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ORIGINAL ARTICLE

Theoretical Study of Relation among Structural Parameter and Water Decontamination Behaviors of some Drugs in Presence of Carbon Nanotube

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KEYWORDS

Purification of wastewater; Pharmaceutical pollution; Carbon nanotubes; Fuzzy-Neural Adaptive Inference System; Artificial Neural Network

ABSTRACT: The shortage and extremely high utilization of water resources and the necessity of water with optimal quality for drinking and agricultural use and the preservation of the environment, human has led to the purification of industrial waste and wastewater by preventing the entrance of pollutants into surface water and underground water and creating a trusted cycle. One of the most dangerous pollutants that threating human health and the environment is Pharmaceutical pollution. Due to the high solubility of drugs, conventional purification cannot completely eliminate these contaminants, and the researchers have noted the use of new techniques such as the use of nanotechnology in water treatment, which entails high initial costs. For this reason, one has to look for a solution to these costs; one of the most commonly used methods of using theoretical methods. In this study, an effective method for treating carbon nanotubes in artificial nanotubes using the artificial neural network (ANN) system and the fuzzy-nerve adaptive inference system (ANFIS) has been used. Some structural descriptors Such as polar surface area, LUMO, HOMO and molecular volume were calculated and studied for more influential performance in experimental experiments. In this regard, the control error and the test error were analyzed and the correlation between the effective parameters was determined. Then, a parameter that has a greater impact on water contamination has been identified in the presence and absence of carbon nanotubes. As a result, the polar surface has the greatest impact.

INTRODUCTION

The shortage of water, especially in arid and semi-arid areas, and the excessive use of water resources and providing good water quality for drinking, agricultural and environmental purposes, has led humans to find recovery and reuse of Industrial wastewater, sewage, and floods and also create a reliable and effective cycle [1]. Drug contaminants are one of the important issues of today's life. Many researchers, especially in advanced countries, have reported the presence of these pollutants even in drinking water, and have been mentioned their negative effects on the environment and human health [2]. Nowadays, medicines are an essential element in modern life. Medicines are used in the treatment of humans, veterinary, agriculture and

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aquaculture [2, 3]. The presence of drugs in the environment is increasing greatly around the world. Humans and animals are the main source of infection due to the use of drugs. Some medicines are widely used in treatment, which is due to active metabolite, which has a high percentage of consumption, so they constantly discharge in the sewage. Due to the long half-life of these medicines in the environment and the accumulation and active biological levels, these drugs cause environmental contamination [4]. Recent studies indicate that many of the drug substances are inadequately removed in the refinery, and the presence of drugs in surface water, groundwater and even marine systems shows low concentration to high concentrations [4]. Studies show that medicines are consumed extensively by manufacturers of medicines, also expired medicines and overdose medicines, and drugs that are consumed by humans and animals, are entering to environment. Drugs used by humans are the main source of contamination. Due to the high solubility of drugs, the possibility of their occurrence in aquatic resources is much higher. Unfortunately, conventional water purification is not able to eliminate these contaminants and medicines that have a high half-life, especially antibiotics accumulate in water, and reinstate the human body and mutation human body and mutation Microorganisms have dangerous consequences. In recent decades, only a few scientists have been interested in finding out the fate of these drugs and their effects on living organisms that are emitted in large quantities in the environment [2]. Active drug substances (APIs) are known from the time of preparation and used as pollutants in the environment. Environmental impacts can range from invisible to obvious in multiple environments (such as aquatic environments) and even at higher and more severe levels (such as wildlife consumption). Reducing (APIs) in the environment relies on pollution control at the outlet of the refinery [5]. By the 1990s, the possibility of the occurrence of a drug in the environment (PIE) and its fate was thought to be normal. This lack of scientific interest in pharmacy appears to be confusing as an environmental pollutant [3]. The first comprehensive scientific research in the 1990s were done on the presence of drugs in local rivers and sewage treatment systems, and in some studies in 2002 there were more than 60 drug compounds in rivers and sewage treatment systems [2]. Pharmaceutical materials must have a very high solubility in the body of (human, animal, plant) for absorbing to the target cells [2]. Drugs are essentially "biological, active, and often complex. They often have a stable biologically analysis, and also stable metabolism. Some medicines are highly water soluble. Due to the lack of degradation and biological composition, their removal in the refinery is limited and, as a result, they enter into the body of living organisms by entering aquatic environments [3]. Modifying long norms for prescribing clinical drugs can be a less costly and effective way to prevent environmental pollution by drugs. For example, it can be prevented by reducing the dosage of the drug or the use and prescription of some low-risk drugs from environmental contamination. These approaches, called the Permanent and Sustainable Drugs to Environment (EDSP), can lead to reduce Active Potential Ingredients (APIs) and their entry into the environment, and can be largely eliminated (waste of unwanted foods and drugs) and manages the exclusion decrease of (APIs) metabolism [5]. In this article, the keyword of Pharmaceutical pollution in environment was investigated by the Google scholar search engine, Springer and Elsevier. In this way, some articles were achieved that investigated the various aspects of Pharmaceutical pollution in the environment experimentally. Searching Persian articles, the keyword "Pharmaceutical pollution in the environment" but unfortunately, an article was not received. Atrazine, antipyrin, aspirin, benzocaine, chlordane, and chlorpyrifos have the high risk for the environment and the health of humans and living organisms. With regard to the serious research on the global drug contamination in the world and the

necessity of starting empirical studies in our country, effective parameters were selected. These parameters were investigated with theoretical studies in order to compensate the high cost of experimental studies and time, so we could identify the most effective parameter that has the highest efficiency with the new treatment method with carbon nanotubes [6-7].

MATERIALS AND METHODS

Artificial neural networks perform the learning process based on the human learning pattern (repeating error correction by encouraging desired states) [8]. The important point is that artificial neural networks educate and operate on the basis of numerical inputs and outputs and do not need any mathematical equations of the system [8]. Learning and generalizing are the most important features of these networks, which has led to use them widely [8]. A neural network that can calculate any arithmetical and logical function is only be done using mathematics and algorithms [8, 11]. The key element of this pattern is the new structure of its information processing system, and is linked to a large number of elements (neurons) with strong internal communications called weight communications, and work together to solve a particular problem have been formed [8-12]. A neural network is a very parallel and distributed processor that consists of small processor units and has an inherent tendency to store experimental data and prepare it for use [10-12].

The purpose of this project is to use carbon nanotubes to investigate their ability to purify wastewater from the hospital theoretically [10-12]. For this purpose, the effects of different factors such as length of nanotubes and its diameter will be studied and effective structural parameters on the solubility of drugs in water will be studied [10-12]. Several cases have been used for the treatment of various contaminants, most of which are technical aspects [10-12]. The application of optimization methods along with testing and modeling designs to predict the conditions and reduce the number of required water purification tests is considered as an innovation aspect of this research. The ANFIS uses a trained input-output information set to further predict various phenomena by constructing an FIS which membership function parameters are redeployed in a post-propagation mode alone or in conjunction with the least squares method. So this model comes from a variety of neural networks along with an error post propagation algorithm and a controlled learning capability that can only support sogne type fuzzy systems [10-12]. The most obvious problem with the use of the Fuzzy Inference System is to optimize the FIS parameters, which is solved using comparative networks. Therefore, this type of network is also used in this research. The design of drugs and carbon nanotubes in a two-dimensional environment was carried out in the chem office draw professional software (version 16.0.0.82), and then they were transferred to the Chem3D software (version 16.0.0.82) to design drugs in the three dimensional environment and by analyzing the total energy of drugs and nanotubes the polar carbon was calculated and then the input file of Gaussian software (version 7.0) was prepared. Then the drugs were placed in the vicinity of the carbon nanotubes and all the processes of the calculation and preparation of the Gaussian file were repeated again. The calculation results at this stage are shown in Figures 1 to 6.

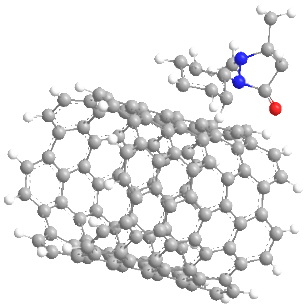

Figure 2. ANTIPYRIN with Nanotube 6.6

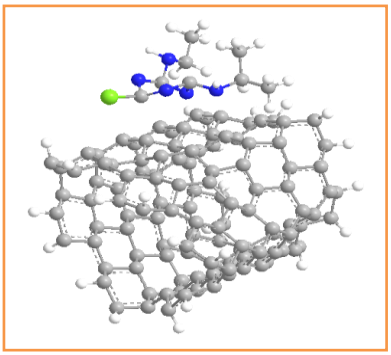

Figure 1. ATRAZIN with Nanotube 6.6

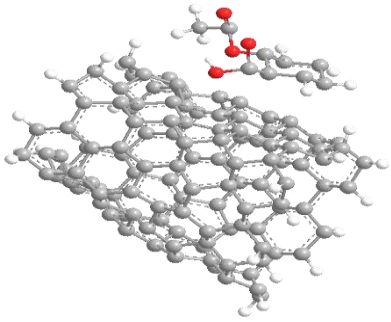

Figure 4. ASPIRIN with Nanotube 6.6

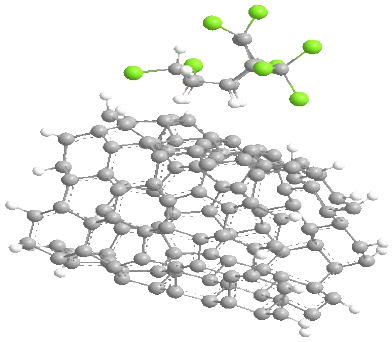

Figure 3. CHLORDANE with Nanotube 6.6

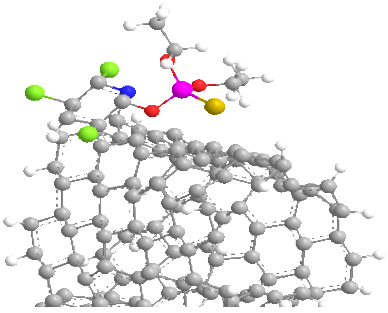

Figure 6. CHLORPYRIFOS with Nanotube 6.6

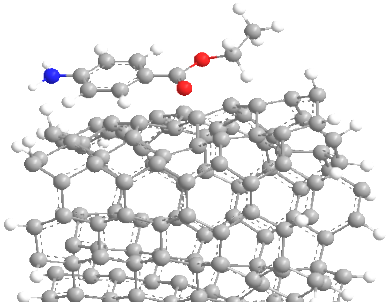

Figure 5. BENZOCAIN with Nanotube 6.6

The Gaussian software analyzed the target drug and its proximity with two carbon nanotubes and prepared the fch file and then the parameters of HOMO and LUMO were calculated using the Gaussian View software **(version 5)**. HOMO and LUMO are varieties of molecular orbitals, in chemistry. These acronyms are "the highest occupied molecular orbitals" and "the lowest unoccupied molecular orbitals" respectively. The energy difference between HOMO and LUMO is called the HOMO-LUMO cavity. The difference in the energy of the HOMO-LUMO cavity represents the stability of the molecule, and the higher the difference, the greater the stability of the molecule in the test conditions. The fch file, which was prepared in Gaussian software, was transferred to Multiwfn software (version 3.3.6), and after executing the executable software, the molecular volume of the drugs and the molecular volume of their combination with carbon nanotubes were calculated. Now using the drug solubility and the parameters obtained in the

preceding steps mentioned above, the corresponding tables are prepared and then analyzed using the fuzzy logic of the nervous system and the ANFIS algorithm in MATLAB software (version 7.8) . Two or more neurons can form a layer together. The simplest neural network is the single-layer network. The neural network includes the input layer, the hidden layer, and the output layer. Figure 7 shows a single-layer network with R input and S output of the neuron [13].

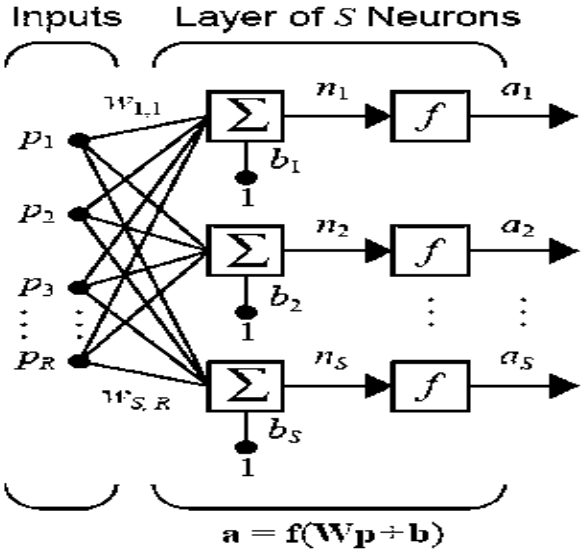

Figure 7. single-layer network

RESULTS AND DISCUSSION

Results of analysis of the ANFIS algorithm with the ANFIS algorithm in fuzzy logic-neural network were presented using MATLAB software and coding program and presented tables and diagrams for discussion of the results. The data calculated by the software in the form of a table as input parameters for the MATLAB software were prepared as follows for continuing calculations. (Tables 1-3).

Table1. Values of calculated properties for the drugs studied in the absence of nanotubes *Solubility

Name	Homo(a.u)	Lumo(a.u)	V(cm^3.mol)	Polar surface area	Logs*
ANTIPYRIN	-0.01259	0.08004	142.684	26.71	0.39
ASPIRIN	-0.03663	0.08258	119.684	69.92	-1.61
ATRAZIN	-0.04092	0.03206	152.603	60.15	-3.55
BENZOCAIN	-0.01835	0.05093	122.729	55.48	-2.32
CHLORDANE	-0.01805	0.00449	214.054	0.00	-5.35
CHLORPYRIFOS	-0.00240	0.01499	215.539	39.72	-5.67

Table 2. Values of calculated properties for the drugs studied in the presence of nanotubes 5.5 s*Solubility

Name	Homo(a.u)	Lumo(a.u)	V(cm^3.mol)	polar surface area	logs*
ANTIPYRIN- 5.5	-0.00381	0.00082	879.990	26.71	0.39
ASPIRIN- 5.5	-0.00014	0.00329	857.400	69.92	-1.61
ATRAZIN- 5.5	-0.00240	0.00485	889.932	60.15	-3.55
BENZOCAIN- 5.5	-0.00376	0.00147	855.356	55.48	-2.32
CHLORDANE- 5.5	-0.00181	0.00171	949.510	0.00	-5.35
CHLORPYRIFOS-5.5	-0.00311	0.00273	947.640	39.72	-5.67

Table 3. Values of calculated properties for the drugs studied in the presence of nanotubes 6.6 s*Solubility

Name	Homo(a.u)	Lumo(a.u)	V(cm^3.mol)	polar surface area	logs*
ANTIPYRIN- 6.6	-0.00517	0.00240	882.768	26.71	0.39
ASPIRIN- 6.6	-0.00001	0.00196	989.933	69.92	-1.61
ATRAZIN- 6.6	-0.00205	0.00152	1040.203	60.15	-3.55
BENZOCAIN- 6.6	-0.00179	0.00284	983.728	55.48	-2.32
CHLORDANE- 6.6	-0.00163	0.00206	1102.388	0.00	-5.35
CHLORPYRIFOS-6.6	-0.00490	0.00136	1103.765	39.72	-5.67

By examining the reported values in Table 4 and diagram 1 in the absence of carbon nanotubes, the test error for the polarized surface parameter is lower than other parameters, which means that the contamination of the studied compounds Parameters of other molecular volume parameters, LUMO, HOMO are more important.

Table 4. The values of train and test error for drugs in the absence of carbon nanotubes with a parameter

Selected parameter	Error trn	Error chk
HOMO	0.0757	3.0512
LUMO	0.0001	1.3351
V	0.0007	8.8942
SF	0.000٠	3.0668

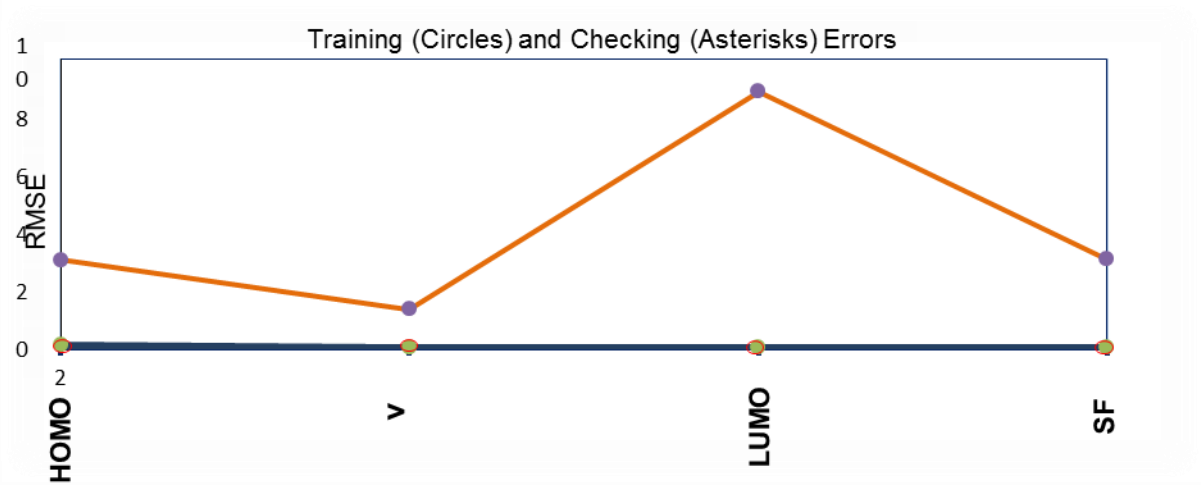

Diagram 1. Training (Circles) and Checking (Asterisks) Errors in the absence of carbon nanotubes with a parameter. The most important parameter selected in the calculations: SF

Due to the reported values in Table 5 and diagram 2, in the presence of Armchair 5.5 carbon nanotubes, the test error value for the polarized surface parameter is lower than other parameters, which means that the contamination of the studied compounds of this parameter is more important than other molecular volume parameters, LUMO, HOMO

Table 5. The values of train and test error for drugs in the presence of carbon nanotubes 5.5 with a parameter

Selected parameter	error trn	error chk
HOMO	0.0344	3.9746
LUMO	1.7257	1.8106
V	0.001٠	2.2154
SF	0.00٠٠	3.0668

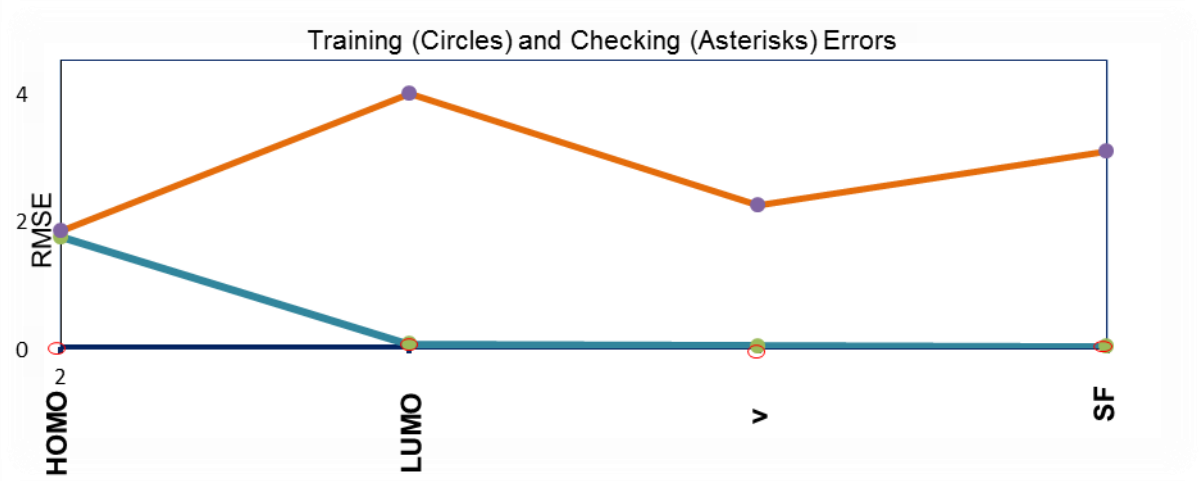

Diagram 2. Training (Circles) and Checking (Asterisks) Errors in the presence of carbon nanotubes 5.5 with two parameter The most important parameter selected in the calculations: SF

Regarding the values reported in Tables 6 and diagram 3, to determine the dependency among the parameters in terms of the effect on the contamination in water with neural network model for one parametric dependencies in the presence of Armchair 6.6 carbon nanotubes were done, and observed that the test error value for the polarized surface parameter is lower than other parameters, which means that the contamination of the studied compounds is more important than other molecular volume parameters, LUMO, HOMO.

Table 6. The values of train and test error for drugs in the presence of carbon nanotubes ۶.۶ with a parameter

Selected parameter	error trn	error chk
HOMO	0.3786	3.6852
LUMO	1.8512	1.3363
V	0.0000	0.6671
SF	0.0000	3.0668

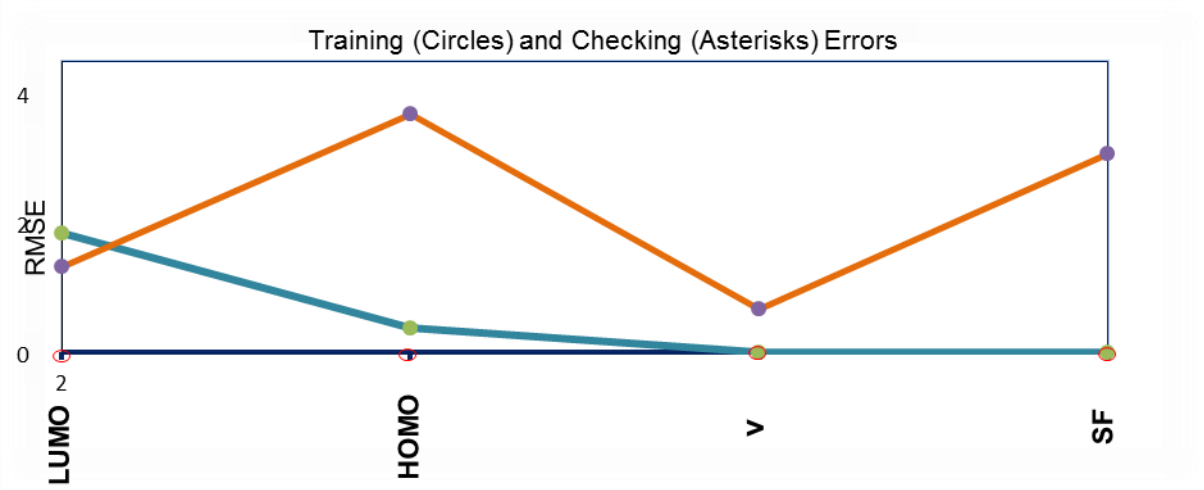

Diagram 3. Training (Circles) and Checking (Asterisks) Errors in the presence of carbon nanotubes 6.6 with a parameter The most important parameter selected in the calculations: SF

CONCLUSIONS

In this research, the ability to predict artificial neural network and non-fuzzy adaptive inference system in predicting the effective parameter of drugs contamination in the absence and presence of carbon nanotubes in water was investigated. As seen from the results, the polarized surface parameter of the other parameters studied in the absence and presence of various carbon nanotubes has a greater effect on water contamination, which means that concentration can be achieved for experimental experiments in this regard. The experiments were conducted on a polarized surface parameter to achieve better and faster results in this field. The type of carbon nanotubes from 5.5 to 6.6 did not change as a result and the polarized surface parameter is more important contamination.

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