_1}\right) - 2(m-p),$$

where the equality is attained if G *is either a regular or star graph.*

Theorem 4.7. [35] *Let* G *be a connected* n*-order graph such that the complement* $\overline{G}$ *of* G *is also connected. If* δ_1*,* p *and* $\overline{\delta_1}$*,* $\overline{p}$ *are the minimum non-pendent vertex degree and number of pendent vertices of* G *and* $\overline{G}$*, respectively, then*

$$SDD(G) \geq n(n-1) + (p + \overline{p})\left(\alpha + \frac{1}{\alpha} - 2\right) - SDD(\overline{G}), \qquad (2)$$

where $\alpha = \min\left\{\overline{\delta_1}, \delta_1\right\}$*. Equality in* (2) *holds only if* G *is a* k*-regular graph with* $2k+1$ *vertices.*

In [28], not only the chemical applicability of the SDD index was examined thoroughly but also inequalities involving this index and several other molecular descriptors were derived.

Theorem 4.8. [28] *Consider a graph* G*.*

(i). *If* G *has size* $m \geq 1$ *and maximum degree* Δ*, then*

$$SDD(G) \geq m\left(\left(\frac{{}^0R_2(G)}{\Delta \cdot m}\right)^2 - 2\right)$$

with equality if and only if G *is regular.*

(ii). *If the order of* G *is at least* 3*, then*

$$SDD(G) > \frac{3}{2}ABC(G)$$

(iii). *If the size of* G *is* $m \geq 1$*, then*

$$SDD(G) \geq \frac{2m^2}{GA(G)}$$

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

(iv). *It holds that* $SDD(G) \geq 2\,GA(G)$*; however, if* G *is connected then the aforementioned inequality becomes equality if and only if* G *is regular.*

The next result gives a lower bound on the SDD index in terms of the second Zagreb index R_1, Albertson's irregularity index irr and the size of a graph.

Theorem 4.9. [55] *If* G *is a graph of size* $m \geq 1$*, then*

$$SDD(G) \geq \frac{\big(irr(G)\big)^2}{R_1(G)} + 2m,$$

with equality if and only if there exists a number r *such that the equation* $|d_u - d_v|/(d_u d_v) = r$ *holds for every edge* $uv \in E(G)$*.*

A graph G is said to be an edge-transitive graph if for every pair of edges $e_1, e_2 \in E(G)$, there is an automorphism that maps e_1 to e_2.

Theorem 4.10. [33] *If* G *is a graph with* $m \geq 1$ *edges, then*

$$SDD(G) \geq \frac{m^2}{ISSD(G)},$$

where the equality holds whenever G *is either a regular or an edge-transitive graph. Also, it holds that*

$$SDD(G) \geq ISDD(G) + \frac{3m}{2},$$

with equality if and only if G *is a regular graph. Moreover, it holds that*

$$SDD(G) \geq \frac{4}{m}\big(AG(G)\big)^2 - 2m,$$

where

$$AG(G)=\sum_{uv\in E(G)}\frac{d_u+d_v}{2\sqrt{d_ud_v}}.$$

Theorem 4.11. [20] *Let G be a connected graph with size $m\geq 2$. Then*

$$SDD(G)\geq \frac{\left({}^{0}R_2(G)\right)^2}{R_1(G)}-2m$$

with equality if and only if G is a regular graph or a semiregular bipartite graph. Also, it holds that

$$SDD(G)\geq 2m\left(\frac{2m^2}{\left(GA(G)\right)^2}-1\right)$$

and

$$SDD(G)\geq \frac{4m^4}{(m-1)(GA(G))^2}-\frac{m\left(\Pi_1^*(G)\right)^{\frac{2}{m}}}{(m-1)\left(\Pi_2(G)\right)^{\frac{1}{m}}}-2m$$

where the equality holds in either of the two inequalities if and only if

$$\frac{d_{v_i}}{d_{v_j}}+\frac{d_{v_j}}{d_{v_i}}=\frac{d_{v_k}}{d_{v_\ell}}+\frac{d_{v_\ell}}{d_{v_k}}$$

for every pair of edges $v_iv_j, v_kv_\ell\in E(G)$. Moreover, it holds that

$$SDD(G)\geq \frac{m}{m-1}\left(2(m+1)-\frac{\left(\Pi_1^*(G)\right)^{\frac{2}{m}}}{\left(\Pi_2(G)\right)^{\frac{1}{m}}}\right)$$

with equality if and only if G is regular.

Theorem 4.12. [20,41] *Let G be a connected graph of size $m\geq 2$, minimum edge degree δ_e and maximum edge degree Δ_e. Then*

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

with equality if and only if

$$\frac{d_u}{d_v} + \frac{d_v}{d_u} = \frac{d_w}{d_x} + \frac{d_x}{d_w}$$

for every pair of edges $uv, wx \in E(G)$ *and* $d_y + d_z - 2 = \Delta_e$ *or* δ_e *for every edge* $yz \in E(G)$.

Theorem 4.13. [20] *Let* G *be a connected graph with size* $m \geq 2$ *and minimum edge degree* δ_e. *Then*

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

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

Theorem 4.14. [20] *Let* G *be a non-trivial connected* n*-order graph of size* m. *Then*

$$SDD(G) \geq \frac{n^2}{R_{-1}(G)} - 2m$$

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

Theorem 4.15. [54] *If* G *is a connected graph of maximum degree* δ, *then* $SDD(G) \geq \delta^2 \cdot {}^0R_{-1}(G)$, *with equality if and only if* G *is regular.*

Theorem 4.16. [54] *Let* G *be a connected graph of size* m, *where* $m \geq 1$.

(i). *If* G *has minimum degree* δ, *then for* $\alpha > 0$, *it holds that*

$$SDD(G) \geq \frac{2\delta^2 m^{\frac{\alpha+1}{\alpha}}}{(R_\alpha(G))^{\frac{1}{\alpha}}},$$

with equality if and only if G *is regular.*

(ii). *If* G *has minimum degree* δ *and maximum degree* Δ, *then for* $\alpha > 0$, *it holds that*

$$SDD(G) \geq \frac{\delta^2 (2m)^{\frac{\alpha+1}{\alpha}}}{\Delta \left({}^0R_\alpha(G) \right)^{\frac{1}{\alpha}}}$$

with equality if and only if G *is regular.*

(iii). *The following inequalities hold*

$$SDD(G) \geq \frac{2m^2}{R_1(G)} \quad \text{and} \quad SDD(G) \geq \frac{4m^2}{{}^0R_3(G)},$$

where the equality in either of these two inequalities holds if and only if $G = K_2$.

Theorem 4.17. [60] *If T is a non-trivial n-order tree, then*

$$SDD(T) \geq n^2 - \overline{SDD}(T) - 2,$$

with equality if and only if $T = P_n$, where

$$\overline{SDD}(T) = \sum_{uv \notin E(T)} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u} \right).$$

Theorem 4.18. [60] *For $n \geq 4$, if T is an n-order tree of maximum degree Δ, then*

$$SDD(T) \geq 2(n-1)\left(\frac{1}{\Delta} + 2 + \frac{(n-3)^2}{2n - \Delta - 4} \right) - n - \overline{SDD}(T),$$

with equality if and only if the degree set of T has at most three elements, where $\overline{SDD}(T)$ is defined in Theorem 4.17.

Theorem 4.19. [58, 59] *If G is a connected non-trivial graph, then*

$$SDD(G) \geq \frac{\big(SO(G)\big)^2}{R_1(G)}$$

with equality if and only if there exists a constant r such that the equation $(d_u)^{-2} + (d_v)^{-2} = r$ holds for every edge $uv \in E(G)$, where SO is the Sombor index [38] defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{(d_u)^2 + (d_v)^2}.$$

The extended adjacency matrix (introduced in [85]) of a graph G with the vertex set $\{v_1, v_2, \cdots, v_n\}$ is denoted by $A_{ex}(G)$ and is defined as the matrix whose (i, j)-th entry is

$$\frac{1}{2}\left(\frac{d_{v_i}}{d_{v_j}}+\frac{d_{v_i}}{d_{v_j}}\right)$$

whenever $v_iv_j \in E(G)$ and 0 whenever $v_iv_j \notin E(G)$. Denote by $\eta_1(G)$ and $\eta_n(G)$ the largest and the least eigenvalues, respectively, of $A_{ex}(G)$.

Theorem 4.20. [32] *If G is an n-order graph, then* $SDD(G) \geq n \cdot \eta_n(G)$.

Theorem 4.21. [31] *Let G be a connected graph and*

$$k = \max\left\{\frac{1}{2}\left(\frac{d_u}{d_v}+\frac{d_v}{d_u}\right) : uv \in E(G)\right\},$$

then

$$SDD(G) \geq \frac{(2\,\eta_1(G)+k)^2-k^2}{4k}.$$

The arithmetic-geometric matrix of a graph G with the vertex set $\{v_1, v_2, \cdots, v_n\}$ is denoted by $A_{AG}(G)$ and is defined as the matrix whose (i, j)-th entry is

$$\frac{d_{v_i}+d_{v_j}}{2\sqrt{d_{v_i}d_{v_j}}}$$

whenever $v_iv_j \in E(G)$ and 0 whenever $v_iv_j \notin E(G)$. The sum of the absolute eigenvalues of $A_{AG}(G)$ is known as the arithmetic-geometric of G, which is denoted by $\mathcal{E}_{AG}$. The next lower bound is obtained from an inequality reported in [19] that was derived by using a slightly different definition of the SDD index.

Theorem 4.22. [19] *If G is an n-order graph of size* $m \geq 1$ *and minimum degree at least* 1*, then*

$$SDD(G) \geq 2\left(\frac{(\mathcal{E}_{AG}(G))^2}{n} - m\right).$$

Additional lower bounds on the SDD index can be found in [56, 61, 63, 73] as well as from the inequalities, involving SDD index, reported in [52]. Lower bounds on the SDD index of the graphs generated by applying some operations on graphs can be found in [54, 61, 62, 69].

4.2 Upper Bounds

We start this section by listing a simple but notable upper bound on the SDD index established in [79].

Theorem 4.23. [79] *If G is a non-trivial n-order graph of maximum degree Δ, then the inequality $SDD(G) \leq n\,\Delta$ holds with equality if and only if G is δ-regular.*

The bound given in the next result was first reported in [35] without the characterization of the graphs attaining this bound.

Theorem 4.24. [54] *If G is a connected graph of size m, minimum degree δ and maximum degree Δ, then*

$$SDD(G) \leq m\left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta}\right),$$

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

The next result is a notable corollary of Theorem 4.24.

Corollary 4.25. [54] *If G is a connected n-order graph of size m, then*

$$SDD(G) \leq m\left(\frac{1}{n-1} + n - 1\right),$$

with equality if and only if $G = K_{n-1,1}$.

Theorem 4.26. [35] *If G is a connected graph with size m, minimum non-pendent vertex degree δ_1, number of pendent vertices p and maximum degree Δ, then*

$$SDD(G) \leq p\left(\Delta + \frac{1}{\Delta}\right) + (m-p)\left(\frac{\Delta}{\delta_1} + \frac{\delta_1}{\Delta}\right),$$

with equality if and only if G is any of the following graphs:
(i) a regular graph,
(ii) a graph having the degree set $\{1, \Delta\}$ such that at least one end-vertex of every edge of G has degree Δ,

(iii) a graph having the degree set $\{1, \delta_1, \Delta\}$ such that exactly one end-vertex of every edge of G has degree Δ.

We remark here that the graphs attaining the bound given in Theorem 4.26 were not fully characterized in [35]; the same case is with the next result, however we are stating the next result without any changes and leaving to readers the exercise of characterizing graphs (in the following result).

Theorem 4.27. [35] *If G is a connected graph with order n, size m, number of pendent vertices p, maximum degree Δ, hyper Zagreb index H_Z and minimum non-pendent vertex degree δ_1, then*

$$SDD(G) \leq \frac{H_Z - p(\delta_1 + 1)^2}{\delta_1^2} + p\left(\Delta + \frac{1}{\Delta}\right) - 2(m - p),$$

where the equality is attained if G is either a regular or star graph.

Theorem 4.28. [35] *If G is a connected n-order graph of minimum degree δ and maximum degree Δ such that the complement $\overline{G}$ of G is also connected, then*

$$SDD(G) \leq \binom{n}{2}\left(k + \frac{1}{k}\right) - SDD(\overline{G}),$$

with equality if and only if G is regular, where

$$k = \max\left\{\frac{\Delta}{\delta}, \frac{\overline{\Delta}}{\overline{\delta}}\right\};$$

while $\overline{\delta}$ and $\overline{\Delta}$ are the minimum and maximum degrees, respectively, of $\overline{G}$.

Theorem 4.29. [28] *Let G be a graph having size $m \geq 1$.*

(i). *It holds that $SDD(G) \leq {}^0R_2(G)$ and $SDD(G) \leq {}^0R_3(G)$ where the equality in any of these two inequalities holds if and only if the maximum degree of G is 1.*

(ii). *If G is connected having order n such that $4m \geq 5(n-1)$, then $SDD(G) < R_1(G)$.*

(iii). *Let G be connected and its minimum degree is at least 8. If the inequality $d_u \leq d_v \leq \sqrt{2}\, d_u$ holds for every edge $uv \in (G)$, then $SDD(G) < ISI(G)$.*

(iv). *If the minimum degree of G is $\delta \geq 1$, then*

$$SDD(G) \leq \frac{\sigma(G)}{\delta^2} + 2m. \tag{3}$$

If G is connected then the equality in (3) holds if and only if G is regular.

Theorem 4.30. [65] *If G is an n-order graph of size m, then*

$$SDD(G) \leq 2m\big({}^0R_{-1}(G) + 1\big) - n^2,$$

with equality if and only if $d_u = d_v$ for every $uv \notin E(G)$. Also, it holds that

$$SDD(G) \leq 2m \left(\frac{Kf(G) + n}{n-1}\right) - n^2,$$

with equality if G is either complete or complete bipartite, where $Kf(G)$ is the Kirchhoff index of G (see for example [66]).

In [66], it was indicated that the equality in the second inequality of Theorem 4.30 holds also for the graphs K_n^- and K_n^{--} for $n \geq 5$, where K_n^- is the graph obtained from the complete graph K_n by removing an edge and K_n^{--} is the graph deduced also from K_n by removing two non-adjacent edges.

Theorem 4.31. [54] *If G is a connected graph of maximum degree Δ, then $SDD(G) \leq \Delta^2 \cdot {}^0R_{-1}(G)$, with equality if and only if G is regular.*

Theorem 4.32. [65] *If G is an n-order graph of size m, minimum degree δ and maximum degree Δ, then*

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

with equality if G is regular.

Recall the definition of the extended adjacency matrix $A_{ex}(G)$ of a graph G given in the previous subsection. The sum of the absolute eigenvalues of $A_{ex}(G)$ is known as the extended energy of G, which is denoted by $\mathcal{E}_{ex}(G)$. Recall also that $\eta_1(G)$ and $\eta_n(G)$ denote the largest and least eigenvalues, respectively, of $A_{ex}(G)$.

Theorem 4.33. [52] *If G is an n-order graph of size at least one, then $SDD(G) \leq n \cdot \eta_1(G)$ with equality if and only if G is regular. Also, it holds that*

$$SDD(G) \leq \frac{n}{2}\, \mathcal{E}_{ex}(G)$$

with equality if and only if G is either the complete graph K_n or the complete bipartite graph $K_{n/2,n/2}$.

The first bound on the SDD index given in Theorem 4.33 was obtained also in [31, 32] independently.

Theorem 4.34. [31] *If G is an n-order graph of size at least one, then*

$$SDD(G) \leq -n(n-1) \cdot \eta_n(G)$$

and equality holds if and only if G is the complete graph.

Theorem 4.35. [33] *If T is an n-order tree with maximum degree Δ number of pendent vertices p, then*

$$SDD(T) \leq \frac{(n-1)\Delta^2 + p}{2}$$

Theorem 4.36. [33] *If G is a graph with size $m \geq 1$, minimum degree δ and maximum degree Δ edges, then*

$$SDD(G) \leq \frac{\left(\sqrt{\frac{\delta}{\Delta} + \frac{\Delta}{\delta}} + \sqrt{2}\right)^2 \left(AG(G)\right)^2}{\sqrt{2}m\sqrt{\frac{\delta}{\Delta} + \frac{\Delta}{\delta}}} - 2m.$$

Theorem 4.37. [20] *Let G be a graph of size $m \geq 1$, maximum degree Δ*

and minimum degree δ. Then

$$SDD(G) \leq (a_1+a_2)\sqrt{(m-1)^0R_2(G) + m\left(\Pi_1^*(G)\right)^{1/m}} - 2m - a_1a_2ISI(G),$$

with equality if and only if G is regular, where

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

However, if G connected and $m \geq 2$, then

$$SDD(G) \leq m\left(\left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2 - 2\right).$$

Theorem 4.38. [20] *If G is a connected graph with size $m \geq 2$, then*

$$SDD(G) \leq 4(AG(G))^2 - \frac{m(m-1)\left(\Pi_1^*(G)\right)^{\frac{2}{m}}}{\left(\Pi_2(G)\right)^{\frac{1}{m}}} - 2m. \qquad (4)$$

If the following equation holds for every pair of edges $v_iv_j, v_kv_\ell \in E(G)$ then the equality in (4) holds:

$$\frac{d_{v_i}}{d_{v_j}} + \frac{d_{v_j}}{d_{v_i}} = \frac{d_{v_k}}{d_{v_\ell}} + \frac{d_{v_\ell}}{d_{v_k}}.$$

Theorem 4.39. [20] *Let G be a non-trivial connected n-order graph of size m, minimum edge degree δ_e and maximum edge degree Δ_e. Then*

$$SDD(G) \leq \frac{n^2R_1(G)}{4m^2}\frac{\left(\Delta_e+\delta_e+4\right)^2}{(\Delta_e+2)(\delta_e+2)} - 2m$$

and

$$SDD(G) \leq n\left(\delta_e+\Delta_e+4\right) - \frac{m^2(\delta_e+2)(\Delta_e+2)}{R_1(G)} - 2m,$$

where the equality in either of these two inequalities holds if and only if G is regular or semiregular bipartite. Also,

$$SDD(G) \leq \frac{n^2}{4R_{-1}(G)}\frac{\left(\Delta_e+\delta_e+4\right)^2}{(\Delta_e+2)(\delta_e+2)} - 2m,$$

with equality holding if and only if G is a regular graph or a semiregular bipartite graph, or $\Delta_e \neq \delta_e$ provided that $d_u + d_v - 2 \in \{\Delta_e, \delta_e\}$ for every edge $uv \in E(G)$ with

$$(\Delta_e + 2) \sum_{uv \in E(G);\, d_u + d_v - 2 = \Delta_e} \frac{1}{d_u d_v} = (\delta_e + 2) \sum_{uv \in E(G);\, d_u + d_v - 2 = \delta_e} \frac{1}{d_u d_v}.$$

Moreover,

$$SDD(G) \leq n\,(\delta_e + \Delta_e + 4) - (\delta_e + 2)(\Delta_e + 2) R_{-1}(G) - 2m$$

with equality if and only if G is regular or semiregular bipartite, or $\Delta_e \neq \delta_e$ provided that $d_u + d_v - 2 \in \{\Delta_e, \delta_e\}$ for every edge $uv \in E(G)$. Furthermore, if S is a subset of $E(G)$ which minimizes the expression

$$\left| \sum_{uv \in S} \frac{1}{d_u d_v} - \frac{1}{2} R_{-1}(G) \right|$$

and if $m \geq 2$, then

$$SDD(G) \leq \frac{n^2}{R_{-1}(G)} - 2m + (\Delta_e - \delta_e)^2 \alpha(S) R_{-1}(G)$$

and

$$SDD(G) \leq \frac{n^2}{R_{-1}(G)} - 2m + \frac{(\Delta_e - \delta_e)^2 R_{-1}(G)}{4},$$

with equality holding in either of these two inequalities if and only if G is regular or semiregular bipartite, where

$$\alpha(S) = \frac{\sum_{uv \in S} \frac{1}{d_u d_v}}{R_{-1}(G)} \left(1 - \frac{\sum_{uv \in S} \frac{1}{d_u d_v}}{R_{-1}(G)} \right).$$

Theorem 4.40. [60] *If T is a non-trivial n-order tree, then*

$$SDD(T) \leq 2n^2 - 5n - \overline{SDD}(T) + 4,$$

with equality if and only if $T = K_{n-1,1}$, where $\overline{SDD}(T)$ is defined in Theorem 4.17.

Theorem 4.41. [60] *If T is a non-trivial n-order tree of maximum degree Δ, then*

$$SDD(T) \leq 2(n-1)\left(n - \frac{n-2}{\Delta}\right) - n - \overline{SDD}(T).$$

with equality if and only if the degree set of T has at most two elements, where $\overline{SDD}(T)$ is defined in Theorem 4.17.

Theorem 4.42. [72] *If G is a connected non-trivial graph of size m, then*

$$SDD(G) \leq \sqrt{\big({}^0R_3(G) - 2R_1(G)\big)\big({}^0R_{-1}(G) - 2R_{-1}(G)\big)} - 2m.$$

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

Additional upper bounds on the SDD index can be found in [12, 56, 61, 63, 73]. Several upper bounds on the SDD index of the graphs generated by applying different operations on graphs can be found in [36, 54, 61, 62].

5 Open Problems

Although various open problems can be posed concerning the SDD index, we mention here some of them related to existing results. In addition to Problems 1–4 and Conjecture 2 mentioned in Section 3, we propose here the following open problems.

Problem 5. *Characterize graphs having the maximum SDD index among all n-order molecular graphs for $n \geq 6$.*

Note that Corollary 3.20 gives a solution to the minimal version of Problem 5 for the case when the minimum degree is at least 2.

The next problem can be considered as a variant of Problem 1.

Problem 6. *Characterize graphs attaining the minimum and maximum values of the SDD index among all n-order molecular k-cyclic graphs (especially, molecular trees) with a given*
(i) domination number,
(ii) number of segments, or
(iii) diameter (and hence radius).

The next problem can be considered as a variant of Problem 2.

Problem 7. *Characterize graphs attaining the maximum SDD index among all n-order molecular k-cyclic graphs with a given number of pendent vertices for $k \geq 1$.*

We end this article with the remark that the minimal version of Problem 7 was attacked in [24].

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