THE SECOND MATHEMATICAL CONFERENCE OF REPUBLIC OF SRPSKA
Trebinje, 8. and 9. june 2012.

Minimal values of the detour index of bicyclic graphs

Žana Kovijanić Vukićević

Faculty of Natural Sciences and Mathematics, University of Montenegro
zanak@t-com.me and

Vladimir Božović

Faculty of Natural Sciences and Mathematics, University of Montenegro
vladobozovic@yahoo.com

Abstract. In this paper, we give an overview of the problem of the minimal detour index in the class of connected bicyclic graphs. For the fixed number of vertices, we split the problem into two cases: bicyclic graphs without common edges between cycles and the complement of it. In both cases, we find graphs with minimal detour index.

1. Introduction

Topological indices are the numbers that reflect certain structural characteristics of organic molecules, obtained from the respective graphs. One of the oldest and the most completely analyzed is the Wiener index or the Wiener number.

Let $G = (V, E)$ be a simple connected graph. The distance between vertices $u, v \in V$ in G is the length of the shortest path between them denoted by $d(u, v)$ or $d_G(u, v)$. The Wiener index of the graph G is defined as

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

That is

$$W(G) = \frac{1}{2} \sum_{u \in V} D_G(u)$$

where $D_G(u)$ is the sum $D_G(u) = \sum_{v \in V} d_G(u, v)$, for any vertex $u \in V$.

The Wiener index was first proposed by Harold Wiener [**3**] as an aid to determining the boiling point of paraffin. In particular, he mentions in his article that the boiling point t_B can be quite closely approximated by the formula

$$t_B = aw + bp + c,$$

where w is the Wiener index, p the polarity number and a, b and c are constants for a given isomeric group. Since then, it was observed that the Wiener index has a connection to a host of other properties of molecules (viewed as graphs). For more information about the Wiener index in chemistry and mathematics see [**5**] and [**4**], respectively.

Another topological index, called the *detour index*, is conceptually close to Wiener index, except that its definition refers to *the longest distance* instead of *the shortest distance* between two graph vertices. The detour index $\omega(G)$, where G denotes the underlying graph, has been introduced by Amić and Trinajstić [**8**] and by John [**9**] independently

$$\omega(G) = \sum_{\{u,v\}\subseteq V(G)} l_G(u,v),$$

where $l_G(u,v)$ is the length of the longest path between two vertices.

The length $l_G(u,v)$ of the longest path is also called *detour distance* between vertices $u, v \in V$ in G. When it is clear from a context which underlying graph G is assumed, we simply write $l(u,v)$ instead of $l_G(u,v)$. Also, we define

$$\omega(G) = \frac{1}{2}\sum_{u\in V} L_G(u)$$

where $L_G(u)$ is the sum $L_G(u) = \sum_{v\in V} l_G(u,v)$, for any vertex $u \in V$.
Recently, as for Wiener index, it's been presented significance of detour index in the structure-boiling point relation [**6**], [**7**].

The main goal of this paper is to find graphs with minimal detour index among the class of connected bicyclic graphs with n vertices. For the rest of paper, we treat exclusively connected type of graphs.

In the Section 2 we give review of important terminology and theory regarding main problem, mostly based on papers [**1**] and [**2**].

The case of bicyclic graphs without common edges between two cycles is treated in Section 3. We found, by Theorem 3.3, that the smallest detour index in the corresponding class is $n^2 + 2n - 7$. It is attained at so called $n-$vertex butterfly, that looks like two triangles having one vertex in common and all other $n-5$ vertices are attached as pendent vertices to that common vertex (Figure 1).

The most interesting and consequently the most complex case, subject of Section 4, is about bicyclic graphs with common edges between two cycles. The central role in this section has a Theorem 4.1 which brings out an iterative procedure of converting given graph to the one with smaller detour index. According to our result, the smallest detour index for this class has the graph that looks like two glued triangles by one side, making a parallelogram, and all other $n-4$ pendent vertices are attached to one of two common vertices of those triangles (Figure 3).

2. Preliminaries

Let $H = (V(H), E(H))$ be graph without pendent vertices and $V(H) = \{v_1, v_2, \dots, v_n\}$. Let $T_1, T_2, \dots, T_n$ be vertex disjoint trees such that H and T_i have exactly one vertex v_i in common, for $1 \leqslant i \leqslant n$. Such graph is denoted by $H(T_1, T_2, \dots, T_n)$. Let S_n and P_n be the n-vertex star and path, respectively. Let C_n be a cycle graph with n vertices.

The next assertion is valid for arbitrary cyclic graph. The proof of the following lemma is proved in paper by Zhou and Chai [**1**].

Lemma 2.1. *Let $H = (V(H), E(H))$ be graph without pendent vertices and $G = H(T_1, T_2, \dots, T_n)$. Then*

$$\omega(G) = \sum_{i=1}^{n} W(T_i) + \sum_{1 \leqslant i < j \leqslant n} [|T_i| D_{T_j}(v_j) + |T_j| D_{T_i}(v_i) + |T_i||T_j| l_H(v_i, v_j)].$$

We will also use the following lemmas.

Lemma 2.2. [**2**] *Let T be n-vertex tree different from n-vertex star S_n. Then*

$$(n-1)^2 = W(S_n) < W(T).$$

Lemma 2.3. [**1**] *Let T be n-vertex tree where $n \geqslant 3$ and $u \in V(T)$. Let x be the center of star S_n. Then*

$$n - 1 = D_{S_n}(x) \leqslant D_T(u).$$

Equality holds exactly when $T = S_n$ and $u = x$.

Denote by $\mathcal{U}_{n,r}$ the class of unicyclic graphs with n vertices and cycle length r, where $3 \leqslant r \leqslant n$. Subclass of $\mathcal{U}_{n,r}$ where all $n-r$ pendent vertices are attached to a single vertex of the cycle C_r is denoted by $\mathcal{S}_{n,r}$. For fixed n and r, all graphs from $\mathcal{S}_{n,r}$ are isomorphic, so concrete instance of this class we denote by $S_{n,r}$.

Proposition 2.1. [**1**] *Among n-vertex unicyclic graphs, $S_{n,3}$ for $n \geqslant 3$ is the unique graph with the smallest detour index, which is equal to $n^2 - 3$.*

3. Bicyclic graphs with cycles without common edges

Let $\mathcal{B}_{n;k,m}$ be a class of bicyclic graphs with $n-$vertices, whose cycles have k and m vertices and don't have common edges. We are going to prove that the smallest detour index in $\bigcup_{3 \leqslant k \leqslant m} \mathcal{B}_{n;k,m}$, for $n \geqslant 5$, has the so called n-vertex butterfly $B \in \mathcal{B}_{n;3,3}$, the graph presented in the following figure

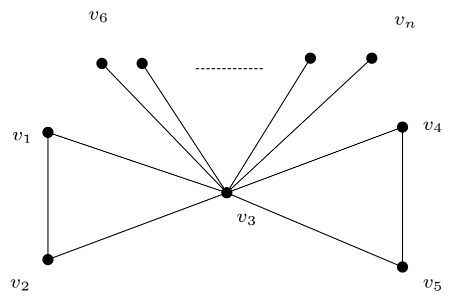

FIGURE 1. n-vertex butterfly $B \in \mathcal{B}_{n;3,3}$.

THEOREM 3.1. *Let G be unicyclic graph with n vertices. Then for each $u \in V(G)$*

$$L_G(u) \geqslant n+1$$

with equality if and only if $G = S_{n,3}$ and u is the vertex at the cycle with $n-3$ attached pendent vertices.

PROOF. Let G be unicyclic graph with n vertices. Then, there is a $r \in N$ and vertex disjoint trees $T_1, T_2, \ldots, T_r$, such that $G = C_r(T_1, T_2, \ldots, T_r)$ and $n = |T_1| + |T_2| + \ldots + |T_r|$. We are going to prove that for each $u \in V(G)$

$$L_G(u) \geqslant \frac{1}{4}(3r^2 - 4r + r_0) + n - r,$$

where $r_0 = 1$ if r is odd, and $r_0 = 0$ if r is even. Equality holds if and only if there is an $i \in \{1, 2, \ldots, r\}$ such that $u = v_i$ and all other $n - r$ vertices are pendent and attached to u.

Let $u = v_i$ for some $i \in \{1, 2, \ldots, r\}$. Then, for odd r

$$L_{C_r}(u) = \sum_{j \neq i} l(u, v_j) = 2\left[(r-1) + (r-2) + \ldots + (r - \frac{r-1}{2})\right],$$

and for even r

$$L_{C_r}(u) = \sum_{j \neq i} l(u, v_j) = 2\left[(r-1) + (r-2) + \ldots + (r - \frac{r}{2} + 1)\right] + (r - \frac{r}{2}).$$

Hence,

$$L_{C_r}(u) = \frac{1}{4}(3r^2 - 4r + r_0), \tag{3.1}$$

where $r_0 = 1$ if r is odd, and $r_0 = 0$ if r is even.

It is clear that $L(u) > L(v_i)$ for $i \in \{1, 2, \ldots, r\}$ and $u \in T_i \backslash \{v_i\}$. Let $u = v_i$, for some $i \in \{1, 2, \ldots, r\}$. Then

$$L_G(u) = L_{C_r}(u) + \sum_{t \in T_i, t \neq u} l(u,t) + \sum_{t \in T_j \backslash \{v_j\}, j \neq i} l(u,t). \tag{3.2}$$

For the second summand of the right hand side of equality (3.2) we have

$$\sum_{t \in T_i, t \neq u} l(u,t) \geqslant |T_i| - 1, \tag{3.3}$$

where equality holds if and only if each vertex in $T_i \backslash \{v_i\}$ is pendent. For the third summand of the right hand side of equality (3.2), it holds

$$\begin{aligned}
\sum_{t \in T_j \backslash \{v_j\}, j \neq i} l(u,t) &= \sum_{t \in T_j \backslash \{v_j\}, j \neq i} [l(u,v_j) + l(v_j,t)] \\
&= (|T_j| - 1) \cdot l(u,v_j) + \sum_{t \in T_j \backslash \{v_j\}, j \neq i} l(v_j,t) \\
&\geqslant (|T_j| - 1) \cdot l(u,v_j),
\end{aligned}$$

where equality holds if

$$\sum_{t \in T_j \backslash \{v_j\}, j \neq i} l(v_j,t) = 0. \tag{3.4}$$

However, in that case we have that $T_j = \{v_j\}$ for $j \neq i$ which implies that

$$\sum_{t \in T_j \backslash \{v_j\}, j \neq i} l(u,t) = 0.$$

It means that all vertices out of cycle C_r are pendent and attached to one single vertex v_i implying

$$L_G(u) = L_{C_r}(u) + |T_i| - 1 = \frac{1}{4}(3r^2 - 4r + r_0) + n - r.$$

Note that the functions

$$f_1(r) = \frac{1}{4}(3r^2 - 4r + 1) + n - r \text{ and } f_0(r) = \frac{1}{4}(3r^2 - 4r) + n - r$$

are increasing for $r \geqslant 3$ and $r \geqslant 4$, respectively. As

$$f_1(3) = n + 1 \text{ and } f_0(4) = n + 4,$$

it follows that

$$L_G(u) \geqslant n + 1$$

with equality iff $r = 3$ and u is the vertex at triangle with $n - 3$ attached pendent vertices. □

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be vertex-disjoint graphs and $a_1 \in V_1$, $a_2 \in V_2$. Denote by $G_1^{a_1} * G_2^{a_2}$ graph obtained by "gluing" vertices a_1 and a_2 into a new vertex a^*, that is:

$$V(G_1^{a_1} * G_2^{a_2}) = V_1 \backslash \{a_1\} \cup V_2 \backslash \{a_2\} \cup \{a^*\},$$

$$E(G_1^{a_1} * G_2^{a_2}) = \{(u,a^*) | (u,a_1) \in E_1\} \cup \{(u,a^*) | (u,a_2) \in E_2\} \cup$$

$$\cup \{(u,v) | (u,v) \in E_1,\ u,v \neq a_1\} \cup \{(u,v) | (u,v) \in E_2,\ u,v \neq a_2\}.$$

THEOREM 3.2. *Let* $G_1 = (V_1, E_1)$, $G_2 = (V_2, E_2)$ *and* $G = G_1^{a_1} * G_2^{a_2}$. *Then*

$$\omega(G) = \omega(G_1) + \omega(G_2) + L_{G_1}(a_1)|V_2 - 1| + L_{G_2}(a_2)|V_1 - 1|$$

PROOF.

$$\begin{aligned}
\omega(G) &= \sum_{\{u,v\}\subseteq V_1} l(u,v) + \sum_{\{u,v\}\subseteq V_2} l(u,v) + \\
&+ \sum_{u\in V_1\setminus\{a_1\}, v\in V_2\setminus\{a_2\}} l(u,v) \\
&= \omega(G_1) + \omega(G_2) + \sum_{u\in V_1\setminus\{a_1\}} \sum_{v\in V_2\setminus\{a_2\}} (l(u,a^*) + l(a^*,v)) \\
&= \omega(G_1) + \omega(G_2) + L_{G_1}(a_1)|V_2 - 1| + L_{G_2}(a_2)|V_1 - 1|.
\end{aligned}$$

□

THEOREM 3.3. *Let G be a n-vertex bicyclic graph whose cycles have no common edges and $n \geqslant 5$. Then*

$$\omega(G) \geqslant \omega(B) = n^2 + 2n - 7,$$

where B is the $n-$vertex butterfly (Figure 1).

PROOF. Let G be an arbitrary bicyclic graph with n vertices whose cycles have no common edges. Then $G = G_1^{a_1} * G_2^{a_2}$ for some unicyclic graphs $G_1 \in \mathcal{U}_{n_1,p}$ and $G_2 \in \mathcal{U}_{n_2,q}$ such that $n = n_1 + n_2 - 1$. Due to previous theorem

$$\omega(G) = \omega(G_1) + \omega(G_2) + L_{G_1}(a_1)(n_2 - 1) + L_{G_2}(a_2)(n_1 - 1).$$

By Proposition 2.1 we have

$$\omega(G_1) \geqslant \omega(S_{n_1,3}) \text{ and } \omega(G_2) \geqslant \omega(S_{n_2,3}),$$

with equalities if and only if

$$G_1 = S_{n_1,3} \text{ and } G_2 = S_{n_2,3}.$$

From Theorem 3.1 it follows

$$L_{G_1}(a_1) \geqslant n_1 + 1 \text{ and } L_{G_2}(a_2) \geqslant n_2 + 1,$$

with equalities if and only if a_1 and a_2 are vertices in $S_{n_1,3}$ and $S_{n_2,3}$ with $n_1 - 2$ and $n_2 - 2$ pendent vertices, respectivelly. Hence

$$\begin{aligned}
\omega(G) &\geqslant \omega(S_{n_1,3}) + \omega(S_{n_2,3}) + \\
&\quad +(n_1+1)(n_2-1) + (n_2+1)(n_1-1) \\
&= n_1^2 - 3 + n_2^2 - 3 + 2n_1 n_2 - 2 \\
&= n^2 + 2n - 7.
\end{aligned}$$

We conclude that $\omega(G) = n^2 + 2n - 7$ if and only if $G_i = S_{n_i,3}$ and a_i has $n_i - 2$ pendent vertices, for $i = 1, 2$. In this case, G is actually B, the n-vertex butterfly.

□

4. Bicyclic graphs with cycles with common edges

Denote by $\mathcal{E}_n(s, p_1, p_2),\ s \geqslant p_1 \geqslant p_2 \geqslant 1,\ p_1 \geqslant 2$, the class of $n-$vertex bicyclic graphs, $n \geqslant 4$, whose cycles R_1, R_2 have at least one common edge, where

$$s = |E(R_1) \cap E(R_2)|,\ p_1 = |E(R_1) \setminus E(R_2)| \text{ and } p_2 = |E(R_2) \setminus E(R_1)|.$$

Described class is illustrated in the following figure

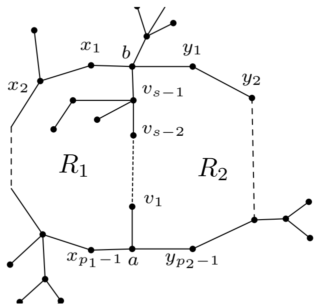

FIGURE 2. Graph $G \in \mathcal{E}_n(s, p_1, p_2)$

We prove that minimal detour index in $\bigcup\limits_{\substack{s\geqslant p_1\geqslant p_2\geqslant 1\\ p_1\geqslant 2}} \mathcal{E}_n(s, p_1, p_2)$, has the graph depictured in the following figure

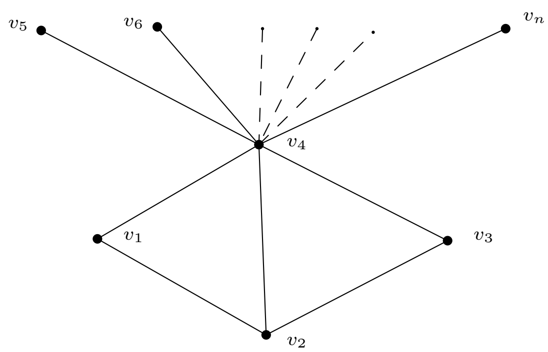

FIGURE 3. A graph $E \in \mathcal{E}_n(2, 2, 1)$.

with

$$\omega(E) = n^2 + 3n - 11.$$

Based on lemmas 2.1 - 2.3, it is easy to see that if any tree on a graph $G \in \mathcal{E}_n(s, p_1, p_2)$ is replaced by a star with the same number of vertices, then the detour index will be decreased. Since we are looking for the graph with the least detour index, we can begin with the assumption that all attached trees are stars. Denote by $\mathcal{E}_n^*(s, p_1, p_2)$, $s \geqslant p_1 \geqslant p_2 \geqslant 1$, $p_1 \geqslant 2$, the family of bicylic graphs from $\mathcal{E}_n(s, p_1, p_2)$ whose all attached trees are stars.

Following theorem has central role in the course of getting bicyclic graph with minimal detour index. We omit the lengthy, technically complex proof and refer the interested reader to [**10**] for more details.

THEOREM 4.1. *Let $G \in \mathcal{E}_n^*(s, p_1, p_2)$ be a bicyclic graph whose cycles R_1 and R_2 have a common $s-$path $P = \{(a, v_1), (v_1, v_2), \ldots, (v_{s-1}, b)\}$ and let*

$$G' = G \cdot (v_{s-1}, b) + (b, v_{s-1})$$

be the graph formed from G merging the edge (v_{s-1}, b) into a vertex b and attaching a new pendent vertex v_{s-1} at b. Then $\omega(G) > \omega(G')$.

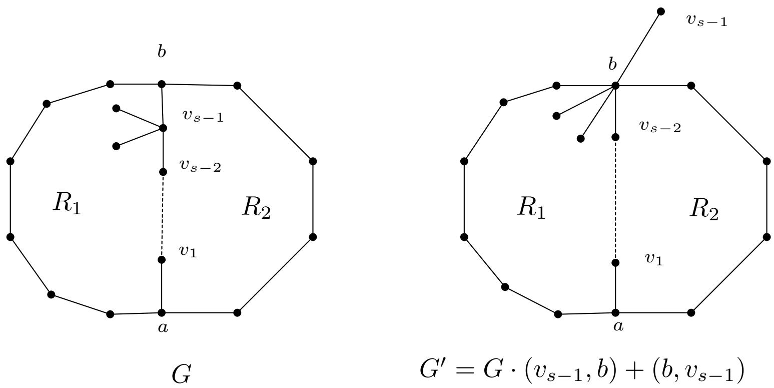

FIGURE 4. Transformation of G into G'

Previous theorem introduces, in a subtle way, the procedure of iterative reducing cycles R_1 and R_2 by absorbing two vertices into one. Namely, every bicyclic graph with common edges between two cycles, could be isomorphically transformed into graph that belongs to class $\mathcal{E}_n(s, p_1, p_2)$, i.e. that middle path is the longest one. For example, two graphs in the following picture there are two isomorphic graphs that belong to $\mathcal{E}_4(2, 2, 1)$.

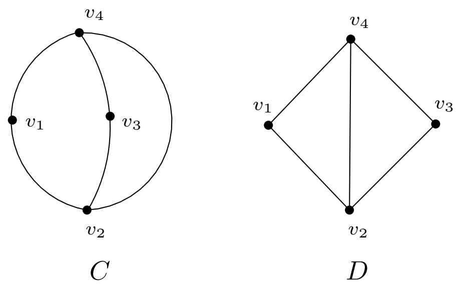

FIGURE 5. Two isomorphic graphs (C and D) from $\mathcal{E}_4(2,2,1)$.

Clearly, we can always isomorphically transform graph G in a such fashion that cycles R_1 or R_2 have the longest "piece" in common. Therefore, at the end of the procedure established in the Theorem 4.1, the cycles of original graph G will be reduced to a graph D (Figure 5) belonging to $\mathcal{E}_4(2,2,1)$ and all trees (stars in our case) will be shifted and attached to the four vertices of D. The following figure corresponds to the described situation

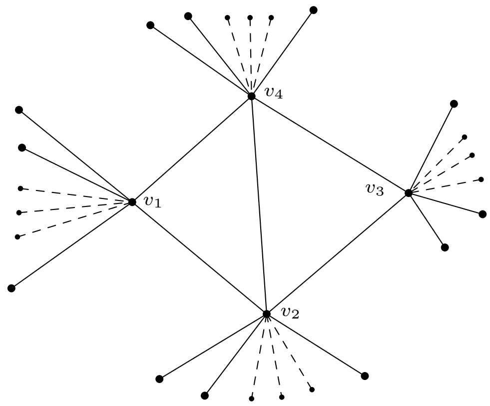

FIGURE 6. A graph F from $\mathcal{E}_n(2,2,1)$.

Let D be the graph from $\mathcal{E}_4(2,2,1)$ depictured in the Figure 5. Then,

$$l_D(v_i,v_j) = \begin{cases} 2 & , \quad \{i,j\} = \{2,4\} \\ 3 & , \quad \text{otherwise} \end{cases} \tag{4.1}$$

Let T_1, T_2, T_3 and T_4 be vertex disjoint stars such that v_1, v_2, v_3 and v_4 are their respective roots. Such bicyclic graph will be denoted by $D(T_1,T_2,T_3,T_4)$. For $n = |T_1| + |T_2| + |T_3| + |T_4|$, $D(T_1,T_2,T_3,T_4)$ is n-vertex graph (Figure 6). The following theorem is the final step in showing that the graph E (Figure 3) has the minimal detour index.

THEOREM 4.2. *Let $G = D(T_1, T_2, T_3, T_4)$ such that $|T_2| \leqslant |T_4|$. For any fixed $i \in \{1, 2, 3\}$ let G' be a graph obtained from G removing all pendent vertices from the vertex v_i to the vertex v_4. Then $\omega(G) > \omega(G')$.*

PROOF.

$$\begin{aligned}
\omega(G) - \omega(G') &= \sum_{\substack{t \in T_i \\ t \neq v_i}} \sum_{j \neq i} \sum_{u \in T_j} [l_G(t,u) - l_{G'}(t,u)] \\
&= \sum_{\substack{t \in T_i \\ t \neq v_i}} \sum_{j \neq i} \sum_{u \in T_j} [(1 + l_D(v_i, v_j) + l(v_j, u)) \\
&- \sum_{\substack{t \in T_i \\ t \neq v_i}} \sum_{j \neq i} \sum_{u \in T_j} (1 + l_D(v_4, v_j) + l(v_j, u))] \\
&= \sum_{\substack{t \in T_i \\ t \neq v_i}} \sum_{j \neq i} \sum_{u \in T_j} [l_D(v_i, v_j) - l_D(v_4, v_j)]
\end{aligned}$$

Due to (4.1), $l_D(v_i, v_j) - l_D(v_4, v_j) > 0$, so $\omega(G) > \omega(G')$.

□

5. Conlusions

In this paper we studied detour index of connected bicyclic graphs. The main goal was to find the graphs with minimal detour index in the defined class. The problem was separated into two cases: bicyclic graphs without and with common edges between two cycles.

In the first case, we realized that every connected bicyclic graph G, without common edges, is made by merging two vertices of unicyclic graphs G_1 and G_2 into single vertex, as described in Section 3. That observation helped us to find the graph, so called $n-$vertex butterfly $B_{n;3,3}$, with minimal detour index $n^2 + 2n - 7$.

The second case, problem of bicyclic graphs with common edges, is mainly resolved in the Theorem 4.1. In that theorem we introduced iterative procedure of removing a common edge between two cycles and attaching to the specific node which resulted in getting a new graph with smaller detour index. Once we reduced the problem to the case of parallelogram with attached stars to the four parallelogram vertices, as showed in the Figure 6, then Theorem 4.2 resolves that the smallest detour index has the graph represented in the Figure 3.

For the future research, it might be worth trying of finding the exact values of detour index for some particular type of graphs. It looks that the case of bicyclic graphs without common edges or the case of bicyclic graphs with just one edge in common could be, with some lengthy algebraic calculations, finally resolved. If that is achieved, then some of the results of this paper would be easily obtained.

References

[1] B. Zhou, X. Cai *On detour index*, MATCH Commun. Math. Comput. Chem 63 (2010), 199-210

[2] A. A. Dobrynin, R. Entringer, I. Gutman, *Wiener index of trees: Theory and application*, Acta Appl. Math. 6 (2001), 211-249.

[3] H. Wiener, *Structural determination of paraffin boiling points*, J. Amer. Chem. Soc. 69 (1947), 1720.

[4] I. Gutman and O. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, Germany, 1986.

[5] F. Buckley and F. Harary, *Distance in Graphs*, Addison-Wesley, Redwood, CA, 1990.

[6] N. Trinajstić, S. Nikolić, B. Lučić, D. Amić, Z. Mihalić, Z. *The Detour Matrix in Chemistry*, J. Chem. Inf. Comput. Sci. 1997, 37, 631-638.

[7] I. Lukovits, *The Detour Index*, Croat. Chem. Acta 1996, 69, 873- 882.

[8] D. Amić, N. Trinajstić, *On the Detour Matrix*, Croat. Chem. Acta 1995, 68, 53-62.

[9] P. John, *On the computation of the Wiener index of selected Delta-dimensional lattice structures*, MATCH Commun. Math. Chem. 1995, 32, 207-219.

[10] Žana Kovijanić Vukićević and Vladimir Božović, *Bicyclic graphs with minimal values of the detour index*, 2012, Filomat 26:6 (2012), 12631272.