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Degree Distance Index of the Mycielskian and its Complement

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ABSTRACT Let G be a finite connected simple graph. The degree distance index $DD(G)$ of G is defined as $\sum_{\{u,v\}\subseteq V(G)} d_G(u,v)(\deg_G(u)+\deg_G(v))$, where $\deg_G(u)$ is the degree of vertex u in G and $d_G(u,v)$ is the distance between two vertices u and v in G. In this paper, we determine the degree distance of the complement of arbitrary Mycielskian graphs. It is well known that almost all graphs have diameter two. We determine this graphical invariant for the Mycielskian of graphs with diameter two.

KEYWORDS Degree distance • Zagreb indices • Mycielskian.

1. INTRODUCTION

Throughout this paper we consider (non trivial) simple graphs, that are finite and undirected graphs without loops or multiple edges. Let $G=(V(G),E(G))$ be a connected graph of order n = |V(G)| and of size m = |E(G)|. The distance between two vertices u and v is denoted by $d_G(u,v)$ and is the length of a shortest path between u and v in G. The diameter of G is $\max\{d_G(u,v) : u,v\in V(G)\}$. It is well known that almost all graphs have diameter two. The degree of vertex u is the number of edges adjacent to u and is denoted by $\deg_G(u)$.

A ***chemical graph*** is a graph whose vertices denote atoms and edges denote bonds between those atoms of the underlying chemical structure. A ***topological index*** for a (chemical) graph G is a numerical quantity invariant under automorphisms of G and it does not depend on the labeling or pictorial representation of the graph. Topological indices and graph invariants based on the distances between vertices of a graph or vertex degrees are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making their chemical applications.

The concept of topological index came from work done by Harold Wiener in 1947 while he was working on boiling point of paraffin. The ***Wiener index*** of G is defined as $W(G)=\sum_{\{u,v\}\subseteq V(G)} d_G(u,v)$. Two important topological indices introduced about forty years ago by Ivan Gutman and Trinajstić [5] are the ***first Zagreb index*** $M_1(G)$ and the ***second Zagreb index*** $M_2(G)$ which are defined as

$$M_1(G)=\sum_{uv\in E(G)}(\deg_G(u)+\deg_G(v))=\sum_{u\in V(G)}(\deg_G(u))^2,\ M_2(G)=\sum_{uv\in E(G)}\deg_G(u)\ \deg_G(v).$$

The ***degree distance*** was introduced by Dobrynin and Kochetova [1] and Gutman [4] as a weighted version of the Wiener index. The degree distance of G, denoted by $DD(G)$, is defined as follows and it is computed for important families of graphs (see[8] and [12] for instance):

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

For a graph $G=(V,E)$, the ***Mycielskian*** of G is the graph $\mu(G)$ (or simply, μ) with the disjoint union $V\cup X\cup\{x\}$ as its vertex set and $E\cup\{v_ix_j : v_iv_j\in E\}\cup\{xx_i : 1\le i\le n\}$ as its edge set, where $V=\{v_1,v_2,...,v_n\}$ and $X=\{x_1,x_2,...,x_n\}$, see [9]. The Mycielskian and generalized Mycielskians have fascinated graph theorists a great deal. This has resulted in studying several graph parameters of these graphs. Fisher et al. [3] determine the domination number of the Mycielskian in 1998, Taeri et al. [2] determine the Wiener index of the Mycielskian in 2012, and Ashrafi et al. [6] determine Zagreb coindices of the Mycielskian in 2012.

In this paper we determine the degree distance index of the Mycielskian of each graph with diameter two. Also, we determine the degree distance of the complement of Mycielskian of arbitrary graphs.

2. DEGREE DISTANCE OF THE MYCIELSKIAN

In order to determine the degree distance index of Mycielskian graphs, we need the following observations. From now on we will always assume that G is a connected graph,

$$V(G)=\{v_1,v_2,...,v_n\},\ X=\{x_1,x_2,...,x_n\},\ V(G)\cap X=\phi,\ x\notin V(G)\cup X,$$

and μ is the Mycielskian of G, where

$$V(\mu)=V(G)\cup X\cup\{x\},\ E(\mu)=E(G)\cup\{v_ix_j : v_iv_j\in E(G)\}\cup\{xx_i : 1\le i\le n\}.$$

Observation 1. *Let μ be the Mycielskian of G. Then for each $v \in V(\mu)$ we have*

$$\deg_{\mu}(v) = \begin{cases} n & v = x \\ 1 + \deg_G(v_i) & v = x_i \\ 2\deg_G(v_i) & v = v_i \end{cases}$$

Observation 2. *In the Mycielskian μ of G, the distance between two vertices $u, v \in V(\mu)$ are given as follows.*

$$d_{\mu}(u,v) = \begin{cases} 1 & u = x, v = x_i \\ 2 & u = x, v = v_i \\ 2 & u = x_i,\ v = x_j \\ d_G(v_i,v_j) & u = v_i,\ v = v_j,\ d_G(v_i,v_j) \le 3 \\ 4 & u = v_i,\ v = v_j,\ d_G(v_i,v_j) \ge 4 \\ 2 & u = v_i, v = x_j, i = j \\ d_G(v_i,v_j) & u = v_i, v = x_j, i \ne j, d_G(v_i,v_j) \le 2 \\ 3 & u = v_i, v = x_j, i \ne j, d_G(v_i,v_j) \ge 3. \end{cases}$$

Specially, the diameter of the Mycielskian graph is at most four.

There are $|E(G)|$ unordered pairs of vertices in $V = V(G)$ whose distance is one, and

$$\sum_{\substack{(u,v)\in V\times V \\ d_G(u,v)=1}} (\deg_G(u) + \deg_G(v)) = 2 \sum_{uv\in E(G)} (\deg_G(u) + \deg_G(v)) = 2M_1(G).$$

Lemma 1. *Let G be a graph of size m whose vertex set is $V = \{v_1, v_2, ..., v_n\}$. Then,*

$$\sum_{\{v_i,v_j\}\subseteq V} (\deg_G(u) + \deg_G(v)) = (n-1)2m.$$

Proof. For each $i \in [n] = \{1,2,...,n\}$, $|\{\ \{i, j\} \subseteq [n] : j \ne i\}| = n-1$. Therefore,

$$\sum_{\{i,j\}\subseteq[n]} (\deg_G(v_i) + \deg_G(v_j)) = \sum_{i=1}^{n} (n-1)\ \deg_G(v_i) = (n-1)2m.$$

□

Lemma 2. *For each graph G of size m we have*

$$\sum_{\{v_i,v_j\}\notin E(G)} (\deg_G(v_i) + \deg_G(v_j)) = 2m(n-1) - M_1(G).$$

Proof. Since each vertex $v_i \in V(G)$ has $\deg_G(v_i)$ neighbors in G, the number of non-adjacent vertices to v_i in G equals $n-1-\deg_G(v_i)$. This implies that

$$\begin{aligned}\sum_{\{v_i,v_j\}\notin E(G)}(\deg_G(v_i)+\deg_G(v_j)) &= \sum_{i=1}^{n}(n-1-\deg_G(v_i))\ \deg_G(v_i)\\ &= (n-1)\sum_{i=1}^{n}\deg_G(v_i)-\sum_{i=1}^{n}(\deg_G(v_i))^2\\ &= 2m(n-1)-M_1(G).\end{aligned}$$

□

It is a well known fact that almost all graphs have diameter two. This means that graphs of diameter two play an important role in the theory of graphs and their applications.

Theorem 1. *Let G be an n-vertex graph of size m whose diameter is 2. If μ is the Mycielskian of G, then the degree distance index of μ is given by*

$$DD(\mu) = 4\,DD(G) - M_1(G) + (7n-1)n + (8n+12)m.$$

Proof. By the definition of degree distance index, we have

$$DD(\mu(G)) = \sum_{\{u,v\}\subseteq V(\mu)} d_\mu(u,v)\ (\deg_\mu(u)+\deg_\mu(v)).$$

Regarding to the different possible cases which u and v can be chosen from the set $V(\mu)$, the following cases are considered. In what follows, the notations are as before and two observations 1 and 2 are applied for computing degrees and distances in μ.

Case 1. $u = x$ and $v \in X$:

$$\sum_{i=1}^{n} d_\mu(x,x_i)\ (\deg_\mu(x)+\deg_\mu(x_i)) = \sum_{i=1}^{n}\ (n+1+\deg_G(v_i)) = n(n+1)+2m.$$

Case 2. $u = x$ and $v \in V(G)$:

$$\sum_{i=1}^{n} d_\mu(x,v_i)\ (\deg_\mu(x)+\deg_\mu(v_i)) = \sum_{i=1}^{n}\ 2(n+2\deg_G(v_i)) = 2(n^2+4m).$$

Case 3. $\{u,v\} \subseteq X$:

Using Lemma 1 we see that

$$\begin{aligned}\sum_{\{x_i,x_j\}\subseteq X} d_\mu(x_i,x_j)(\deg_\mu(x_i)+\deg_\mu(x_j)) &= \sum_{\{x_i,x_j\}\subseteq X} 2(2+\deg_G(v_i)+\deg_G(v_j))\\ &= 4\binom{n}{2}+2\sum_{\{i,j\}\subseteq[n]}(\deg_G(v_i)+\deg_G(v_j))\\ &= 2n^2-2n+4(n-1)m.\end{aligned}$$

Case 4. $\{u,v\}\subseteq V(G)$. Since the diameter of G is two, Observation 2 implies that $d_\mu(v_i,v_j)=d_G(v_i,v_j)$. Hence,

$$\sum_{\{v_i,v_j\}\subseteq V(G)} d_\mu(v_i,v_j)\ (\deg_\mu(v_i)+\deg_\mu(v_j)) = \sum_{\{v_i,v_j\}\subseteq V(G)} d_G(v_i,v_j)\ (2\deg_G(v_i)+2\deg_G(v_j))$$
$$=2DD(G).$$

Case 5. $u=v_i$ and $v=x_i$, $1\le i\le n$.

$$\sum_{i=1}^{n} d_\mu(v_i,x_i)\ (\deg_\mu(v_i)+\deg_\mu(x_i)) = \sum_{i=1}^{n} 2\ (3\deg_G(v_i)+1)$$
$$=2n+12m.$$

Case 6. $u=v_i$ and $v=x_j$, $i\ne j$.

$$\sum_{\substack{\{v_i,x_j\}\subseteq V(\mu)\\ i\ne j}} d_\mu(v_i,x_j)\ (\deg_\mu(v_i)+\deg_\mu(x_j)) = \sum_{\substack{\{v_i,x_j\}\subseteq V(\mu)\\ i\ne j}} d_\mu(v_i,x_j)\ (2\deg_G(v_i)+\deg_G(v_j)+1)$$
$$= \sum_{\substack{\{v_i,x_j\}\subseteq V(\mu)\\ i\ne j}} d_\mu(v_i,x_j)\ (\deg_G(v_i)+\deg_G(v_j))$$
$$+ \sum_{\substack{\{v_i,x_j\}\subseteq V(\mu)\\ i\ne j}} d_\mu(v_i,x_j)\ (\deg_G(v_i)+1).$$

Since $d_\mu(v_i,x_j)=d_\mu(v_j,x_i)$, $d_\mu(v_i,v_i)=0$, and using Observation 2, we have

$$\sum_{\substack{\{v_i,x_j\}\subseteq V(\mu)\\ i\ne j}} d_\mu(v_i,x_j)\ (\deg_G(v_i)+\deg_G(v_j)) = 2\sum_{\substack{\{v_i,v_j\}\subseteq V(G)\\ i\ne j}} d_\mu(v_i,x_j)\ (\deg_G(v_i)+\deg_G(v_j))$$
$$=2\sum_{\{v_i,v_j\}\subseteq V(G)} d_G(v_i,v_j)\ (\deg_G(v_i)+\deg_G(v_j))$$
$$=2DD(G).$$

Each edge $v_iv_j=v_jv_i\in E(G)$ corresponds to two pairs $\{v_i,x_j\}$ and $\{v_j,x_i\}$ of distance 1 in the Mycielskian graph μ. Since the diameter of G is two and using Lemma 2 we get

$$\sum_{\substack{\{v_i,x_j\}\subseteq V(\mu)\\ i\ne j}} d_\mu(v_i,x_j)\ (\deg_G(v_i)+1) = \sum_{\substack{\{v_i,x_j\}\subseteq V(\mu)\\ v_iv_j\in E(G)}} 1\ (1+\deg_G(v_i)) + \sum_{\substack{\{v_i,x_j\}\subseteq V(\mu)\\ v_iv_j\notin E(G)}} 2\ (1+\deg_G(v_i))$$
$$=2m+\sum_{v_iv_j\in E(G)} (\deg_G(v_i)+\deg_G(v_j)).$$
$$+4(\binom{n}{2}-m)+2\sum_{v_iv_j\notin E(G)} (\deg_G(v_i)+\deg_G(v_j))$$
$$=2n(n-1)+2m(2n-3)-M_1(G).$$

Now the result follows through these six cases.

□

3. DEGREE DISTANCE OF THE COMPLEMENT OF MYCIELSKIAN

In order to determine the degree distance index of the complement of Mycielskian graphs, we need two following observations.

Observation 3. *Let $\overline{\mu}$ be the complement of Mycielskian μ of G. Then for each $v \in V(\overline{\mu})$ we have*

$$\deg_{\overline{\mu}}(v) = \begin{cases} n & v = x \\ 2n - (1 + \deg_G(v_i)) & v = x_i \\ 2n - 2\deg_G(v_i) & v = v_i \end{cases}$$

Observation 4. *In the complement of Mycielskian μ of G, the distance between two vertices $u, v \in V(\overline{\mu})$ are given as follows.*

$$d_{\overline{\mu}}(u,v) = \begin{cases} 2 & u = x, v = x_i \\ 1 & u = x, v = v_i \\ 1 & u = x_i,\ v = x_j \\ 1 & u = v_i,\ v = v_j,\ d_G(v_i,v_j) > 1 \\ 2 & u = v_i,\ v = v_j,\ d_G(v_i,v_j) = 1 \\ 1 & u = v_i, v = x_j, i = j \\ 1 & u = v_i, v = x_j, i \neq j, d_G(v_i,v_j) > 1 \\ 2 & u = v_i, v = x_j, i \neq j, d_G(v_i,v_j) = 1. \end{cases}$$

Specially, the diameter of $\overline{\mu}$ is exactly 2.

Theorem 2. *Let G be an n-vertex graph of size m and let $\overline{\mu}$ be the complement of the Mycielskian μ of G. Then, the degree distance index of $\overline{\mu}$ is given by*

$$DD(\overline{\mu}) = n(6n^2 + 10n - 5) - 4m - 5M_1(G).$$

Proof. By the definition of degree distance, we have

$$DD(\overline{\mu}) = \sum_{\{u,v\} \subseteq V(\overline{\mu})} d_{\overline{\mu}}(u,v)\ (\deg_{\overline{\mu}}(u) + \deg_{\overline{\mu}}(v)).$$

We consider the following cases. For computing degrees and distances in $\overline{\mu}$ we use two observations 3 and 4.

Case 1. $u = x$ and $v \in X$.

$$\sum_{i=1}^{n} d_{\overline{\mu}}(x, x_i)\ (\deg_{\overline{\mu}}(x) + \deg_{\overline{\mu}}(x_i)) = \sum_{i=1}^{n} 2(3n - \deg_G(v_i) - 1) = 6n^2 - 2n - 4m.$$

Case 2. $u = x$ and $v \in V(G)$.

$$\sum_{i=1}^{n} d_{\overline{\mu}}(x, v_i)\ (\deg_{\overline{\mu}}(x) + \deg_{\overline{\mu}}(v_i)) = \sum_{i=1}^{n} (3n - 2\deg_G(v_i)) = 3n^2 - 4m.$$

Case 3. $\{u, v\} \subseteq X$. Using Lemma 1 we see that

$$\begin{aligned}\sum_{\{x_i, x_j\} \subseteq X} d_{\overline{\mu}}(x_i, x_j)(\deg_{\overline{\mu}}(x_i) + \deg_{\overline{\mu}}(x_j)) &= \sum_{\{i, j\} \subseteq [n]} (4n - 2 - (\deg_G(v_i) + \deg_G(v_j))) \\ &= 4n^2 - 2n - 2m(n-1).\end{aligned}$$

Case 4. $\{u, v\} \subseteq V(G)$. Using Lemma 2 we have

$$\begin{aligned}\sum_{\{v_i, v_j\} \subseteq V(G)} d_{\overline{\mu}}(v_i, v_j)\ (\deg_{\overline{\mu}}(v_i) + \deg_{\overline{\mu}}(v_j)) &= \sum_{v_i v_j \notin E(G)} (4n - 2(\deg_G(v_i) + \deg_G(v_j))) \\ &\quad + 2 \sum_{v_i v_j \in E(G)} (4n - 2(\deg_G(v_i) + \deg_G(v_j))) \\ &= 4n(\binom{n}{2} - m) - 2(2m(n-1) - M_1(G)) \\ &\quad + 8mn - 4M_1(G) \\ &= 2n^2(n-1) + 4m - 2M_1(G).\end{aligned}$$

Case 5. $u = v_i$ and $v = x_i$, $1 \le i \le n$.

$$\sum_{i=1}^{n} d_{\overline{\mu}}(v_i, x_i)\ (\deg_{\overline{\mu}}(v_i) + \deg_{\overline{\mu}}(x_i)) = \sum_{i=1}^{n} (4n - 3\deg_G(v_i) - 1) = 4n^2 - n - 6m.$$

Case 6. $u = v_i$ and $v = x_j$, $i \neq j$. By Observation 4, $d_{\overline{\mu}}(v_i, x_j) = d_{\overline{\mu}}(v_j, x_i)$ is 1 when $v_i v_j \notin E(G)$, otherwise is 2. Thus,

$$\begin{aligned}\sum_{\substack{\{v_i, x_j\} \subseteq V(\overline{\mu}) \\ i \neq j}} d_{\overline{\mu}}(v_i, x_j)\ (\deg_{\overline{\mu}}(v_i) + \deg_{\overline{\mu}}(x_j)) &= \sum_{\substack{(v_i, v_j) \\ v_i v_j \notin E(G)}} (4n - 1 - 2\deg_G(v_i) - \deg_G(v_j)) \\ &\quad + \sum_{\substack{(v_i, v_j) \\ v_i v_j \in E(G)}} 2(4n - 1 - 2\deg_G(v_i) - \deg_G(v_j))\end{aligned}$$

Each vertex v_i can be paired with $n-1-\deg_G(v_i)$ vertices v_j as (v_i,v_j) with the condition $v_iv_j \notin E(G)$. Also, note that $\sum_{(v_i,v_j)}(\deg_G(v_i)+\deg_G(v_j))$ is equal to $2\sum_{\{v_i,v_j\}}(\deg_G(v_i)+\deg_G(v_j))$. Hence, using Lemma 2 we obtain

$$\begin{aligned}\sum_{\substack{(v_i,v_j)\\ v_iv_j\notin E(G)}}(4n-1-2\deg_G(v_i)-\deg_G(v_j)) &= 2\left(\binom{n}{2}-m\right)(4n-1)-\sum_{\substack{(v_i,v_j)\\ v_iv_j\notin E(G)}}(\deg_G(v_i)+\deg_G(v_j))\\ &\quad-\sum_{\substack{(v_i,v_j)\\ v_iv_j\notin E(G)}}\deg_G(v_i)\\ &=(n^2-n-2m)(4n-1)-2(2m(n-1)-M_1(G))-(2m(n-1)-M_1(G)).\end{aligned}$$

Note that $|\{(v_i,v_j):\ v_iv_j \in E(G)\}|=2m$ and

$$\sum_{(v_i,v_j):v_iv_j\in E(G)}\deg_G(v_i)=\sum_{i=1}^{n}(\deg_G(v_i))^2,$$

because each vertex v_i has $\deg_G(v_i)$ neighbors and appears $\deg_G(v_i)$ times in the desired summation. Thus, using similar arguments we see that

$$\sum_{\substack{(v_i,v_j)\\ v_iv_j\in E(G)}} 2(4n-1-2\deg_G(v_i)-\deg_G(v_j))=4m(4n-1)-6M_1(G).$$

Now the result follows through these cases.

□

By considering Observation 3, it's not hard to check that

$$M_1(\overline{\mu})=5M_1(G)+8n^3-3n^2-24mn+4m+n.$$

Thus, Theorems 1 and 2 imply the following result.

Corollary 4. Let G be an n-vertex graph of size m and let H be the complement of the Mycielskian of G. Then, $DD(\mu(H))=16n^3+73n^2+5n+20m+56mn-25M_1(G)$.

□

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A Note on Vertex–Edge Wiener Indices of Graphs

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ABSTRACT The vertex-edge Wiener index of a simple connected graph *G* is defined as the sum of distances between vertices and edges of *G*. Two possible distances $D_1(u,e|G)$ and $D_2(u,e|G)$ between a vertex *u* and an edge *e* of *G* were considered in the literature and according to them, the corresponding vertex-edge Wiener indices $W_{ve_1}(G)$ and $W_{ve_2}(G)$ were introduced. In this paper, we present exact formulas for computing the vertex-edge Wiener indices of two composite graphs named splice and link.

KEYWORDS Distance in graph • vertex–edge Wiener index • Splice • Link.

1. INTRODUCTION

The graphs considered in this paper are undirected, finite and simple. A *topological index* (also known as *graph invariant*) is any function on a graph that does not depend on a labeling of its vertices. The oldest topological index is the one put forward in 1947 by Harold Wiener [1,2] nowadays referred to as the *Wiener index*. Wiener used his index for the calculation of the boiling points of alkanes. The Wiener index $W(G)$ of a connected graph *G* is defined as the sum of distances between all pairs of vertices of *G*:

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v|G),$$

where $d(u,v|G)$ denotes the distance between the vertices *u* and *v* of *G* which is defined as the length of any shortest path in *G* connecting them. Details on the mathematical properties of the Wiener index and its applications in chemistry can be found in [1–8].

In analogy with definition of the Wiener index, the vertex-edge Wiener indices are defined based on distance between vertices and edges of a graph [9,10]. Two possible distances between a vertex *u* and an edge *e=ab* of a connected graph *G* can be considered.

The first distance is denoted by $D_1(u,e|G)$ and defined as [9]:

$$D_1(u,e|G) = \min\{d(u,a|G), d(u,b|G)\},$$

and the second one is denoted by $D_2(u,e|G)$ and defined as [10]:

$$D_2(u,e|G) = \max\{d(u,a|G), d(u,b|G)\}.$$

Based on these two distances, two vertex-edge versions of the Wiener index can be introduced. The first and second *vertex–edge Wiener indices* of G are denoted by $W_{ve_1}(G)$ and $W_{ve_2}(G)$, respectively, and defined as $W_{ve_i}(G) = \sum_{u \in V(G)} \sum_{e \in E(G)} D_i(u, e|G)$, where $i \in \{1,2\}$. It should be explained that, the vertex-edge Wiener index introduced in [9] is half of the first vertex-edge Wiener index W_{ve_1}. However, in the above summation, for every vertex u and edge e of G, the distance $D_i(u, e|G)$ is taken exactly one time into account, so the summation does not need to be multiplied by a half. The first and second vertex-edge Wiener indices are also known as *minimum and maximum indices*, and denoted by $Min(G)$ and $Max(G)$, respectively. Since these indices are considered as the vertex-edge versions of the Wiener index, their present names and notations seem to be more appropriate.

In [10,11], the vertex–edge Wiener indices of some chemical graphs were computed and in [12,13], the behavior of these indices under some graph operations were investigated. In this paper, we present exact formulas for the first and second vertex-edge Wiener indices of two composite graphs named splice and link. Readers interested in more information on computing topological indices of splice and link of graphs, can be referred to [12,14–20].

2. RESULTS AND DISCUSSION

In this section, we compute the first and second vertex–edge Wiener indices of splice and link of graphs. We start by introducing some notations.

Let G be a connected graph. For $u \in V(G)$, we define:

$$d(u|G) = \sum_{v \in V(G)} d(u, v|G),$$

$$D_i(u|G) = \sum_{e \in E(G)} D_i(u, e|G), \qquad i \in \{1,2\}.$$

With the above definitions,

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

$$W_{ve_i}(G) = \sum_{u \in V(G)} D_i(u|G), \qquad i \in \{1,2\}.$$

2.1 SPLICE

Let G_1 and G_2 be two connected graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$, respectively. For given vertices $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$, a *splice* [17] of G_1 and G_2 by vertices a_1 and a_2 is denoted by $(G_1.G_2)(a_1, a_2)$ and defined by identifying the vertices a_1 and a_2 in the union of G_1 and G_2. We denote by n_i and m_i the order and size of the graph G_i, respectively. It is easy to see that, $|V((G_1.G_2)(a_1, a_2))| = n_1 + n_2 - 1$ and $|E((G_1.G_2)(a_1, a_2))| = m_1 + m_2$.

In the following lemma, the distance between two arbitrary vertices of $(G_1.G_2)(a_1,a_2)$ is computed. The result follows easily from the definition of the splice of graphs, so its proof is omitted.

Lemma 2.1 Let $u,v\in V((G_1.G_2)(a_1,a_2))$. Then

$$d(u,v|(G_1.G_2)(a_1,a_2))=\begin{cases} d(u,v|G_1) & u,v\in V(G_1)\\ d(u,v|G_2) & u,v\in V(G_2)\\ d(u,a_1|G_1)+d(a_2,v|G_2) & u\in V(G_1),\ v\in V(G_2)\end{cases}.$$

In the following lemma, the distances D_1 and D_2 between vertices and edges of $(G_1.G_2)(a_1,a_2)$ are computed.

Lemma 2.2 Let $u\in V((G_1.G_2)(a_1,a_2))$ and $e\in E((G_1.G_2)(a_1,a_2))$. Then

$$D_i(u,e|(G_1.G_2)(a_1,a_2))=\begin{cases} D_i(u,e|G_1) & u\in V(G_1),\ e\in E(G_1)\\ D_i(u,e|G_2) & u\in V(G_2),\ e\in E(G_2)\\ d(u,a_1|G_1)+D_i(a_2,e|G_2) & u\in V(G_1),\ e\in E(G_2)\\ d(u,a_2|G_2)+D_i(a_1,e|G_1) & u\in V(G_2),\ e\in E(G_1)\end{cases},$$

where $i\in\{1,2\}$.

Proof. Using Lemma 2.1, the proof is obvious. ■

In the following theorem, the first and second vertex-edge Wiener indices of $(G_1.G_2)(a_1,a_2)$ are computed.

Theorem 2.3 The first and second vertex-edge Wiener indices of $G=(G_1.G_2)(a_1,a_2)$ are given by:

$$\begin{aligned}W_{ve_i}(G)&=W_{ve_i}(G_1)+W_{ve_i}(G_2)+m_2d(a_1|G_1)+m_1d(a_2|G_2)\\&+(n_2-1)D_i(a_1|G_1)+(n_1-1)D_i(a_2|G_2),\end{aligned}$$

where $i\in\{1,2\}$.

Proof. By definition of the vertex-edge Wiener indices,

$$W_{ve_i}(G)=\sum_{u\in V(G)}\sum_{e\in E(G)}D_i(u,e|G),\qquad i\in\{1,2\}.$$

Now, we partition the above sum into four sums as follows:

The first sum S_1 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)$ and edges from $E(G_1)$. Using Lemma 2.2, we obtain:

$$S_1=\sum_{u\in V(G_1)}\sum_{e\in E(G_1)}D_i(u,e|G)=\sum_{u\in V(G_1)}\sum_{e\in E(G_1)}D_i(u,e|G_1)=W_{ve_i}(G_1).$$

The second sum S_2 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)$ and edges from $E(G_2)$. Similar to the previous case, we obtain:

$$S_2 = \sum_{u \in V(G_2)} \sum_{e \in E(G_2)} D_i(u,e|G_2) = W_{ve_i}(G_2).$$

The third sum S_3 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)\setminus\{a_1\}$ and edges from $E(G_2)$. Using Lemma 2.2, we obtain:

$$S_3 = \sum_{u \in V(G_1)\setminus\{a_1\}} \sum_{e \in E(G_2)} D_i(u,e|G) = \sum_{u \in V(G_1)\setminus\{a_1\}} \sum_{e \in E(G_2)} [d(u,a_1|G_1) + D_i(a_2,e|G_2)]$$
$$= m_2 d(a_1|G_1) + (n_1-1)D_i(a_2|G_2).$$

The last sum S_4 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)\setminus\{a_2\}$ and edges from $E(G_1)$. Similar to the previous case, we obtain:

$$S_4 = \sum_{u \in V(G_2)\setminus\{a_2\}} \sum_{e \in E(G_1)} [d(u,a_2|G_2) + D_i(a_1,e|G_1)]$$
$$= m_1 d(a_2|G_2) + (n_2-1)D_i(a_1|G_1).$$

Now the formula of $W_{ve_i}(G)$, $i \in \{1,2\}$, is obtained by adding the quantities S_1, S_2, S_3 and S_4. ■

2.2 LINK

Let G_1 and G_2 be two connected graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$, respectively. For vertices $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$, a *link* [17] of G_1 and G_2 by vertices a_1 and a_2 is denoted by $(G_1 \sim G_2)(a_1,a_2)$ and obtained by joining a_1 and a_2 by an edge in the union of these graphs. We denote by n_i and m_i the order and size of the graph G_i, respectively. It is easy to see that, $|V((G_1 \sim G_2)(a_1,a_2))| = n_1 + n_2$ and $|E((G_1 \sim G_2)(a_1,a_2))| = m_1 + m_2 + 1$.

In the following lemma, the distance between two arbitrary vertices of $(G_1 \sim G_2)(a_1,a_2)$ is computed. The result follows easily from the definition of the link of graphs, so its proof is omitted.

Lemma 2.4 Let $u,v \in V((G_1 \sim G_2)(a_1,a_2))$. Then

$$d(u,v|(G_1 \sim G_2)(a_1,a_2)) = \begin{cases} d(u,v|G_1) & u,v \in V(G_1) \\ d(u,v|G_2) & u,v \in V(G_2) \\ d(u,a_1|G_1) + d(a_2,v|G_2) + 1 & u \in V(G_1),\ v \in V(G_2) \end{cases}.$$

In the following lemma, the distances D_1 and D_2 between vertices and edges of $(G_1 \sim G_2)(a_1,a_2)$ are computed.

Lemma 2.5 Let $u \in V((G_1 \sim G_2)(a_1,a_2))$ and $e \in E((G_1 \sim G_2)(a_1,a_2))$. Then

$$D_i(u,e|(G_1 \sim G_2)(a_1,a_2)) = \begin{cases} D_i(u,e|G_1) & u \in V(G_1),\ e \in E(G_1) \\ D_i(u,e|G_2) & u \in V(G_2),\ e \in E(G_2) \\ d(u,a_1|G_1) + D_i(a_2,e|G_2) + 1 & u \in V(G_1),\ e \in E(G_2) \\ d(u,a_2|G_2) + D_i(a_1,e|G_1) + 1 & u \in V(G_2),\ e \in E(G_1) \\ d(u,a_1|G_1) + i - 1 & u \in V(G_1),\ e = a_1a_2 \\ d(u,a_2|G_2) + i - 1 & u \in V(G_2),\ e = a_1a_2 \end{cases},$$

where $i \in \{1,2\}$.

Proof. Using Lemma 2.4, the proof is obvious. ■

In the following theorem, the first and second vertex-edge Wiener indices of $(G_1 \sim G_2)(a_1,a_2)$ are computed.

Theorem 2.6 The first and second vertex-edge Wiener indices of $G = (G_1 \sim G_2)(a_1,a_2)$ are given by:

$$W_{ve_i}(G) = W_{ve_i}(G_1) + W_{ve_i}(G_2) + (m_2+1)d(a_1|G_1) + (m_1+1)d(a_2|G_2)$$
$$+ n_2D_i(a_1|G_1) + n_1D_i(a_2|G_2) + n_1m_2 + n_2m_1 + (n_1+n_2)(i-1),$$

where $i \in \{1,2\}$.

Proof. By definition of the vertex-edge Wiener indices,

$$W_{ve_i}(G) = \sum_{u\in V(G)} \sum_{e\in E(G)} D_i(u,e|G), \quad i \in \{1,2\}.$$

Now, we partition the above sum into six sums as follows:

The first sum S_1 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)$ and edges from $E(G_1)$. Using Lemma 2.5, we obtain:

$$S_1 = \sum_{u\in V(G_1)} \sum_{e\in E(G_1)} D_i(u,e|G) = \sum_{u\in V(G_1)} \sum_{e\in E(G_1)} D_i(u,e|G_1) = W_{ve_i}(G_1).$$

The second sum S_2 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)$ and edges from $E(G_2)$. Similar to the previous case, we obtain:

$$S_2 = \sum_{u\in V(G_2)} \sum_{e\in E(G_2)} D_i(u,e|G_2) = W_{ve_i}(G_2).$$

The third sum S_3 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)$ and edges from $E(G_2)$. Using Lemma 2.5, we obtain:

$$S_3 = \sum_{u\in V(G_1)} \sum_{e\in E(G_2)} D_i(u,e|G) = \sum_{u\in V(G_1)} \sum_{e\in E(G_2)} [d(u,a_1|G_1) + D_i(a_2,e|G_2) + 1]$$
$$= m_2d(a_1|G_1) + n_1D_i(a_2|G_2) + n_1m_2.$$

The fourth sum S_4 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)$ and edges from $E(G_1)$. Similar to the previous case, we obtain:

$$S_4 = \sum_{u\in V(G_2)} \sum_{e\in E(G_1)} [d(u,a_2|G_2) + D_i(a_1,e|G_1) + 1]$$
$$= m_1 d(a_2|G_2) + n_2 D_i(a_1|G_1) + n_2 m_1 .$$

The fifth sum S_5 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)$ and the edge a_1a_2 of G. By Lemma 2.5, we obtain:

$$S_5 = \sum_{u\in V(G_1)} \sum_{e=a_1a_2} D_i(u,e|G) = \begin{cases} \sum_{u\in V(G_1)} d(u,a_1|G_1) & i=1 \\ \sum_{u\in V(G_1)} (d(u,a_1|G_1)+1) & i=2 \end{cases}$$
$$= \begin{cases} d(a_1|G_1) & i=1 \\ d(a_1|G_1)+n_1 & i=2 \end{cases}.$$

The last sum S_6 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)$ and the edge a_1a_2 of G. Similar to the previous case, we obtain:

$$S_6 = \sum_{u\in V(G_2)} \sum_{e=a_1a_2} D_i(u,e|G) = \begin{cases} d(a_2|G_2) & i=1 \\ d(a_2|G_2)+n_2 & i=2 \end{cases}.$$

Now the formula of $W_{ve_i}(G)$, $i \in \{1,2\}$, is obtained by adding the quantities S_1, S_2, S_3, S_4, S_5 and S_6. ■

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Electro–Spunorganic Nanofibers Elaboration Process Investigations using BPs Operational Matrices

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ABSTRACT In this paper operational matrix of Bernstein Polynomials (BPs) is used to solve Bratu equation. This nonlinear equation appears in the particular elecotrospun nanofibers fabrication process framework. Elecotrospun organic nanofibers have been used for a large variety of filtration applications such as in non-wovens and filtration industries. By using operational matrix of integration and multiplication the investigated equations are turned into set of algebraic equations. Numerical solutions show both accuracy and simplicity of the suggested approach.

KEYWORDS Bratu equation • Elecotrospun nanofibers • Bernstein polynomials • Operational matrix.

1. INTRODUCTION

Electrospinning has been recognized as one of the most convenient, direct and economical methods for the fabrication of polymer nanofibers. Various polymers have been successfully electrospun into ultrafine fibers in recent years mostly in solvent solution and some in melt form. Electrospinning is a process for elaborating nanofibers with diameters about $20nm$ by forcing a fluidified polymer through a spinneret by an electric field. The elements required for electrospinning include a polymer source, a high-voltage supply (HV), and a collector (as shown in Fig. 1) [4]. Through several different collection methods, this process yields nonwoven, nanoporous materials. The basis of electrospinning is derived from a large change in electric potential. Many electrospinning device were designed in vibration-electrospinning [14, 9], magneto-electrospinning [18], bubble-electrospinning [12, 10].

In this paper, a mathematical model of the electrospinning process has been associated to Bratu equation through thermo-electro-hydrodynamics balance equations. This model is considered in terms of fluid velocity at the level of the outer edge of the syringue. It has been showed that the problem can be expressed through second-order nonlinear ordinary differential Bratue quation:

$$u''(x) + \lambda e^{u(x)} = 0,\ \ 0 < x < 1, \qquad \lambda \text{ is constant} \tag{1}$$

with initial conditions $u(0) = b_0 = 0$ and $u'(0) = b_1 = 0$ will be investigated.

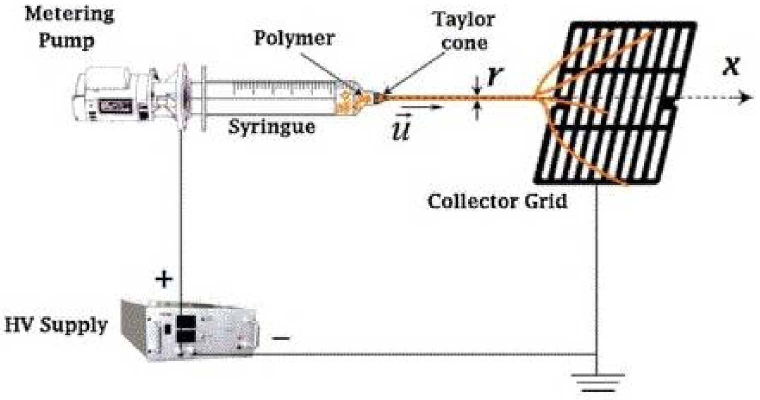

Figure 1. Electrospinning process setup.

Colantoni and Boubaker established a model which is the monodimensional Bratu equation as following [4]:

$$\begin{cases} \dfrac{\partial^2 u}{\partial x^2} - \lambda e^u = 0, \\ with\text{: } \lambda = \dfrac{18\, E^2 (I - r^2 k E)^2}{\rho^2 r^4}. \end{cases}$$

where ρ is material density, $r$is is the radius of the jet atxial coordinate x (Fig. 1), $I$is the electrical current intensity, $k$is a constant which depend only on temperature in the case of an in compressible and E is electric field in the axial direction.

The approximation and numerical techniques are utilized to solve this equation. Some of these methods were B–spline method [3], Chebyshev wavelets method [16], Adomian decomposition method [15], Variational iteration method [1, 8] and other method [6,7,13].

In this study, we will generalize the operational matrix for fractional integration and multiplication within Bernstein Polynomials. Bernstein polynomials (B-polynomials) have many useful properties. They play a prominent role in various areas of mathematics and have frequently been used in the solution of integral equations, differential equations and approximation theory; see e.g., [5, 17]. The core of this approach is to convert the given problem into a system of algebraic equations. This transformation is possible by expanding the unspecified function within Bernstein Polynomials. The speed of the computation increases. To evaluate the unknown coefficients which appear in this approach, we utilized the operational matrix of integral and multiple.

Now we are ready to present the organization of our wok: In Section 2, some properties of Bernstein polynomials is presented. The operational matrix is computed for integration and produc in section 3. The suggested approach is used to approximate the Bratu equation in the next section. After that we apply the proposed technique to Bratu equation in section 5. A conclusion part in Section 6 closed the manuscript.

2. BERNSTEIN POLYNOMIALS AND THEIR PROPERTIES

2.1 DEFINITION OF BERNSTEIN POLYNOMIALS

The Bernstein polynomials of the mth degree on the interval $[0,1]$ are defined as [2]:

$$B_{i,m}(x) = \binom{m}{i} x^i (1-x)^{m-i}, \quad 0 \leq x \leq m. \tag{2}$$

The following Bernstein polynomials satisfy recursive definition:

$$B_{i,m}(x) = (1-x)B_{i,m-1}(x) + xB_{i-1,m-1}(x), \qquad i = 0,1,\cdots,m. \tag{3}$$

It can easily be shown that each of the Bernstein polynomials is positive and also the sum of all the Bernstein polynomials is unity for all real $x \in [0,1]$, i.e., $\sum_{i=0}^{m} B_{i,m}(x) = 1$. By using the binomial expansion of $(1-x)^{m-i}$, Bernstein polynomials can be show in terms of linear combination of the basis functions

$$\begin{aligned} B_{i,m}(x) &= \binom{m}{i} x^i (1-x)^{m-i} = \binom{m}{i} x^i \left(\sum_{k=0}^{m-i} (-1)^k \binom{m-i}{k} x^k\right) \\ &= \sum_{k=0}^{m-i} (-1)^k \binom{m}{i} \binom{m-i}{k} x^{i+k}, \qquad i = 0,1,\cdots,m. \end{aligned} \tag{4}$$

We can show the Bernstein polynomials by $B_{i,m}(x) = A_{i+1}T_m(x)$, for $i = 0,1,\cdots,m$, where

$$A_{i+1} = \left[\overbrace{0,0,\cdots,0}^{i\ times}, (-1)^0\binom{m}{i}, (-1)^1\binom{m}{i}\binom{m-i}{1}, \cdots, (-1)^{m-i}\binom{m}{i}\binom{m-i}{m-i}\right],$$

and

$$T_m(x) = \begin{bmatrix} 1 \\ x \\ \vdots \\ x^m \end{bmatrix}.$$

Now if we define $(m+1) \times (m+1)$ matrix A such that

$$A = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_{m+1} \end{bmatrix},$$

then we have $\phi(x) = AT_m(x)$, where $\phi(x) = \left[B_{0,m}(x), B_{1,m}(x), \cdots, B_{m,m}(x)\right]^T$ and A is an upper triangular matrix given by:

$$A = \begin{bmatrix} (1)^0\binom{m}{0} & (1)^1\binom{m}{0}\binom{m-0}{1-0} & \cdots & (1)^{m-0}\binom{m}{0}\binom{m-0}{m-0} \\ 0 & (1)^0\binom{m}{i} & \cdots & (1)^{m-i}\binom{m}{i}\binom{m-i}{m-i} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & (1)^0\binom{m}{m} \end{bmatrix},$$

and $|A| = \prod_{i=0}^{m} m\binom{m}{i}$, so A is an invertible matrix.

2.2 APPROXIMATION OF FUNCTION

The set of Bernstein polynomials$\{B_{0,m}, B_{1,m}, \cdots, B_{m,m}\}$ in Hilbert space $L^2[0,1]$ is a complete basis [11]. Therefore, any polynomial of degree $m$can be expanded in terms of linear combination of $B_{i,m}$:

$$f(x) = \sum_{i=0}^{m} c_i B_{i,m} = C^T \phi, \tag{5}$$

where $\phi^T = [B_{0,m}, B_{1,m}, \cdots, B_{m,m}]$ and $C^T = [c_0, c_1, \cdots, c_m]$. Then C^Tcan be obtained by

$$C^T \langle \phi, \phi \rangle = \langle f, \phi \rangle, \tag{6}$$

where

$$\langle f, \phi \rangle = \int_0^1 f(x)\phi(x)^T dx = [\langle f, B_{0,m}\rangle, \langle f, B_{1,m}\rangle, \cdots, \langle f, B_{m,m}\rangle], \tag{7}$$

and $\langle \phi, \phi \rangle$ is called dual matrix of ϕ which is showed by Q, and the Q is obtained as:

$$Q = \langle \phi, \phi \rangle = \int_0^1 \phi(x)\phi(x)^T dx, \tag{8}$$

and then

$$C^T = \left(\int_0^1 f(x)\phi(x)^T dx\right) Q^{-1}. \tag{9}$$

The elements of the dual matrix, Q, are easily computed by

$$\begin{aligned}(Q)_{i+1,j+1} &= \int_0^1 B_{i,m}(x)\, B_{j,m}(x) dx \\ &= \binom{n}{i}\binom{n}{j} \int_0^1 (1-x)^{2n-(i+j)} x^{i+j}\, dx \\ &= \frac{\binom{n}{i}\binom{n}{j}}{(2n+1)\binom{2n}{i+j}}, \qquad i,j = 0,1,\cdots,m.\end{aligned}$$

3. OPERATIONAL MATRIX OF BERNSTEIN POLYNOMIALS

3.1 THE OPERATIONAL MATRIX OF INTEGRAL

In this section, we describe breifley operational matrix for the Riemann-Liouville integral on the basis of BPs from order m as[17]:

$$\int_0^x \phi(t)dt \simeq P\phi(x), \tag{10}$$

by substituting $\phi(x) = AT_m(x)$ in Eq. (10) we get:

$$\begin{aligned}\int_0^x \phi(t)dt &= A\int_0^x T_m(t)\, dt = A\left[\int_0^x 1\, dt, \int_0^x t\, dt, \cdots, \int_0^x t^m\, dt\right]^T \\ &= A\left[x, \frac{x^2}{2}, \cdots, \frac{x^{m+1}}{m+1}\right]^T = AD\overline{T}_m,\end{aligned} \tag{11}$$

where D is an $(m+1)\times(m+1)$ matrix given by

$$D=\begin{bmatrix}1 & 0 & \cdots & 0\\ 0 & \frac{1}{2} & \cdots & 0\\ \vdots & \vdots & \ddots & 0\\ 0 & 0 & \cdots & \frac{1}{m+1}\end{bmatrix},$$

and

$$\overline{T}_m=\begin{bmatrix}x\\ x^2\\ \vdots\\ x^{1+m}\end{bmatrix}.$$

Now we approximate x^{i+1} by $m+1$ terms of the Bernstein basis:

$$x^{i+1}\simeq E_i^T\phi(x). \tag{12}$$

Therefore we have

$$\begin{aligned}E_i &= Q^{-1}\left(\int_0^1 x^{i+1}\phi_m(x)dx\right) \\ &= Q^{-1}\left[\int_0^1 x^{i+1}B_{0,m}(x)dx, \int_0^1 x^{i+1}B_{1,m}(x)dx,\cdots,\int_0^1 x^{i+1}B_{m,m}(x)dx,\right]^T \\ &= Q^{-1}\overline{E}_i.\end{aligned} \tag{13}$$

where $\overline{E}_i=\left[\overline{E}_{i,0},\overline{E}_{i,1},\cdots,\overline{E}_{i,m}\right]$ and

$$\overline{E}_{i,j}=\int_0^1 x^{i+1}B_{i,j}(x)dx=\frac{m!\Gamma(i+j+2)}{j!\Gamma(i+m+3)},\quad i,j=0,1,\cdots,m, \tag{14}$$

where E is an $(m+1)\times(m+1)$ matrix that has vector $Q^{-1}\overline{E}_i$ for ith columns. Therefore, we can write

$$P\phi(x)=AD[E_0^T\phi(x),E_1^T\phi(x),\cdots,E_m^T\phi(x)]^T=ADE^T\phi(x). \tag{15}$$

Finally, we obtain

$$\int_0^1\phi(t)\,dt\simeq P\phi(x), \tag{16}$$

where

$$P=ADE, \tag{17}$$

is called the Bernstein polynomials operational matrix of fractional integration.

3.2 B–POLYNOMIALS OPERATIONAL MATRIX OF PRODUCT

It is always necessary to evaluate the product of $\phi(x)$ and $\phi(x)^T$, which is called the product matrix for the Bernstein polynomials basis. The operational matrices for the product $\hat{C}$ is given by

$$C^T\phi(x)\phi(x)^T\simeq\phi(x)^T\hat{C}, \tag{18}$$

where $\hat{C}$ is an $(m+1)\times(m+1)$ matrix. So we have

$$\begin{aligned}C^T\phi(x)\phi(x)^T &= C^T\phi(x)(T_m(x)^TA^T)=\left[C^T\phi(x),x\left(C^T\phi(x)\right),\cdots,x^m\left(C^T\phi(x)\right)\right]A^T \\ &= \left[\textstyle\sum_{i=0}^m c_i\,B_{i,m},\sum_{i=0}^m c_ix\,B_{i,m},\cdots,\sum_{i=0}^m c_i\,x^mB_{i,m}\right]\end{aligned} \tag{19}$$

Now, we approximate all functions $x^k B_{i,m}(x)$ in terms of $\{B_{i,m}(x)\}_{i=0}^{m}$ for $i,k = 0,1,\cdots,m$. By (5), we have

$$x^m B_{i,m} \simeq e_{k,i}^T \phi_m(x) \tag{20}$$

that $e_{k,i} = \left[e_{k,i}^0, e_{k,i}^1, \cdots, e_{k,i}^m\right]^T$, then we obtain the components of the vector of $e_{k,i}$

$$\begin{aligned} e_{k,i} &= Q^{-1}\left(\int_0^1 x^k B_{i,m}(x)\phi(x)dx\right) \\ &= Q^{-1}\left[\int_0^1 x^k B_{i,m}(x)B_{0,m}(x)dx\,, \int_0^1 x^k B_{i,m}(x)B_{1,m}(x)dx, \cdots, \int_0^1 x^k B_{i,m}(x)B_{m,m}(x)dx\right]^T \\ &= \frac{Q^{-1}}{2m+k+1}\left[\frac{\binom{m}{0}}{\binom{2m+k}{i+k}}, \frac{\binom{m}{1}}{\binom{2m+k}{i+k+1}}, \cdots, \frac{\binom{m}{m}}{\binom{2m+k}{i+k+m}}\right]^T, \qquad i,k = 0,1,\cdots,m. \end{aligned} \tag{21}$$

Thus we obtain finally

$$\begin{aligned} \sum_{i=0}^{m} c_i x^k B_{i,m}(x) &= \sum_{i=0}^{m} c_i\left(\sum_{j=0}^{m} e_{k,i}^j\, B_{j,m}(x)\right) = \sum_{j=0}^{m} B_{j,m}(x)\left(\sum_{i=0}^{m} c_i e_{k,i}^j\right) \\ &= \phi(x)^T\left[\sum_{i=0}^m c_i e_{k,i}^0\,, \sum_{i=0}^m c_i e_{k,i}^1, \cdots, \sum_{i=0}^m c_i e_{k,i}^m\right]^T \\ &= \phi(x)^T\left[e_{k,0}, e_{k,1}, \cdots, e_{k,m}\right]C = \phi(x)^T V_{k+1} C\,, \end{aligned} \tag{22}$$

where $V_{k+1}(k = 0,1,\cdots,m)$ is an$(m+1)\times(m+1)$ matrix that has vectors $e_{k,i}(i = 0,1,\cdots,m)$ given, for each columns. If we choose an $(m+1)\times(m+1)$ matrix $\bar{C} = [V_1 c, V_2 c, \cdots, V_{m+1} c\ ]$, from (19) and (22) we can write:

$$C^T\phi(x)\phi(x)^T \simeq \phi(x)^T \bar{C} A^T \tag{23}$$

and therefore we obtain the operational matrix of product, $\hat{C} = A^T$.

4. SOLUTION OF BRATU EQUATION

Consider Bratu equation given in (1). We first approximate derivative by the Bernstein basis ϕ as follows:

$$u''(x) = C^T\phi(x) \tag{24}$$

where

$$C^T = [c_0, c_1, \cdots, c_m], \tag{25}$$

$$\phi^T = \left[B_{0,m}, B_{1,m}, \cdots, B_{m,m}\right], \tag{26}$$

are unknowns. Using initial conditions $u(x)$ can be represented as

$$u(x) = C^T P^2 \phi = G^T \phi, \tag{27}$$

where $C^T P^2 = G^T$and P is the operational matrix of integration. Here we use the Taylor expansion of the strongly nonlinear term as:

$$e^u = 1 + u + \frac{u^2}{2} + \frac{u^3}{3!} + \frac{u^4}{4!}$$

Also using (5) and (23) we approximate constant functions 1 and nonlinear terms by the Bernstein basis as:

$$1 = d^T\phi, \tag{28}$$

$$u^2(x) = G^T\phi\phi^T G = \phi^T \hat{G} G, \tag{29}$$

$$u^3(x) = \phi^T \hat{G}^2 G, \tag{30}$$

$$u^4(x) = \phi^T \hat{G}^3 G, \tag{31}$$

Now, by substituting (27) and (28)–(31), into (1) we have

$$\phi^T C = \lambda\left(\phi^T d + \phi^T G + \frac{1}{2}\phi^T \hat{G} G + \frac{1}{3!}\phi^T \hat{G}^2 G + \frac{1}{4!}\phi^T \hat{G}^3 G\right) \tag{32}$$

or

$$\phi^T - \left(C - \lambda\left(\phi^T d + \phi^T G + \frac{1}{2}\phi^T \hat{G} G + \frac{1}{3!}\phi^T \hat{G}^2 G + \frac{1}{4!}\phi^T \hat{G}^3 G\right)\right) = 0. \tag{33}$$

Finally, we obtain the following linear system of algebraic equations:

$$\left(C - \lambda\left(\phi^T d + \phi^T G + \frac{1}{2}\phi^T \hat{G} G + \frac{1}{3!}\phi^T \hat{G}^2 G + \frac{1}{4!}\phi^T \hat{G}^3 G\right)\right) = 0, \tag{34}$$

that by solving this system we can obtain the vector C. Consequently determine the approximate value of $u(x)$ can be calculated from (27).

5. ILLUSTRATIVE EXAMPLE

Below we use the presented approach in order to solve a Bratu equation.

Example. *Consider the second-order initial value problem [1,3,15]*

$$u''(x) - \lambda e^{u(x)} = 0, \qquad 0 < x < 1, \tag{35}$$

subject to the initial condition $u(0) = u'(0) = 0$. The exact solution is $u(x) = 2\ln(\cos(x))$. By applying the technique described in Section 4, in Figure 2 the exact solution together with the approximate solutions $u(x)$ show for different values of $m = 6, 8, 12$ and $\lambda = 2$. The approximate values of $u(x)$ converge to the exact solutions with increase in the number of the Bernstein basis. In Table 1, the obtained results of BPs with $m = 12$ and methods in [4] are showed.

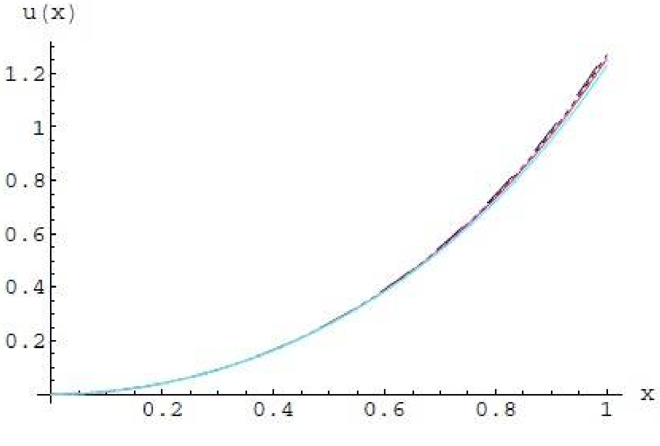

Figure 2. The exact solution: (blue line) and when $\lambda = 2$ approximation solutions for m = *12* (red line), m = *8* (dotted) and m = *6* (Long–dashed).

Table 1. Solution of Bratu equation.

x	Exact	BPEs	EVIM	BPs
0.03448	0.00118911	0.00118	0.00117	0.00118912
0.10345	0.010721	0.01061	0.0105	0.0107219
0.17241	0.0298737	0.02958	0.02929	0.0298804
0.24138	0.058839	0.05825	0.05766	0.0588668
0.31034	0.097897	0.09692	0.09592	0.0979798
0.37931	0.147465	0.14689	0.14632	0.147662
0.44828	0.20807	0.20599	0.20391	0.208484
0.51724	0.280393	0.27761	0.27483	0.281178
0.58621	0.365339	0.36178	0.35822	0.366712
0.65517	0.464004	0.45943	0.45485	0.466255
0.72414	0.577847	0.57211	0.56638	0.581339
0.79313	0.708731	0.70165	0.69462	0.713882
0.86207	0.858899	0.85038	0.84186	0.866119
0.93103	1.03165	1.02144	1.01122	1.04121
1	1.23125	1.21906	1.20687	1.24298

6. CONCLUSION

In this work we have performed an accurate and efficient approachbased using the Bernstein polynomials for solving the second-order initial value problems of Bratu–type. The Bernstein polynomials operational matrixes of integration and multiplication are used to reduce the problem to the solution of nonlinear algebraic equations. Illustrative example are presented to demonstrate the applicability and validity of the approach. We used Mathematica for computations.

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Hosoya Polynomials of Random Benzenoid Chains

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ABSTRACT Let G be a molecular graph with vertex set $V(G)$ and $d_G(u,v)$ be the topological distance between vertices u and v in G. The Hosoya polynomial $H(G,x)$ of G is a polynomial $\sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$ in variable x. In this paper, we obtain an explicit analytical expression for the expected value of the Hosoya polynomial of a random benzenoid chain with n hexagons. Furthermore, as corollaries, the expected values of the well-known topological indices: Wiener index, hyper-Wiener index and Tratch–Stankevitch–Zefirov index of a random benzenoid chain with n hexagons can be obtained by simple mathematical calculations, which generates the results given by I. Gutman et al. [Wiener numbers of random benzenoid chains, *Chem. Phys. Lett.* **173** (1990) 403–408].

KEYWORDS Wiener index • random benzenoid chain • Hosoya polynomial • expected value • generating function.

1. INTRODUCTION

A molecular graph (or chemical graph) is a representation of the structural formula of a chemical compound in terms of graph theory. Specifically, a *molecular graph* is a simple graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Note that hydrogen atoms are often omitted. For example, *benzenoid chains* are molecular graphs of unbranched catacondensed benzenoid hydrocarbons. *Molecular structure descriptors* (or *topological indices*) of molecular graphs are graph invariants and are used for Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies, which mainly focus on structure-dependent chemical behaviours of molecules [4, 18].

Let G be a molecular graph with vertex set $V(G)$, $d_G(u,v)$ be the *topological distance* (or *distance* for short) between vertices u and v in G, i.e., the length of a shortest path connecting u and v in G. The subscript is omitted when there is no risk of confusion. The *Hosoya polynomial}* in variable x of G, introduced by Hosoya [12], is defined as $H(G,x)= \sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$, where the sum is taken over all unordered pairs of (not necessarily distinct) vertices in G. Hence the polynomial contains the number of vertices as the constant term.

The Hosoya polynomial not only contains more information concerning distance in the molecular graph than any of the hither to proposed distance-based molecular structure descriptors, which were extensively studied in chemical graph theory, see for instance the surveys [16, 17], but also deduces some of them. For example, Wiener index $W(G)$ of a molecular graph G [20], the oldest and most well-studied molecular structure descriptor so far, is equal to the first derivative of the Hosoya polynomial in $x=1$, i.e.,

$$W(G)=\frac{d}{d_x}H(G,x)\Big|_{x=1}. \tag{1}$$

The chemical applications and mathematical properties of $W(G)$ are well documented [5, 6, 9, 10]. Moreover, hyper-Wiener index $WW(G)$ [14], Tratch–Stankevitch–Zefirov index $TSZ(G)$ [19] can be deduced from $H(G,x)$ as follows:

$$WW(G)=\frac{1}{2}\frac{d^2}{dx^2}xH(G,x)\Big|_{x=1}, \tag{2}$$

$$TSZ(G)=\frac{1}{3!}\frac{d^3}{dx^3}x^2H(G,x)\Big|_{x=1}. \tag{3}$$

Two classes of general molecular structure descriptors

$$\frac{1}{k!}\frac{d^k}{dx^k}x^{k-1}H(G,x)\Big|_{x=1} \text{ and } \frac{1}{k!}\frac{d^k}{dx^k}H(G,x)\Big|_{x=1}$$

for positive integers k were also studied in Refs. [2, 15]. On the other hand, recently Brückler etc. [2] proposed a new class of distance-based molecular structure descriptors: Q-indices, which can reflect the fact that any kind of interaction between physical objects (in particular, between atoms in a molecule) decrease with increasing distance, and showed that Q-indices are equal to the Hosoya polynomial. So the Hosoya polynomial and the quantities derived from it will play a significant role in QSAR and QSPR researches, and abundant literature appeared on this topic [3, 8,21, 22, 23].

Let B_{n+1} denote a benzenoid chain with $n+1$ hexagons ($n \geq 0$). There are obviously unique benzenoid chains B_{n+1} for $n = 0,1$. More generally, a benzenoid chain B_{n+1} can be regarded as a benzenoid chain B_n to which a new terminal hexagon $u_n, y_1, y_2, y_3, y_4, v_n$ has been adjoined. However, when $n \geq 2$, the terminal hexagon can be attached in three ways, resulting in the local arrangements we describe as B^1_{n+1}, B^2_{n+1}, B^3_{n+1}, according to the related position of the terminal hexagon shown in Figure 1.

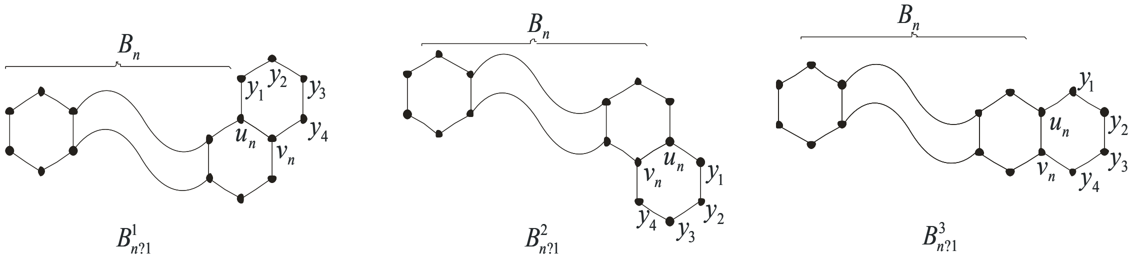

Figure 1. The three types of local arrangements in benzenoid chains B_{n+1}

A *random benzenoid chain*, R_{n+1} with $n+1$ hexagons, is a benzenoid chain obtained by stepwise additions of terminal hexagons. As the initial steps, $R_1 = B_1$, $R_2 = B_2$, and for each step k ($2 \leq k \leq n$) a random selection is made from one of the three possible constructions:

$B_k \rightarrow B^1_{k+1}$, with probability p_1,

$B_k \rightarrow B^2_{k+1}$, with probability p_2 or

$B_k \rightarrow B^3_{k+1}$, with probability $q=1-p_1-p_2$.

We assume the probabilities p_1 and p_2 are constants, invariant to the step parameter k. That is, the process described is a Markov chain of order zero with a state space consisting of three states [7].

In the present paper, we calculate the expected value of the Hosoya polynomial of a random benzenoid chain R_n and give an explicit analytical expression by using the mathematical method: generating function. As corollaries, formulae for the expected values of some topological indices deduced from the expression can be obtained by using simple mathematical operators.

2. RECURSION RELATIONS OF HOSOYA POLYNOMIALS OF RANDOM BENZENOID CHAINS

Let G be a connected graph with vertex set $V(G)$. For the simplicity, we define one notation as follows: for a vertex $u \in V(G)$,

$$H_G(u;x) = \sum_{v \in V(G)} x^{d(u,v)},$$

i.e., the contribution of the vertex u to the Hosoya polynomial $H(G,x)$ of G. As described above in the previous section, a benzenoid chain B_{n+1} is obtained by attaching to a benzenoid chain B_n a terminal hexagon consisting of vertices u_n, y_1, y_2, y_3, y_4, v_n (see Figure 1). For this construction the following relations are easily obtained [10]:

$$H_{B_{n+1}}(y_1;x) = xH_{B_n}(u_n;x) + x^3 + x^2 + x + 1 \tag{4a}$$

$$H_{B_{n+1}}(y_2;x) = x^2 H_{B_n}(u_n;x) + x^2 + 2x + 1, \tag{4b}$$

$$H_{B_{n+1}}(y_3;x) = x^2 H_{B_n}(v_n;x) + x^2 + 2x + 1, \tag{4c}$$

$$H_{B_{n+1}}(y_4;x) = xH_{B_n}(v_n;x) + x^3 + x^2 + x + 1, \tag{4d}$$

and

$$H(B_{n+1},x) = H(B_n,x) + \sum_{i=1}^{4} H_{B_{n+1}}(y_i;x) - (x^3 + 2x^2 + 3x). \tag{5}$$

Note that the last term on the right-hand side of Eq. (5) appears because the contribution of pairs of vertices y_i and y_j $(1 \le i < j \le 4)$ to $H(B_{n+1},x)$ are calculated twice in the second term on the right-hand side of Eq. (5). Substituting Eq. (4) for Eq.(5), we get

$$H(B_{n+1},x) = H(B_n,x) + x(x+1)(H_{B_n}(u_n;x) + H_{B_n}(v_n;x)) + x^3 + 2x^2 + 3x + 4. \tag{6}$$

In fact, the equations discussed above associated with a concrete benzenoid chain are valid for a random benzenoid chain, i.e., Eqs. (4)-(6) still hold when we simultaneously replace B_{n+1} for $R_{n+1}$and B_n for R_n.

In the following we consider contributions of u_{n+1} and v_{n+1} to $H(B_{n+1},x)$ according to the positions of u_{n+1} and v_{n+1}. There are three cases to consider:

Case 1. $B_{n+1} \rightarrow B^1_{n+2}$. In this case, $u_{n+1} = y_1$ and $v_{n+1}=y_2=$. Consequently, $H_{B_{n+1}}(u_{n+1};x) = H_{B_{n+1}}(y_1;x)$ and $H_{B_{n+1}}(v_{n+1};x) = H_{B_{n+1}}(y_2;x)$, which are given by Eqs. (4a) and (4b), respectively.

Case 2. $B_{n+1} \to B^2_{n+2}$. In this case, $u_{n+1} = y_3$ and $v_{n+1} = y_4$. Consequently, $H_{B_{n+1}}(u_{n+1};x) = H_{B_{n+1}}(y_3;x)$ and $H_{B_{n+1}}(v_{n+1};x) = H_{B_{n+1}}(y_4;x)$,, which are given by Eqs. (4c) and (4d), respectively.

Case 3. $B_{n+1} \to B^3_{n+2}$. In this case, $u_{n+1}=y_2$ and $v_{n+1} = y_3$. Consequently, $H_{B_{n+1}}(u_{n+1};x) = H_{B_{n+1}}(y_2;x)$, and $H_{B_{n+1}}(v_{n+1};x) = H_{B_{n+1}}(y_3;x)$,, which are given by Eqs. (4b) and (4c), respectively.

For a random benzenoid chain R_{n+1}, $H(R_{n+1},x)$, $H_{R_{n+1}}(u_{n+1};x)$ and $H_{R_{n+1}}(v_{n+1};x)$ are random variables and we denote their expected values by $H_{n+1}(x), U_{n+1}(x)$ and $V_{n+1}(x)$, respectively, i.e.,

$$H_{n+1}(x) = E(H(R_{n+1},x)), U_{n+1}(x) = E(H_{R_{n+1}}(u_{n+1};x)),$$
$$V_{n+1}(x) = E(H_{R_{n+1}}(v_{n+1};x)).$$

Since the above three cases occur in random benzenoid chains with probabilities p_1, p_2 and $1-p_1-p_2$, respectively, by the definition of the expected value we immediately obtain

$$U_{n+1}(x) = p_1 H_{R_{n+1}}(y_1;x) + p_2 H_{R_{n+1}}(y_3;x) + qH_{R_{n+1}}(y_2;x), \tag{7a}$$
$$V_{n+1}(x) = p_1 H_{R_{n+1}}(y_2;x) + p_2 H_{R_{n+1}}(y_4;x) + qH_{R_{n+1}}(y_3;x), \tag{7b}$$

Substituting the corresponding analogues associated with random benzenoid chains R_n and R_{n+1} to Eq. (4) for Eq. (7), we get

$$U_{n+1}(x) = (p_1 x + qx^2) H_{R_n}(u_n;x) + p_2 x^2 H_{R_n}(v_n;x) + (x^3 - x)p_1 + (x+1)^2, \tag{8a}$$
$$V_{n+1}(x) = (p_2 x + qx^2) H_{R_n}(v_n;x) + p_1 x^2 H_{R_n}(u_n;x) + (x^3 - x)p_2 + (x+1)^2, \tag{8b}$$

By applying the expectation operator to Eq. (8), and noting that $E(U_{n+1}(x)) = U_{n+1}(x)$ and $E(V_{n+1}(x)) = V_{n+1}(x)$, we obtain

$$U_{n+1}(x) = (p_1 x + qx^2) U_n(x) + p_2 x^2 V_n(x) + (x^3 - x)p_1 + (x+1)^2 \ , \tag{9a}$$
$$V_{n+1}(x) = (p_2 x + qx^2) V_n(x) + p_1 x^2 U_n(x) + (x^3 - x)P_2 + (x+1)^2 \tag{9b}$$

A recursion relation for the expected value of the Hosoya polynomial of a random benzenoid chain can be obtained from Eq. (6) by using R_k in place of B_k ($k=n, n+1$) and by using the expectation operator:

$$H_{n+1}(x) = H_n(x) + (x + x^2)(U_n(x) + V_n(x)) + x^3 + 2x^2 + 3x + 4. \tag{10}$$

The system of recursion equations (9) and (10) holds for $n \geq 0$, and has boundary conditions:

$$H_0(x) = x+2,\, U_0(x) = x+1,\;\; V_0(x) = x+1. \tag{11}$$

3. SOLUTION FOR THE SYSTEM OF RECURSION EQUATIONS

To solve the recursion equations (9) and (10), we use the method of the generating function [1]. First define the following generating functions in variable *t*. Let

$$U(t) = \sum_{n\geq 0} U_n(x)t^n\;,\;\; V(t) = \sum_{n\geq 0} V_n(x)t^n,\;\; H(t) = \sum_{n\geq 0} H_n(x)t^n, \qquad 0 < t < 1.$$

From Eqs. (9)–(11), we get relations of their generating functions as follows:

$$U(t) = t(p_1x + qx^2)U(t) + p_2tx^2V(t) + \frac{t(x^3 - x)p_1 + t(x+1)^2}{1-t} + x + 1 \tag{12a}$$

$$V(t) = t(p_2x + qx^2)V(t) + p_1tx^2U(t) + \frac{t(x^3 - x)p_2 + t(x+1)^2}{1-t} + x + 1, \tag{12b}$$

$$H(t) = tH(t) + (x + x^2)t(U(t) + V(t)) + \frac{t(x^3 + 2x^2 + 3x + 4)}{1-t} + x + 2 \tag{12c}$$

As Eqs. (12a) and (12b) comprise a system of two linear equations in two variables *U*(*t*) and *V*(*t*), a straight forward calculation results in

$$U(t) = \frac{p_1x(x+1)^2}{(x-1)(1-xt)} + \frac{(1-p_1)x(x+1)}{(x-1)(1-x^2t)} + \frac{(p_1x^2+1)(x+1)}{(1-x)(1-t)} + \frac{p_2(p_1-p_2)t^2x^3(x+1)^2}{(1-t)(1-qt)}\left(\frac{1}{1-x^2t} - \frac{1}{1-xt}\right), \tag{13a}$$

$$V(t) = \frac{p_2x(x+1)^2}{(x-1)(1-xt)} + \frac{(1-p_2)x(x+1)}{(x-1)(1-x^2t)} + \frac{(p_2x^2+1)(x+1)}{(1-x)(1-t)} + \frac{p_1(p_2-p_1)t^2x^3(x+1)^2}{(1-t)(1-qt)}\left(\frac{1}{1-x^2t} - \frac{1}{1-xt}\right). \tag{13b}$$

Substituting Eq. (13) for Eq. (12) and then rearranging, we can easily get:

$$\begin{aligned} H(t) = {} & \frac{x+2}{1-t} + \frac{(x^3+2x^2+3x+4)t}{(1-t)^2} + \frac{(1-q)x^2(x+1)^3t}{(x-1)(1-t)(1-xt)} + \frac{(1+q)x^2(x+1)^2t}{(x-1)(1-t)(1-x^2t)} \\ & + \frac{(x+1)^2((1-q)x^3+2x)t}{(1-x)(1-t)^2} - \frac{(p_1-p_2)^2x^4(x+1)^3t^3}{(1-at)(1-t)^2}\left(\frac{1}{1-x^2t} - \frac{1}{1-xt}\right). \end{aligned} \tag{14}$$

Applying two special cases of Newton's generalized binomial theorem

$$\frac{1}{1-y}=\sum_{n=0}^{+\infty} y^n \quad \text{and} \quad \frac{1}{(1-y)^2}=\sum_{n=0}^{+\infty}(n+1)\,y^n$$

to Eq. (14) and then rearranging it, we get

$$\begin{aligned} H(t) &= x+2+3(x^3+2x^2+2x+2)t+(2x^5+6x^4+12x^3+14x^2+11x+10)t^2+ \\ &\sum_{n=3}^{+\infty}[x+2+n(x^3+2x^2+3x+4)+\frac{n(x+1)^2((1-q)x^3+2x)}{1-x}+\frac{(1-q)x^2(x+1)^3(x^n-1)}{(x-1)^2} \;.. \\ &+\frac{(1+q)x^2(x+1)(x^{2n}-1)}{(x-1)^2}-(p_1-p_2)^2x^4(x+1)^3\sum_{l=0}^{n-3}q^l(\sum_{k=0}^{n-3-l}(n-l-k-2)(x^{2k}-x^k))]t^n. \end{aligned} \tag{15}$$

4. RESULTS AND DISCUSSION

From Eq. (15), we have the following main theorem.

Theorem 4.1. Let $H_n(x)$ be the expected value of the Hosoya polynomial of a random benzenoid chain with n hexagons. Then

$$H_1(x)=3x^3+6x^2+6x+6;$$

$$H_2(x)=2x^5+6x^4+12x^3+14x^2+11x+10;$$

and when and $n \geq 3$,

$$\begin{aligned} H_n(x) &= x+2+n(x^3+2x^2+3x+4)+\frac{n(x+1)^2((1-q)x^3+2x)}{1-x}+ \\ &\frac{(1-q)x^2(x+1)(x^{2n}-1)}{(x-1)^2}-(p_1-p_2)^2x^4(x+1)^3\sum_{l=0}^{n-3}q^l(\sum_{k=0}^{n-3-l}(n-l-k-2)(x^{2k}-x^k)). \end{aligned}$$

We can obtain some corollaries by taking parameters as special values or Eqs. (1)–(3). When $q=1$ (in this case $p_1 = p_2 = 0$), a random benezoid chain is definitely a linear benzenoid chain, i.e., a benzoid chain without no turns. So from Theorem 4.1 we have

Corollary 4.2. [21] Let G be a benzenoid chain with n hexagons. If G has no turns, then the Hosoya polynomial of G is

$$H(G,x)=x+2+\frac{n(x^2-x-4)(x^2+1)}{x-1}+\frac{2x^2(x+1)(x^{2n}-1)}{(x-1)^2}.$$

If p_1=1 or p_2=2, a random benzenoid chain with n hexagons is definitely a helicene with n hexagons, then we get

Corollary 4.3. [21] Let G be a helicene with n hexagons. Then the Hosoya polynomial of G is

$$H(G,x)=x+2+\frac{x^2(x+1)((x+1)^3x^n-(n-1)x^5-x^4+(n-3)x^3-x^2-2x-2)}{(x-1)^2}$$
$$+\frac{n(x^5+x^4+2x^3+3x^2+x+4)}{1-x}$$

In addition, from Eqs. (1)–(3), we can obtain the expected values of some molecular structure descriptors from Theorem 4.1.

Corollary 4.4. [13] The expected value W_n of the Wiener index of a random benzenoid chain with n hexagons is

$$W_n=4n^3+16n^2+6n+1+\frac{4}{3}q(n^3-3n^2+2n)-\frac{4}{3}(p_1-p_2)^2\sum_{l=0}^{n-3}l(l+1)(l+2)q^{n-3-l}$$

Corollary 4.5. The expected value WW_n of the hyper-Wiener index of a random benzenoid chain with n hexagons is

$$WW_n=\frac{1}{3}[3+(11+26q)n+(79-33q)n^2+(28+4q)n^3+(5+3q)n^4]-$$
$$(p_1-p_2)^2\sum_{l=0}^{n-3}l(l+1)(l+2)(l+9)q^{n-3-l}$$

Corollary 4.6. The expected value TSZ_n of the Tratch-Stankevitch-Zefirov index of a random benzenoid chain with n hexagons is

$$TSZ_n=\frac{1}{30}[30+(-58+566q)n+(1185-635q)n^2+(490-10q)n^3+(135+65q)n^4$$
$$+(18+14q)n^5-(p_1-p_2)^2\sum_{l=0}^{n-3}l(l+1)(l+2)(14(l+3)^2+139(l+3)+510)q^{n-3-l}$$

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Complete Forcing Numbers of Polyphenyl Systems

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ABSTRACT The idea of "forcing" has long been used in many research fields, such as colorings, orientations, geodetics and dominating sets in graph theory, as well as Latin squares, block designs and Steiner systems in combinatorics [D. Donovan, E. S. Mahmoodian, C. Ramsay, A. P. Street, Defining sets in combinatorics: A survey, in: C. D. Wensley (Ed.), Surveys in Combinatorics, Cambridge Univ. Press, 2003, pp. 115–174]. Recently, the forcing on perfect matchings has been attracting more researchers' attention. A forcing set of a perfect matching M of a graph G is a subset of M contained in no other perfect matchings of G. A global forcing set of G, introduced by Vukičević et al., is a subset of E(G) on which there are distinct restrictions of any two different perfect matchings of G. Combining the above "forcing" and "global" ideas. Xu et al. in [Complete forcing numbers of catacondensed benzenoid, *J. Combin. Optim.* **29** (2015) 803–814.] introduced a complete forcing set of G defined as a subset of E(G) on which the restriction of any perfect matching M of G is a forcing set of M. The minimum cardinality of complete forcing sets is the complete forcing number of G. In this paper, we give the explicit expressions for the complete forcing number of several classes of polyphenyl systems.

KEYWORDS Complete forcing number • polyphenyl system • global forcing number.

1. INTRODUCTION

The molecular graphs (or more precisely, the graphs representing the carbon-atoms) of polyphenyls are called the polyphenyl systems. This kind of macrocyclic aromatic hydrocarbons called polyphenyls and their derivatives attracted the attention of chemists for many years [3, 4, 5]. The derivatives of polyphenyls are very important organic chemicals, which can be used in organic synthesis, drug synthesis, heat exchanger, etc. Biphenyl compounds also have extensive industrial applications. For example, 4,4–bis (chloromethyl) biphenyl can be used for the synthesis of brightening agents. Especially, polychlorinated biphenyls (PCBs) can be applied in print and dyeing extensively [6, 7]. On the other side, PCBs are dangerous organic pollutants, which lead to global pollution. Many years ago, a series of physical properties were discussed [8–13].

A perfect matching M (or Kekulé structure, 1-factor) of a graph G is a set of independent edges such that every vertex of G is incident with exactly one edge in M.

Let G be a graph with edge set $E(G)$ that admits a perfect matching M. A forcing set of M is a subset S of M contained in no other perfect matchings of G. The minimum possible cardinality of forcing set S is called the forcing number of M.

The notions of a forcing edge and the forcing number of a perfect matching first appeared in 1991 in a paper of Harary, Klein and Živković [14]. The root of these concepts can be traced to the works [15, 16] by Randić and Klein in 1985−1987, where the forcing number was introduced under the name of "innate degree of freedom" of a Kekulé structure, which plays an important role in the resonance theory in chemistry.

Over the past two decades, more and more mathematicians were attracted to the study on forcing sets (including forcing edges and forcing faces, etc) and the forcing numbers of perfect matchings of a graph. The scope of graphs in consideration has been extended from polyhexes to various bipartite graphs and non-bipartite graphs.

Some varied topics such as global (or total) forcing matchings and anti-forcing matching also emerged.

Klein and Randić [15] proposed the degree of freedom of a graph from the global point of view, defined as the sum of forcing numbers over all perfect matchings of a graph, and showed by evidence that the degree of freedom of a chemical graph actually measures graphical characteristics distinct from those measured by a couple of common resonance energy estimators. Because of extensive industrial and medical applications, one class of chemical graph-macrocyclic aromatic hydrocarbons called polyphenyls and their derivatives attracted the attention of chemists for many years [3, 4, 5]. A series of linear and branched polyphenyls and their derivatives were synthesized and some physical properties were discussed [8−13].

Gutman [17] showed that the values which the Wiener indices of isometric polyphenyls may assume are all congruent modulo 36. Bian and Zhang [18, 19] determined the polyphenyl chain with minimum and maximum Wiener (or edge-Wiener) indices among all the polyphenyl chains with n hexagons. Li and Bian [20] gave the extremal polyphenyl chains concerning k-matchings and k-independent sets. In 2013, Ma and Bian [21] also gave the extremal polyphenyl spiders concerning k-matchings and k-independent sets. A complete forcing set of G, introduced by Xu et al. [2] recently, is a subset of $E(G)$ on which the restriction of any perfect matching is a forcing set of the perfect matching. The minimum possible cardinality of complete forcing sets of G is the complete forcing number of G, denote it by $cf(G)$. Xu et al. gave an expression for the complete forcing number of a hexagonal chain and a recurrence relation for complete forcing number of cata-condensed hexagonal system. In 2014, Xu et al. [22] by the constructive proof, gave an explicit analytical expression for the complete forcing number of a primitive coronoid, a circular single chain consisting of congruent regular hexagons.

Based on these works, in this paper, we give the explicit expressions for the complete forcing number of several classes of polyphenyl systems.

2. PRELIMINARIES

All graphs in this paper are simple connected and have perfect matchings. For all terms and notations used but not defined here, we refer the reader to the textbooks [23, 24].

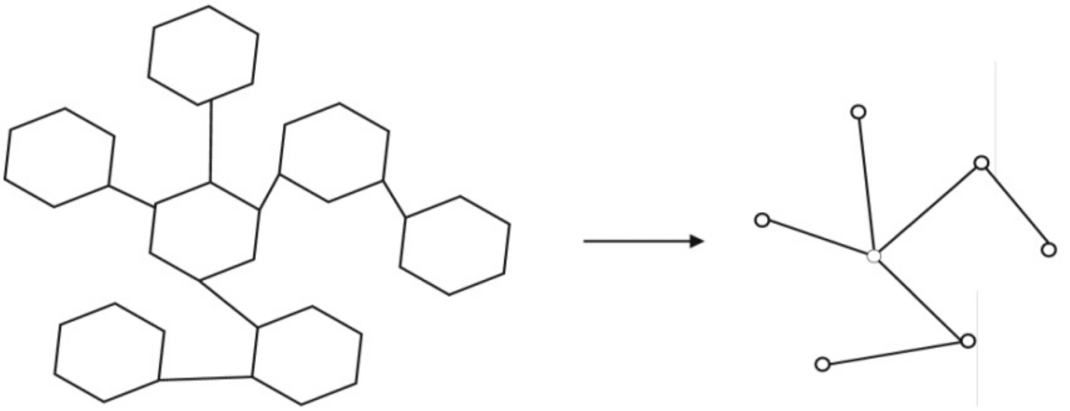

Figure 1. A tree-like polyphenyl system and corresponding tree.

A polyphenyl system H is said to be tree-like (see Figure 1), if each vertex of H lies in a hexagon and the graph obtained by contracting every hexagon into a vertex in original molecular graph is a tree.

A hexagon r of a tree-like polyphenyl system may have one, two, three, four, five or six neighboring hexagons. If r has one neighboring hexagon, then it is said to be terminal, and internal otherwise. Also it is branched if it has three or more neighboring hexagons.

Definition 1. If every hexagon in a polyphenyl system has exactly two neighboring hexagons, then it is called primitive coronoid polyphenyl system. The set of primitive coronoid polyphenyl systems with n hexagons is denoted by CH_n (see Figure 2).

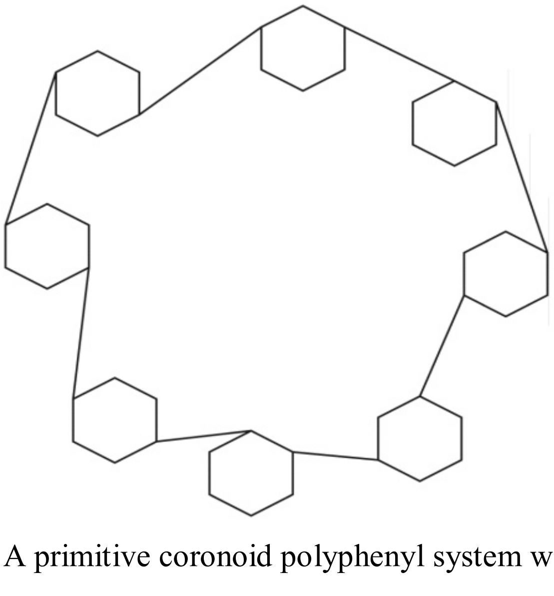

Figure 2. A primitive coronoid polyphenyl system with 8 hexagons.

Definition 2. A tree-like polyphenyl system without branched hexagons is called a polyphenyl chain. A polyphenyl chain with n hexagons is denoted by H_n (see Figure 3).

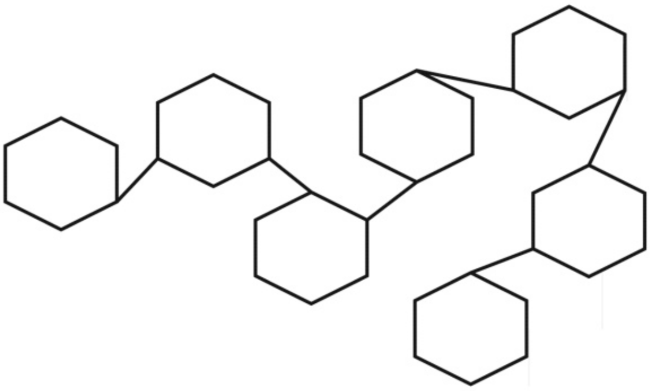

Figure 3. A polyphenyl chain with 7 hexagons.

For a hexagon C, two vertices u and v of C are said to be in ortho–position if they are adjacent in C. If two vertices are at distance 2, they are in meta–position. Finally, if u and v are at distance 3, we say that they are in para–position. Examples of pairs of vertices in ortho–, meta–, and para–position are shown in Figure 4.

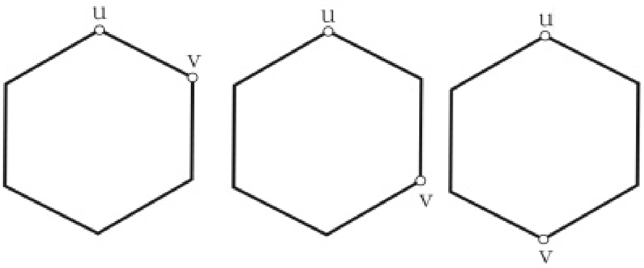

Figure 4. Orhto–, meta–, and para–positions of vertices u and v in C.

An internal hexagon C in a polyphenyl chain is called ortho–hexagon, meta–hexagon, or para–hexagon, if the two vertices of C incident with two edges which connect other two hexagons are in ortho–, meta–, or para–position, respectively.

Following Lovász and Plummer [24], an edge of G is said to be allowed if it is contained in some perfect matching of G and forbidden otherwise.

Theorem 1. *Let H be a tree-like polyphenyl system with n hexagons. Then we have $cf(H) = 2n$.*

Proof. Suppose that H is a tree-like polyphenyl system with n hexagons.

First we claim that every edge incident with the terminal hexagons is forbidden edge. In fact, if an edge incident with a terminal hexagon C is allowed edge, then it lies in some perfect matching M of H, hence, the number of the rest of vertices in C besides the vertex incident with the allowed edge is odd, which contradicts that H has the perfect matching.

We can delete all edges incident with terminal hexagons, and obtain the resulting graph, which consists of a small tree-like polyphenyl system and some independent hexagons.

Now we consider the small tree-like polyphneyl system, we also can show that every edge incident with the terminal hexagons of the small polyphenyl system is forbidden edge, then we delete all edges incident with terminal hexagons of the small tree-like polyphenyl system again. By iterating the same proceed, until the resulting graph is an independent hexagon. We can conclude that all edges between the two hexagons are forbidden edges, and the edges lie in every hexagon are allowed edges of H. Moreover, there are two perfect matchings in each hexagon, the union of perfect matching of each hexagon will be a perfect matching of H, and the number of perfect matching of H is $2n$.

By definition of complete forcing number, we take any two adjacent edges in every hexagon, the set of these edges will be a complete forcing set of H. Then we have $cf(H) = 2n$. ■

Since the polyphenyl chain can be viewed as a special tree-like polyphenyl system, as a corollary of Theorem 1, we easily have the following result.

Corollary 2. *Let H_n be any polyphenyl chain with n hexagons. Then we have $cf(H_n) = 2n$.*

For a primitive coronoid polyphenyl system CH, the meta–hexagon in CH will affect the number of perfect matchings of CH, according to whether CH has meta–hexagons or not, we distinguish the following two cases.

Theorem 3. *Let CH_n be a primitive coronoid polyphenyl system with n hexagons such that CH_n has no meta–hexagons. Then we have $cf(CH_n) = 2n + 1$.*

Proof. By the assumption, any hexagon C of CH_n is either ortho–hexagon or para–hexagon, so the two vertices of C incident with two edges which connect other two hexagons are in ortho–position or para–position.

First, we claim that G has a perfect matching M consisting of edges connecting two hexagons with the remainder two independent edges of every hexagon by deleting the two ortho– (or para–) position vertices of C. Moreover, every hexagon has two perfect matchings, the union of a perfect matching of every hexagon will be a perfect matching of CH_n. So the number of perfect matchings of CH_n is $2n + 1$.

We can obtain a complete forcing set of CH_n by taking any one edge connecting two hexagons and two adjacent edges of every hexagon in CH_n. Hence, the complete forcing number of CH_n is $2n + 1$. ■

Theorem 4. *Let CH_n be any primitive coronoid polyphenyl system with n hexagons such that CH_n has at least one meta–hexagon. Then we have $cf(CH_n) = 2n$.*

Proof. According to assumption, CH_n has at least one meta–hexagon C. We claim that none of the two edges incident with the two meta-position vertices of C is allowed edge. In fact, if one of the two edges is allowed edge, then it must be matched by some perfect matching M of CH_n, in this case, the remainder vertices of C besides the vertex incident with the allowed edge cannot be completely matched by M, which contradicts that M is a perfect matching of CH_n.

So, the vertices of every hexagon in CH_n must be matched by themselves in M, namely, any edge connecting two hexagons must be forbidden edge of CH_n. The resulting graph is the set of independent hexagons by deleting all the forbidden edges of CH_n. It is clear that the number of perfect matchings of CH_n is $2n$, and we can obtain the complete forcing set of CH_n by taking two adjacent edges of every hexagon of CH_n. Hence, the complete forcing number of CH_n is $2n$. ■

4. CONCLUDING REMARKS

In this section, we discuss the global forcing number of the polyphenyl system. For a simple connected graph G with a perfect matching, let $\mathrm{M}(G)$ denote the set of all perfect matchings in G, and $f : \mathrm{M}(G) \to \{0, 1\}^{|E(G)|}$ a characteristic function of perfect matchings of G. Any set $S \subseteq E(G)$ such that $f|S$ is an injection is called a global forcing set in G, and the cardinality of smallest such S is called the global forcing number of G. Tomislav Došlić et al. showed that the global forcing number of graph G has lower bound $\lceil \log_2|\mathrm{M}(G)| \rceil$ and upper bound $|E(G)| - |V(G)| + 1$. We can easily show that the lower and upper bounds of the global forcing number for a tree-like polyphenyl system with n hexagons (in particular a polyphenyl chain with n hexagons) and a primitive coronoid polyphenyl system with n hexagons which has no meta- hexagons are all tight. And the global forcing number of a tree-like polyphenyl system with n hexagons (in particular a polyphenyl chain with n hexagons) is n, the global forcing number of a primitive coronoid polyphenyl system with n hexagons which has no meta–hexagons is $n+1$. For a primitive coronoid polyphenyl system with n hexagons which has at least one meta–hexagon, only the lower bound of the global forcing number for this primitive coronoid polyphenyl system is tight, and the global forcing number of it is n. These results are similar to that of the complete forcing number of the polyphenyl system.

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Quantitative Structure Activity Relationship Study of Inhibitory Activities of 5–Lipoxygenase and Design new Compounds by Different Chemometrics Methods

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ABSTRACT A quantitative structure-activity relationship (QSAR) study was conducted for the prediction of inhibitory activity of 1-phenyl[2H]-tetrahydro-triazine-3-one analogues as inhibitors of 5-Lipoxygenase. The inhibitory activities of the 1-phenyl[2H]-tetrahydro-triazine-3-one analogues modeled as a function of molecular structures using chemometrics methods such as multiple linear regression (MLR) and least squares support vector machines (LS-SVM). The obtained models were applied to predict the inhibitory activity of compounds which were not in the modeling procedure. The results of models showed high prediction ability with root mean square error of prediction of 0.167 and 0.061 for MLR and LS-SVM, respectively. The LS-SVM method was used for prediction of inhibitory activity of the new inhibitor derivatives.

KEYWORDS QSAR • 1–phenyl[2H]–tetrahydro–triazine–3–oneanalogues • MLR • LS–SVM.

1. INTRODUCTION

Lipoxygenases (LOs) are a class of widely occurring, non-heme iron-containing oxygenases that can be isolated from animals, higher plants, and fungi. Currently, three distinct mammalian LOs have been characterized, 5-LO, 12-LO, and 15-LO, which oxygenate arachidonic acid at specific carbon centers (C5, C12, and C15, respectively) [1].The 5-Lipoxygenase is the first dedicated enzyme in the biosynthetic pathway leading to the leukotrienes. Since leukotrienes have been implicated as important mediators in such diseases as asthma, psoriasis, ulcerative colitis, and rheumatoid arthritis, inhibition of 5-Lipoxygenase offers a potential approach for the therapy of these diseases [2].

In the present study, the inhibitory activity data of 1-phenyl[2H]-tetrahydro-triazine-3-one analogues as inhibitors of 5-Lipoxygenase were used to construct a mathematical model with structural information, a so-called QSAR (quantitative structure–activity relationship). Quantitative structure-activity relationships (QSAR) are an important tool in agrochemistry, pharmaceutical chemistry, toxicology, and eventually most facts of chemistry [3, 4]. QSAR models are mathematical equations which relate chemical structure of a compound to its physical, chemical, biological and technological properties. The main goal of QSAR studies is to establish an empirical rule or function to relate the structural descriptors of compounds under investigation to bioactivities. This rule or function is then utilized to predict the same bioactivities of compounds which are not involved in the training set from their structural descriptors. Model development in QSAR studies comprises different critical steps as (1) descriptor generation, (2) data splitting to calibration (or training) and prediction (or validation) sets, (3) variable selection, (4) finding appropriate model between selected variables and activity and (5) model validation [5].

Among the investigation of QSAR, one of the most important factors affecting the quality of the model is the method to build the model. Many multivariate data analysis methods such as multiple linear regression (MLR) [6, 7], artificial neural network (ANN) [8] and partial least squares (PLS) [9] have been used in QSAR studies. MLR, as most commonly used chemometrics method, has been extensively applied to QSAR investigations. The artificial neural network (ANN) offers satisfactory accuracy in most cases but tends to over fit the training data. The PLS method is based on factor analysis that is originally suggested and chemically applied by Wold et al [10]. The support vector machine (SVM) is a popular algorithm developed from the machine learning community. Due to its advantages and remarkable generalization performance over other methods, SVM has attracted attention and gained extensive applications [11, 12]. As a simplification of traditional SVM, Suykens and Vandewalle [13, 14] have proposed the use of least-squares SVM (LS-SVM). LS-SVM encompasses similar advantages as SVM, but its additional advantage is that it requires solving a set of linear equations (linear programming), which is much easier computationally [15, 16]. In this study, the MLR and LS-SVM methods were proposed to model and predict the inhibitory activity of 1-phenyl[2H]-tetrahydro-triazine-3-one analogues as inhibitors of 5-Lipoxygenase.

2. THEORY

The LS-SVM [13] is capable of dealing with linear and nonlinear multivariate calibration. In LS-SVM a linear estimation is made in kernel-induced feature space ($y = w^T\phi(x) + b$). As in SVM, it is necessary to minimize a cost function (C) containing a penalized regression error, as follow:

$$C = \frac{1}{2}w^T w + \frac{1}{2}\gamma\sum_{i=1}^{N} e_i^2 \tag{1}$$

such that:

$$y_i = w^T\phi(x_i) + b + e_i \tag{2}$$

for all $i = 1,\ldots,N$, where ϕ denotes the feature map.

The first part of this cost function is a weight decay which is used to regularize weight sizes and penalize large weights. Due to this regularization, the weights converge to similar value. Large weights deteriorate the generalization ability of the LS-SVM because they can cause excessive variance. The second part of Eq. (1) is the regression error for all training data. The parameter γ, which has to be optimized by the user, gives the relative weight of this part as compared to the first part. The restriction supplied by Eq. (2) gives the definition of the regression error. Eq. (1) and its restriction given by Eq. (2), could be concluded to be a typical problem of convex optimization [14] which might be solved by the Lagrange multipliers method, as follow:

$$L = \frac{1}{2}\|w\|^2 + \gamma\sum_{i=1}^{N} e_i^2 - \sum_{i=1}^{N} \alpha\{w^T \phi(x_i) + b + e_i - y_i\} \tag{3}$$

where

$$y_i = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}, \quad e_i = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_N \end{bmatrix} \quad and \quad \alpha_i = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix}.$$

Obtaining the optimum, that is, carrying out $\partial L(w,b,e_i,\alpha_i)/\partial w$, $\partial L(w,b,e_i,\alpha_i)/\partial b$, $\partial L(w,b,e_i,\alpha_i)/\partial e_i$, $\partial L(w,b,e_i,\alpha_i)/\partial \alpha_i$ and setting all partial first derivatives to zero, generates the weights that are the linear combinations of the training data:

$$\frac{\partial L(w,b,e,\alpha)}{\partial w} = w - \sum_{i=1}^{N} \alpha_i \phi(x_i) = 0 \therefore w = \sum_{i=1}^{N} \alpha_i \phi(x_i) \tag{4}$$

$$\frac{\partial L(w,b,e,\alpha)}{\partial e} = \sum_{i=1}^{N} \gamma e - \alpha = 0 \tag{5}$$

and then

$$w = \sum_{i=1}^{N} \alpha_i \phi(x_i) = \sum_{i=1}^{N} \gamma e_i \phi(x_i) \tag{6}$$

where a positive definite kernel is used as follows:

$$K(x_i, x_j) = \phi(x_i)^T \phi(x_j) \tag{7}$$

An important result of this approach is that the weights (w) can be written as linear combinations of the Lagrange multipliers with corresponding data training (x_i). Substituting the result of Eq. (6) into the original regression line $(y = w^T \phi(x) + b)$, the following result is obtained:

$$y = \sum_{i=1}^{N} \alpha_i \phi(x_i)^T \phi(x) + b = \sum_{i=1}^{N} \alpha_i \langle (\phi(x_i)^T, \phi(x) \rangle + b \tag{8}$$

for a point y_i to be evaluated it is:

$$y_i = \sum_{i=1}^{N} \alpha_i \phi(x_i)^T \phi(x_j) + b = \sum_{i=1}^{N} \alpha_i \langle (\phi(x_i), \phi(x_j) \rangle + b \tag{9}$$

The α vector follows from solving a set of linear equation:

$$M\begin{bmatrix} \alpha \\ b \end{bmatrix} = \begin{bmatrix} y \\ 0 \end{bmatrix} \tag{10}$$

where M is a square matrix given by:

$$M = \begin{bmatrix} K + \frac{I}{\gamma} & 1_N \\ 1_N^T & 0 \end{bmatrix} \tag{11}$$

Where K denotes the kernel matrix with $ijth$ element $K = (x_i, x_j) = \phi(x_i)^T \phi(x_j)$ and I denotes the identity matrix $N \times N$, $1_N = [1 \quad 1 \quad \cdots \quad 1]^T$. Hence, the solution is given by:

$$\begin{bmatrix} \alpha \\ b \end{bmatrix} = M^{-1} \begin{bmatrix} y \\ 0 \end{bmatrix} \tag{12}$$

As demonstrated in Eqs. (11) and (12), all Lagrange multipliers (the support vectors) are usually nonzero, which means that all training objects contribute to the solution. In contrast, with standard SVM the LS-SVM solution is usually not sparse. However, as described by Suykens and J. Vandewalle [13] a sparse solution can be easily achieved via pruning or reduction techniques. Depending on the number of training data set either direct solvers or iterative solvers such as conjugate gradients methods (for large data sets) can be used in both cases with numerically reliable methods.

In applications involving nonlinear regression, it is enough to change the inner product $\langle \phi(x_i), \phi(x_j) \rangle$ of Eq. (9) by a kernel function and the $ijth$ element of matrix K equals $K_{ij} = \phi(x_i)^T \phi(x_j)$. If this kernel function meets Mercer’s condition, the kernel implicitly determines both a nonlinear mapping, $x \to \phi(x)$ and the corresponding inner product $\phi(x_i)^T \phi(x_j)$. This leads to the following nonlinear regression function:

$$y = \sum_{i=1}^{N} \alpha_i K(x_i, x) + b \tag{13}$$

for a point x_j to be evaluated it is:

$$y_j = \sum_{i}^{N} \alpha_i K(x_i, x_j) + b \tag{14}$$

The attainment of the kernel function is cumbersome and it will depend on each case. However, the kernel function is more used as the radial basis function (RBF), $\exp(-(\|x_i - x_j\|^2)/2\sigma^2)$, a simple Gaussian function, and polynomial functions $\langle x_i, x_j \rangle^d$, where σ^2 is the width of the Gaussian function and d is the polynomial degree, which should be optimized by the user, to obtain the support vector. For α of the RBF kernel and d of the polynomial kernel it is of significant importance to do a careful model selection of the tuning parameters, in combination with the regularization constant γ, in order to achieve a good generalization model.

3. MATERIALS AND COMPUTATIONAL METHODS

3.1. HARDWARE AND SOFTWARE

The computations were made with the ASUS Personal Computer (1 GB RAM) that was equipped with the Windows 7 operating system and MATLAB (Version 9.0, Mathwork Inc.). The LS-SVM optimization and model results were obtained using the LS-SVM lab toolbox (Matlab/C Toolbox for Least-Squares Support Vector Machines). The MLR analysis with a stepwise forward selection method was carried out by using the SPSS 21 software. Kennard-Stones program was written in MATLAB according to the algorithm [17, 18]. ChemOffice package (Version 2010) was used to draw the molecular structure and optimization by the AM1. Descriptors were calculated using Dragon software (Milano Chemometrics and QSAR research group, http://www.disat.unimib.it/chm/). These descriptors are calculated using two-dimensional representation of the molecules and therefore geometry optimization is not essential for calculating these types of descriptors.

3.2. DATA SET

The inhibitory activity values of 1-phenyl[2*H*]-tetrahydro-triazine-3-one analogues were taken from literature [2]. The chemical structures of 1-phenyl[2*H*]-tetrahydro-triazine-3-one analogues (Figure 1) and their corresponding inhibitory activity values have been listed in Table 1. In order to assure that training and prediction sets cover the total space occupied by the original data set, it was divided into parts of training and prediction set according to the Kennard-Stones algorithm [17, 18]. The Kennard-Stones algorithm is known as one of the best ways of building training and prediction sets and it has been used in many QSAR studies.

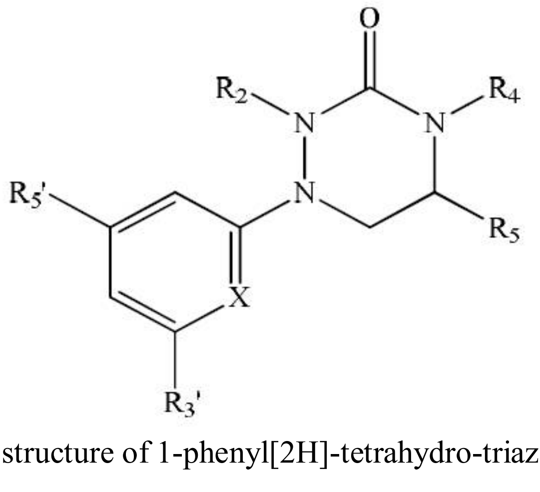

Figure 1. Chemical structure of 1-phenyl[2H]-tetrahydro-triazine-3-one analogues.

Table 1. Structures and observed inhibitory activity of 5-Lipoxygenase of 1-phenyl[2H]-tetrahydro-triazine-3-one analogues.

No.	Substitution						$\log(1/IC_{50})$
	X	R_3'	R_5'	R_2	R_4	R_5	obs[a]
1	CH	H	H	H	H	CH_2OCH_2Ph	6.00
2	CH	H	H	H	H	Bu	5.82
3	CH	H	H	H	H	i-Pr	5.17
4	CH	H	H	H	H	Me(R)	5.17
5[b]	CH	H	H	H	H	Me_2	5.17

6	CH	H	H	H	H	Et	5.16
7[b]	CH	H	H	H	H	Me	4.94
8	CH	H	H	H	H	$CH_2OC_2H_4OMe$	4.85
9	CH	H	H	H	H	Me(S)	4.85
10	CH	H	H	H	H	CO_2Me	4.70
11[b]	CH	H	H	H	H	H	4.68
12	CH	H	OCH_2Ph	H	H	H	5.96
13	CH	H	Br	H	H	H	5.31
14	CH	H	Cl	H	H	H	5.20
15	CH	H	Et	H	H	H	4.89
16	CH	H	SMe	H	H	H	4.85
17[b]	CH	H	Me	H	H	H	4.82
18	CH	H	CF_3	H	H	H	4.77
19	CH	H	F	H	H	H	4.72
20	CH	H	CN	H	H	H	4.43
21	CH	H	OMe	H	H	H	4.33
22	CH	H	NO_2	H	H	H	4.31
23	CH	H	NH_2	H	H	H	3.75
24	CH	H	Br	H	H	Me	5.59
25	CH	H	Cl	H	H	Me	5.57
26	CH	H	F	H	H	Me	5.20
27[b]	CH	H	Me	H	H	Me	4.72
28	CH	H	H	H	C(=O)-i-Pr	H	5.89
29	CH	H	H	H	C(=O)Et	H	5.59
30	CH	H	H	H	C(=O)Me	Me	5.48
31	CH	H	H	H	C(=O)Me	H	5.47
32	CH	H	H	H	OCH_2Ph	Me	5.37
33	CH	H	H	H	OH	Me	5.22
34	CH	H	H	H	OEt	Me	5.13
35	CH	H	H	H	OCH_2Ph	H	5.08
36	CH	H	H	C(=O)Et	C(=O)Et	H	4.90
37	CH	H	H	H	OMe	Me	4.65
38	CH	H	H	C(=O)Me	C(=O)Me	H	4.40
39	N	Br	H	H	H	Me	5.62
40	N	Br	H	H	H	H	5.46
41	N	Cl	H	H	H	Me	5.46
42[b]	N	Me	H	H	H	Me	5.42
43	N	Me	H	H	H	H	5.26
44	N	OMe	H	H	H	Me	5.26
45	N	Cl	H	H	H	H	5.25
46	N	F	H	H	H	Me	5.18
47	N	F	H	H	H	H	5.04
48	N	OMe	H	H	H	H	5.02
49	N	H	H	H	H	Me	4.66
50	N	H	H	H	H	H	4.59
51	CH	H	Cl	H	C(=O)Me	H	5.89
52	CH	H	Cl	H	OH	Me	5.41
53	CH	H	F	H	OH	Me	5.16
54	CH	Me	Me	H	OH	H	5.08
55	CH	F	F	H	H	H	5.05
56	CH	Me	Me	H	H	H	4.92
57[b]	N	Cl	H	H	H	H	5.48
58[b]	CH	H	Cl	H	H	H	5.35
59[b]	CH	H	H	H	H	H	4.77
60	CH	Cl	Me	H	H	H	5.48

[a] Observed inhibitory activity .

[b] The compounds selected as the test set.

3.3. MOLECULAR DESCRIPTORS

A major step in constructing QSAR model is generation of the corresponding numerical descriptors of the molecular structures. Molecular descriptors define the molecular structure and physicochemical properties of molecules by a single number. To calculate the different kinds of theoretical descriptors for each molecule, the Dragon (Milano Chemometrics and QSAR research group, http://www.disat.unimib.it/chm/) software was utilized. The Dragon is able to calculate different molecular descriptors such as constitutional, topological, molecular walk counts, BCUT, Galvez topol. Charge indices, 2D autocorrelations, charge, aromaticity indices, Randic molecular profiles, geometrical, RDF, 3D-MoRSE, WHIM, GETAWAY, functional groups, atom-centered fragments, properties and empirical. In this study, just GETAWAY (geometry, topology, and atom-weights assembly) and WHIM (weighted holistic invariant molecular) descriptors were used. Here, 293 descriptors were calculated by Dragon for each molecule, therefore we have 60×293 data matrix X. The rows and columns of this matrix are the number of molecules and molecular descriptors respectively.

4. RESULTS AND DISCUSSION

4.1. PRINCIPAL COMPONENT ANALYSIS OF THE DATA SET

Principal components analysis (PCA) was performed on the calculated structural descriptors to the whole data set (Table1), for investigation the distribution in the chemical space, which shows the spatial location of samples to assist the separation of the data into training and prediction sets. The PCA results show that three PCs (PC1, PC2 and PC3) describe 81.35% of the overall variances (Figure 2). Since almost all variables can be accounted for the first three PCs, their score plot is a reliable presentation of the spatial distribution of the points for the data set. As can be seen in Figure 2, there is not a clear clustering between compounds. The data separation is very important in the development of reliable and robust QSAR models. The quality of the prediction depends on the data set used to develop the model. For regression analysis, data set was separated into two groups, a training set (51 data) and a prediction set (9 data) according to Kennard-Stones algorithm. As shown in Figure 2, the distribution of the compounds in each subset seems to be relatively well-balanced over the space of the principal components.

4.2. MLR ANALYSIS

The multivariate calibration is a powerful tool for modeling, because it extracts more information from the data and allows building more robust models. Among the descriptors calculated, the most significant molecular descriptors were identified using multiple linear regression analysis with a stepwise forward selection method. According to inhibitory activity data (Table 1), the data classified to training and prediction sets according to Kennard-Stones algorithm and the MLR model was run.

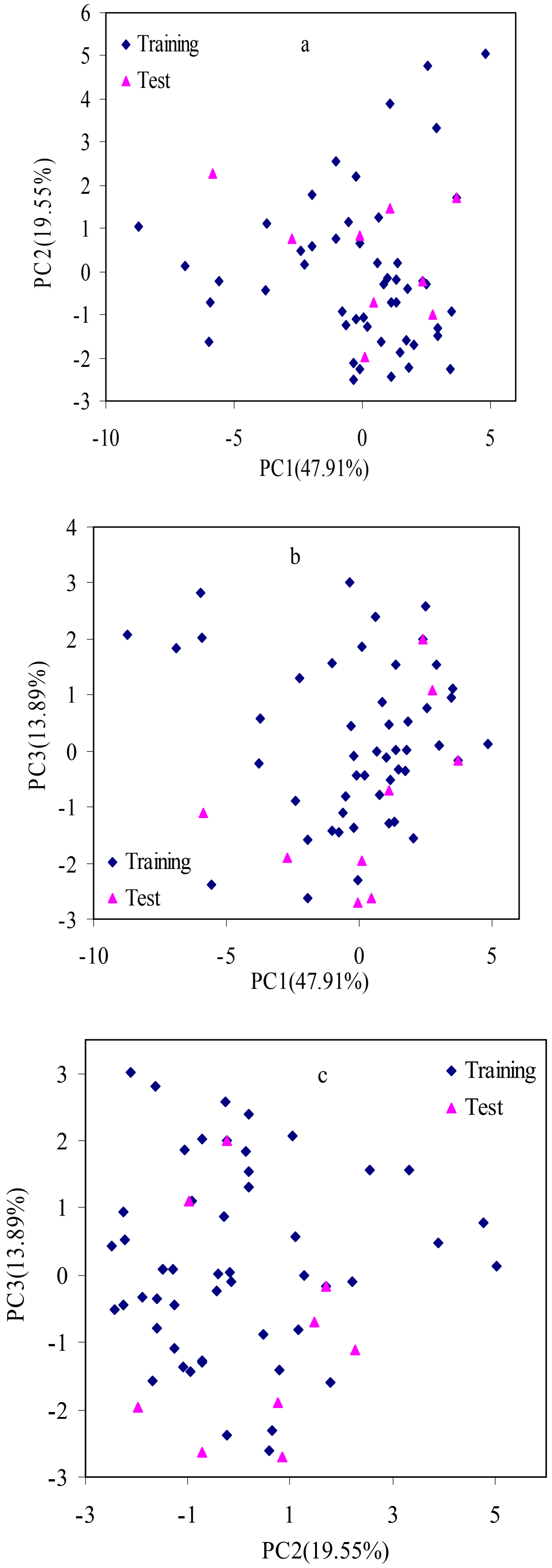

Figure 2. Principal components analysis of the descriptors for the data set, (a) PC2 versus PC1, (b) PC3 versus PC1 and (c) PC3 versus PC2.

The best equation obtained for the inhibitory activity of 1-phenyl[2H]-tetrahydro-triazine-3-one analogues derivatives was:

$$\log(1/IC_{50}) = 3.095 - 1.131R7e - 38.269R6U^{+} - 4.942R1u + 4.897R2u - 5.247P2u + 3.787H2v + 18.425G3e - 0.008Vu$$

As seen, the resulting model has eight significant descriptors. Table 2 shows the calculated descriptors for each molecule, the descriptors coefficients, the standard error of coefficients, the t values for null hypothesis, and their related P values.

Table 2. Results of multiple linear regression analysis.

Notation	Descriptors	Coefficient	S.E.[a] of coefficient	t value	P value
Intercept	-	3.095	2.358	1.312	0.197
R7e	R autocorrelation of lag 7 / weighted by Sanderson electronegativity	-1.131	0.282	-4.018	0.000
$R6U^{+}$	R maximal autocorrelation of lag 6 / unweighted	-38.269	8.865	-4.317	0.000
R1u	R autocorrelation of lag 1 / unweighted	-4.942	0.747	-6.613	0.000
R2u	R autocorrelation of lag 2 / unweighted	4.897	0.794	6.169	0.000
P2u	2nd component shape directional WHIM index / unweighted	-5.247	1.147	-4.575	0.000
H2v	H autocorrelation of lag 2 / weighted by van der Waals volume	3.787	0.455	8.330	0.000
G3e	3rd component symmetry directional WHIM index / weighted by Sanderson electronegativity	18.425	5.821	3.165	0.003
Vu	V total size index / unweighted	-0.008	0.003	-2.209	0.033

[a] Standard error.

4.3. LS–SVM ANALYSIS

LS-SVM was performed with radial basis function (RBF) as a kernel functions. In the model development using LS-SVM and RBF kernel, γ and σ^2 parameters were a manageable task. To determine the optimal parameters, a grid search was performed based on leave-one-out cross-validation on the original training set for all parameter combinations of γ and σ^2 from 0.1 to 10 and 1 to 100, respectively. In Table 3 is shown the optimum γ and σ^2 parameters for the LS-SVM and RBF kernel, using the training sets for 51 inhibitory activity data.

Table 3. Observation and calculation values of log(1/IC_{50}) using MLR and LS-SVM models.

No. of compounds (Table 1)	Observation log(1/IC_{50})	MLR		LS-SVM	
		Predicted	Error (%)	Predicted	Error (%)
5	5.170	4.980	-3.675	5.081	-1.721
7	4.940	4.792	-2.996	4.856	-1.700
11	4.680	4.836	3.333	4.716	0.769
17	4.820	4.851	0.643	4.832	0.249
27	4.720	4.916	4.152	4.771	1.080
42	5.420	5.189	-4.262	5.356	-1.181
57	5.480	5.327	-2.792	5.389	-1.660
58	5.350	5.227	-2.299	5.309	-0.766
59	4.770	4.966	4.109	4.746	-0.503
γ				0.500	
σ^2				10.000	
RMSEP		0.167		0.061	
RSEP (%)		3.315		1.212	

4.4. MODEL VALIDATION AND PREDICTION OF INHIBITORY ACTIVITY

The predictive ability of these methods (MLR and LS-SVM) were investigated by prediction of inhibitory of 9 molecules (their structures are given in Table 1). Validation of predictive ability is another key step in QSAR studies. Several statistical parameters have been used for the evaluation of the suitability of the developed QSAR models for prediction of the property of the studied compounds this include the root mean square error of prediction (RMSEP) and relative standard error of prediction (RSEP), validation through an external prediction set.

$$RMSEP = \sqrt{\frac{\sum_{i=1}^{n}(y_{i,pred} - y_{i,obs})^2}{n}} \tag{15}$$

$$RSEP(\%) = 100 \times \sqrt{\frac{\sum_{i=1}^{n}(y_{i,pred} - y_{i,obs})^2}{\sum (y_{i,obs})^2}} \tag{16}$$

where $y_{i,pred}$ is the predicted of the inhibitory activity using different model, $y_{i,obs}$ is the observed value of the inhibitory activity, and n is the number of compounds in the prediction set. The statistical parameters obtained by these methods are listed in Table 3.

Table 3 shows RMSEP, RSEP and the percentage error for prediction of inhibitory activity of 1-phenyl[2H]-tetrahydro-triazine-3-one analogues. As can be seen, the good results were achieved in LS-SVM model with percentage error ranges from -1.721 to 1.080 for inhibitory activity of 1-phenyl[2H]-tetrahydro-triazine-3-one analogues. The plots of the predicted inhibitory activity versus actual values are shown in Figure 3 for each model (line equations and R^2 values are also shown). The correlation coefficients (R^2) for LS-SVM model were better than the MLR model. Also, it is possible to see that LS-SVM presents excellent prediction abilities when compared with MLR model.

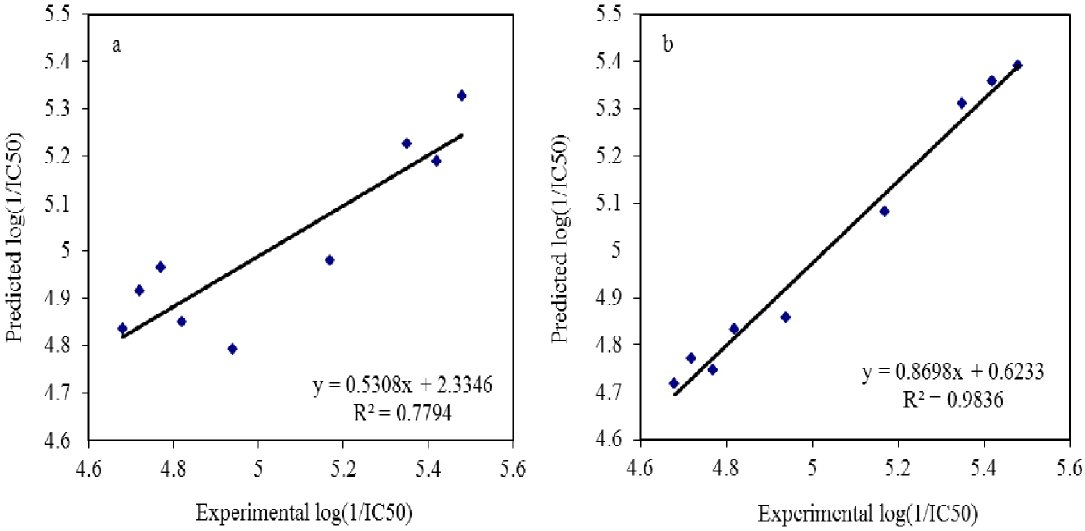

Figure 3. Plots of predicted versus actual log(1/IC_{50}), (a) MLR and (b) LS-SVM.

4.5. MOLECULAR DESIGN

As an application of proposed method, we investigated LS-SVM model to predict the inhibitory activity of four new 1-phenyl[2*H*]-tetrahydro-triazine-3-one analogues whose biological tests were not performed with them yet. Table 4 shows the chemical structure of four new compounds and their inhibitory activity calculated by this proposed method.

Table 4. New structures of 1-phenyl[2H]-tetrahydro-triazine-3-one analogues and predicted log(1/IC_{50}) by LS-SVM.

Number of Design	Substitution						log(1/IC_{50}) Calc.[a]
	X	R_3'	R_5'	R_2	R_4	R_5	
1	N	H	Me	H	H	Me	4.617
2	N	F	H	H	H	Br	6.138
3	CH	Br	H	H	H	Cl	5.856
5	CH	H	OH	H	Cl	H	5.149

[a] Calculated by LS-SVM model.

5. CONCLUSION

Using LS-SVM, a QSAR model has been successfully developed for the prediction of inhibitory activity for 60 compounds. The results well illustrate the power of descriptors in prediction of inhibitory activity of 1-phenyl[2*H*]-tetrahydro-triazine-3-one analogues. The model could predict the inhibitory activity of 1-phenyl[2*H*]-tetrahydro-triazine-3-one analogues derivatives not existed in the modeling procedure accurately. The work, shows that descriptors are capable to recognize the physicochemical information and be can useful to predict the inhibitory activity of the new compounds.

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Three–Center Harary Index and its Applications

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ABSTRACT The Harary index H can be viewed as a molecular structure descriptor composed of increments representing interactions between pairs of atoms, such that their magnitude decreases with the increasing distance between the respective two atoms. A generalization of the Harary index, denoted by H_k, is achieved by employing the Steiner-type distance between k-tuples of atoms. We show that the linear combination $H + \lambda H_3$ is significantly better correlated with a variety of physico-chemical properties of alkanes than H itself.

KEYWORDS Harary index • multicenter Harary index • Steiner distance • molecular graph.

1. INTRODUCTION

Let G be a molecular graph [1] and $v_1, v_2, \ldots, v_n$ be its vertices. The distance [1,2] between the vertices v_i and v_j, denoted by $d(v_i, v_j)$, is the number of edges in (= the length of) a shortest path that connects v_i and v_j. The oldest distance-based molecular structure descriptor is the Wiener index, defined as [3,4]

$$W = W(G) = \sum_{i<j} d(v_i, v_j) . \qquad (1)$$

Although this topological index found numerous chemical applications, a general objection to it is that pairs of vertices at the greatest distance have the greatest contributions to the numerical value of W. Bearing in mind that vertices of a molecular graph represent atoms [1], this property of the Wiener index seemingly contradicts the fact that the interaction between near-lying atoms are greatest. Several attempts were made to eliminate this difficulty [5-7], but the simplest and more efficient solution was achieved by modifying Eq. (1) as

$$H = H(G) = \sum_{i<j} \frac{1}{d(v_i, v_j)} . \qquad (2)$$

Formula (2) was independently conceived by Ivanciuc at al. [8] and Plavšić et al. [9]. The molecular structure descriptor H was named "*Harary index*" (in honor of Frank Harary [10]). Eventually, this index attracted much attention; see the surveys [11,12], the recent book [13], and the recent papers [14–16].

Same as the Wiener index, Eq. (1), the Harary index H, Eq. (2), may also be viewed as a sum of structural increments representing *pairs* of atoms, i.e., *two-center* interatomic interactions. Following an idea outlined in a recent paper [17], one could think of three-center, four-center, etc. interactions that would lead to the following evident multicenter extension of the Harary-index concept:

$$H_3 = H_3(G) = \sum_{i<j<k} \frac{1}{d(v_i, v_j, v_k)} \tag{3}$$

$$H_4 = H_4(G) = \sum_{i<j<k<l} \frac{1}{d(v_i, v_j, v_k, v_l)}$$

and in the general case,

$$H_k = H_k(G) = \sum_{i_1<i_2<\cdots<i_k} \frac{1}{d(v_{i_1}, v_{i_2}, \ldots, v_{i_k})} .$$

In the above formulas, for the multiple-vertex distances we take the standard *Steiner distance* (introduced in graph theory as early as in the 1980s [18]). For details on the Steiner distance see the recent paper [17] or in appropriate monographs [19-21].

In nutshell: The Steiner distance $d(v_{i_1}, v_{i_2}, \ldots, v_{i_k})$ of k distinct vertices $v_{i_1}, v_{i_2}, \ldots, v_{i_k}$ of a graph G, is the number of edges of a connected subgraph of G, with smallest number of edges, containing all the vertices $v_{i_1}, v_{i_2}, \ldots, v_{i_k}$.

The multicenter Harary indices, based on Steiner distances of k-tuples of vertices, will be denoted as H_k. For reasons explained in the subsequent section, in what follows we shall be concerned only with the three-center Harary index H_3.

2. AN AUXILIARY LEMMA

In the general case, the calculation of the Steiner distance $d(v_{i_1}, v_{i_2}, \ldots, v_{i_k})$ of a k-tuple of vertices of a molecular graph is a difficult and computation-extensive task. In the case $k = 3$, this calculation is significantly simplified by means of the following Lemma:

Lemma 1. Let G be a (connected) graph and x, y, z its three distinct vertices. Then the Steiner distance of x, y, z is related to the ordinary distance of these vertices as:

$$d(x, y, z) = \frac{1}{2}\left[d(x, y) + d(x, z) + d(y, z)\right] . \tag{4}$$

Proof. Any connected subgraph of G with the smallest number of edges is necessarily a tree (i.e., it is acyclic). We have to distinguish between two cases: when the three vertices x, y, z are not collinear and when these are collinear, see Figure 1.

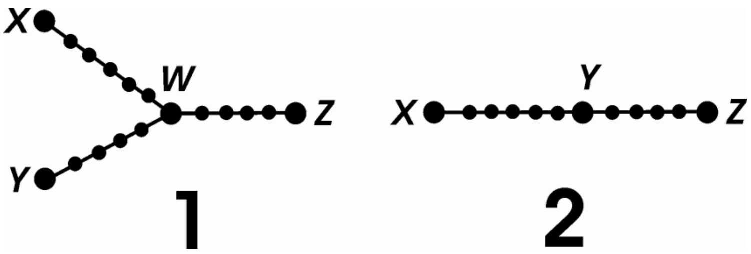

Figure 1. Two different arrangements of the vertices x, y, z in a molecular graph; for details see the proof of Lemma 1.

Case 1: x, y, z are not collinear. Then, using the notation specified in Fig. 1,

$$d(x,y,z) = d(x,w) + d(y,w) + d(z,w) \,. \tag{5}$$

On the other hand,

$$d(x,y) = d(x,w) + d(y,w)$$
$$d(x,z) = d(x,w) + d(z,w)$$
$$d(y,z) = d(y,w) + d(z,w)$$

which yields $d(x,y) + d(x,z) + d(y,z) = 2\left[d(x,w) + d(y,w) + d(z,w)\right]$. Then Eq. (4) follows by bearing in mind (5).

Case 2: x, y, z are collinear. Then, using the notation specified in Fig. 1,

$$d(x,y,z) = d(x,z) \,. \tag{6}$$

Then we have

$$d(x,z) = \frac{1}{2}\left[d(x,z) + d(x,z)\right] = \frac{1}{2}\left[d(x,y) + d(y,z) + d(x,z)\right]$$

and Eq. (4) directly follows from (6).

This completes the proof of Lemma 1.

By means of Lemma 1, the calculation of the three-center Harary index, Eq. (3), becomes quite easy and is of equal (low) complexity as the calculation of the respective Wiener index. Unfortunately, results analogous to Lemma 1 could not be established for $k \geq 4$.

3. NUMERICAL WORK

We first present two results that look rather discouraging. In Figure 2 is shown the correlation between the Harary and three-center Harary indices in the case of isomeric octanes. In Figure 3a is shown the correlation between Harary index and standard enthalpy of formation (ΔH_f^o) of the same set of octanes [22]. In Figure 3b is displayed the analogous plot for the three-center Harary index. In view of the very good linear correlation between H and H_3 (cf. Figure 2), there is no statistical difference between the two correlations shown in Figure 3, and both are disappointingly weak.

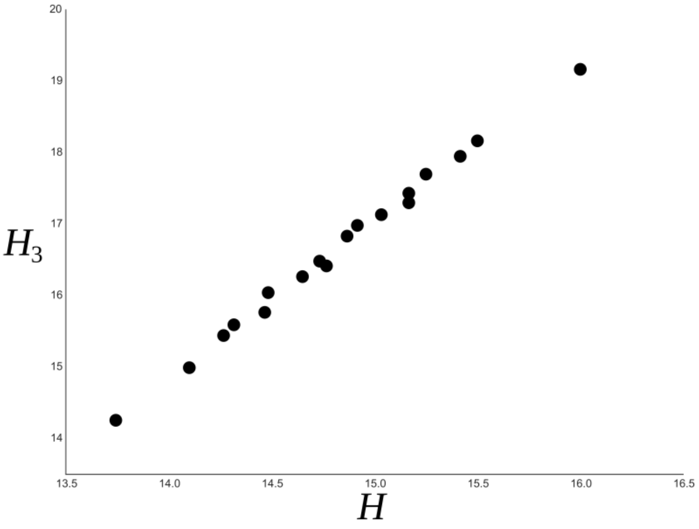

Figure 2. Correlation between the three-center Harary index H_3 , Eq. (3), and the ordinary Harary index H, Eq. (2) for the set of isomeric octanes (18 data points); the correlation coefficient is $R = 0.9980$.

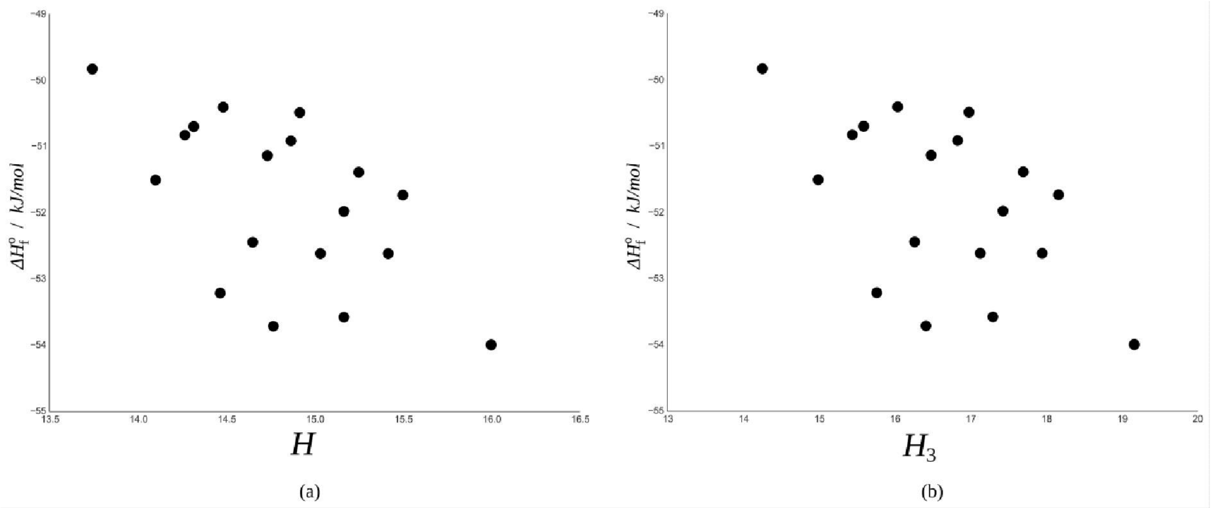

Figure 3. (a) Correlation between the standard enthalpy of formation (ΔH_f^o) of isomeric octanes [22] and the ordinary Harary index H ; $R = -0.576$.
(b) Analogous correlation with the three-center Harary index H_3 ; $R = -0.528$.

A remarkable improvement is obtained by means of the linear combination of the two Harary indices, namely $H + \lambda H_3$, shown in Figure 4, where the optimized value $\lambda = -0.443$ is used for the parameter λ .

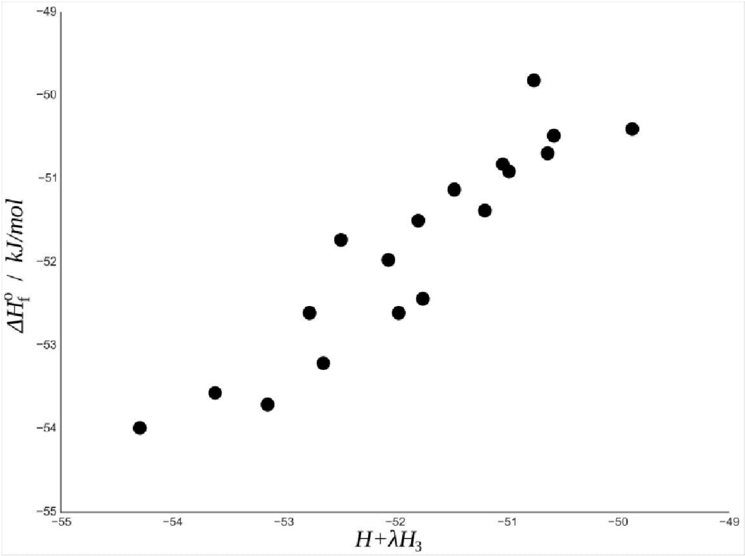

Figure 4. Correlation between the standard enthalpy of formation (ΔH_f^o) of isomeric octanes [22] and the linear combination $H + \lambda H_3$ of the two Harary indices. The best results are obtained for $\lambda = -0.433$ in which case the correlation coefficient increases to $R = 0.928$.

Analogous improvements have been found also in the case of a number of other physico-chemical properties of octanes. The respective statistical data are collected in Table 1.

Property	$R(H)$	$R(H_3)$	$R(H+\lambda H_3)$	λ
ΔH_f^o	–0.576	–0.542	0.928	–0.433
S^o	–0.929	–0.914	0.954	–0.356
ΔH_{ev}	–0.779	–0.745	0.928	–0.414
BP	–0.573	–0.533	0.831	–0.429
CT	–0.111	–0.063	0.756	–0.451
CP	0.505	0.540	0.754	–0.483
$\log P$	–0.184	–0.192	0.223	–0.503

Table 1. Correlation coefficients for the correlation between physico-chemical properties of octane isomes [22] and Harary index ($R(H)$), three-center Harary index ($R(H_3)$), and the linear combination thereof ($R(H+\lambda H_3)$); ΔH_f^o = standard enthalpy of formation, S^o = standard entropy, ΔH_{ev} = enthalpy of evaporation, BP = boiling point at atmospheric pressure, CT = critical temperature, CP = critical pressure, $\log P$ = logarithm of octanol/water partition coefficient; in the last column is the optimized value of the parameter λ for which $R(H+\lambda H_3)$ is maximal.

4. DISCUSSION AND CONCLUDING REMARKS

If the topological indices H and H_3 were exactly linearly correlated, then their linear combination would not result in any improvement. From the data shown in Table 1 we see that in some cases significant improvements are obtained, which may be viewed as a kind of (convenient) surprise. This especially is the case for formation enthalpy, critical temperature, and critical pressure. Remarkably, whereas the indices H and H_3 are completely uncorrelated with critical temperature, i.e., $R(H) \approx R(H_3) \approx 0$, their linear combination results in a moderately good correlation, $R(H + \lambda H_3) > 0.75$.

In all cases, the linear combination of H and H_3 improves the quality of the correlations. However, in some cases, the gain is minor and insignificant. This (necessarily) happens for properties that are well correlated with H and H_3 (e.g., entropy), but also when the initial correlations are weak (e.g. partition coefficient).

A noteworthy fact is that the optimized value of the parameter λ is nearly equal for all physico-chemical properties examined, and is always negative-valued.

The Harary index is constructed so as to take into account (in a rather rough manner) interactions between pairs of atoms. In the case of usually employed molecular graphs, these are pairs of carbon atoms. At the first glance, by means of the three-center version of the Harary index, some more subtle interatomic interactions might be also taken into account. However, the fact that the parameter λ is relatively large and always negative, indicates that the ordinary Harary index seems to overestimate the interactions between pairs of atoms. Thus, the principal role of H_3 would be to provide a compensation for the intrinsic error of the Harary index. As we could see, this compensation is often very efficient.

From a practitioner's point of view, neither the original Harary index, nor its version improved by the three-center index, are sufficient to accurately reproduce a physico-chemical (or any other) property of the considered organic compounds. This is clearly seen by inspecting Figures 2 and 3. This apparent deficiency of graph-based structure descriptors is nowadays well understood and individual descriptors are nowadays hardly ever used for modeling properties of organic molecules. The successful strategy is to simultaneously use several such descriptors and construct QSPR/QSAR models [4,23–25]. The interested reader is referred to the recent survey [25] in which the design of several commercially interesting pharmacologically active substances (including those with anti-cancer activity) is described.

The present studies indicate that the efficiency of QSPR/QSAR models would be much improved if instead of the Harary index, its combination with three-center Harary index would be utilized.

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Investigation the Effect of Nanocomposite Material on Permeation Flux of Polyerthersulfone Membrane using a Mathematical Approach

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ABSTRACT Integrally skinned asymmetric membranes based on nanocomposite polyethersulfone were prepared by the phase separation process using the supercritical CO_2 as a nonsolvent for the polymer solution. In present study, the effects of temperature and nanoparticle on selectivity performance and permeability of gases has been investigated. It is shown that the presence of silica nanoparticles not only disrupts the original polymer chain packing but also alters the chemical affinities of penetrants in polyethersulfone matrices. Because, in the presence of hydrophilic silica, CO_2 affinity filler, hydrogen-bond interactions between the oxygen atoms of carbon dioxide and the hydrogen atoms of hydroxyl group on the nanosilica surface would take place at the interface and thus solubility and consequently permeability towards CO_2 are higher in comparison with CH_4 for the membranes. Furthermore, in present study, a novel mathematical approach has been proposed to develop a model for permeation flux and selectivity performance of the membrane using Support Vector Machine.

SVM is employed to develop model to estimate process output variables of a nanocomposite membrane including permeation flux and selectivity performance. Model development that consists of training, optimization and test was performed using randomly selected 80%, 10%, and 10% of available data respectively. Test results from the SVM based model showed to be in better agreement with operating experimental data compared to other developed mathematical model. The minimum calculated squared correlation coefficient for estimated process variables is 0.99. Based on the results of this case study SVM proved that it can be a reliable accurate estimation method.

KEYWORDS Nanocomposite material • polyerthersulfone membrane • silica nanoparticles • Support Vector Machine (SVM).

1. INTRODUCTION

Support Vector Machine introduced first by Vapnik, is a supervised learning method with associated learning algorithm that analyzes data and recognizes patterns of input/output data. In recent years, ANN has been demonstrated to be a substitute for deterministic modeling and estimation methods with good potentials to be explored.

SVM is based on the structural risk minimization principle from computational learning theory. It is one of the most sophisticated non-parametric supervised classifiers available today, with many different configurations depending on kernel function used to generate transform function that maps input space into output space. Commonly, several functions including linear, polynomial, Radial Basis Function (RBF) and multilayer perceptron are used as the kernel function in SVM. By the use of kernels necessary computations are performed directly in the input space .Although, it is mostly considered as a linear algorithm in a high dimensional feature space, it does not necessitate the practical input/output mapping problem to be a high dimensional space problem. A brief discussion on mathematical basis of SVM is presented here that helps understanding the way SVM works and the features that render it superiority over other learning algorithms.

2. MATHEMATICAL MODEL

Pattern recognition or classification can be performed by SVM in a data set consisting of N data point $\{x_k, y_k\}$ $k = 1,2, \ldots, N$ where x_k is a p-dimensional vector and y_k can take one of the two values, either +1 or -1 (i.e., $y_k \epsilon \{+1, -1\}$ indicating the class to which the point x_k belongs. In their basic form, they learn a linear hyperplane that separates a set of positive samples from a set of negative samples with maximum margin. Consider Figure 1 which shows two possible separating hyperplanes and their associated margins. Both hyperplanes can correctly classify all the given data. However, we expect the hyperplane with the larger margin to be more accurate in classifying new data than the hyperplane with the smaller margin. This is the reason that SVM searches for the hyperplane with the largest margin.

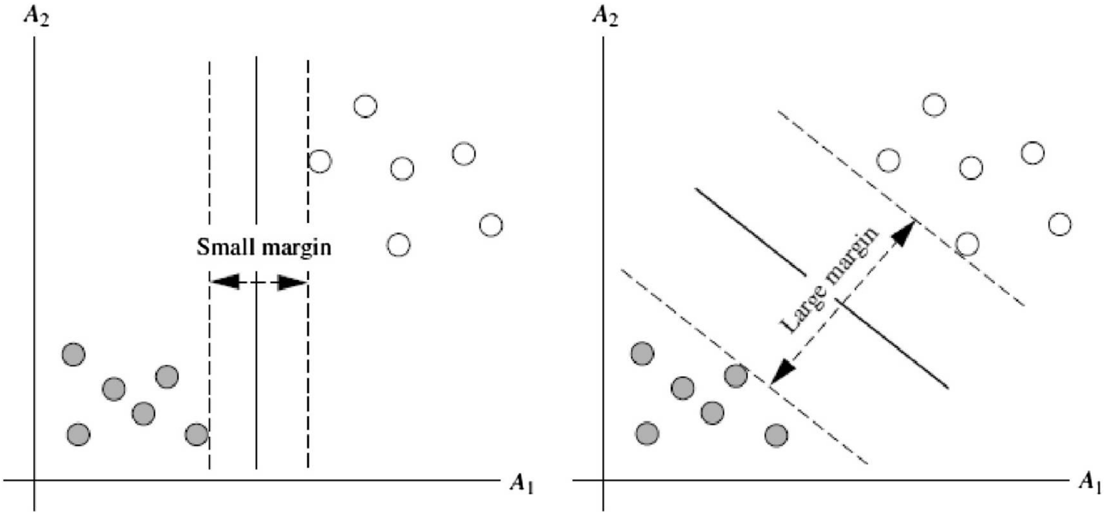

Figure 1. Support Vector Machine Classifier.

A separating hyperplane can be written as $w.x - b = 0$ [1, 2], where w is the normal vector to the hyperplane and b represents the offset of the hyperplane from origin that is referred to as bias. The offset along the vector w from the origin can be determined by $b/_{||w||}$. As shown in Figure 2, for the cases that the training data are linearly separable, two hyperplanes can separate the data in a way that there are no data points between them. Obviously these hyperplanes can be described as:

$$w.x - b = 1 \tag{2}$$

$$w.x - b = -1 \tag{3}$$

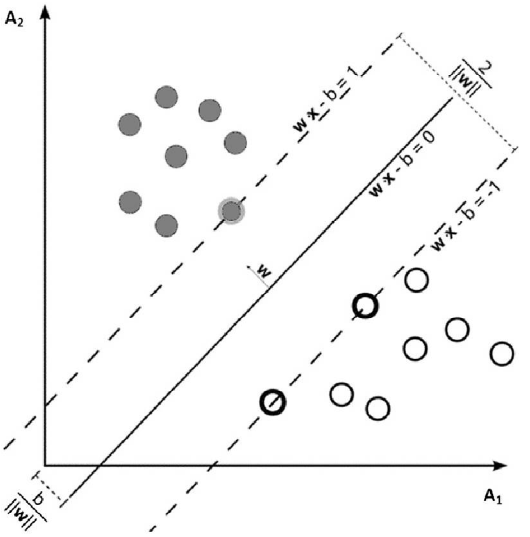

Figure 2. Hyperplane Definition.

By using geometry, one can show that distance between these two hyperplanes is $^{2}/_{||w||}$, so the problem of ||w|| minimization is required to maximize hyperplane margin. It is also required to prevent data points from falling into the margin, and other necessary constraints are imposed as:

w.x_k–b ≥ 1	For x_k of the first class	(4)
w.x_k–b ≤ –1	For x_k of the second class	(5)

That can be rewritten as:

$$y_i(w.x_k - b) \geq 1 \qquad \text{For } all \;\; 1 \leq k \leq N \tag{6}$$

Constraint minimization of ||w|| is thus required to develop an ideal classifier. Such minimization problem is difficult to solve, however it is possible to substitute 0.5 $||w||^2$ instead of ||w|| in problem. It was shown that, minimization problem can be formulated as:

$$\min_{w,b}\max_{a\geq 0}\left\{\frac{1}{2}||w||^2 - \sum_{i=1}^{N} a_i\,(y_i(wx - b) - 1)\right\} \tag{7}$$

where α_i is Lagrangian multiplier that helps in finding the local minimum or maximum of a function. The problem of Eq. 7 can be solved by standard quadratic programming techniques that results in finding normal vector to the hyperplane as presented in Eq. 8:

$$w = \sum_{k=1}^{n} a_i \, y_i x_i \tag{8}$$

Input/output support vector machine model with the general form of $y = f(x)$ takes the form of Eq.9 in feature space:

$$f(x) = \sum_{k=1}^{N} a_i \, . K(x, x_k) + b \tag{9}$$

where $f(x)$ represents output vector and $K(x, x_k)$ is the kernel function calculated from the inner product of the two vectors x and x_k in the feasible region built by the inner product of the vectors $\Phi(x)$ and $\Phi(x_k)$ as follows:

$$K(x, x_k) = \Phi(x)^{r} . \, \Phi(x_k) \tag{10}$$

Among choices for Kernel function the Radial Basis Function (RBF) Kernel that is used extensively has been applied in this work that is presented in Eq. 11,

$$K(x, x_k) = \exp\left(\frac{-||x_k - \mathrm{x}||^2}{\sigma^2}\right) \tag{11}$$

where σ is kernel parameter to be determined by an external optimization algorithm during the internal SVM calculations. Bias, b, is usually determined by using primal constraints as:

$$\mathrm{b} = -\left(\tfrac{1}{2}\right)\left[\max_{\{i, y_i = -1\}}\left(\textstyle\sum_{j \epsilon \{SV\}}^{m} y_i a_i \, K(x_i, x_j)\right)\right] + \min_{\{i, y_i = -1\}}\left(\textstyle\sum_{j \epsilon \{SV\}}^{m} y_i a_i \, K(x_i, x_j)\right) \tag{12}$$

Lagrangian multipliers, a_i, can be calculated by solving following quadratic programming problem:

$$\omega(a) = \textstyle\sum_{i=1}^{N} a_i - \frac{1}{2}\sum_{i,j=1}^{N} a_i a_j y_i y_j K(x_i, x_j) \tag{13}$$

Subject to constraints $0 \leq a_i \leq \gamma$, $i = 1, \ldots, N$, where γ is regularization parameter and controls the tradeoff between complexity of the support vector machine model and the number of non-separable points. This compact formulation of quadratic optimization has been proved to have a unique solution. In conclusion, the SVM takes the form of the constrained optimization problem of Eq. 14 in order to obtain the optimum value of γ

$$\min_{\omega, \beta, \xi_i \xi_i^*} \frac{1}{2} ||\omega||^2 + \gamma . \textstyle\sum_{i=1}^{N} (\xi_i, \xi_i^*) \tag{14}$$

Subject to

$$\begin{array}{ll} y_i - \omega^T x_i - b \leq \varepsilon + \xi_i & t = 1, \ldots, N \\ \omega^T x_i + b - y_i \leq \varepsilon + \xi_i^* & t = 1, \ldots, N \\ \xi \geq 0 & t = 1, \ldots, N \\ \xi_i \geq 0 & t = 1, \ldots, N \end{array}$$

where ε is the precision threshold and ξ_i, ξ_i^* represent the slack variables with nonnegative values to ensure feasible constraints. The first term in Eq. 14 represents model complexity while the second term represents the model accuracy or error tolerance. The Mean Square Error (MSE) and Mean Absolute Error (MAE) as defined by Eqs. 15 and 16 are used to calculate prediction error of the developed SVM model.

$$\mathrm{MSE} = \frac{\sum_{i=1}^{n}(O_i - T_i)^2}{n} \tag{15}$$

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}|O_i - T_i| \tag{16}$$

where O_i is the simulation results of SVM model, T_i represents real time plant data of the natural gas sweetening plant and n denotes the number of the data used for model evaluation.

3. RESULTS AND DISCUSSION

The Figurs 3, 4 show the effect of nanoparticle on the CO_2 permeation of an integrally skinned asymmetric polyethersulfone membrane formed at T=45°C, P=100 bar, DMAc/PES mass ratio of 2.5 and the depressurization rate of 1.83 bar/min. The incorporation of silica nanoparticle in the membranes results in further increase in permeability towards CO_2 compared to CH_4 and thus increases the membrane selectivity. It is believed that the presence of silica nanoparticles not only disrupts the original polymer chain packing but also alters the chemical affinities of penetrants in polyethersulfone matrices. Because, in the presence of hydrophilic silica, CO_2 affinity filler, hydrogen-bond interactions between the oxygen atoms of carbon dioxide and the hydrogen atoms of hydroxyl group on the nanosilica surface would take place at the interface and thus solubility and consequently permeability towards CO_2 are higher in comparison with CH_4 for the membranes.

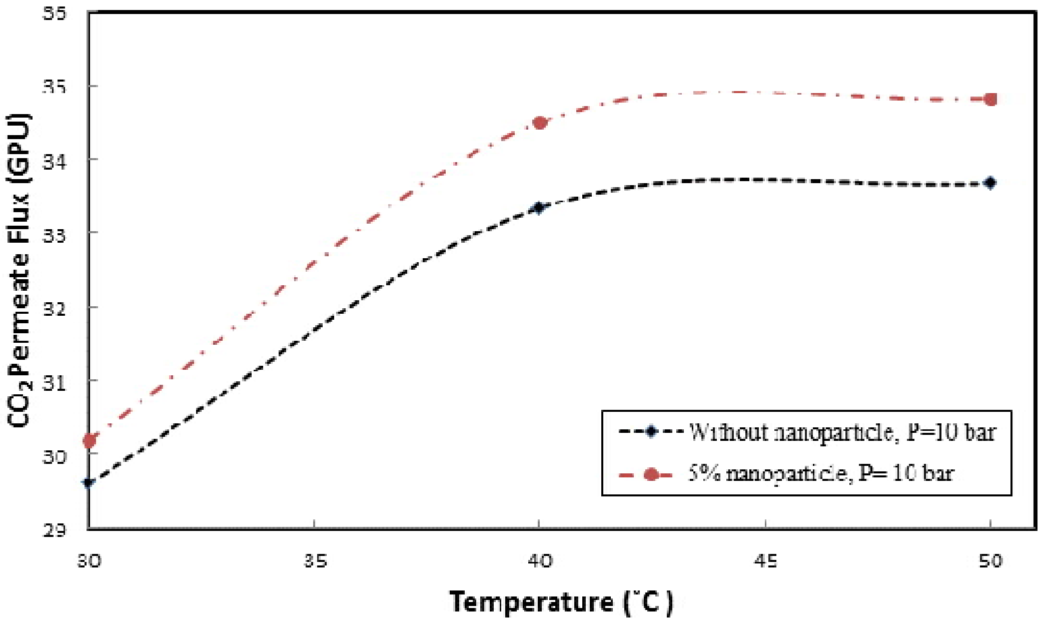

Figure 3. Effect of silica nanoparticle on the CO_2 permeation of the integrally skinned polyethersulfone membrane.

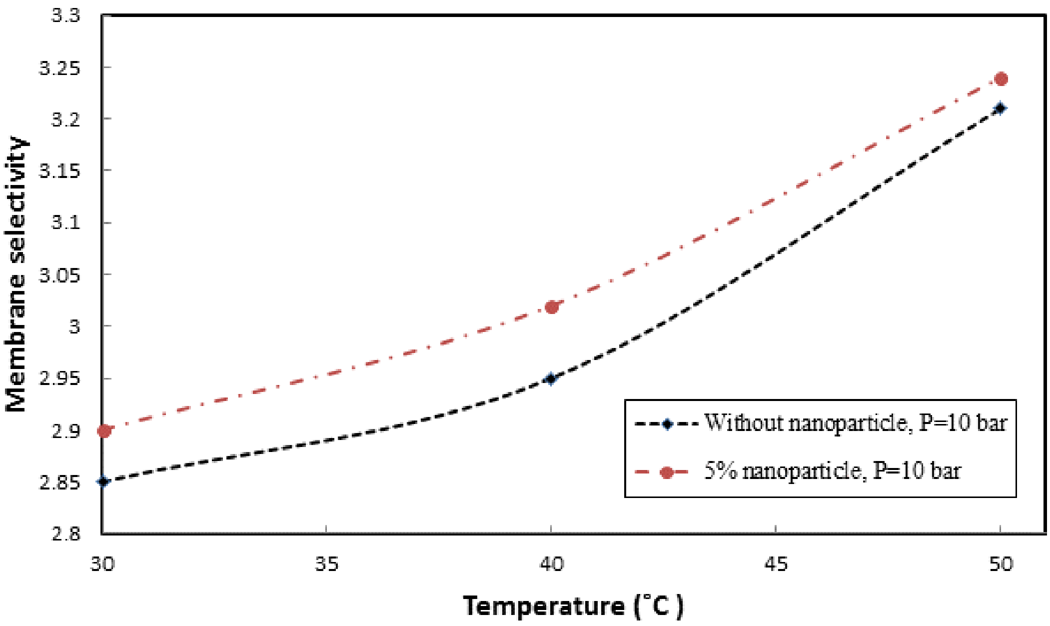

Figure 4. Effect of silica nanoparticle on membrane selectivity of the integrally skinned polyethersulfone membrane.

The operating plant data collected over the span of one year is used in this case study. The data has been normalized between -1 and +1 to prevent truncation error due to wide ranges of numerical values for input/output variables to be included in the SVM model. Since the model development is based on normalizing data, it is necessary to map input data to normalized space accordingly. Normalized model output should also be mapped into the space of real values for output variable to be compared to operating plant data. To develop input/output model the calculation procedure of section 3 that is programmed in Matlab environment is executed on an Intel dualcore2.40 GHz processor accompanied by 4G RAM that it took around 12 hours to get convergence. Convergence indicates that optimum model is achieved; however, it does not guarantee accuracy of model predictions. To ensure model reliability the input variables of test data subset are entered to the developed model and model predictions are validated against experimental data and are also compared with ANN model prediction where available. The ANN based model is of feed-forward back propagation type and was developed using the same training data that is used in this research work.

4. CONCLUSION

The effects of experimental operating conditions such as the temperature and the presence of silica nanoparticles in the structure of dense nanocomposite layers were investigated. It was found that, it is possible to induce a very-controlled asymmetry in a dense film and pore sizes by changing the temperature and pressure. Also, presence of silica nanoparticle proved to increase the permeability of CO_2 and thus the membrane selectivity. Also this study demonstrates the applicability of SVM to develop accurate input/output model of the operational variables of ananocomposite membrane. The kernel parameters for developed model are determined and model predictions are compared with those obtained from another mathematical model. Beside the general advantages that are cited for SVM over ANN as an input/output modeling tool, the predicted data in this study showed better performance of support vector machine over artificial neural networks in terms of accuracy. The numerical values of AAD% calculated showed a minimum 12% improvement gained by SVM over ANN that is of great importance if the predicted data are to be used for monitoring and/or control purposes. This study reveals some the application potentials of SVM as a modeling tool in oil and gas industries that requires much more attention to be fully understood.

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On The Generalized Mass Transfer with a Chemical Reaction: Fractional Derivative Model

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ABSTRACT: In this article using the inverse Laplace transform, we show analytical solutions for the generalized mass transfers with (and without) a chemical reaction. These transfers have been expressed as the Couette flow with the fractional derivative of the Caputo sense. Also, using the Hankel contour for the Bromwich's integral, the solutions are given in terms of the generalized Airy functions.

Keywords: Lévêque Problem, Laplace transform, Generalized Airy functions, Fractional derivative.

1. INTRODUCTION

The mass transfer operations play a critical role in chemistry and other related science especially in chemical engineering. These operations are closely connected with the analogous problems of the convective heat transfer from non-isothermal surfaces. When a system contains more than one component whose concentration varies from one location to another, there is a natural propensity for mass to be transferred. There are many transfer operations in the literature such as solid dissolving in a liquid, gas absorption in a liquid and etc. which provides wide class of researches in chemical and energy sciences. For example in [7], analytical solutions and asymptotic expressions are proposed for homogenous and heterogeneous chemical reactions. Elperin et al. [11] have been solved the problem of mass transfer with a heterogeneous chemical reaction of the first order in boundary layer flows on non-newtonian power-low fluids.

Luchko and Punzi presented physical behavior behind the anomalous processes described by the continuous time random walk (CTRW) model and discussed on its feasibility for modeling of heat transform processes heterogeneous media [13]. Also, they deduce a macroscopic model in form of a generalized fractional diffusion equation from the CTRW model on the microscopic level. Oldham demonstrated that that the electric current is linearly related to the temporal semiderivative of the concentrations at the electrode of the species involved in the electrochemical reaction [14].

The problem of mass transfer with (without) an irreversible chemical reaction in different flows has been discussed in the literature and has been mostly presented in the Newtonian and non-Newtonian liquids, or in the case of permeable surfaces. This problem can be formulated in the following form [7], [9, 10], [11]

$$(b+\alpha y)\frac{\partial u}{\partial x}=D\frac{\partial^2 u}{\partial y^2}-ku,\ \ D>0, a, b, k\in \mathrm{R}, \tag{1–1}$$

$$u(0,y)=0, u(x,0)=u_0, \tag{1–2}$$

$$\lim_{y\to\infty} u(x,y)<\infty. \tag{1–3}$$

A short treatise of the above equation with different situations may be considered as [7]:

- In case $a=0$ and $b\neq 0$, it is known as the uniform (plug) flow.
- In case $a\neq 0$ and $b=0$, it is known as the Couette flow.
- In case $a\neq 0$ and $b\neq 0$, it is known as the Couette flow with moving interface.

For the above three cases, if we set $k=0$, then this mass transfer is interpreted without a chemical reaction and for $k\neq 0$, it is considered as a homogenous chemical reaction. For solving this problem, the Laplace integral transform method has been proposed which leads to the analytical solutions with the closed form and corresponding asymptotic expressions. For these solutions, the Airy function of the first kind [19]

$$Ai(y)=\frac{1}{\pi}\int_0^\infty \cos(yr+\frac{r^3}{3})dr, \tag{1–4}$$

plays an important role for determining the structures and forms of them. This function is appeared in the inverse Laplace transform of the Bromwich's integral on the Hankel contour, see Figure 1 and references [7],[18].

As generalization of the problem (1–1), in this paper, first we consider the following partial differential equation with the higher order derivatives

$$\left(b+ay\right)\frac{\partial u}{\partial x}=D_n\frac{\partial^{2n} u}{\partial y^{2n}}-ku,\ \ D_n=\left(-1\right)^{n+1}, a, b, k\in \mathrm{R},\ n\in \bullet, \tag{1–5}$$

$$u(0,y)=0, u(x,0)=u_0, \tag{1–6}$$

$$\lim_{y\to\infty} u(x,y)<\infty. \tag{1–7}$$

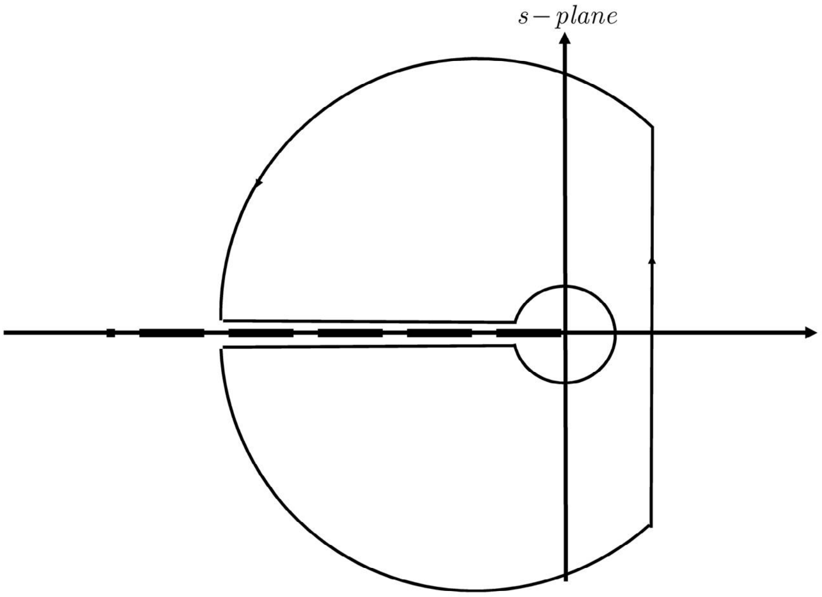

Figure 1. The Hankel Contour.

and show that the solution of this problem is writhen in terms of the generalized Airy function [1]

$$\mathrm{A}_{2n+1}(y)=\frac{1}{\pi}\int_0^{\infty}\cos(yr+\frac{r^{2n+1}}{2n+1})\,dr. \qquad (1-8)$$

In second step, we modify the solution of problem (1−5) with respect to the fractional derivative in the Caputo sense [17]

$$({}^{C}D_x^{\alpha}f)(x)=\frac{1}{\Gamma(n-\alpha)}\int_0^x(x-s)^{n-\alpha-1}f^{(n)}(s)ds,\, n-1<\alpha\le n, \qquad (1-9)$$

for the following problem

$$\left(b+ay\right){}^{C}D_a^{\alpha}u=D\frac{\partial^{2n}u}{\partial y^{2n}}-ku, 0<\alpha\le 1. \quad (1-10)$$

To express our motivation, in Section 2 we survey the preliminaries properties of the generalized Airy functions (1−8) and in next sections we solve the problems (1−5) and (1−10) in different cases of parameters a,b,k using the Laplace transform. The solutions are obtained with respect to the Bromwich's integral on the Hankel contour in terms of the generalized Airy functions.

Table 1. Positive zeros of $\mathrm{A}_{2n+1}(x)$ function for $n = 1,2,3,4$.

$n=1$	$A_3(x)$	-
$n=2$	$A_5(x)$	$\lambda_{21} = 2.754254$
$n=3$	$A_7(x)$	$\lambda_{31} = 2.65450, \lambda_{32} = 5.35923$
$n=4$	$A_9(x)$	$\lambda_{41} = 2.65927, \lambda_{42} = 5.33275, \lambda_{43} = 7.97432$

2. THE GENERALIZED AIRY FUNCTIONS

The generalized Airy function (1–8) is the solution of ordinary differential equation of order $2n$

$$(-1)^{n+1} y^{(2n)} - xy = 0, \quad x \in \mathrm{P}. \tag{2–1}$$

This solution can be obtained using the Laplace integral method

$$y(x) = \int_C e^{xz} v(z) dz, \tag{2–2}$$

as

$$y(x) = \int_C e^{xz - \frac{z^{2n+1}}{2n+1}} dz, \tag{2–3}$$

where contour C is chosen such that the function $v(z)$ must vanish at boundaries. After deformation and normalization of integral (2-3), we rewrite the y as the $\mathrm{A}_{2n+1}(x)$ function as follows

$$\mathrm{A}_{2n+1}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ixz + i\frac{z^{2n+1}}{2n+1}} dz, \tag{2–4}$$

$$= \frac{1}{\pi} \int_0^{\infty} \cos(xz + \frac{z^{2n+1}}{2n+1}) dz, \tag{2–5}$$

with value [1]

$$\mathrm{A}_{2n+1}(0) = \frac{\Gamma(\frac{1}{2n+1}) \cos(\frac{\pi}{2(2n+1)})}{(2n+1)^{\frac{2n}{2n+1}}}. \tag{2–6}$$

Figure 2 shows the behavior of the $A_{2n+1}(x)$ function for $n = 1,2,3,4$ which is similar to the Airy function. It is obvious that the $\mathrm{A}_{2n+1}(x)$ function has infinite negative roots on the negative semiaxes and $n-1$ positive roots on positive semiaxes, see Table 1 for some positive roots of the $\mathrm{A}_{2n+1}(x)$ function. Also, for more applications and contributions of this function in partial fractional differential equations especially higher order heat equation

$$\frac{\partial}{\partial t}u(x,t)=\frac{\partial^n}{\partial x^n}u(x,t),\quad u(x,0)=u_0(x),\tag{2–7}$$

see [2–5], [6], [12] [15, 16].

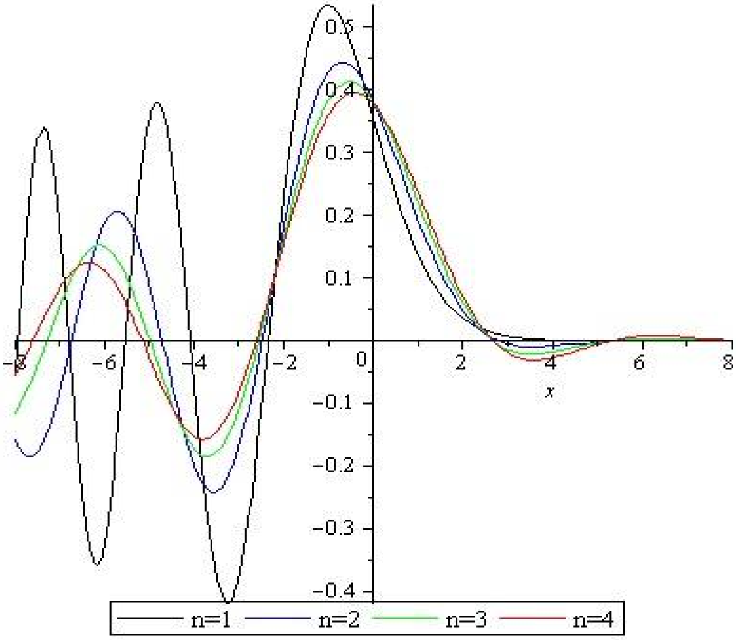

Figure 2. The generalized Airy functions for $n=1,2,3,4$

3. THE GENERALIZED MASS TRANSFER IN COUETTE FLOW

In this section we start with a theorem for the inverse Laplace transform of multi-valued function $F(s)$. We assume that the point $s=0$ is a branch point and F has no poles, then the inverse Laplace transform of $F(s)$, can be computed by means of the integral of a real-valued function.

Theorem 3.1 (***Titchmarsh theorem*** [*8*]) Let $F(s)$ be an analytic function which has a branch cut on the real negative semiaxis, furthermore $F(s)$ has the following properties

$$F(s)=O(1),\qquad |s|\to\infty,$$

$$F(s)=O\left(\frac{1}{|s|}\right),\qquad |s|\to 0,$$

for any sector $|arg(s)| < \pi - \eta$ where $0 < \eta < \pi$. Then the inverse Laplace transform of $F(s)$, can be written as the Laplace transform of the imaginary part of the function $F(re^{-i\pi})$

$$f(x) = L^{-1}\{F(s);x\} = \frac{1}{2\pi}\lim_{s\to 0}\int_{-\pi}^{\pi} \varepsilon F(\varepsilon e^{i\theta})e^{i\theta + x\varepsilon e^{i\theta}}d\theta - \frac{1}{\pi}\int_0^{\infty} e^{-rx}\Im(F(re^{-i\pi}))dr. \quad (3\text{–}1)$$

3.1 THE COUETTE FLOW WITHOUT CHEMICAL REACTION: THE GENERALIZED LÉVÊQUE PROBLEM

Problem 3.2 *We consider a mass transfer without chemical reaction which is known as the Lévêque problem in the literature* [7]. *In this case we generalize and reformulate it with equation* (*1–5*) *as*

$$\frac{\partial u}{\partial x} = D_n \frac{\partial^{2n} u}{\partial y^{2n}}, \quad n \in \mathrm{N}, \quad (3\text{–}2)$$

$$u(0,y) = 0, u(x,0) = u_0, \quad (3\text{–}3)$$

$$\lim_{y\to\infty} u(x,y) < \infty. \quad (3\text{–}4)$$

For solving this problem, we apply the Laplace transform on both sided of equation (3–2) with respect to x

$$\tilde{u}(s,y) = \int_0^{\infty} e^{-sx}u(x,y)dx, \quad (3\text{–}5)$$

and use the boundary condition to derive the relation

$$D_n \frac{\partial^{2n}\tilde{u}}{\partial y^{2n}} - sy\tilde{u} = 0. \quad (3\text{–}6)$$

In view of the finiteness of solution and $2n$ linear independent solutions of the above differential equation, we get the solution with respect to the $\mathrm{A}_{2n+1}(x)$ function in the following form

$$\tilde{u}(s,y) = C(s)\mathrm{A}_{2n+1}(s^{\frac{1}{2n+1}}y). \quad (3\text{–}7)$$

Applying other boundary condition, we obtain the unknown coefficient $C(s)$, that is

$$\tilde{u}(s,y) = \frac{u_0}{s\mathrm{A}_{2n+1}(0)}\mathrm{A}_{2n+1}(s^{\frac{1}{2n+1}}y). \quad (3\text{–}8)$$

The inverse of (3–8) is obtained by considering the Bromwich's integral

$$u(x,y) = \frac{u_0}{2\pi i\mathrm{A}_{2n+1}(0)}\int_{c-i\infty}^{c+i\infty} \frac{1}{s}\mathrm{A}_{2n+1}(s^{\frac{1}{2n+1}}y)e^{sx}ds, \quad (3\text{–}9)$$

which has a branch point at the origin. By using the suitable change of the Bromwich contour of integration (Figure 1) and applying the Titchmarsh Theorem 3.1, we get the solution as

$$u(x,y) = u_0 - \frac{u_0}{\pi \mathrm{A}_{2n+1}(0)} \int_0^\infty \frac{1}{r} e^{-rx} \Im\{\mathrm{A}_{2n+1}(r^{\frac{1}{2n+1}} e^{-i\frac{\pi}{2n+1}} y)\} dr. \tag{3-10}$$

For simplification of the above solution for $n = 1$ in terms of the Bessel functions, first consider the following identity in terms of the modified Bessel functions [7]

$$Ai(x) = \frac{\sqrt{x}}{3}\left(I_{-\frac{1}{3}}\left(\frac{2}{3}x^{\frac{3}{2}}\right) - I_{\frac{1}{3}}\left(\frac{2}{3}x^{\frac{3}{2}}\right)\right),$$

and use the Theorem 3.1 to obtain the solution in terms of the imaginary parts of Airy function as follows

$$u(x,y) = u_0 - \frac{u_0 3^{\frac{1}{6}} \Gamma(\frac{2}{3})}{2\pi} \int_0^\infty \frac{1}{r^{\frac{5}{6}}} e^{-rx} y^{\frac{1}{2}} J_{\frac{1}{3}}\left(\frac{2}{3} r^{\frac{1}{2}} y^{\frac{3}{2}}\right) dr. \tag{3-11}$$

Also, the solution of equation (3–2), can be generalized by replacing the term $\frac{\partial u}{\partial x}$ by ${}^{C}D_x^{\alpha}u$ as the Caputo fractional derivative. In the sense, by using the fact [17]

$$\Lambda\{{}^{C}D_x^{\alpha}u(x,y); s\} = s^{\alpha}\tilde{u}(s,y) - s^{\alpha-1}u(0,y), \quad 0 < \alpha \le 1, \tag{3-12}$$

and applying the similar procedure for solving the new problem, we obtain the solution (3–10) in the following form

$$u(x,y) = u_0 - \frac{u_0}{\pi \mathrm{A}_{2n+1}(0)} \int_0^\infty \frac{1}{r} e^{-rx} \Im\{\mathrm{A}_{2n+1}(r^{\frac{\alpha}{2n+1}} e^{-i\frac{\pi}{2n+1}} y)\} dr. \tag{3-13}$$

Problem 3.3 *We consider other type of the generalized Lévêque problem as*

$$(1+y)\frac{\partial u}{\partial x} = D_n \frac{\partial^{2n} u}{\partial y^{2n}}, \; n \in \mathrm{N}, \tag{3-14}$$

$$u(0,y) = 0, u(x,0) = u_0, \tag{3-15}$$

$$\lim_{y \to \infty} u(x,y) < \infty. \tag{3-16}$$

In similar procedure to the previous problem, after applying the Laplace transform we get

$$\tilde{u}(s,y) = \frac{u_0}{s \mathrm{A}_{2n+1}(s^{\frac{1}{2n+1}})} \mathrm{A}_{2n+1}(s^{\frac{1}{2n+1}}(1+y)), \tag{3-17}$$

which its inverse is obtained by the following Bromwich's integral

$$u(x,y) = \frac{u_0}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{1}{s \mathrm{A}_{2n+1}(s^{\frac{1}{2n+1}})} \mathrm{A}_{2n+1}(s^{\frac{1}{2n+1}} y) e^{sx} ds. \tag{3-18}$$

The integrand of the Bromwich's integral has the branch point at the origin and infinite number of poles s_n as

$$\mathrm{A}_{2n+1}(s_j^{\frac{1}{2n+1}})=\mathrm{A}_{2n+1}(\lambda_{nj})=0,\ j=1,2,\cdots, \tag{3–19}$$

where λ_{nj} are the zeros of the A_{2n+1} function. It is evident that the all poles $s_j=\lambda_{nj}^{2n+1}$ are outside the contour of integration except $n-1$ positive roots of them. Some of these positive zeros has been shown in Table 1. Therefore, for obtaining the residues at the simple poles $s_j, j=1,\cdots,n-1,$ we have

$$\begin{aligned}I_n&=\sum_{i=1}^{n-1}Res\{\frac{1}{s\mathrm{A}_{2n+1}(s^{\frac{1}{2n+1}})}\mathrm{A}_{2n+1}(s^{\frac{1}{2n+1}}y)e^{sx};s_i=\lambda_{ni}^{2n+1}\}\\&=\sum_{i=1}^{n-1}\frac{(2n+1)}{\lambda_{ni}\mathrm{A}_{2n+1}'(\lambda_{ni})}\mathrm{A}_{2n+1}(\lambda_{ni}y)e^{\lambda_{ni}^{2n+1}x}.\end{aligned} \tag{3–20}$$

According to the above value and Titchmarsh theorem, we finally get the solution of Problem 2 as

$$u(x,y)=(1+I_n)u_0-\frac{u_0}{\pi}\int_0^\infty\frac{1}{r}e^{-rx}\Im\{\frac{\mathrm{A}_{2n+1}(r^{\frac{1}{2n+1}}e^{-i\frac{\pi}{2n+1}}y)}{\mathrm{A}_{2n+1}(r^{\frac{1}{2n+1}}e^{-i\frac{\pi}{2n+1}})}\}dr. \tag{3–21}$$

Also, in the case of the fractional derivative model of problem with respect to x, we get the solution of problem in the following form

$$u(x,y)=(1+I_{n,\alpha})u_0-\frac{u_0}{\pi}\int_0^\infty\frac{1}{r}e^{-rx}\Im\{\frac{\mathrm{A}_{2n+1}(r^{\frac{\alpha}{2n+1}}e^{-i\frac{\pi}{2n+1}}y)}{\mathrm{A}_{2n+1}(r^{\frac{\alpha}{2n+1}}e^{-i\frac{\pi}{2n+1}})}\}dr, \tag{3–22}$$

where

$$I_{n,\alpha}=\sum_{i=1}^{n-1}\frac{(2n+1)}{\alpha\lambda_{ni}\mathrm{A}_{2n+1}'(\lambda_{ni})}\mathrm{A}_{2n+1}(\lambda_{ni}y)e^{\lambda_{ni}^{\frac{2n+1}{\alpha}}x}. \tag{3–23}$$

For simplification of the solution (3-21) in $n=1$ in terms of the Bessel functions, similar to the previous procedure in (3-11), we use Theorem 3.1 to obtain

$$u(x,y)=u_0-\frac{u_0 3^{\frac{1}{2}}(1+y)^{\frac{1}{2}}}{2\pi}\int_0^\infty\frac{1}{r}e^{-rx}\frac{J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}}(1+y)^{\frac{3}{2}})J_{-\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}})-J_{-\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}}(1+y)^{\frac{3}{2}})J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}})}{J_{\frac{1}{3}}^2(\frac{2}{3}r^{\frac{1}{2}})+J_{-\frac{1}{3}}^2(\frac{2}{3}r^{\frac{1}{2}})-J_{-\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}})J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}})} \tag{3–24}$$

3.2. THE COUETTE FLOW WITH A CHEMICAL REACTION

At this point, we consider the Couette flow in the presence of a chemical reaction.

Problem 3.4 *We consider the following Couette flow with a chemical reaction*

$$y\frac{\partial u}{\partial x}=D_n\frac{\partial^{2n}u}{\partial y^{2n}}-u,\ n\in\mathrm{N}, \tag{3–25}$$

$$u(0,y)=0, u(x,0)=u_0, \tag{3–26}$$

$$\lim_{y\to\infty} u(x,y)<\infty. \tag{3–27}$$

For this problem similar to the previous problem, after applying the Laplace transform and boundary conditions, we get the solution as

$$\tilde{u}(s,y)=\frac{u_0}{sA_{2n+1}\left(\frac{1}{s^{\frac{2n}{2n+1}}}\right)}A_{2n+1}\left(\frac{1+sy}{s^{\frac{2n}{2n+1}}}\right). \tag{3–28}$$

In view of the $n-1$ positive simple poles $s_i=\frac{1}{\lambda_{ni}^{\frac{2n+1}{2n}}}, i=1,2,\cdots,n-1$, the inverse Laplace transform of the above function is given by

$$u(x,y)=(1+I_n)u_0-\frac{u_0}{\pi}\int_0^\infty \frac{1}{r}e^{-rx}\Im\left\{\frac{A_{2n+1}\left[\frac{1+re^{-i\pi}}{(re^{-i\pi})^{\frac{2n}{2n+1}}}\right]}{A_{2n+1}\left[\frac{1}{(re^{-i\pi})^{\frac{2n}{2n+1}}}\right]}\right\}dr, \tag{3–29}$$

where

$$I_n=\sum_{i=1}^{n-1} Res\left\{\frac{A_{2n+1}\left(\frac{1+sy}{s^{\frac{2n}{2n+1}}}\right)}{sA_{2n+1}\left(\frac{1}{s^{\frac{2n}{2n+1}}}\right)}e^{sx}; s_i=\frac{1}{\lambda_{ni}^{\frac{2n+1}{2n}}}\right\}$$

$$=-\sum_{i=1}^{n-1}\frac{(2n+1)}{2n\lambda_{ni}A_{2n+1}'(\lambda_{ni})}A_{2n+1}\left(\frac{1+\frac{y}{\lambda_{ni}^{\frac{2n+1}{2n}}}}{\lambda_{ni}}\right)e^{\frac{x}{\lambda_{ni}^{\frac{2n+1}{2n}}}}. \tag{3–30}$$

Also, in the case of the fractional derivative model of problem, we get the solution of problem in the following form

$$u(x,y)=(1+I_n)u_0-\frac{u_0}{\pi}\int_0^\infty\frac{1}{r}e^{-rx}\Im\left\{\frac{A_{2n+1}\left[\dfrac{1+r^{\alpha}e^{-i\pi\alpha}y}{(re^{-i\pi})^{\frac{2n\alpha}{2n+1}}}\right]}{A_{2n+1}\left[\dfrac{1}{(re^{-i\pi})^{\frac{2n\alpha}{2n+1}}}\right]}\right\}dr, \tag{3–31}$$

where

$$I_{n,\alpha}=-\sum_{i=1}^{n-1}\frac{(2n+1)}{2n\alpha\lambda_{ni}\mathrm{A}_{2n+1}'(\lambda_{ni})}\mathrm{A}_{2n+1}\left(\frac{1+\dfrac{y}{\lambda_{ni}^{\frac{2n\alpha}{2n+1}}}}{\lambda_{ni}}\right)e^{\left(\frac{x}{\lambda_{ni}^{\frac{2n\alpha}{2n+1}}}\right)}. \tag{3–32}$$

Moreover, for simplification of the solution (3–29) in $n=1$ in terms of the Bessel functions, we get

$$u(x,y)=u_0e^{-y}-\frac{u_0 3^{\frac{1}{2}}}{2\pi}\int_0^\infty\frac{(1-ry)^{\frac{1}{2}}}{r}e^{-rx}\frac{J_{\frac{1}{3}}\left(\frac{2}{3r}(1-ry)^{\frac{3}{2}}\right)J_{-\frac{1}{3}}\left(\frac{2}{3r}\right)-J_{-\frac{1}{3}}\left(\frac{2}{3}(1-ry)^{\frac{3}{2}}\right)J_{\frac{1}{3}}\left(\frac{2}{3r}\right)}{J_{\frac{1}{3}}^2\left(\frac{2}{3r}\right)+J^2_{-\frac{1}{3}}\left(\frac{2}{3r}\right)-J_{-\frac{1}{3}}\left(\frac{2}{3r}\right)J_{\frac{1}{3}}\left(\frac{2}{3r}\right)}dr. \tag{3–33}$$

4. CONCLUDING REMARKS

This paper provides new results in obtaining the analytical solutions of some generalized partial differential equations. These equations have been interpreted as the Couette flows with (without) chemical reactions. We considered fractional derivative models (in Caputo sense) for these PDEs and solved them by the Laplace transform. We encountered with the generalized Airy functions in the Bromwich's integral of inverse Laplace transform. Zeros of these functions were the first steps in obtaining the solutions as the simple poles of integrands. Finally, the desired solutions have been written in terms of the Laplace transform of the imaginary parts of the generalized Airy functions.

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A Note on Hyper–Zagreb Index of Graph Operations

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ABSTRACT In this paper, the hyper-Zagreb index of the Cartesian product, composition and corona product of graphs are computed. These results correct some errors in G. H. Shirdel et al. [*Iranian J. Math. Chem.* **4** (2) (2013) 213–220].

KEYWORDS Hyper-Zagreb index • Zagreb index • graph operation.

1. INTRODUCTION

Throughout this paper, we consider only simple connected graphs. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $w \in V(G)$ is the number of vertices adjacent to w and is denoted by $d_G(w)$. We refer to [11] for unexplained terminology and notation.

In theoretical chemistry, the physico-chemical properties of chemical compounds are often modeled by means of molecular-graph-based structure-descriptors, which are also referred to as topological indices [10, 15]. The Zagreb indices are widely studied degree-based topological indices, and were introduced by Gutman and Trinajstic′ [9] in 1972. The first and the second Zagreb indices of a graph G are respectively defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

The first Zagreb index can also be expressed as a sum over edges of G,

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)].$$

Recently, G.H. Shirdel, H. Rezapour and A.M. Sayadi [14] introduced a new version of Zagreb index named hyper-Zagreb index which is defined for a graph G as

$$HM(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))^2.$$

Some new results on the hyper-Zagreb index can be found in [7, 8].

The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$. If (a, x) is a vertex of $G \times H$, then $d_{G \times H}((a, x)) = d_G(a) + d_H(x)$.

The composition $G[H]$ of graphs G and H with disjoint vertex sets $V(G)$ and $V(H)$ and edge sets $E(G)$ and $E(H)$ is the graph with vertex set $V(G) \times V(H)$ and (a, x) is adjacent to (b, y) whenever a is adjacent to b or $a = b$ and x is adjacent to y. If (a, x) is a vertex of $G[H]$, then $d_{G[H]}((a, x)) = |V(H)| d_G(a) + d_H(x)$.

The corona product $G \circ H$ is defined as the graph obtained from G and H by taking one copy of G and $|V(G)|$ copies of H and then by joining with an edge each vertex of the i^{th} copy of H which is named (H, i) with the i^{th} vertex of G for $i = 1,2,\ldots,|V(G)|$. If u is a vertex of $G \circ H$, then

$$d_{G\circ H}(u) = \begin{cases} d_G(u) + |V(H)| & if\ u \in V(G), \\ d_H(u) + 1 & if\ u \in V(H,i). \end{cases}$$

G. H. Shirdel et al. [14] computed the hyper-Zagreb index of some graph operations. However, the formulae of Theorem 2, Theorem 3, and Theorem 4 of their paper for computing the hyper-Zagreb index of Cartesian product, composition, and corona product are incorrect. In this paper, we give correct expressions for the hyper-Zagreb index of the Cartesian product, composition and corona product of graphs. Readers interested in more information on computing topological indices of graph operations can be referred to [1–6, 12, 13].

2. RESULTS

Theorem 2.1 *Let G and H be graphs. Then*

$$HM(G \times H) = |V(G)|HM(H) + |V(H)|HM(G) + 12M_1(G)|E(H)| + 12M_1(H)|E(G)|.$$

Proof. By definition of the hyper-Zagreb index, we have

$$\begin{aligned} HM(G \times H) &= \textstyle\sum_{(a,x)(b,y)\in E(G\times H)} [d_{G\times H}((a,x)) + d_{G\times H}((b,y))]^2 \\ &= \textstyle\sum_{a\in V(G)} \sum_{xy\in E(H)} [d_G(a) + d_H(x) + d_G(a) + d_H(y)]^2 \\ &\quad + \textstyle\sum_{x\in V(H)} \sum_{ab\in E(G)} [d_H(x) + d_G(a) + d_H(x) + d_G(b)]^2 \\ &= \textstyle\sum_{a\in V(G)} \sum_{xy\in E(H)} [2d_G(a) + d_H(x) + d_H(y)]^2 \\ &\quad + \textstyle\sum_{x\in V(H)} \sum_{ab\in E(G)} [2d_H(x) + d_G(a) + d_G(b)]^2 \\ &= \textstyle\sum_{a\in V(G)} \sum_{xy\in E(H)} [4d_G(a)^2 + (d_H(x) + d_H(y))^2 + 4d_G(a)(d_H(x) + d_H(y))] \\ &\quad + \textstyle\sum_{x\in V(H)} \sum_{ab\in E(G)} [4d_H(x)^2 + (d_G(a) + d_G(b))^2 + 4d_H(x)(d_G(a) + d_G(b))] \\ &= 4|E(H)|M_1(G) + |V(G)|HM(H) + 8|E(G)|M_1(H) \\ &\quad + 4|E(G)|M_1(H) + |V(H)|HM(G) + 8|E(H)|M_1(G). \end{aligned}$$

□

As an application of Theorem 2.1, we list explicit formulae for the hyper-Zagreb index of the rectangular grid $P_r \times P_s$, C_4 –nanotube $P_r \times C_q$, and C_4 –nanotorus $C_p \times C_q$. The formulae follow from Theorem 2.1 by using the expressions $M_1(P_n) = 4n - 6$, $n > 1$; $M_1(C_n) = 4n$; $HM(P_n) = 16n - 30, n > 2$ and $HM(C_n) = 16n$.

Corollary 2.2 $HM(P_r \times P_s) = 128rs - 150r - 150s + 144, r, s > 2$;

$$HM(P_r \times C_q) = 128rq - 150q, r > 2; HM(C_p \times C_q) = 128pq.$$

Theorem 2.3 *Let G and H be graphs. Then*

$$\begin{aligned} HM(G[H]) &= |V(H)|^4 HM(G) + |V(G)|HM(H) \\ &\quad + 12|V(H)|^2|E(H)|M_1(G) + 10|V(H)||E(G)|M_1(H) + 8|E(H)|^2|E(G)|. \end{aligned}$$

Proof. Using the definition of the hyper-Zagreb index, we have

$$\begin{aligned}
HM(G[H]) &= \sum_{(a,x)(b,y)\in E(G[H])} [d_{G[H]}((a,x)) + d_{G[H]}((b,y))]^2 \\
&= \sum_{x\in V(H)} \sum_{y\in V(H)} \sum_{ab\in E(G)} [|V(H)|d_G(a) + d_H(x) + |V(H)|d_G(b) + d_H(y)]^2 \\
&\quad + \sum_{a\in V(G)} \sum_{xy\in E(H)} [|V(H)|d_G(a) + d_H(x) + |V(H)|d_G(a) + d_H(y)]^2 \\
&= \sum_{x\in V(H)} \sum_{y\in V(H)} \sum_{ab\in E(G)} [|V(H)|^2(d_G(a) + d_G(b))^2 + d_H(x)^2 + d_H(y)^2 \\
&\quad +2d_H(x)d_H(y) + 2|V(H)|(d_G(a) + d_G(b))(d_H(x) + d_H(y))] \\
&\quad +\sum_{a\in V(G)} \sum_{xy\in E(H)} [4|V(H)|^2 d_G(a)^2 + (d_H(x) + d_H(y))^2 \\
&\quad +4|V(H)|d_G(a)(d_H(x) + d_H(y))] \\
&= |V(H)|^4 HM(G) + |V(H)||E(G)|M_1(H) + |V(H)||E(G)|M_1(H) + 8|E(H)|^2|E(G)| \\
&\quad +2|V(H)|^2 M_1(G)(2|E(H)| + 2|E(H)|) + 4|V(H)|^2|E(H)|M_1(G) + |V(G)|HM(H) \\
&\quad +8|V(H)||E(G)|M_1(H).
\end{aligned}$$

□

As an application of Theorem 2.3, we present formulae for the hyper-Zagreb index of the fence graph $P_n[K_2]$ and the closed fence graph $C_n[K_2]$.

Corollary 2.4 $HM(P_n[K_2]) = 500n - 816$, $n > 2$; $HM(C_n[K_2]) = 500n$.

Theorem 2.5 *Let G and H be graphs. Then*

$$\begin{aligned}
HM(G \circ H) &= HM(G) + |V(G)|HM(H) + 5|V(H)|M_1(G) + 5|V(G)|M_1(H) + \\
&4|V(H)|^2|E(G)| + 4|V(G)||E(H)| + 8|E(G)||E(H)| + |V(G)||V(H)|(|V(H)| + 1)^2 \\
&+ 4(|V(H)| + 1)(|E(G)||V(H)| + |E(H)||V(G)|).
\end{aligned}$$

Proof. By definition of the hyper-Zagreb index, we have

$$\begin{aligned}
HM(G \circ H) &= \sum_{uv\in E(G\circ H)} [d_{G\circ H}(u) + d_{G\circ H}(v)]^2 \\
&= \sum_{uv\in E(G)} [d_G(u) + |V(H)| + d_G(v) + |V(H)|]^2 \\
&\quad + \sum_{uv\in E(H)} \sum_{i=1}^{|V(G)|} [d_H(u) + 1 + d_H(v) + 1]^2 \\
&\quad + \sum_{u\in V(G)} \sum_{v\in V(H)} [d_G(u) + |V(H)| + d_H(v) + 1]^2.
\end{aligned}$$

It is easy to see that

$$\begin{aligned}
\sum_{uv\in E(G)} [d_G(u) + d_G(v) + 2|V(H)|]^2 &= \sum_{uv\in E(G)} [(d_G(u) + d_G(v))^2 + 4|V(H)|^2 \\
&\quad +4|V(H)|(d_G(u) + d_G(v))] = HM(G) + 4|V(H)|^2|E(G)| + 4|V(H)|M_1(G).
\end{aligned} \tag{2.1}$$

$$\begin{aligned}
\sum_{uv\in E(H)} \sum_{i=1}^{|V(G)|} [d_H(u) + d_H(v) + 2]^2 &= \sum_{uv\in E(H)} \sum_{i=1}^{|V(G)|} [(d_H(u) + d_H(v))^2 + 4 \\
&\quad +4(d_H(u) + d_H(v))] = |V(G)|\big(HM(H) + 4|E(H)| + 4M_1(H)\big).
\end{aligned} \tag{2.2}$$

$$\begin{aligned}
\sum_{u\in V(G)} \sum_{v\in V(H)} [d_G(u) + d_H(v) + |V(H)| + 1]^2 &= \sum_{u\in V(G)} \sum_{v\in V(H)} [d_G(u)^2 + d_H(v)^2 \\
&\quad +2d_G(u)d_H(v) + (|V(H)| + 1)^2 + 2(|V(H)| + 1)(d_G(u) + d_H(v))] \\
&= |V(H)|M_1(G) + |V(G)|M_1(H) + 8|E(G)||E(H)| + |V(G)||V(H)|(|V(H)| + 1)^2
\end{aligned}$$

$$+4(|V(H)|+1)(|E(G)||V(H)|+|E(\mathrm{H})||V(G)|). \qquad (2.3)$$

By adding Eqs. (2.1), (2.2), and (2.3) the proof is completed. □

Using Theorem 2.5, we can compute the hyper-Zagreb index of the k −thorny cycle $C_n \circ \overline{K}_k$.

Corollary 2.6 $HM(C_n \circ \overline{K}_k) = 16n + 25nk + 10nk^2 + nk^3$.

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QSPR Study on Benzene Derivatives to some Physico–Chemical Properties by using Topological Indices

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ABSTRACT QSPR study on benzene derivatives have been made using recently introduced topological methodology. In this study the relationship between the Randic' (^1x), Balaban (J), Szeged (Sz),Harary (H), Wiener (W), HyperWiener(WW) and Wiener Polarity (W_P) to the thermal energy (E_{th}), heat capacity (C_V) and entropy (S) of benzene derivatives is represented. Physicochemical properties are taken from the quantum mechanics methodology with HF level using the ab initio 6-31G basis sets. The multiple linear regressions (MLR) and back ward methods (with significant at the 0.05 level) were employed to give the QSPR models. The satisfactory obtained results show that combining the two descriptors (Sz, WW) are useful topological descriptors for predicted (C_V) and (S) of the 45 benzene derivatives. The training set models established by MLR method have not good correlation of (E_{th}), which means QSPR models could not predict the thermal energy of compounds.

KEYWORDS QSPR • Topological index • benzene derivatives • graph theory • multiple linear regressions (MLR).

1. INTRODUCTION

Benzene derivatives compounds are widely used industrial chemicals and thus have a high potential for environmental pollution. The eventual release and accumulation of these compounds into the environment in both terrestrial and aquatic systems requires an assessment of their environmental risk. Science experimental measurements of physicochemical properties are extremely time- consuming and expensive.

Quantitative structure – property relationships (QSPRs) have provided a valuable approach in research into physicochemical properties of organic chemicals [1]. Many investigators have used quantum – chemical parameters [2–5].Among the different approaches employing computational chemistry, those based on chemical graph theory have been useful in establishing QSPR [6].

The basic strategy of QSPR is to find the optimum quantitative relationship which can then be used for the prediction of the properties of molecular structures including those unmeasured or even unknown [7–9].

The premise of QSPR is that physicochemical properties can be correlated with molecular structure characteristics (geometric and electronic) expressed in terms of appropriate molecular descriptors [10].

QSPR have been traditionally developed by selecting, a priori, an analytical model (typically) linear, polynomial or lag–linear to quantity the correlation between selected molecular indices and desired physicochemical properties, followed by regression analysis to determine model parameters [11–13].

In the present study, the multiple linear regression (MLR) techniques and back ward methods are used for modeling the thermal energy (E_{th}), heat capacity (C_V) and entropy (S) of 45 benzene derivatives.

The proposed QSPR models were based on molecular descriptors (topological indices) that can be calculated for any compound utilizing only the knowledge of its molecular structure (molecular graph).

The topological indices used for the QSPR analysis were Wiener [14], Szeged [15], first order molecular connectivity [16], Balaban [17], HyperWiener [18], Wiener Polarity [19] and Harary [20] indices.

2. MATERIALS AND METHODS

2.1. QUANTUM CHEMISTRY CALCULATIONS

The thermal energy (E_{th}), heat capacity (C_V) and entropy (S) of 45 benzene derivatives are taken from the quantum mechanics methodology with Hartree–Fock (HF) level using the ab initio 6–31G basis sets. The quantum chemistry data of the 45 congeners are listed in Table 1.

2.2. TOPOLOGICAL INDICES

All the used topological indices were calculated using all hydrogen suppressed graph by deleting all the carbon hydrogen as well as heteroatomic hydrogen bonds from the structure of the benzene derivatives. The descriptors were calculated with chemicalize software [21]. Six topological indices tested in the present study are recorded in Table 2.

2.3. STATISTICAL ANALYSIS

Structure- Property models (MLR models) are generated using the multilinear regression procedure of SPSS version 16. The thermal energy $(E_{th}\frac{kcal}{mol})$, heat capacity $(Cv\frac{cal}{molK})$ and entropy $(S\frac{cal}{molK})$ are used as the dependent variable and ^1x, J, Sz, H, W_P and WW indices as the independent variables. The models are assessed with R value (correlation coefficient), the R^2(coefficient of determination), the R^2- adjusted, the SD value (root of the mean square of errors), the F value (Fischer statistic) and the sig (significant).

3. RESULTS

Several linear QSPR models involving one, two, three, four and five descriptors are established and strongest multivariable correlations are identified by the back ward method are significant at the 0.05 level and regression analysis of the SPSS program.

In the first of this study we drown scattering plots of C_V, S and E_{th} versus the six topological indices, ^1x, J, W, Sz, WW and W_P. Some of these plots are given in Fig. (1–8), respectively. Distribution of the dependent variable against the independent variable for 45 chemicals employed in developing quantitative structure–properties relationship.

3.1. QSPR MODELS FOR HEAT CAPACITY (CV)

Model 1

$C_V = 18.000 – 0.573{}^1x - 4.038\ J – 0.051\ H – 0.103\ WW – 0.006\ WP + 0.257\ Sz$

N= 45 R= 0.966 R^2 =0.933 $R^2_{adj} = 0.922$ SD=2.342

F= 88.125 sig = 0.000 (1)

Model 2

$C_V = 18.045 – 0.574{}^1x - 4.048\ J – 0.051\ H – 0.103\ WW - 0.256Sz$

N= 45 R= 0.966 R^2 =0.933 $R^2_{adj} = 0.924$ SD=2.312

F= 108.531 sig = 0.000 (2)

Model 3

C_V= 18.351 – 0.556^{1}x - 4.180 J – 0.106 WW - 0.266 Sz

N= 45 R= 0.966 R^2 =0.933 R^2_{adj} = 0.926 SD=2.284

F= 138.960 sig = 0.000 (3)

Model 4

C_V = 16.779– 3.975 J – 0.102 WW - 0.252 Sz

N= 45 R= 0.966 R^2 =0.933 R^2_{adj} = 0.928 SD=2.261

F= 188.938 sig = 0.000 (4)

Model 5

C_V = 10.629– 0.085 WW + 0.216 Sz

N= 45 R= 0.964 R^2 =0.929 R^2_{adj} = 0.926 SD=2.292

F= 274.854 sig = 0.000 (5)

It turns out that the heat capacity (C_V) has a good correlation with all six topological indices as well as with WW and Sz (Eq. (5)).

3.2. QSPR MODELS FOR THERMAL ENERGY (ETH)

Model 6

E_{th} = 112.146 – 1.952^{1}x - 16.645 J + 1.496 H – 0.167 WW – 0.702 W_P -0.356 Sz

N= 45 R= 0.425 R^2 =0.181 R^2_{adj} = 0.052 SD=18.837

F= 1.400 sig = 0.240 (6)

Model 7

E_{th} = 106.705- 15.971 J + 1.473 H + 0.180 WW + 0.689 W_P - 0.396 Sz

N= 45 R= 0.425 R^2 =0.180 R^2_{adj} = 0.075 SD=18.603

F= 1.715 sig = 0.154 (7)

Model 8

E_{th} = 102.046- 14.980 J + 1.454 H + 0.130 WW - 0.271 Sz

N= 45 R= 0.422 R^2 =0.178 R^2_{adj} = 0.096 SD=18.396

F= 2.162 sig = 0.091 (8)

Model 9

E_{th} = 112.147- 22.272 J + 0.666 H + 0.021 WW

N= 45 R= 0.414 R^2 =0.171 R^2_{adj} = 0.111 SD=18.240

F= 2.828 sig = 0.050 (9)

Model 10

E_{th} = 108.116- 23.268 J + 1.190 H

N= 45 R= 0.408 R^2 =0.167 R^2_{adj} = 0.127 SD=18.074

F= 4.199 sig = 0.022 (10)

Model 11

E_{th} = 66.730+0.699 H

N= 45 R= 0.365 R^2 =0.134 R^2_{adj} = 0.113 SD=18.214

F= 6.629 sig = 0.014 (11)

It turns out that the correlation coefficient values of all models for E_{th}, is less than 0.2, which means that there is no strong linear relation between E_{th} and descriptors.

3.3. QSPR MODELS FOR ENTROPY (S)

Model 12

$S = 72.845 - 0.598\,{}^{1}x - 4.788\,J + 0.259\,H - 0.116\,WW + 0.334\,W_P + 0.272\,Sz$

$N = 45$ $R = 0.948$ $R^2 = 0.898$ $R^2_{adj} = 0.882$ $SD = 4.008$

$F = 55.810$ $sig = 0.000$ (12)

Model 13

$S = 71.179 - 4.581\,J + 0.252\,H - 0.112\,WW - 0.33\,W_P - 0.259\,Sz$

$N = 45$ $R = 0.948$ $R^2 = 0.898$ $R^2_{adj} = 0.885$ $SD = 3.960$

$F = 68.590$ $sig = 0.000$ (13)

Model 14

$S = 72.903 - 5.259\,J - 0.130\,WW - 0.322\,W_P + 0.312\,Sz$

$N = 45$ $R = 0.947$ $R^2 = 0.897$ $R^2_{adj} = 0.887$ $SD = 3.930$

$F = 86.936$ $sig = 0.000$ (14)

Model 15

$S = 70.664 - 4.772\,J - 0.153\,WW + 0.369\,Sz$

$N = 45$ $R = 0.946$ $R^2 = 0.895$ $R^2_{adj} = 0.888$ $SD = 3.910$

$F = 116.931$ $sig = 0.000$ (15)

Model 16

$S = 63.280 - 0.133\,WW + 0.324\,Sz$

$N = 45$ $R = 0.945$ $R^2 = 0.893$ $R^2_{adj} = 0.888$ $SD = 3.911$

$F = 174.741$ $sig = 0.000$ (16)

It turns out that the entropy(S) has a good correlation with all six topological indices as well as with WW and Sz (Eq. (16)).

4. DISCUSSION

We studied the relationship between topological indices and the thermal energy (E_{th}), heat capacity (C_V) and entropy (S).

The elaborated QSPR models (Eqs 1 – 5) reveal that the heat capacity of the benzene derivatives could be explained by two, three, four, five and six parameter. All of models can explain about 93% of the experimental variance of the dependent variable C_V. The combination of the two parameters (WW, Sz) increases remarkably the predictive power of the QSPR model given by Eq. (5) ($R^2 = 0.929$, $R^2_{adj} = 0.926$, SD = 2.29, F = 274.854).

As can be seen from the statistical parameters of the above equation, a high F of Fischer (F = 274.854) which confirms that the model (5) predicts the heat capacity (dependent variable) in a statistically satisfactory significant manner.

The back ward values of the entropy shows that all of models (Eqs 12 – 16) can explain about 0.90% of the variance of the entropy. The combination of two parameters (WW, Sz) recorded in Eq (16) has highest F of Fischer (F = 174.741) which explain that the model (16) for predict entropy is better than another models. The QSPR models (Eqs 6 – 11) explains only 18% of the variance of the thermal energy besides a low F and a low standard deviation (SD) which confirms that all of models (Eqs 6 – 11) could not use to predicts the thermal energy.

The comparison between the observed data and predicted values using Eq (16) of entropy (S) is presented in Table 3. The linear relations between the observed and predicted values of the entropy of 45 benzene derivatives show in Figure (9).

The comparison between the observed data and predicted values using Eq (5) of C_V is presented in Table 3. The linear relations between the observed and predicted values of the heat capacity of 45 benzene derivatives show in Figure (10).

5. CONCLUSION

The aforementioned results and discussion lead us to conclude that combining the two descriptors (Sz, WW) can be used successfully for modeling and predicting the heat capacity (C_V) and entropy (S) of 45benzene derivatives. The training set models established by MLR method have not good correlation of the thermal energy (E_{th}), which means QSPR models could not predict the thermal energy of compounds.

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Table 1. Benzene derivatives and their thermal energy (E_{th}), heat capacity (C_V) and entropy (S)

compounds	No.	$E_{th}\ {kcal}/{mol}$	$Cv\ {cal}/{molK}$	$S\ {cal}/{molK}$
Bromobenzene	1	65.29	18.974	77.412
Phenol	2	74.241	19.556	73.301
1,2-Dichlorobenzene	3	59.638	22.459	81.422
3-Chlorotoluene	4	84.812	24.561	86.151
1,3-Dihydroxybenzene	5	77.539	24.356	78.827
3-Hydroxyanisole	6	97.706	28.52	85.825
4-Methyl-3-nitroaniline	7	103.88	36.498	97.218
2,4-Dimethylphenol	8	113.333	31.213	95.395
2,6-Dimethylphenol	9	113.476	30.971	88.024
3-Nitrotoluene	10	93.604	28.973	92.842
2,6-Dinitrotoluene	11	93.307	39.695	104.851
4-Methyl-2,6-dinitroaniline	12	105.713	44.947	114.965
5-Methyl-2,6-dinitroaniline	13	105.837	44.81	107.737
5-Methyl-2,4-dinitroaniline	14	105.62	45.252	109.238
2,4-Dinitrotoluene	15	93.169	39.727	105.107
4-Nitrophenol	16	77.413	27.692	86.473
4-Chlorotoluene	17	77.206	31.85	96.426
2,4,6-Trichlorophenol	18	57.376	30.862	93.417
Toluene	19	82.941	27.892	89.047
3-Methyl-6-nitroaniline	20	104.149	35.841	96.864
4-Methyl-2-nitroaniline	21	106.04	33.951	94.282
1,2,4-Trichlorobenzene	22	53.93	26.321	88.346
3,4-Dichlorotoluene	23	79.161	28.303	93.362
2,4-Dichlorotoluene	24	79.266	28.227	88.762
Chlorobenzene	25	65.308	18.726	74.858
1,3,5-Trinitrobenzene	26	74.783	43.544	111.19
1,2,3,4-Tetrachlorobenzene	27	48.143	29.99	94.375

Table 1. (Continued).

2,3,4,5,6-Pentachlorophenol	28	45.776	38.209	105.427
1,3-Dichlorobenzene	29	59.625	22.593	81.815
2-Chlorophenol	30	68.741	23.201	79.752
3-Methylphenol	31	93.75	25.379	83.997
2,3-Dinitrotoluene	32	93.312	39.473	103.012
1,4-Dimethylbenzene	33	109.926	26.47	90.836
2,3,4,5-Tetrachlorophenol	34	51.504	34.552	99.256
2,3,6-Trinitrotoluene	35	96.277	47.777	115.335
4-Methylphenol	36	93.737	25.413	83.681
4-Methyl-3,5-dinitroaniline	37	105.556	45.32	110.557
1,3,5-Trichlorobenzene	38	53.896	26.473	88.731
Benzene	39	70.931	14.87	67.85
2-Nitrotoluene	40	93.788	28.598	87.958
1,4-Dinitrobenzene	41	75.38	32.677	96.457
2-Methyl-3,6-dinitroaniline	42	107.521	43.693	107.087
2-Methyl-4,6-dinitrophenol	43	96.803	43.786	108.582
2,5-Dinitrotolueno	44	93.252	39.676	105.278
1,2-Dinitrobenzene	45	75.477	32.524	95.425

Table 2. Benzene derivatives and their topological indices used in present study

Comp. No.	$^1\chi$	J	H	HW	WP	Sz
1	3.39	1.82	12.92	71	5	78
2	3.39	1.82	12.92	71	5	78
3	3.8	2.28	16.17	106	8	106
4	3.79	2.23	16.08	110	7	108
5	3.79	2.23	16.08	110	7	108
6	4.33	1.98	19.15	176	9	146
7	5.11	2.25	26.67	315	14	232
8	4.2	2.09	19.53	160	10	144
9	4.22	2.15	19.67	151	11	140
10	4.7	2.32	22.72	245	11	186
11	6.04	2.4	34.6	545	19	348
12	6.43	2.7	39.2	669	31	420
13	6.45	2.72	39.13	667	22	418
14	6.43	2.65	38.83	698	21	430
15	6.02	2.33	34.3	576	18	360
16	4.7	2.26	22.6	262	11	192
17	3.79	2.19	16.03	115	7	110
18	4.61	2.49	23.28	215	13	184
19	3.39	1.82	12.92	71	5	78
20	5.11	2.22	26.6	327	14	236
21	5.11	2.27	26.67	315	14	232
22	4.2	2.09	19.53	160	10	144
23	4.2	2.09	19.53	160	10	144
24	4.2	2.09	19.53	160	10	144
25	3.39	1.82	12.92	71	5	78
26	6.91	2.46	42.6	906	21	516
27	4.63	2.52	23.37	211	14	182
28	5.46	2.76	31.6	357	21	282
29	3.79	2.23	16.08	110	7	108
30	3.8	2.28	6.17	106	8	106
31	3.79	2.23	16.08	110	7	108
32	6.04	2.47	34.83	511	19	336
33	3.79	2.19	16.03	115	7	110
34	5.04	2.39	27.32	281	17	230
35	7.36	2.83	47.97	1036	26	588
36	2.18	2.19	16.3	115	7	110
37	6.43	2.7	39.02	669	21	420
38	4.18	2.08	19.5	159	9	144
39	3	2	10	42	3	54
40	4.72	2.4	22.9	231	12	180
41	5.61	2.3	29.74	521	15	314
42	6.45	2.64	38.87	717	22	434
43	6.43	2.66	38.85	691	21	428
44	6.02	2.28	34.14	616	18	372
45	5.63	2.54	30.43	416	16	278

Table 3. Comparison between predicted and observed values of entropy and heat capacity of respect benzene derivatives.

Comp. No.	Observed (S)	Predicted (S)	Residual	Observed (Cv)	Predicted (Cv)	Residual
1	77.41	79.11	1.70	18.97	21.44	2.47
2	73.30	79.11	5.81	19.57	21.44	1.87
3	81.42	83.53	2.11	22.46	24.52	2.06
4	86.15	83.64	-2.51	24.56	24.61	0.05
5	78.83	83.64	4.81	24.36	24.61	0.25
6	85.82	87.18	1.36	28.52	27.20	-1.32
7	97.22	96.55	-0.67	36.50	33.97	-2.53
8	95.40	88.66	6.74	31.21	28.13	-3.08
9	88.02	88.56	0.54	30.97	28.03	-2.94
10	92.84	90.96	-1.88	28.97	29.98	1.01
11	104.85	103.55	-1.30	39.70	39.47	-0.23
12	114.96	110.38	-4.58	44.95	44.48	-0.47
13	107.74	110.00	2.26	44.81	44.22	-0.59
14	109.24	109.77	0.53	45.25	44.18	-1.07
15	105.11	103.31	-1.80	39.73	39.43	-0.30
16	86.47	90.64	4.17	27.69	29.83	2.14
17	96.43	83.62	12.81	31.85	24.61	-7.24
18	93.42	94.30	0.88	30.86	32.09	1.23
19	89.05	79.11	-9.94	27.89	21.44	-6.45
20	96.86	96.25	-0.61	35.84	33.81	-2.03
21	94.28	96.55	2.27	33.95	33.97	0.02
22	88.35	88.66	0.31	26.32	28.13	1.81
23	93.36	88.66	-4.70	28.30	28.13	-0.17
24	88.76	88.66	-0.10	28.23	28.13	-0.10
25	74.86	79.11	4.25	18.73	21.44	2.71
26	111.19	109.97	-1.22	43.54	45.08	1.54
27	94.38	94.18	-0.20	29.99	32.01	2.02
28	105.43	107.17	1.74	38.21	41.20	2.99
29	81.82	83.64	1.82	22.59	24.61	2.02
30	79.75	83.53	3.78	23.20	24.52	1.32
31	84.00	83.64	-0.36	25.38	24.61	-0.77
32	103.01	104.18	1.17	39.47	39.77	0.30
33	90.84	83.49	-7.35	26.47	24.53	-1.94
34	99.26	100.29	1.03	34.55	36.34	1.79
35	115.34	116.00	0.66	47.78	49.58	1.80
36	83.68	83.62	-0.06	25.41	24.61	-0.80
37	110.58	110.38	-0.20	45.32	44.48	-0.84
38	88.73	88.79	0.06	26.47	28.22	1.75
39	67.85	75.19	7.34	14.87	18.72	3.85
40	87.96	90.88	2.92	28.60	29.87	1.27
41	96.46	95.72	-0.74	32.68	34.17	1.49
42	107.09	108.54	1.45	43.69	43.43	-0.26
43	108.58	110.05	1.47	43.79	44.34	0.55
44	105.28	101.88	-3.40	39.68	38.62	-1.06
45	95.42	98.02	2.60	32.52	35.32	2.8

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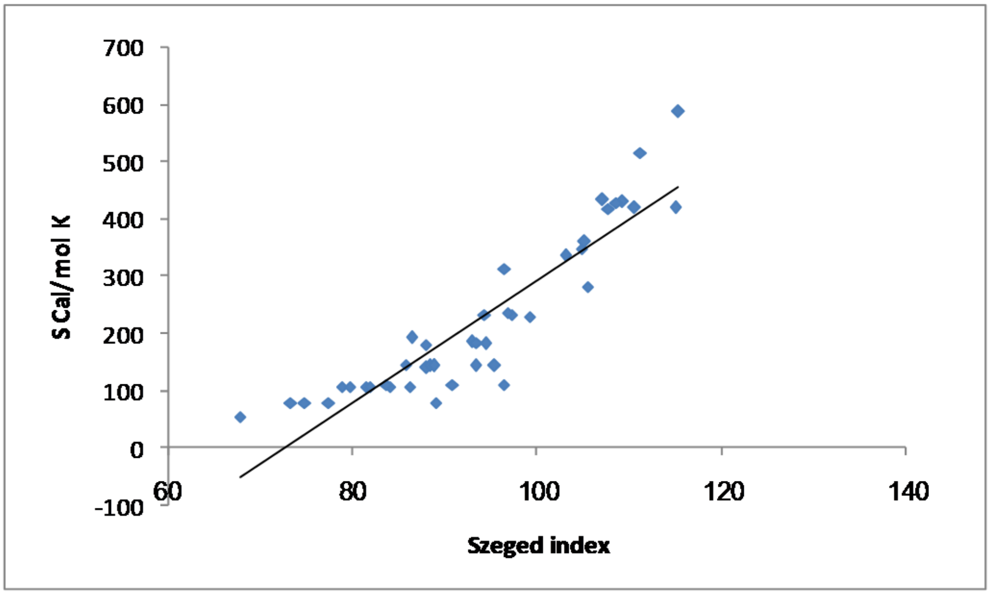

Figure 1. Plots of the Szeged index (Sz) versus entropy of 45 benzene derivatives.

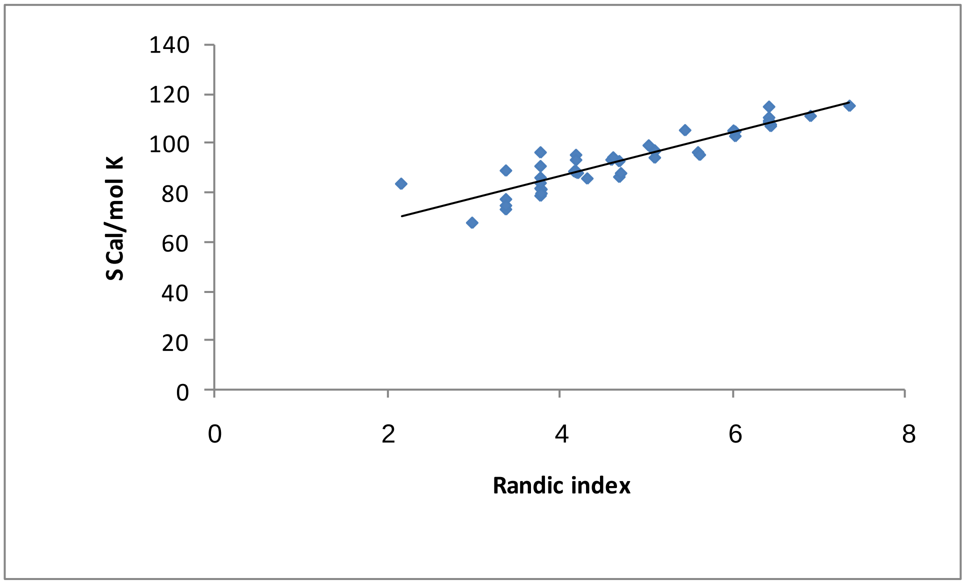

Figure 2. Plots of the Randić index (^{1}x) versus entropy of 45 benzene derivatives.

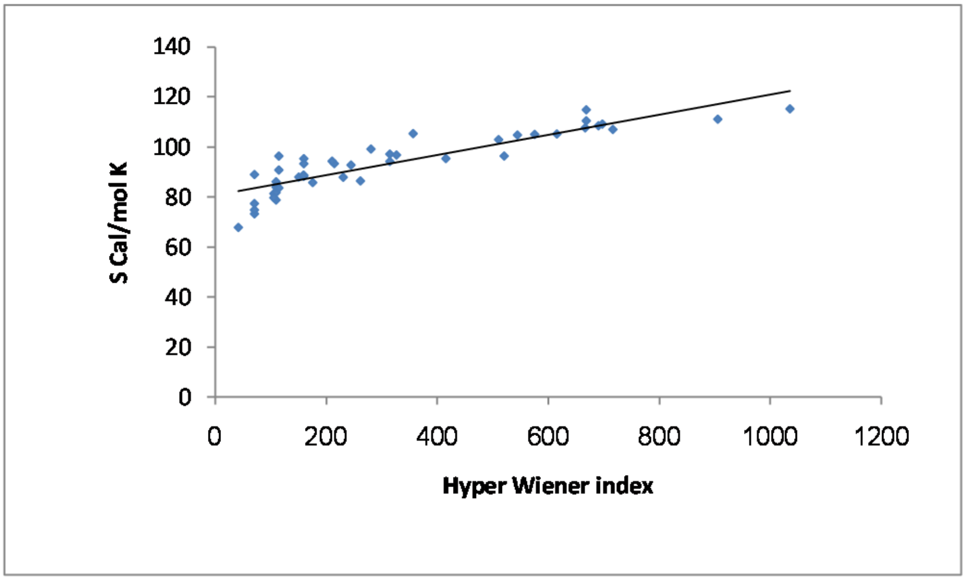

Figure 3. Plots of the Hyper–Wiener (WW) index versus entropy of 45 benzene derivatives.

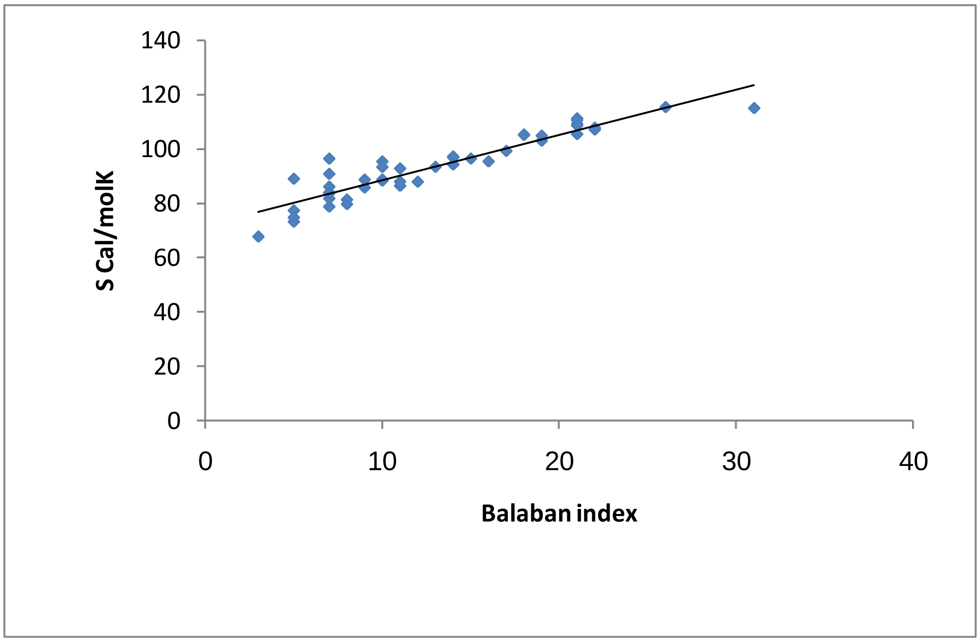

Figure 4. Plots of the Balaban index (J) versus entropy of 45 benzene derivatives.

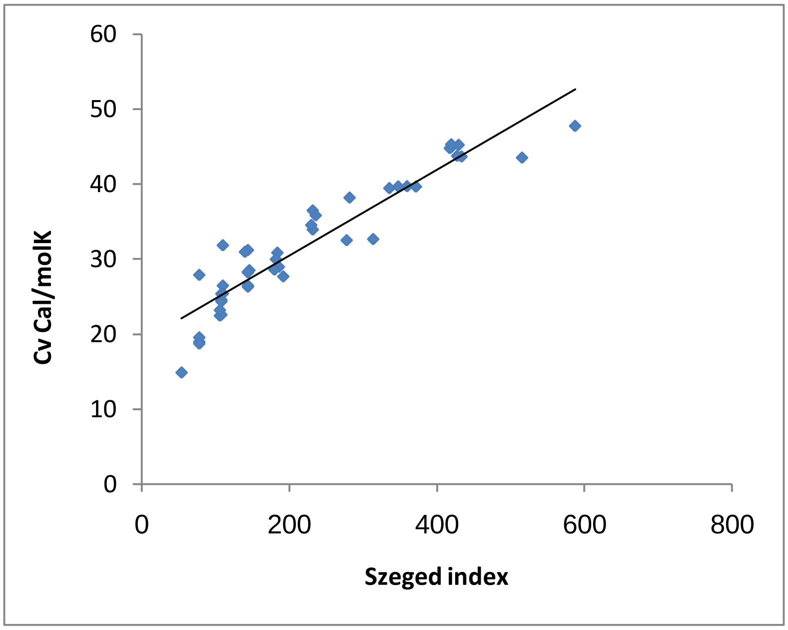

Figure 5. Plots of the Szeged index (Sz) indexversus heat capacity (Cv) of 45 benzene derivatives.

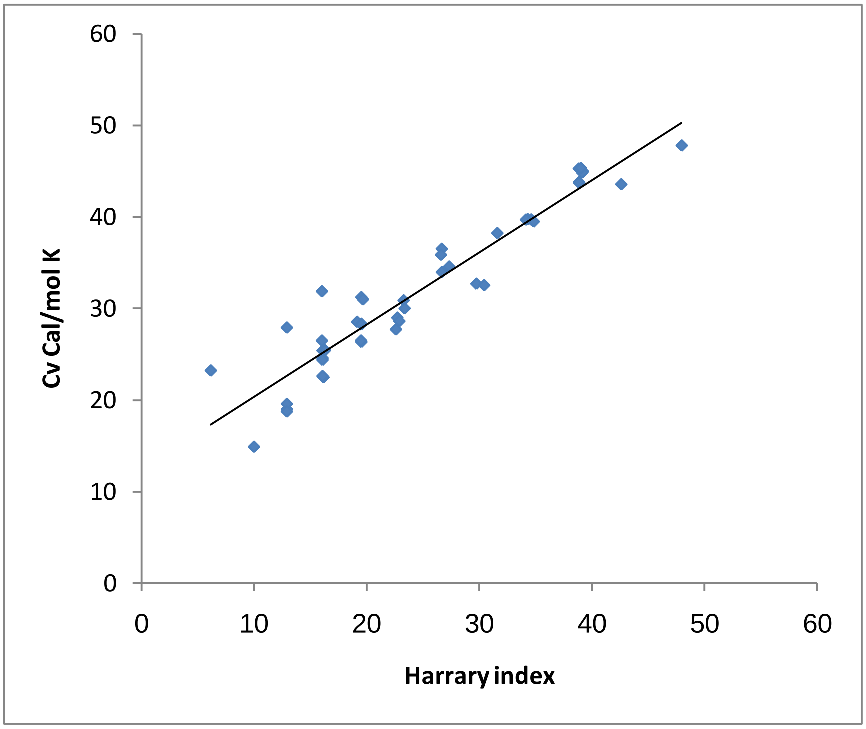

Figure 6. Plots of the Harrary index(H) versus heat capacity (Cv) of 45 benzene derivatives.

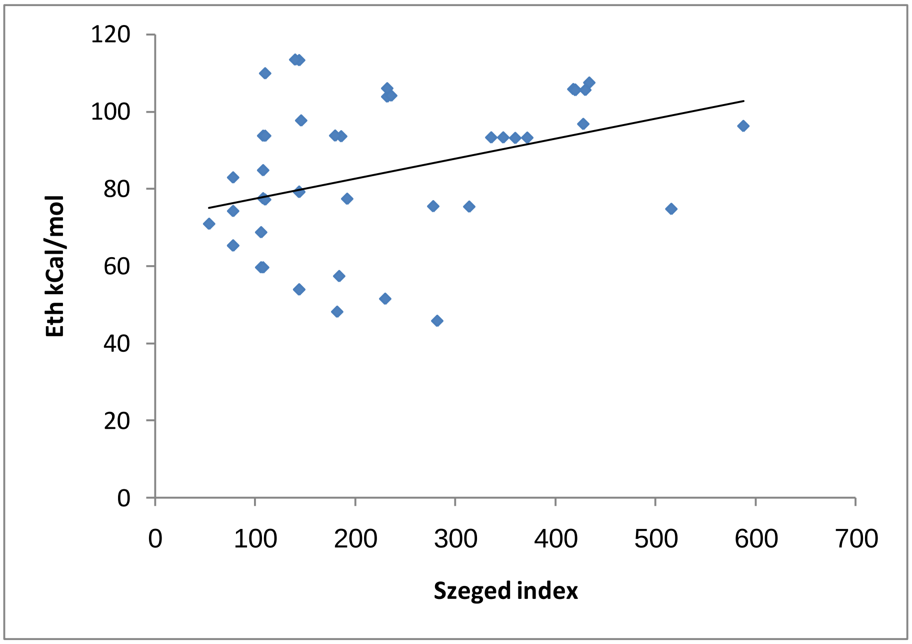

Figure 7. Plots of the Szeged index (Sz) index versus thermal energy (E_{th}) of 45 benzene derivatives .

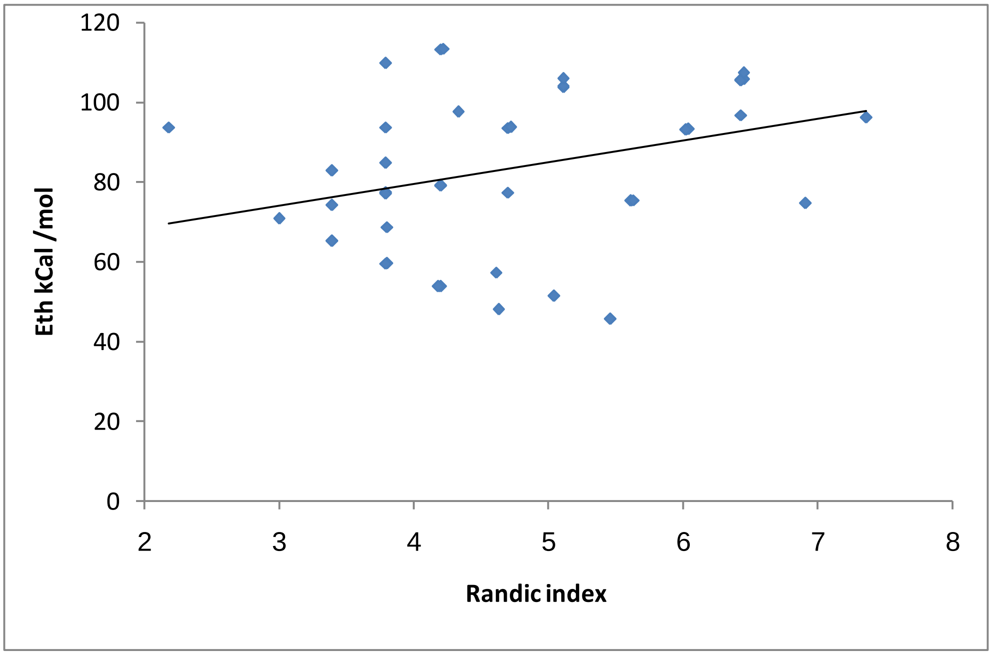

Figure 8. Plots of the Randić index (^{1}x) index versus thermal energy (E_{th}) of 45 benzene derivatives**.**

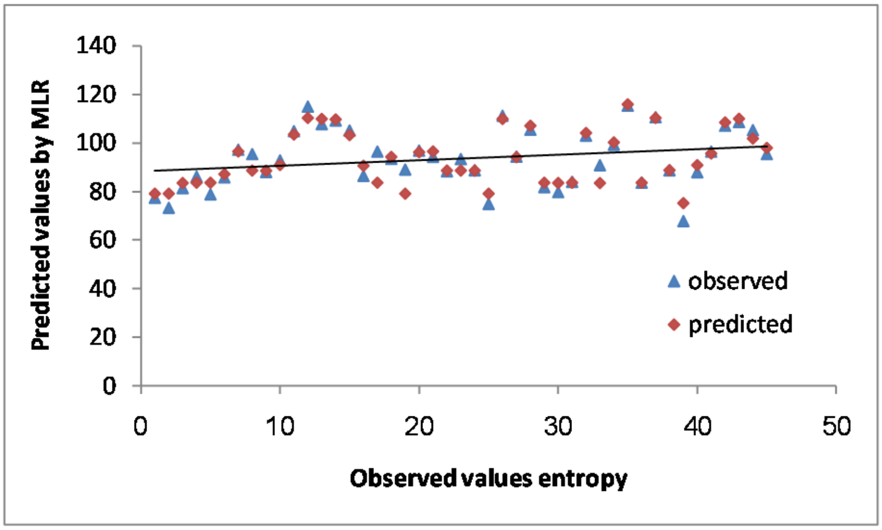

Figure 9. Comparison between the predicted and observed values of entropy by MLR.

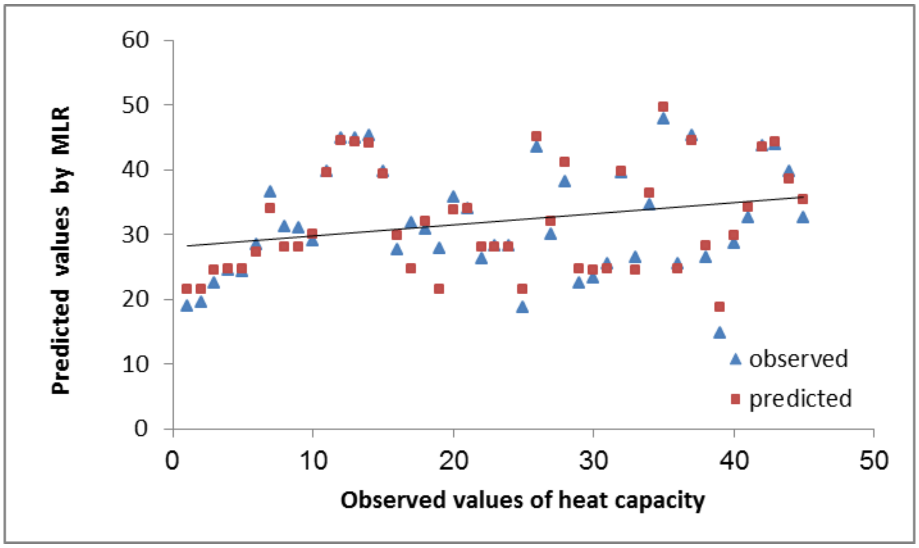

Figure 10. Comparison between the predicted and observed values of thermal energy by MLR

ABSTRACTS
IN
PERSIAN

Degree Distance Index of the Mycielskian and its Complement

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شاخص فاصله-درجه گراف میسیلیسکی و مکمل آن

ادیتور رابط : بیژن طائری

چکیده

در این مقاله ما مقدار دقیق شاخص فاصله-درجه مکمل میسیلیسکی گراف های دلخواه را مشخص می‌نمائیم. قضیه مشهوری وجود دارد مبنی بر این که با دید احتمالاتی تقریبا همه گراف ها با قطر دو هستند. بر این اساس شاخص فاصله-درجه را برای میسیلیسکی گراف های با قطر دو مشخص می‌کنیم.

لغات کلیدی: فاصله-درجه، شاخص های زاگرب، ساختار میسیلیسکی.

A Note on Vertex–Edge Wiener Indices of Graphs

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یادداشتی بر شاخص‌های وینر رأسی-یالی گراف‌ها

ادیتور رابط : علیرضا اشرفی

چکیده

شاخص وینر رأسی-یالی گراف همبند ساده‌ی G به صورت مجموع فواصل بین رأس ها و یال های G تعریف می‌شود. دو فاصله ی ممکن $D_1(u,e|G)$ و $D_2(u,e|G)$ بین رأس u و یال e از G در نوشته‌ها در نظر گرفته شدند و با توجه به آن‌ها شاخص‌های وینر رأسی-یالی مربوط به $W_{ve_1}(G)$ و $W_{ve_2}(G)$ معرفی شدند. در این مقاله فرمول‌های دقیقی برای محاسبه‌ی شاخص‌های وینر رأسی-یالی دو گراف ترکیبی تحت عنوان به‌هم‌پیوستگی و اتصال گراف‌ها ارائه می‌کنیم.

لغات کلیدی: فاصله در گراف، شاخص وینر رأسی-یالی، به‌هم‌پیوستگی، اتصال.

Electro–Spunorganic Nanofibers Elaboration Process Investigations using BPs Operational Matrices

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بررسی فرآیند چرخه تولید نانوفیبرهای الکتروریسی شده ارگانیک با استفاده از ماتریس عملیاتی BP

ادیتور رابط : ایوان گوتمن

چکیده

در این مقاله، ماتریس‌های عملیاتی حاصل از چندجمله‌ای‌های برنشتاین برای حل معادله براتو استفاده شده است. این معادله غیرخطی، در چارچوب فرآیند ساخت نانوفیبرهای الکتروریسی‌شده ویژه ظاهر می‌شود. نانوفیبرهای آلی الکتروریسی‌شده در گستره وسیعی از کاربردهای فیلتراسیون از جمله صنایع فیلترسازی و منسوجات بی‌بافت مورد استفاده قرار می‌گیرند. با استفاده از ماتریس‌های عملیاتی انتگرال و حاصلضرب، معادله مورد بحث به دستگاهی از معادلات جبری تبدیل می‌شود. جواب‌های عددی، دقت و سادگی روش پیشنهادی را نشان می‌دهند.

لغات کلیدی: معادله براتو، نانوفیبرهای الکتروریسی‌شده، چندجمله‌ای برنشتاین، ماتریس‌های عملیاتی.

Hosoya Polynomials of Random Benzenoid Chains

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چندجمله‌ای‌های هوسویای زنجیرهای بنزوئید تصادفی

ادیتور رابط : علی رضا اشرفی

چکیده

فرض کنید G یک گراف مولکولی با مجموعه رأس‌های $V(G)$، و $d_G(u,v)$ فاصله توپولوژیکی بین رأس‌های u و v در گراف G باشد. چندجمله‌ای هوسویای $H(G,x)$ از گراف G یک چندجمله‌ای $\sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$ با متغیر x است. در این مقاله بیان تحلیلی صریحی برای مقدار مورد انتظار از یک زنجیر بنزوئید تصادفی با n-تا شش‌ضلعی ارائه می‌دهیم. همچنین مقادیر مورد انتظار از شاخص‌های توپولوژیکی شناخته شده: شاخص وینر، شاخص هایپر-وینر و شاخص Tratch–Stankevitch–Zefirov از یک زنجیر بنزوئید تصادفی با n شش‌ضلعی می‌تواند توسط محاسبات ساده ریاضی بدست بیاید، که با نتایج بدست آمده توسط ایوان گوتمن تولید می‌شود.

لغات کلیدی: شاخص وینر، زنجیر بنزوئید تصادفی، چند جمله ای هوسویا، مقدار مورد انتظار، تابع تولید کننده.

Complete Forcing Numbers of Polyphenyl Systems

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اعداد نفوذ(اجبار) کامل سیستم‌های پلی‌فنیل

ادیتور رابط : حسن یوسفی آذری

چکیده

ایده " نفوذ(اجبار)" مدت زیادی در بسیاری از شاخه‌های تحقیقاتی وجود داشته است، مانند: رنگ‌آمیزی، جهت‌گیری، کمترین فاصله و مجموعه‌های غالب در نظریه گراف، که به همان خوبی مربع‌های لاتین، طراحی‌های بلوک و سیستم‌های استینر در ترکیبیات می‌باشد. اخیرا بحث نفوذ روی جورسازی‌های کامل توجه بسیاری از محققان را به خود جلب کرده است. یک مجموعه اجباری از یک جورسازی کامل گراف G، زیرمجموعه‌ای از M است که در هیچ جورسازی G مشمول نباشد. یک مجموعه اجباری سراسری G که توسط واکیسویچ و دیگران معرفی شد، یک زیر مجموعه از E(G) با محدودیت‌های ذاتی که برای هر دو جورسازی مختلف G وجود دارد، است. با ترکیب ایده‌های" اجباری" و "سراسری" یک مجموعه، زو و دیگران یک مجموعه اجباری کامل از G را که به صورت زیر مجموعه‌ای از E(G) با محدودیت‌هایی که برای هر جورسازی کامل M از G تعریف می‌شود، معرفی کردند. مینیمم کاردینال مجموعه‌های اجباری کامل، تعداد اجبارهای کامل G است. در این مقاله بیان صریحی برای عدد اجباری کامل برای چندین دسته از سیستم‌های پلی‌فنیل ارائه می‌کنیم.

لغات کلیدی: عدد اجبار کامل، سیستم پلی‌فنیل، عدد اجباری سراسری.

Quantitative Structure Activity Relationship Study of Inhibitory Activities of 5–Lipoxygenase and Design new Compounds by Different Chemometrics Methods

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مطالعه ارتباط کمی فعالیت-ساختار برای فعالیت‌های مهارکنندگی 5-لیپوکسی ژناس و طراحی ترکیبات جدید توسط روش‌های کمومتریک مختلف

ادیتور رابط : ایوان گوتمن

چکیده

مطالعه ارتباط کمی فعالیت-ساختار (QSAR) برای پیش‌بینی بازدارندگی فعالیت 1-فنیل2H تتراهیدرو تریازین3 یک آنالوگ به عنوان مهارکننده 5-لیپوکسی ژناس می‌باشد. فعالیت‌های بازدارندگی فنیل-2Hتتراهیدرو تریازین3 به عنوان تابعی از ساختارهای مولکولی و با استفاده از روش‌های کمومتریک از قبیل رگرسیون خطی چندتایی(MLR) وحداقل مربعات که از ماشین‌های برداری (LS-SVM) حمایت می‌کند، مدل‌سازی می‌شود. مدل‌های به‌دست‌آمده به منظور پیش‌بینی فعالیت مهارکنندگی ترکیباتی که در فرآیند مدلسازی نبودند، به‌کار گرفته شده‌اند. نتایج مدل‌ها نشان داد که توانایی پیش‌بینی بالا با میانگین ریشه خطای مربع برای MLR و LS-SVM به ترتیب برابر است با: 0/167 و 0.061 می‌باشد. روش LS-SVM برای پیش‌بینی فعالیت مهارکننده مشتقات مهارکننده جدید مورد استفاده قرار گرفت.

لغات کلیدی: QSAR، 1-فنیل2H تتراهیدرو تریازین3، MLR، LS-SVM.

Three–Center Harary Index and its Applications

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شاخص هاراری سه‌مرکزی و کاربردهایش

ادیتور رابط : علی رضا اشرفی

چکیده

شاخص هاراری H می‌تواند به عنوان یک توصیف‌گر ساختار مولکولی در نظر گرفته شود که متشکل از افزایش بر همکنش‌های نشان‌داده‌شده بین جفت‌اتم‌ها است، به طوری که مقدارشان با افزایش فاصله بین دو اتم مربوطه، کاهش می‌یابد. یک تعمیم از شاخص هاراری،که با Hk نشان داده می‌شود، با به‌کارگیری فاصله از نوع استینر بین k-تایی از اتم‌ها به دست می‌آید. ما نشان می‌دهیم ترکیب خطی $H+\lambda H3$ به صورت معنی‌داری از نظر تنوع خواص فیزیک-شیمی آلکان ها، نسبت به خود H بهتر است.

لغات کلیدی: شاخص هاراری، شاخص هاراری چند مرکزی، فاصله استینر، گراف مولکولی.

Investigation the Effect of Nanocomposite Material on Permeation Flux of Polyerthersulfone Membrane using a Mathematical Approach

MARJAN ADIB

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بررسی تأثیر مواد نانوکامپوزیت روی نفوذ شار غشاء پلی‌اترسلفون با با رویکرد ریاضی

ادیتور رابط : ایوان گوتمن

چکیده

غشاءهای نامتقارن پوسته‌ای یکپارچه، بر اساس نانوکامپوزیت پلی‌اترسلفون توسط فرآیند جداسازی CO2 فوق‌بحرانی به عنوان یک غیرحلال برای یک محلول پلیمر تهیه شده‌اند. در این پژوهش، اثرات دما و نانوذرات بر عملکرد انتخابی و نفوذپذیری گازها مورد بررسی قرار گرفته است. همچنین نشان داده شده است که حضور نانوذرات سیلیکا نه تنها بسته‌بندی زنجیره‌ای پلیمر اصلی را مختل می‌کند، بلکه باعث ایجاد تغییرات شیمیایی پانسیون‌ها در ماتریس‌های پلی‌پورتسولفون می‌شود. به‌دلیل حضور هیدروفیلیک سیلیکا ، CO2 پرکننده وابستگی، پیوند هیدروژن فعل و انفعالات بین اتم‌های اکسیژن از دی‌اکسیدکربن و اتم‌های هیدروژن از گروه هیدروکسیل روی سطح نانوسیلیکا در پیوند اتفاق می‌افتد و بنابراین حل‌پذیری و در نتیجه نفوذپذیری به سمت CO2 در مقایسه با CH4 برای غشاءها بیشتر است. علاوه بر این، در مطالعه حاضر، یک رویکرد ریاضی جدید پیشنهاد شده است تا یک مدل جدید برای شار نفوذی و عملکرد انتخابی از غشاءای که تحت پشتیبان ماشین برداری استفاده می‌شود، توسعه یابد. SVM برای توسعه مدلی به منظور تخمین فرآیند متغیرهای خروجی از یک غشاء نانوکامپوزیت که شامل شار نفوذی و عملکرد انتخابی است، به‌کار گرفته می شود. توسعه مدل که شامل آموزش، بهینه‌سازی و آزمایشی که به ترتیب برای 80 درصد، 10 درصد انتخاب تصادفی و 10 درصد متغیر ها به کار می‌رود، انجام شد. نتایج آزمایش بر اساس مدل SVM نشان‌دهنده توافق بهتری با داده‌های تجربی در مقایسه با سایر مدل‌های ریاضی پیشرفته است. کمترین مقدار همبستگی مربعی محاسبه‌شده برای فرآیند تخمین متغیرها برابر 0.99 می باشد. بر اساس نتایج این نمونه مطالعه SVM ثابت کرد که این روش تخمین، دقیق و قابل اعتماد است.

لغات کلیدی: مواد نانوکامپوزیت، غشاء پلی‌اترسلفون، نانو ذرات سیلیکا، پشتیبان ماشین برداری (SVM).

On The Generalized Mass Transfer with a Chemical Reaction: Fractional Derivative Model

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در باب انتقال جرم تعمیم‌یافته با یک واکنش شیمیایی: مدل مشتق کسری

ادیتور رابط : علی رضا اشرفی

چکیده

در این مقاله، ما با استفاده از معکوس تبدیل لاپلاس، جوابهای تحلیلی برای انتقال جرم تعمیم یافته با (بدون) یک واکنش شیمیایی را نشان می دهیم. این انتقالات به عنوان جریان کوت با مشتق کسری کاپوتو بیان می‌شوند. همچنین با استفاده از مسیر هنکل برای انتگرال بروموویچ، جوابها بر حسب توابع ایری تعمیم یافته ارائه می شوند.

لغات کلیدی: مساله لِوِک، تبدیل لاپلاس، توابع ایری تعمیم یافته، مشتق کسری.

A Note on Hyper–Zagreb Index of Graph Operations

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یادداشتی درباره شاخص ابرزاگرب عملگرهای گراف

ادیتور رابط : علی رضا اشرفی

چکیده

در این مقاله، شاخص ابرزاگرب حاصل‌ضرب دکارتی، حاصل‌ضرب ترکیبی و حاصل‌ضرب کرونای گراف‌ها محاسبه می‌شود. این نتایج بعضی خطاها در مقاله شیردل و همکارانش را تصحیح می‌کند.

لغات کلیدی: شاخص ابرزاگرب، شاخص زاگرب، عمل گراف.

QSPR Study on Benzene Derivatives to some Physico–Chemical Properties by using Topological Indices

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مطالعه ارتباط کمی ساختار-خاصیت برخی از خواص فیزیکی-شیمیایی مشتقات بنزن با استفاده از شاخص‌های توپولوژیکی

ادیتور رابط : ایوان گوتمن

چکیده

امروزه با استفاده ازروش‌های توپولوژیکی به مطالعه ارتباط کمی ساختار-خاصیت مشتقات بنزن پرداخته شده است. در این تحقیق ارتباط بین شاخص‌های توپولوژیک راندیک اتصال یک(1χ) ، بالابان(J)، سگد(Sz)، هاراری(H)، ابروینر(WW) و وینر پلاریتی (WP) به روش نظریه گراف برای مشتق‌های بنزن موردنظر محاسبه گردید. سپس همبستگی این شاخص‌های توپولوژیک با خواصی نظیر انرژی گرمایی(Eth)، ظرفیت گرمایی در حجم ثابت (Cv) وآنتروپی (S) بدست آمده از روش مکانیک کوانتومی مورد بررسی قرار گرفت. خواص فیزیکی-شیمیایی فوق باکمک نرم‌افزارهای گوس ویو وگوسین 98و با استفاده از یکی از روش‌های آغازین هارتری-فاک و سری پایه 6-31G محاسبه گردید. سپس به منظور مطالعه رابطه کمی ساختار – خاصیت از نرم افزار آماری SPSS، روش برگشتی رگرسیون خطی چند متغیره (MLR) استفاده شد. بدین طریق معین گردید که برای پیشگویی کمیت‌های ظرفیت گرمایی در حجم ثابت (CV) وآنتروپی (S) مشتق های بنزن مورد مطالعه، ترکیبی از دو توصیف‌گر توپولوژیکی، شاخصهای سگد و ابروینر مناسب می‌باشد. اما با توجه به نتایج بدست آمده از روش MLR هیچ‌یک از شاخص‌های مورد مطالعه جهت پیشگویی انرژی گرمایی(Eth)، مناسب نمی‌باشند. بدین ترتیب کارایی شاخص‌های توپولوژیکی مورد استفاده در مدل‌سازی و تعیین خاصیت‌های مولکولی مورد نظر، معین گردید.

لغات کلیدی: بررسی کمی ساختار- خاصیت، شاخص توپولوژیکی، مشتقات بنزن، نظریه گراف، رگرسیون خطی چند متغیره (MLR).

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