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A Theoretical Study of the Size Effect of Carbon Nanotubes on the Removal of Water Chemical Contaminants

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ABSTRACT

The issue of contamination is considered one of the most important and acute issues of human civilization in today's world. In the new decade, humans are facing the problem of clearing natural resources and the environment, including climate. Among the sources of water contaminants are chemical compounds that enter the water naturally through various methods and as a result of human activity. A group of water chemical contaminants is pesticides and herbicides which are widely used in agricultural consumptions. Carbon nanotubes are one of the ways to clean contaminated water, given that carbon nanotubes are in a wide level, they can be very effective in dealing with contaminants, on the other hand, carbon nanotubes can be used as clearing at the site of contamination. In this paper, six chemical contaminants of water including atrazine, simazine, benzoate, ethylbenzene, chloronaphthalene, xylene, have been placed in the vicinity of carbon nanotubes. Adsorption effect has been investigated through parameters such as composition stability, system volume, molecule level and toxicity criterion, polarity level using simulation methods in specialized software, by resizing the carbon nanotubes and finally the most important factor in resizing carbon nanotubes has been introduced.

1. INTRODUCTION

Water is an essential element for life. The amount of fresh water is limited on earth and its quality is under constant pressure. Maintaining freshwater quality is important for the supply of drinking water, food production and the use of recreated water. Water quality can be exposed to risk by the presence of infectious factors, toxic chemicals and radiological hazards. The existence of safe, reliable and free of toxic and hazardous water sources is an essential need for having a healthy and sustainable community. In the new millennium, human is facing the challenge of clearing natural resources, including climate (Zhang, 2003).

Nanotechnology is one of the most important technologies that its applications are associated with lower cost, longer durability and life, lower energy consumption, lower maintenance cost and better properties. Therefore, the application of this knowledge in the field of environmental engineering has been developed as other aspects of human knowledge (Blurchian et al., 2008). Over the past decade, scientists have developed methods to synthesize and describe many new materials with at least one of the dimensions in nanoscale including nanoparticles, nanolayers, and nanotubes. However, the design and synthesis of nanoscale materials with controlled properties is an important and advancing challenge in nano-science and technology (Dahl et al., 2007).

Carbon nanotubes (CNTs) are a new alloform from the carbon family that was reported in 1991 for the first time. Carbon nanotubes (CNTs) have remarkable chemical, physical, mechanical, electrical properties and high length to width ratio [2]. The high length to width ratio of carbon nanotubes (CNTs) places them in the field of one of the refinement materials for wastewater treatment plants [3]. These excellent and unique properties led to various applications in fields such as nanoelectronics, nano-microelectronic devices, field emission, catalyst amplifier, chemical sensors and amplifier of composite materials [2] as well as nanotubes. Carbon nanotubes (CNTs) have more productivity at absorbing organic chemicals compared to activated carbon. The surface of carbon nanotubes, compared to activated carbon in aqueous media, absorbs a large number of inaccessible fine substances such as antibiotics and some drugs. Therefore, carbon nanotubes have a higher absorption capacity to absorb large molecules due to their pores depending on the type of bond and the absorption place.

The area of large surface of carbon nanotubes (CNTs) creates a strong interaction between the nanotubes and dioxins [2] and mainly the large specific surface of carbon nanotubes (CNTs) has a good interaction in the absorption of various contaminants. There are two main types of carbon nanotubes with complete structure. Single-walled carbon nanotubes (SWCNTs) included an integrated graphite sheet as a cylindrical tube and multi-walled carbon nanotubes (MWCNTs) included an array of concentric cylindrical tubes [4 and 2]. Carbon nanotubes as nanostructures have kept the researchers' hope for developing carbon-based nano-materials alive, and researchers are continuing their studies on capacity of absorbing carbon nanotubes [2, 5].

On the other hand, researches have recently been conducted in Stockholm in 2007 in the field of the interactions of carbon nanotubes (CNTs) [1, 6]. According to their effects on cells and organisms, nanomaterials enter the human body through respiration or skin contact, and eventually, if the nanomaterials are present in drugs and foods, they enter the human body by injection or digestion. [7 and 1]. Nanoparticles can

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develop cancer and affect nerve cells and liver, skin and brain cells as well as destruct the integrity of organs and genes. The potential toxicity of the nanoparticles on reproduction and entering into the testes and staying there may have adverse effects on sperm [8, 7, 1].

Nanotechnology is a new and very hopeful trend in science and technology that will shape many new sciences and technologies in the future and will change different aspects of our lives and it will have a great desire to create oneness in all branches of science and technology.

2. RESEARCH METHOD

2.1. Chemical contaminations used

2.1.1. Atrazine

Atrazine is an herbicide widely used by farmers to control weeds. This herbicide is used to remove weeds with the mechanism of stopping photosynthesis in weeds and in some crops in various fields including corn and wheat fields. Recent studies have shown that atrazine has an inhibitory effect on hormone receptors in mammals.

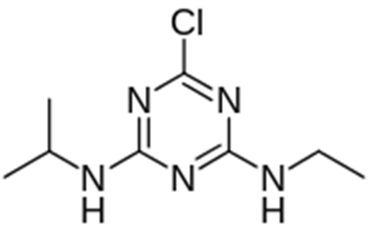

Figure 1. Molecular structure of atrazine

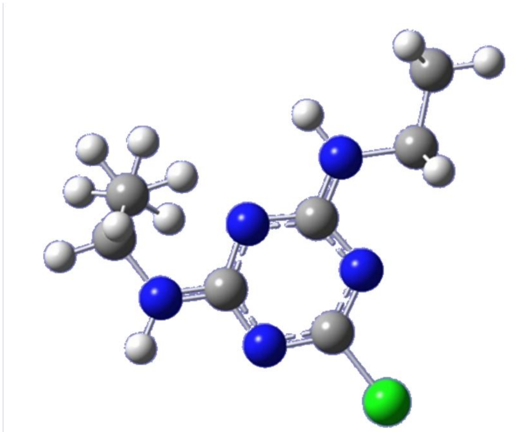

Figure 2. Molecular structure of atrazine in 3D space

Studies have shown that atrazine reduces the activity of 5 alpha-reductase, which itself plays an important role in the metabolism of testosterone. It converts testosterone into an active metabolite called 5 alpha-dihydrotestosterone in the anterior part of pituitary gland and prostate gland.

2.1.2. Benzot

Benzoates are used as preservatives against yeast and mold and have less effect on bacteria. The use of this group of preservatives dates back to the early 1900s. They have synergistic effects with other preservatives such as sorbates, and they are used along with sulfur dioxide, which alone prevents enzymatic activity and browning.

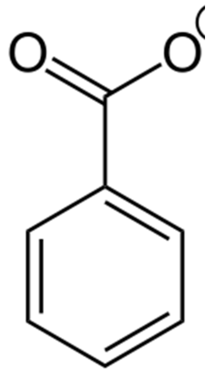

Figure 3. Molecular structure of benzot

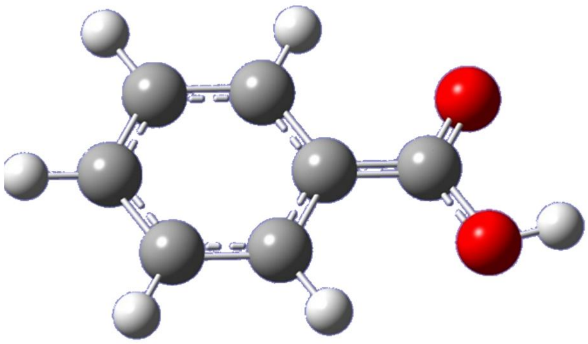

Figure 4. Molecular structure of benzot in 3D space

Sodium benzoate alone can damage and deactivate vital DNA components in cell mitochondria. Mitochondria play a role in energy production in the cell and, if damaged, the cell may be disrupted and may enter apoptosis. Many diseases are attributed to DNA damage, such as Parkinson and other brain and nerve destruction diseases.

2.1.3. Chloronphthalene

Chloronphthalene is an aromatic compound. It is colorless oil that can be used to determine the refractive index of crystals by immersion. The substance is obtained by direct relation with chlorine and naphthalene and it is substituted with dichloro by many derivative compounds.

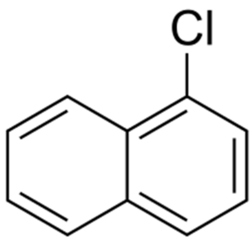

Figure 5. Molecular structure of Chloronphthalene

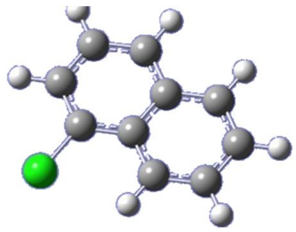

Figure 6. Molecular structure of chloronphthalene in 3D space

This chemical compound is a very toxic and it is sometimes used as a powerful biocide without polymer. Most of times, it is used as insecticides and fungicides on the wooden surface of shipping containers and rivers.

2.1.4. Ethylbenzene

The form of this compound is colorless liquid. Ethylbenzene is a toxic aromatic compound and from petroleum hydrocarbon derivatives that usually entered into the environment through permeation from petroleum industries and activities, waste and wastewater discharge related to pharmaceutical industries, petrochemicals. Complications of ethylbenzene can lead to drowsiness-fatigue-headache-mild pains of eye. If ethylbenzene is present in the water it can lead to diseases such as failure of liver-kidney and the nervous system in long term.

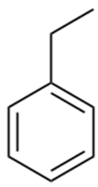

Figure 7. Molecular structure of ethylbenzene

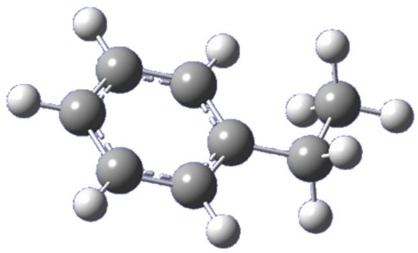

Figure 8. Molecular structure of ethylbenzene in 3D space

Ethylbenzene stimulates the respiratory and nervous system and it is one of the carcinogenic pollutants.

2.1.5. Simazine

Simazine is one of the herbicides of the triazine family which can have a residual and toxic effect on sensitive crops due to its relatively high stability. This compound is used to control broadleaf weeds and annual plants.

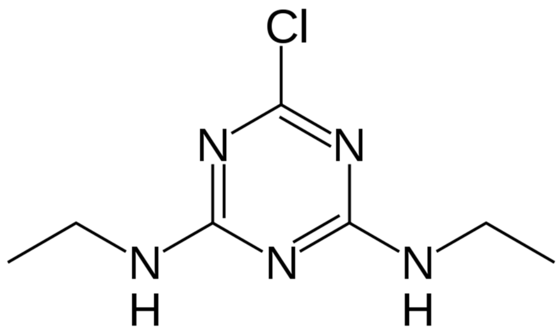

Figure 9. Molecular structure of simazine

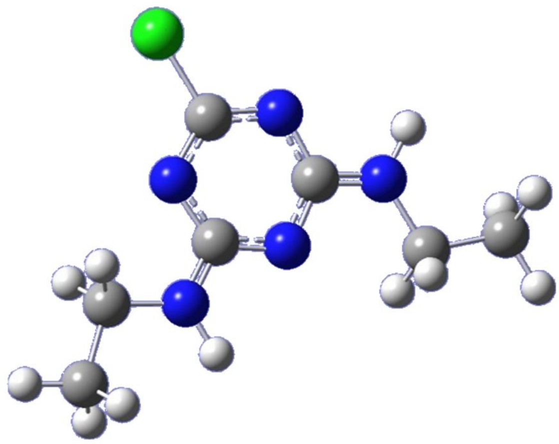

Figure 10. Molecular structure of simazine in 3D space

2.1.6. Xylene

A mixture of three aromatic hydrocarbons is called isomer that has a benzene ring and two methyl groups attached to it. Xylenes are used as solvents in paint and plastic and synthetic adhesive. Xylenes are clear, colorless, fragrant and very flammable liquids. The presence of xylene in the water causes pulmonary edema and its continuous inhalation causes irregular heartbeat. Xylene has nerve effects.

Figure 11. Molecular structure of xylene

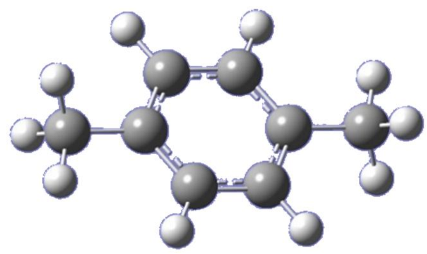

Figure 12. Molecular structure of xylene in 3D space

In case of continuous or long-term period contact, it may cause headaches, muscle weakness, dizziness, and imbalances. Contact with xylene in short time can cause skin, eye, and nose and throat irritation. Xylene is very flammable.

3. SIMULATION AND ENTRY OF DATA INTO SOFTWARE

3.1. Software used

Since it is observed in the title of the article, the research conducted is based on a theoretical study and the neural network method has been used for this purpose. Before entering information to the neural network, a series of specialized chemistry software has been used to obtain some important computational parameters. In the first step, it is referred to the Chem Office Suit software family and it has been used to plot the molecular structure in two-dimensional and three-dimensional spaces. In the second step, it is referred to the Open Babel software and this software has been used to convert suffixes and file recognition to Gauss View software. In the third step, as mentioned above, two parameters of Lumo and Homo were obtained in the Gauss View software as the first outputs. In the fourth step, for converting stored files, Gussian software was used to file recognition to Multiwfn software and finally, three important parameters of volume mass- the available surface and the dipole factor were obtained as subsequent outputs by the help of Multiwfn software. Then the most important factors and parameters in the absorption of contamination have been introduced using the program written by neural network method in Matlab software.

As it can be seen above, there was no word on the presence of carbon nanotubes in the calculations, so after receiving the final outputs from the MATLAB software using the Nanotube Modeler software and the Pymol software, we put each of the contaminants along the lengths 20, 30 and 40 angstroms from carbon nanotubes and we pass all the steps again, then we receive outputs from MATLAB software and compare the obtained tables and finally we introduce the overall conclusion and the most important parameter in resizing carbon nanotubes on the removal of water chemical contaminants.

3.2. Different modes of calculations

In this study, four different modes have been investigated.

Mode One: Contaminants in the absence of carbon nanotubes

Mode Two: Contaminants in the vicinity of a single-wall armchair carbon nanotube with a length of 20 angstroms

Mode Three: Contaminants in the vicinity of single-wall armchair carbon nanotube with a length of 30 angstroms

Mode Four: Contaminants in the vicinity of single-wall armchair carbon nanotube with a length of 40 angstroms

For using neural network, half of the data generated in each mode was selected for network training and the rest of network control.

4. FINDINGS

4.1. The first mode

The structural parameters of the six contaminations were studied and their results are shown in Table 1. After obtaining the results of Table 1 using the neural network, the test error and control error have been calculated in table 2 and diagram 1. Accordingly, the most important parameter is selected using neural network method.

Table 1. Properties of contaminations in the absence of carbon nanotube

LOG'S	Total dipole	Overall surface Area	VOLUME	LUMO	HOMO	Material
-1/25	0/001774	155/31843	147/7109	-0/16580	-0/34293	Atrazine
-1.66	1/6547083	240/57367	238/5106	-0/14484	-0/32664	Benzot
-1.33	1/2388581	143/51814	134/3219	-0/19823	-0/36382	Chloronaphthalene
-1.03	1/8285065	230/67442	221/4988	-0/14364	-0/32676	Ethylbenzene
-1.48	0/3249902	152/25167	146/2514	-0/16559	-0/35306	Simazine
-0.85	0/1007574	180/50024	184/0319	-0/20017	-0/31129	Xylene

Table 2. Values of test and control error for contamination in the absence of nanotubes

Test error	Control error	Selected parameter
0.0103	0.1374	Homo
0.1606	0.17••	LOMO
0.0097	32.3061	Volume
0.0001	0.2218	Overal surface Area
0.0000	0.2413	Total dipole

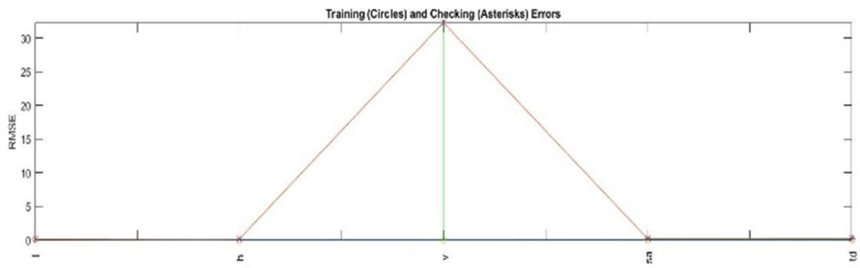

Diagram 1. Test and control error in the absence of carbon nanotubes

The parameter selected in this case is the available polar surface.

4.2. The second mode

The structural parameters of the six contaminations were studied and their results are shown in Table 3. After obtaining the results of Table 3 using the neural network, the test error and control error have been calculated in table 4 and diagram 2. Accordingly, the most important parameter is selected using neural network method.

Table 3. Properties of contaminations in the absence of carbon nanotube with length of 20 angstrom

LOG'S	TOTAL DIPOL	OVERAL SURFACE	VOLUME	LUMO	HOMO	Material
-1/25	1/2434698	250/75817	252/84928	-0/32056	-0/16518	Atrazine
-1.66	1/8827944	162/56373	156/019	-0/2955	-0/19518	Benzot
-1.33	0/4775587	199/63876	208/13891	-0/28038	-0/18913	Chloronaphthalene
-1.03	0/4210947	167/13278	164/11314	-0/29152	-0/16687	Ethylbenzene
-1.48	4/2536142	240/39511	238/18582	-0/29094	-0/19876	Simazine
-0.85	0/0052249	170/43019	165/27999	-0/28547	-0/16824	Xylene

Table 4. Values of test and control error for contamination in the presence of carbon nanotubes with a length of 20 angstroms

Test error	Control error	Selected parameter
0/0641	0/2501	Homo
0/0018	0/2902	LOMO
0/0003	1/4547	Volume
0.0000	0/661۰	Overal surface Area
0.0000	0/134۰	Total dipole

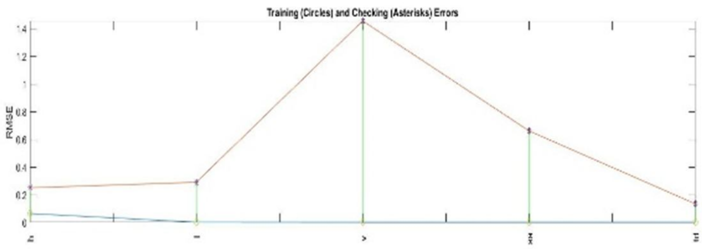

Diagram 2. Test and control error in the presence of carbon nanotubes with a length of 20 angstroms

The parameter selected in this case is the available polar surface.

4.3. The third mode

The structural parameters of the six contaminations were studied and their results are shown in Table 4. After obtaining the results of Table 4 using the neural network, the test error and control error have been calculated in table 5 and diagram 3. Accordingly, the most important parameter is selected using neural network method.

Table 5. Properties of contaminations in the absence of carbon nanotube with length of 30 angstrom

LOG'S	TOTAL DIPOL	OVERAL SURFACE	VOLUME	LUMO	HOMO	Material
-1/25	1/6446375	240/55967	238/49963	-0/32666	-0/14495	Atrazine
-1.66	1/9631981	157/91421	146/84249	-0/32994	-0/18769	Benzot
-1.33	0/2971313	192/15031	197/47864	-0/29109	-0/19673	Chloronaphthalene
-1.03	1/4768851	165/47388	159/5926	-0/31151	-0/19463	Ethylbenzene
-1.48	2/5476806	252/40002	240/4663	-0/27668	-0/19061	Simazine
-0.85	0/0313522	163/08493	161/81474	-0/29502	-0/22032	Xylene

Table 6. Values of test and control error for contamination in the presence of carbon nanotubes with a length of 30 angstroms

Test error	Control error	Selected parameter
0/0001	0/3469	Homo
0/007٠	0/5069	LOMO
0/0137	1/7708	Volume
0/0004	0/107٠	Overal surface Area
0.0000	0/1156	Total dipole

Diagram 3. Test and control error in the presence of carbon nanotubes with a length of 30 angstroms

The parameter selected in this case is the available polar surface.

4.4. The fourth mode

The structural parameters of the six contaminations were studied and their results are shown in Table 5. After obtaining the results of Table 5 using the neural network, the test error and control error have been calculated in table 6 and diagram 4. Accordingly, the most important parameter is selected using neural network method.

Table 7. Properties of contaminations in the presence of carbon nanotube with length of 40 angstrom

LOG'S	TOTAL DIPOL	OVERAL SURFACE	VOLUME	LUMO	HOMO	Material
-1/25	2/8542426	250/8644	253/41226	-0/16671	-0/31368	Atrazine
-1.66	1/9851059	157/71663	146/70546	-0/18718	-0/33012	Benzot
-1.33	0/3004555	192/09331	197/38761	-0/19626	-0/29121	Chloronaphthalene
-1.03	1/3955577	165/49413	159/60979	-0/19949	-0/31184	Ethylbenzene
-1.48	0/5233788	231/52197	223/47829	-0/1561	-0/32103	Simazine
-0.85	0/0186486	162/0946	160/07544	-0/21307	-0/2885	Xylene

Table 8. Values of test and control error for contaminants in the presence of carbon nanotubes with length of 40 angstroms

Test error	Control error	Selected parameter
0/0005	0/19909	Homo
0.0000	0/1604	LOMO
0.0000	1/1745	Volume
0/0002	1/1026	Overal surface Area
0.0000	0/6629	Total dipole

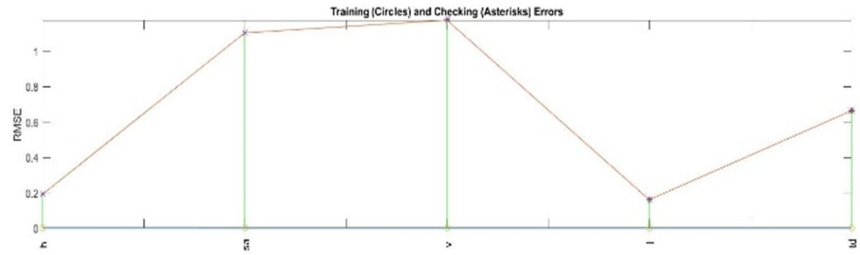

Diagram 4. Test and control error in the presence of carbon nanotubes with a length of 40 angstroms

The parameter selected in this case is the available polar surface.

5. CONCLUSION

As it was observed, according to the inputs and outputs of the software with the neural network model, the armchair carbon nanotube is observed when the test error for the available polar surface parameter is less than the other parameters at all states and lengths. It means that the contaminations of compounds studied of this parameter are more important than other parameters, and the design should be based on this case in the executive state.

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