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Article

Total and Double Total Domination Number on Hexagonal Grid

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Abstract: In this paper, we determine the upper and lower bound for the total domination number and exact values and the upper bound for the double-total domination number on hexagonal grid $H_{m,n}$ with m hexagons in a row and n hexagons in a column. Further, we explore the ratio between the total domination number and the number of vertices of $H_{m,n}$ when m and n tend to infinity.

Keywords: total domination number; double-total domination number; hexagonal grid; molecular graph

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1. Introduction

Graph dominations are widely applied in different problems such as dominating queens, computer network, school bus routing, and social network problems. Specifically, graph dominations have huge applications in chemistry [1–5]. Chemical structures can be represented by graphs, where vertices and edges represent atoms and chemical bonds, respectively. Because of such a correspondence, many chemical and physical properties of molecules are in correlation with graph theoretical invariants. One very important such invariant is the total (double) domination number [2,6–10].

In this paper, we consider hexagonal grids with m hexagons in a row and n hexagons in a column and also infinite hexagonal grids. Hexagonal systems are geometric objects that are obtained by arranging congruent regular hexagons in a plane. They are of significant importance in theoretical chemistry as a natural graph representation of benzenoid hydrocarbons [1,5,11]. Benzenoid hydrocarbons and their derivates are an important class of organic compounds, which have, apart from their chemical importance, great technical and pharmaceutical importance as well and belong to the class of the most serious polluters of the environment.

We explore total and double-total dominations on an arbitrary hexagonal grid. We give upper and lower bound for the totally dominating number and the upper bound for the double-totally dominating number. Furthermore, we explore the ratio between the total domination number and the number of vertices of $H_{m,n}$ when m and n tend to infinity. At this moment, there are only few publications on total and double-total domination on hexagonal chains [3,12], but none dealing with arbitrary grids.

Apart from this Introduction, the rest of the paper is organized as follows. Section 2 lists preliminaries about total and double domination, dominating sets, and hexagonal systems. Section 3 gives upper and lower bounds for total domination number γ_t on arbitrary hexagonal grid $H_{m,n}$. Further, Section 4 is concerned with the ratio between the total domination number and the number vertices of $H_{m,n}$ when m and n tend to infinity. Section 5 deals with double-total domination and gives double-total domination number $\gamma_{\times 2t}$ for linear hexagonal chain $H_{m,1}$ and the upper bound for arbitrary hexagonal grid $H_{m,n}$. The final Section 6 gives conclusions and future work.

2. Preliminaries

Let G be a graph with the vertex set $V(G)$ and edge set $E(G)$. A set $D \subset V(G)$ we call a dominating set of a graph G if every vertex y in $V(G) \setminus D$ is adjacent to some vertex in D. Domination number $\gamma(G)$ is the cardinality of the smallest dominating set. Total domination is the stronger version of domination. A set $D \subset V(G)$ is a totally dominating set of a graph G if every vertex y in $V(G)$ is adjacent to some vertex in D. The total domination number $\gamma_t(G)$ is the cardinality of the smallest totally dominating set.

A set $S \subseteq V$ is a k-tuple dominating set if every vertex $v \in V \setminus S$ satisfies $\deg_S(v) \geq k$ (vertex v is adjacent to at least k vertices from the set S). The k-tuple domination number is the minimum cardinality among all k-tuple dominating sets. A set $S \subseteq V$ is a k-tuple totally dominating set (k-totally dominating set) if every vertex $v \in V$ satisfies $\deg_S(v) \geq k$, e.g., each vertex in V has at least k neighbors in S. In such a case, it must be $k \leq \delta$ where δ is the minimum degree of vertices on G and $|S| \geq k+1$. The k- tuple total domination number $\gamma_{\times kt}(G)$ (k-total domination number $\gamma_{kt}(G)$) is the cardinality of the smallest k-tuple totally dominating set. For $k = 2$, the two-tuple totally dominating set is called the double-totally dominating set.

Each vertex in a hexagonal system has either degree two or degree three. It follows that on the hexagonal grid, there is no $\times k$-total domination for $k \geq 3$.

A vertex shared by three hexagons is called an internal vertex of the respective hexagonal system. A hexagonal system where no three hexagons have an intersection (no internal vertices) is called a catacondensed system, else it is pericondensed.

A catacondensed hexagonal system in which every hexagon is adjacent to at most two hexagons is called a hexagonal chain. A linear hexagonal chain is a hexagonal chain that is a graph representation of linear polyacene. The linear hexagonal chain with m hexagons will be denoted by $H(m,1)$. A double hexagonal chain consists of two condensed identical hexagonal chains ($H(m,2)$).

3. Total Domination Number of a Hexagonal Grid with *m* Hexagons in a Row and *n* Hexagons in a Column

We denote by $H_{m,n}$ a hexagonal grid with m hexagons in a row and n hexagons in a column. For $n = 1$, we have a linear hexagonal chain, and for $n = 2$, a double hexagonal chains. In $H_{m,n}$, any zigzag line with no vertical edges is called a horizontal zigzag line. The horizontal zigzag line of $H_{m,n}$ is denoted by L_i, $(1 \leq i \leq n+1)$, where vertices on L_i are $v_{i,1}, v_{i,2}, \ldots, v_{i,2m}, v_{i,2m+1}$, if $i \in \{1, n+1\}$. Otherwise, for each L_i, $2 \leq i \leq n$, we have vertices $v_{i,1}, v_{i,2}, \ldots, v_{i,2m+2}$. Therefore, on $H_{m,n}$, there are $2(2m+1) + (n-1) \cdot (2m+2) = 2(mn+m+n)$ vertices. See Figure 1 for an example for $H_{4,3}$.

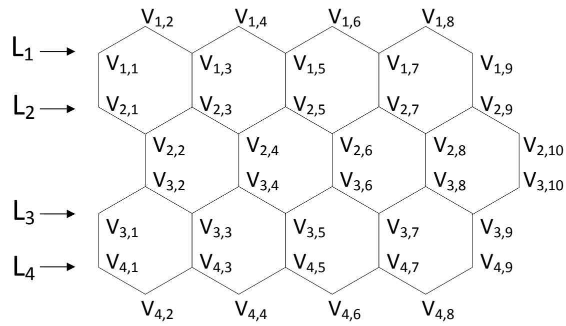

Figure 1. Horizontal zigzag lines denoted by L_i, $i = 1, \ldots 4$, and vertices of $H_{4,3}$. Grid $H_{4,3}$ has $m = 4$ hexagons in a row and $n = 3$ hexagons in a column. As an example, L_1 consists of vertices $v_{1,1}$, $v_{1,2}$, $v_{1,3}$, $v_{1,4}$, $v_{1,5}$, $v_{1,6}$, $v_{1,7}$, $v_{1,8}$, $v_{1,9}$. Similarly, L_2 consists of vertices $v_{2,1}$, $v_{2,2}$, $v_{2,3}$, $v_{2,4}$, $v_{2,5}$, $v_{2,6}$, $v_{2,7}$, $v_{2,8}$, $v_{2,9}$, $v_{2,10}$.

It is known [9] that for the cycle C_n, it holds that:

$$\gamma_t(C_n) = \begin{cases} \frac{n}{2}+1, & n \equiv 2(mod4) \\ \lceil \frac{n}{2} \rceil, & \text{otherwise.} \end{cases}$$

For linear and double hexagonal chains, the following two theorems are proven [3,4]:

Theorem 1. *([4]) For a linear hexagonal chain with m hexagons, it holds that:*

$$\gamma_t(H_{m,1}) = 2m + 2.$$

Theorem 2. *([3]) For a double hexagonal chain with m hexagons, it holds that:*

$$\gamma_t(H_{m,2}) \leq \begin{cases} \frac{5m}{2}+2, & m \equiv 0(mod4) \\ 10\lfloor \frac{m}{4} \rfloor + 6, & m \equiv 1(mod4) \\ 10\lfloor \frac{m}{4} \rfloor + 8, & m \equiv 2(mod4) \\ 10\lceil \frac{m}{4} \rceil, & m \equiv 3(mod4). \end{cases}$$

Now, we will consider $H_{m,n}$ when $n \geq 3$ and give the upper bounds for total domination number $\gamma_t(H_{m,n})$.

Theorem 3. *For a hexagonal grid with m hexagons in a row and n hexagons ($n \geq 3$) in a column $H_{m,n}$, it holds that:*

$$\gamma_t(H_{m,n}) \leq \begin{cases} (n+2)\frac{2m+3}{3} - 1, & m \equiv 0(mod3) \\ (n+2)\frac{2m+4}{3} - 2, & m \equiv 1(mod3) \\ (n+2)\frac{2m+2}{3}, & m \equiv 2(mod3). \end{cases}$$

Proof. We will consider six different cases depending on m modulo three and n modulo two (n is odd or even).

Case 1.1 $m \equiv 0(mod3)$, n odd.

Let us define $S_i = \{v_{i,2+3j}, j = 0, \dots, \frac{2m}{3}\}$, $i = 2, \dots, n$, $S_1 = \{v_{1,5+6j}, j = 0, \dots, \frac{m}{3} - 1\}$ and $S_{n+1} = \{v_{n+1,5+6j}, j = 0, \dots, \frac{m}{3} - 1\}$. See Figure 2 for an example for $H_{9,7}$.

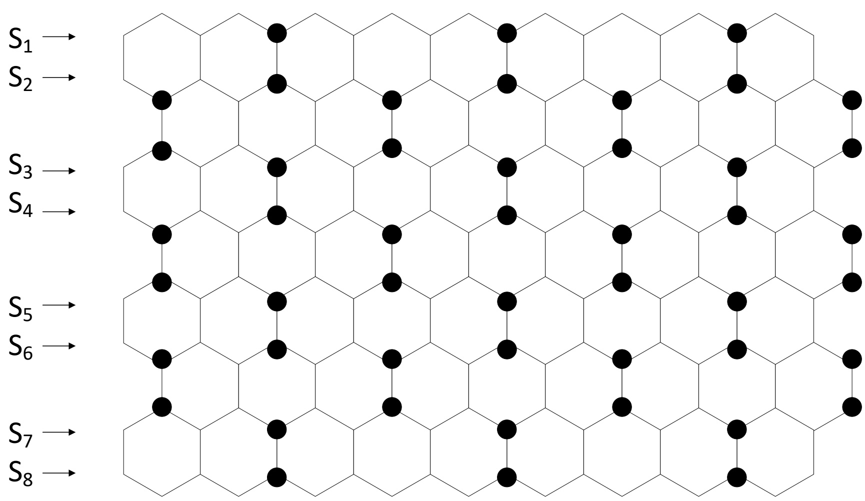

Figure 2. $S_1 \cup S_2 \cup \dots \cup S_8$ on $H_{9,7}$.

$$|S_1 \cup S_2 \cup \cdots \cup S_{n+1}| = (n-1)|S_2| + 2|S_1| = (n-1)(\frac{2m}{3}+1) + 2 \cdot \frac{m}{3} = n(\frac{2m+3}{3}) - 1.$$

These vertices totally dominate all vertices on $L_2, \ldots, L_n$ and also totally dominate both $3(\frac{m}{3}) = m$ vertices on the L_1 and on L_{n+1}.

All vertices are totally dominated by exactly one vertex. Further, all totally dominating vertices totally dominate three vertices except for totally dominating vertices from the last column. The totally dominating vertices from the last column have degree two, so they can totally dominate two vertices at most.

Now, we consider the case on L_1 (it is the same for L_{n+1}). From the previous, m vertices on L_1 are totally dominated, and $m+1$ are not totally dominated. From the structure of S_1, it follows that there exist $\frac{m}{3}$ groups of three consequent vertices, which are not totally dominated. From each such group, we must take two vertices into the totally dominating set D. It follows that we have to take $2 \cdot \frac{m}{3}$ such vertices to dominate L_1 totally. Then, only $v_{1,2m+1}$ is not totally dominated ($v_{n+1,2m+1}$ for L_{n+1}), so we need at least one vertex more to dominate it totally. Finally,

$$\gamma_t(H_{m,n}) \leq n(\frac{2m+3}{3}) - 1 + 4\frac{m}{3} + 2 = (n+2)\frac{2m}{3} + (n+1) = (n+2)\frac{2m+3}{3} - 1.$$

Case 1.2 $m \equiv 0(mod 3)$, n even.

In this case, $S_1, S_2, \ldots, S_n$ are the same as in Case 1.1. Only $S_{n+1} = \{v_{n+1,1+6j}, j = 0, \ldots, \frac{m}{3}\}$. Then, $|S_{n+1}| = \frac{m}{3} + 1$. Therefore,

$$\begin{aligned} |S_1 \cup S_2 \cup \cdots \cup S_{n+1}| &= (n-1)|S_2| + 2|S_1| + 1 = (n-1)(\frac{2m}{3}+1) + 2 \cdot \frac{m}{3} + 1 \\ &= n \cdot (\frac{2m}{3}+1) = n(\frac{2m+3}{3}). \end{aligned}$$

On L_1 and L_{n+1} (same for odd n), we need $2 \cdot \frac{2m}{3} = \frac{4m}{3}$ totally dominating vertices. In this case, only the vertex $v_{1,2m+1}$ is not totally dominated, and we need at least one vertex more to dominate it totally. From this follows:

$$\gamma_t(H_{m,n}) \leq n \cdot (\frac{2m}{3}+1) + 4 \cdot \frac{m}{3} + 1 = (n+2)\frac{2m}{3} + (n+1) = (n+2)\frac{2m+3}{3} - 1.$$

Case 2.1 $m \equiv 1(mod 3)$, n odd.

Let us define $S_i = \{v_{i,2+3j}, j = 0, \ldots, \lfloor \frac{2m}{3} \rfloor\}$, $i = 2, \ldots, n$, $S_1 = \{v_{1,5+6j}, j = 0, \ldots, \lfloor \frac{m}{3} \rfloor - 1\}$, and $S_{n+1} = \{v_{n+1,5+6j}, j = 0, \ldots, \lfloor \frac{m}{3} \rfloor - 1\}$. See Figure 3 for an example for $H_{10,7}$.

$$|S_1 \cup S_2 \cup \cdots \cup S_{n+1}| = (n-1)|S_2| + 2|S_1| = (n-1)(\lfloor \frac{2m}{3} \rfloor + 1) + 2 \cdot \lfloor \frac{m}{3} \rfloor.$$

These vertices totally dominate all vertices on $L_2, \ldots, L_n$ except for the last column. Furthermore, they totally dominate $3(\lfloor \frac{m}{3} \rfloor)$ vertices on L_1 and the same on L_{n+1}.

All vertices in this case are totally dominated by exactly one vertex, and each totally dominating vertex totally dominates three vertices (which is maximum on a hexagon).

Now, we consider the case on L_1 (it is the same on L_{n+1}). On L_1 exist $\lceil \frac{m}{3} \rceil$ groups of three consequent vertices, which are not totally dominated. From each such group, we have to take at least two vertices into the totally dominating set D. It follows that we have to take $2 \cdot \lceil \frac{m}{3} \rceil$ such vertices to dominate L_1 totally.

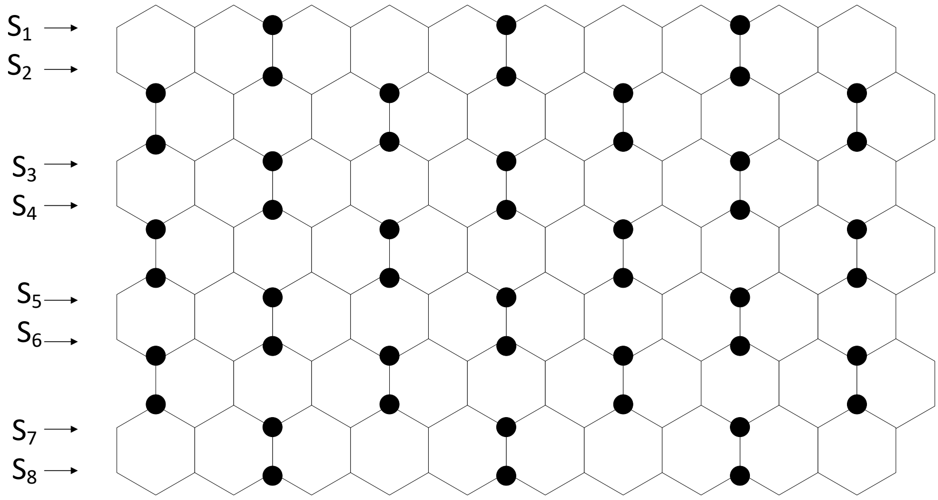

Figure 3. $S_1 \cup S_2 \cup \cdots \cup S_8$ on $H_{10,7}$.

Then, on the last n^{th} column, $2 \cdot \lfloor \frac{n}{2} \rfloor$ vertices are not totally dominated. They are in groups of two consequent vertices:

$$(v_{2,2m+2}, v_{3,2m+2}; v_{4,2m+2}, v_{5,2m+2}; \ldots; v_{n-1,2m+2} v_{n,2m+2}).$$

See Figure 3 for an example for $H_{10,7}$. Therefore, to dominate them totally, we must take all of them in the totally dominating set D. Hence,

$$\begin{aligned}\gamma_t(H_{m,n}) &\leq (n-1)(\lfloor \frac{2m}{3} \rfloor + 1) + 2 \cdot \lfloor \frac{m}{3} \rfloor + 4 \cdot \lceil \frac{m}{3} \rceil + 2 \cdot \lfloor \frac{n}{2} \rfloor \\ &= \frac{2}{3}(mn + 2m + 2n + 1) = (n+2)\frac{2m+1}{3} + n = (n+2)\frac{2m+4}{3} - 2.\end{aligned}$$

Case 2.2 $m \equiv 1 (mod 3)$, n even.

In this case, $S_1, S_2, \ldots, S_n$ are the same as in Case 2.1 for odd n. Only $S_{n+1} = \{v_{n+1,1+6j}, j = 0, \ldots, \lfloor \frac{m}{3} \rfloor\}$. Then, $|S_{n+1}| = \lfloor \frac{m}{3} \rfloor + 1$. Therefore,

$$\begin{aligned}|S_1 \cup S_2 \cup \cdots \cup S_{n+1}| &= (n-1)|S_2| + 2|S_1| + 1 \\ &= (n-1)(\lfloor \frac{2m}{3} \rfloor + 1) + 2 \cdot \lfloor \frac{m}{3} \rfloor + 1.\end{aligned}$$

On L_1, we need $2 \cdot \lceil \frac{m}{3} \rceil$ totally dominating vertices more, and on L_{n+1}, we need $2 \cdot \lfloor \frac{m}{3} \rfloor$ totally dominating vertices more (there is one block more with three undominated vertices on the L_1).

The same as for the case when nis odd, there are $2 \cdot \frac{n}{2}$ vertices, which are not totally dominated on the last n^{th} column. Furthermore, to dominate them totally, we must take all of them in the totally dominating set D. Hence,

$$\begin{aligned}\gamma_t(H_{m,n}) &\leq ((n-1)(\lfloor \frac{2m}{3} \rfloor + 1) + 2 \cdot \lfloor \frac{m}{3} \rfloor + 1) + 2 \cdot \lceil \frac{m}{3} \rceil + 2 \cdot \lfloor \frac{m}{3} \rfloor + 2 \cdot \frac{n}{2} \\ &= \frac{2}{3}(mn + 2m + 2n + 1) = (n+2)\frac{2m+4}{3} - 2.\end{aligned}$$

Case 3.1 $m \equiv 2 (mod 3)$, n odd.

Similar to the previous cases, $S_i = \{v_{i,2+3j}, j = 0,\ldots,\lfloor\frac{2m}{3}\rfloor\}$, $i = 2,\ldots,n$, $S_1 = \{v_{1,5+6j}, j = 0,\ldots,\lfloor\frac{m}{3}\rfloor\}$, and $S_{n+1} = \{v_{n+1,5+6j}, j = 0,\ldots,\lfloor\frac{m}{3}\rfloor\}$. See Figure 4 for an example for $H_{8,7}$.

$$\begin{aligned}|S_1 \cup S_2 \cup \cdots \cup S_{n+1}| &= (n-1)|S_2| + 2|S_1| \\ &= (n-1)(\lfloor\frac{2m}{3}\rfloor + 1) + 2\cdot(\lfloor\frac{m}{3}\rfloor + 1) = n\frac{2m+2}{3}.\end{aligned}$$

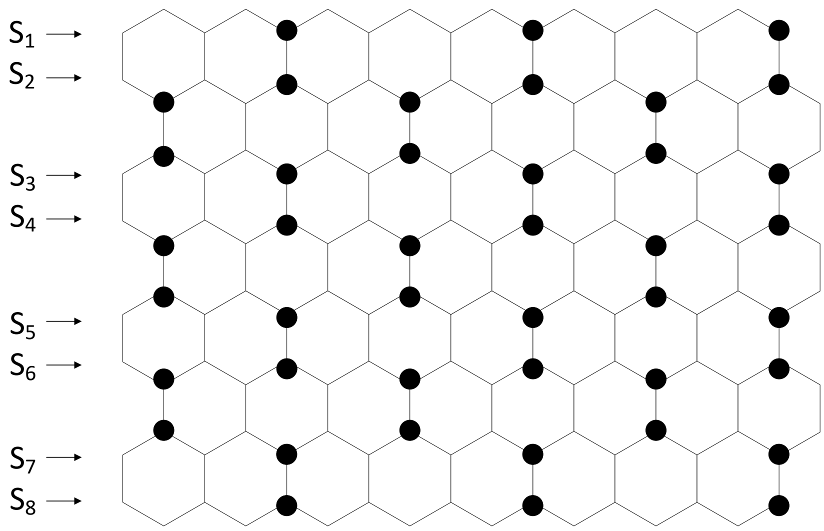

Figure 4. $S_1 \cup S_2 \cup \cdots \cup S_8$ on $H_{8,7}$.

These vertices totally dominate all vertices on $L_2,\ldots,L_n$ and also totally dominate $3\lfloor\frac{m}{3}\rfloor + 2$ vertices both on L_1 and L_{n+1}.

All vertices are totally dominated by exactly one vertex. Further, all totally dominating vertices totally dominate three vertices except for $v_{1,2m+1}$ and $v_{n+1,2m+1}$, which totally dominate two vertices. Vertices $v_{1,2m+1}$ and $v_{n+1,2m+1}$ have degree two, so they can totally dominate two vertices at most.

Now, we consider the case on L_1 (it is the same on L_{n+1}). Similar to the case $m \equiv 1(mod 3)$, on L_1 exist $\lceil\frac{m}{3}\rceil$ groups of three consequent vertices, which are not totally dominated. From each such group, we have to take at least two vertices into the totally dominating set D. It follows that we have to take $2\cdot\lceil\frac{m}{3}\rceil$ such vertices to dominate L_1 totally. Then, all vertices on $H_{m,n}$ are total dominated.

$$\begin{aligned}\gamma_t(H_{m,n}) &\le n\frac{2m+2}{3} + 4\cdot\lceil\frac{m}{3}\rceil \\ &= n\frac{2m+2}{3} + 4\cdot\frac{m+1}{3} = (n+2)\frac{2m+2}{3}\end{aligned}$$

Case 3.2 $m \equiv 2(mod 3)$, n even.

In this case, $S_1, S_2, \ldots, S_n$ are the same as in Case 3.1. Only $S_{n+1} = \{v_{n+1,1+6j}, j = 0,\ldots,\lfloor\frac{m}{3}\rfloor\}$. Then, $|S_{n+1}| = \lfloor\frac{m}{3}\rfloor + 1$. These vertices totally dominate all vertices on $L_2,\ldots L_n$, and each vertex is totally dominated by exactly one vertex.

$$|S_1 \cup S_2 \cup \cdots \cup S_{n+1}| = (n-1)|S_2| + 2|S_1| = (n-1)(\lfloor\frac{2m}{3}\rfloor + 1) + 2\cdot(\lfloor\frac{m}{3}\rfloor + 1).$$

The same as in Case 3.1, we need $2\cdot\lceil\frac{m}{3}\rceil$ vertices to dominate L_1 totally (also for L_{n+1}). From this, it follows:

$$\gamma_t(H_{m,n}) \le (n-1)(\lfloor\frac{2m}{3}\rfloor + 1) + 6\cdot\lceil\frac{m}{3}\rceil = (n+2)\frac{2m+2}{3}.$$

□

Remark 1. *It is easy to check that the bounds are tight for small examples. For example, it holds that* $\gamma_t(H_{2,3}) = 10$, $\gamma_t(H_{2,4}) = 12$, $\gamma_t(H_{3,3}) = 14$, *and* $\gamma_t(H_{4,3}) = 18$. *All these numbers are equal to the upper bound for* $\gamma_t(H_{m,n})$. *See Figure 5 for an example for* $H_{3,3}$.

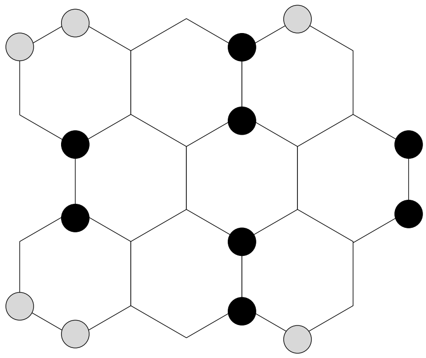

Figure 5. Total dominating set on $H_{3,3}$. Black vertices belong to $S_1 \cup S_2 \cup \cdots \cup S_4$. Gray vertices must be added to the totally dominating set to dominate L_1, L_4 and the last column $n = 3$.

Proposition 1. *For a hexagonal grid with m hexagons in a row and n hexagons (*$n \geq 3$*) in a column* $H_{m,n}$*, it holds that:*

$$\gamma_t(H_{m,n}) > \frac{2nm}{3}.$$

Proof. It follows from Theorem 3 if we take only $S_1 \cup \cdots \cup S_{n+1}$ as a part of the totally dominating set on $H_{m,n}$. Vertices on $H_{m,n}$ are then totally dominated with only one vertex from $S_1 \cup \cdots \cup S_{n+1}$ or are not totally dominated. Then:

$$\gamma_t(H_{m,n}) > |S_1 \cup \cdots \cup S_{n+1}| > \frac{2nm}{3}.$$

□

4. Determining $\lim_{m,n\to\infty} \frac{\gamma_t(H_{m,n})}{2(mn+m+n)}$

Theorem 4. *For a hexagonal grid with m hexagons in a row and n hexagons in a column* $H_{m,n}$*, which has* $2(mn + m + n)$ *vertices, it holds that:*

$$\lim_{m,n\to\infty} \frac{\gamma_t(H_{m,n})}{2(mn+m+n)} = \frac{1}{3}.$$

Proof. From Proposition 1 and Theorem 3, it follows that:

$$\frac{2nm}{3} < \gamma_t(H_{m,n}) < \frac{2(n+2)(m+2)}{3}.$$

If we divide this by $2(mn + m + n) = 2((m + 1)(n + 1) - 1)$ (the number of vertices on $H_{m,n}$), we obtain:

$$\frac{2nm}{3 \cdot 2((m+1)(n+1)-1)} < \frac{\gamma_t(H_{m,n})}{2((m+1)(n+1)-1)} < \frac{2(n+2)(m+2)}{3 \cdot 2((m+1)(n+1)-1)}. \quad (1)$$

For $m, n \to \infty$, the left and the right hand side of (1) tend to $\frac{1}{3}$. Applying the sandwich rule gives us the desired result:

$$\lim_{m,n\to\infty} \frac{\gamma_t(H_{m,n})}{2(mn+m+n)} = \frac{1}{3}.$$

□

The previous limit is no surprise because on a hexagonal grid, one vertex can totally dominate at most three vertices. This means that on very large grids, around one third of their vertices should be in any totally dominating set.

5. Double-Total Domination on a Hexagonal Grid

Theorem 5. *For a linear hexagonal chain with m hexagons, it holds that:*

$$\gamma_{\times 2t}(H_{m,1}) = \begin{cases} 6\lceil \frac{m}{2} \rceil, & m \text{ odd} \\ 6\frac{m}{2}+4, & m \text{ even.} \end{cases}$$

Proof. (a) m is odd.

Because we consider double-total domination, each vertex adjacent to a vertex with degree two must be in any minimal double-totally dominating set D. From this, it follows that all vertices from the first and last hexagon and all other vertices with degree three must be in D. If only these vertices are in D, inner vertices of degree three are not $\times 2$-totally dominated. They are totally dominated only once. We have to take at least two vertices of degree two on each odd hexagon to double-totally dominate them. Then, $\{(v_{i,1+4j}), (v_{i,2+4j}), (v_{i,3+4j});\ i \in \{1,2\};\ j \in \{0,1,\ldots,\lfloor \frac{m}{2} \rfloor\}\}$ are in D. Hence,

$$|D| = 6(\lfloor \frac{m}{2} \rfloor + 1) = 6\lceil \frac{m}{2} \rceil.$$

(b) m is even.

Like in the previous case, any minimal double-totally dominating set must have all vertices that are adjacent to at least one vertex of degree two. If only these vertices are in D, the inner vertices of degree three are not double-totally dominated. Therefore, we have to take into D the remaining two inner vertices from every odd hexagon. Then, $\{(v_{i,1+4j}), (v_{i,2+4j}), (v_{i,3+4j});\ i \in \{1,2\};\ j \in \{0,1,\ldots,\frac{m}{2}-1\}\}$ $\cup\{v_{1,2m}, v_{1,2m+1}, v_{2,2m}, v_{2,2m+1}\}$ are in D. Therefore,

$$|D| = 6\frac{m}{2} + 4.$$

□

Theorem 6. *For a hexagonal grid with m hexagons in a row and n hexagons in a column $H_{m,n}$, it holds that:*

$$\gamma_{\times 2t}(H_{m,n}) \leq \begin{cases} (3n+3)\lceil \frac{m}{2} \rceil + n - 1, & m,n \text{ odd} \\ n(\frac{3m}{2}+2) + 2m + 1, & m,n \text{ even} \\ (n+1)(\frac{3m}{2}+2), & m \text{ even}, n \text{ odd} \\ 3n\left(\frac{m+1}{2}\right) + 2m + n & m \text{ odd}, n \text{ even.} \end{cases}$$

Proof. Case 1. m, n are odd.

By T_i, we denote the subset of the double-totally dominating set on the i^{th} zigzag line of $H_{m,n}$. Let us define:

$$T_1 = \{v_{1,1+4j}, v_{1,2+4j}, v_{1,3+4j}, j = 0,\ldots,\lfloor \frac{m}{2} \rfloor\}$$
$$T_i = \{v_{i,1+4j}, v_{i,2+4j}, v_{i,3+4j}, j = 0,\ldots,\lfloor \frac{m}{2} \rfloor\} \cup v_{i,2m+2},\ i = 2,\ldots,n$$

$$T_{n+1} = \{v_{n+1,1+4j}, v_{n+1,2+4j}, v_{n+1,3+4j}, j = 0, \ldots, \lfloor \frac{m}{2} \rfloor\}.$$

See Figure 6 for an example for $H_{5,5}$. It is easy to see that $T_1 \cup T_2 \cup \cdots \cup T_{n+1}$ is a double-totally dominating set on $H_{m,n}$ for m and n odd.

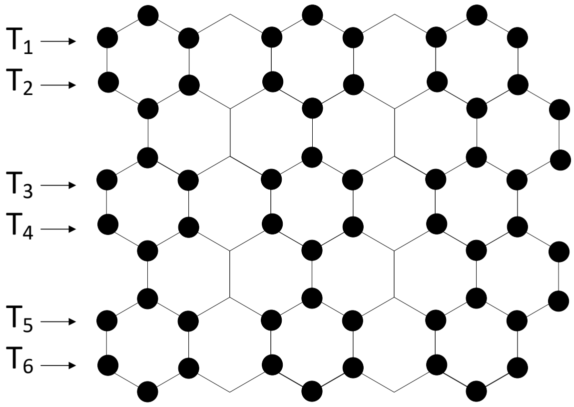

Figure 6. $T_1 \cup T_2 \cup \cdots \cup T_6$ on $H_{5,5}$.

We have $|T_1 \cup T_2 \cup \cdots \cup T_{n+1}| = 2|T_1| + (n-1)|T_i|$. This is $2 \cdot 3\lceil \frac{m}{2} \rceil + (n-1)\left(3\lceil \frac{m}{2} \rceil + 1\right) = (3n+3)\lceil \frac{m}{2} \rceil + (n-1)$. Hence,

$$\gamma_{\times 2t}(H_{m,n}) \leq (3n+3)\lceil \frac{m}{2} \rceil + (n-1).$$

Case 2. m, n are even.
Let us define:

$$\begin{aligned} T_1 &= \{v_{1,1+4j}, v_{1,2+4j}, v_{1,3+4j}, j = 0, \ldots, \frac{m}{2} - 1\} \cup \{v_{1,2m}, v_{1,2m+1}\} \\ T_i &= \{v_{i,1+4j}, v_{i,2+4j}, v_{i,3+4j}, j = 0, \ldots, \frac{m}{2} - 1\} \cup \{v_{i,2m+1}, v_{i,2m+2}\},\ i = 2, \ldots, n \\ T_{n+1} &= \{v_{n+1,1}, v_{n+1,2}, \ldots, v_{n+1,2m+1}\}. \end{aligned}$$

See Figure 7 for an example for $H_{6,6}$. It is easy to see that $T_1 \cup T_2 \cup \cdots \cup T_{n+1}$ is a double-totally dominating set on $H_{m,n}$ for m and n even. $|T_1 \cup T_2 \cup \cdots \cup T_{n+1}| = n|T_1| + |T_{n+1}|$. This is $n\left(\frac{3m}{2} + 2\right) + 2m + 1$. Therefore,

$$\gamma_{\times 2t}(H_{m,n}) \leq n\left(\frac{3m}{2} + 2\right) + 2m + 1.$$

Case 3. m is even, and n is odd.
Let us define:

$$\begin{aligned} T_1 &= \{v_{1,1+4j}, v_{1,2+4j}, v_{1,3+4j}, j = 0, \ldots, \frac{m}{2} - 1\} \cup \{v_{1,2m}, v_{1,2m+1}\} \\ T_i &= \{v_{i,1+4j}, v_{i,2+4j}, v_{i,3+4j}, j = 0, \ldots, \frac{m}{2} - 1\} \cup \{v_{1,2m+1}, v_{1,2m+2}\},\ i = 2, \ldots, n \\ T_{n+1} &= \{v_{n+1,1+4j}, v_{n+1,2+4j}, v_{n+1,3+4j}, j = 0, \ldots, \frac{m}{2} - 1\} \cup \{v_{n+1,2m}, v_{n+1,2m+1}\}. \end{aligned}$$

See Figure 8 for an example for $H_{6,5}$. It is easy to see that $T_1 \cup T_2 \cup \cdots \cup T_{n+1}$ is a double-totally dominating set on $H_{m,n}$ $|T_1 \cup T_2 \cup \cdots \cup T_{n+1}| = (n+1)|T_1|$. This is $(n+1)\left(\frac{3m}{2} + 2\right)$. Hence,

$$\gamma_{\times 2t}(H_{m,n}) \leq (n+1)\left(\frac{3m}{2} + 2\right).$$

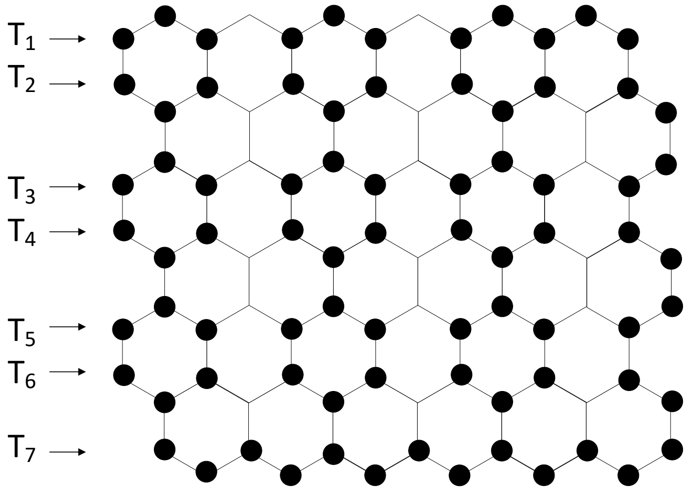

Figure 7. $T_1 \cup T_2 \cup \cdots \cup T_7$ on $H_{6,6}$.

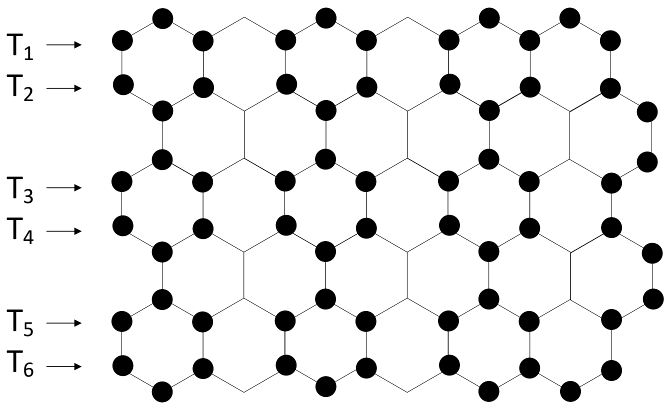

Figure 8. $T_1 \cup T_2 \cup \cdots \cup T_6$ on $H_{6,5}$.

Case 4. m is odd, and n is even.
Let us define:

$$T_1 = \{v_{1,1+4j}, v_{1,2+4j}, v_{1,3+4j}, j = 0, \ldots, \lfloor \frac{m}{2} \rfloor\}$$
$$T_i = \{v_{i,1+4j}, v_{i,2+4j}, v_{i,3+4j}, j = 0, \ldots, \lfloor \frac{m}{2} \rfloor\} \cup \{v_{1,2m+2}\},\ i = 2, \ldots, n$$
$$T_{n+1} = \{v_{n+1,1}, v_{n+1,2}, \ldots, v_{n+1,2m+1}\}.$$

See Figure 9 for an example for $H_{5,6}$. It is easy to see that $T_1 \cup T_2 \cup \cdots \cup T_{n+1}$ is a double-totally dominating set on $H_{m,n}$. Then, it holds $|T_1 \cup T_2 \cup \cdots \cup T_{n+1}| = |T_1| + (n-1)|T_2| + |T_{n+1}|$. This is $3\left(\lfloor \frac{m}{2} \rfloor + 1\right) + (n-1)\left(3(\lfloor \frac{m}{2} \rfloor + 1) + 1\right) + 2m + 1 = 3n\left(\frac{m+1}{2}\right) + 2m + n$.

Therefore,

$$\gamma_{\times 2t}(H_{m,n}) \leq 3n\left(\frac{m+1}{2}\right) + 2m + n.$$

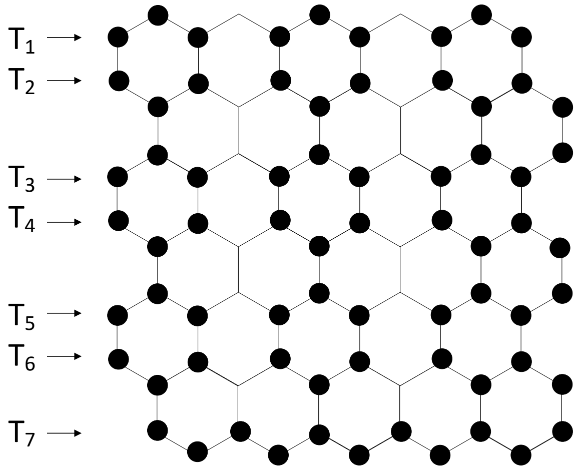

Figure 9. $T_1 \cup T_2 \cup \cdots \cup T_7$ on $H_{5,6}$.

□

6. Conclusions

We determined the upper and lower bounds for the total domination number and exact values and the upper bound for the double-total domination number on hexagonal grid $H_{m,n}$ with m hexagons in a row and n hexagons in a column. Previous works [3,12] explored the total domination on hexagonal chains, but none dealt with arbitrary hexagonal grids. We tried to fill this gap. Further, we showed that the ratio between the total domination number $\gamma_t(H_{m,n})$ and the number of vertices of $H_{m,n}$ when m and n tend to infinity equals $1/3$. This means that for very large grids, around a third of the vertices should be in the totally dominating set. Finally, we showed with multiple examples that the given bounds were tight. Moreover, the given bounds were equal to the exact solution for the given examples. In future work, we plan to determine the exact values for $\gamma_t(H_{m,n})$ and $\gamma_{\times 2t}(H_{m,n})$. We suspect that some of the given bounds are minimal. Furthermore, we plan to explore total and double-total dominations on some other types of chemical graphs.

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