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Theoretical study of Graphene nanoparticles surface effects on Removal of Pharmaceuticals Contaminants from water by neural network computational method

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ABSTRACT

One of the major crises we face is water and wastewater pollution, as the population increases, industries develop and pollution increases. The pharmaceutical industries produce a large amount of polluted wastewater containing the drug. The drugs, due to their antimicrobial properties, inhibit the activity of bacteria in the biological treatment system and disrupt the purification process without being eliminated. Therefore, common methods used in wastewater treatment in the pharmaceutical industries such as biological treatment are not generally effective. Nanotechnology has provided opportunities to develop low-cost, high-cost, environmentally friendly water and wastewater treatment processes. Using Nanotechnology, more studies can be carried out on many water-resistant pollutants, such as water-based pharmaceutical pollutants and pollutants that we cannot disinfect using conventional methods. Also using this technology will have great results. This study was computational and we used Nano-graphene in this study to investigate the Removal of 4 drug contaminants (diazepam - Lindal - phenobarbital - phenytoin - theophylline - diuron) using the smart neural network system, Fuzzy inference system, based on matching and application software (ChemOffice software, Open Babel software, Gaussian & GaussView software, Multiwfn software, and MATLAB software). Molecular parameters of materials (surface, volume, main dipole and molecular orbitals) were calculated by modeling and analyzing compounds. The test error value for the parameter of available polar level in five Tables and the test error value for the size parameter in three Tables is lower than the other parameters. This means that the contamination of the compounds studied by these parameters is more important than other molecular parameters. Considering different conditions, the volume and main dipole parameters have a greater effect on water contamination than the other parameters studied in the presence and absence of carbon Nano-graphene.

1. INTRODUCTION

Iran is one of the regions in the world with low annual rainfall (0-4 mm), which does not enjoy sufficient rainfall and does not have per capita non-renewable water. [1] Most of the areas in the country are covered with arid, semi-arid and low-water areas, and therefore, water had a critical role in the life of our country for a long time. Due to the recent drought and the excessive harvest of groundwater, we are facing a shortage of safe water supplies in the country. [2] For example, neglecting the nature and proper disposal of waste and also the lack of a proper municipal sewage system has now led to the accumulation of large amounts of alluviums with large amounts of sewage sludge in the heart of metropolitan areas. This contamination can penetrate aquifers and even leak into drinking water wells. [3]

The pharmaceutical industry is one of those industries that has expanded in our country and produces a significant amount of contaminated wastewater containing drugs. Drugs enter the environment and mainly the aquatic environment through the wastewater of the pharmaceutical industry and factories, hospitals, human and animal wastewater. These compounds precipitate in the soil and persist in surface and groundwater with runoff from the soil, causing irreparable environmental damage and eventually infiltrating human drinking water. [4] Due to the problems and difficulties of water contamination in communities, many countries have done a great deal in the field of water and wastewater treatment, and there has been a great deal of attention in recent years to new refining technologies. Nanotechnology has provided opportunities for the development of low cost, high cost and environmentally friendly water and wastewater treatment processes. Using Nanotechnology, more studies can be carried out on many water-resistant pollutants, such as water-based pharmaceutical contaminants and contaminants that we cannot disinfect using conventional methods and applying this technology will have great results. Nanoparticles are the most common elements in nanotechnology and their interesting properties have made them widely used in various industries such as medicine and pharmaceutical industries, agriculture, industry, water, and wastewater.

Nanotechnology in water and wastewater treatment examines various areas including pollution monitoring, water desalination, wastewater treatment, and water recovery and purification. [5]

2. RESEARCH METHODOLOGY

In this study, we investigated the removal of water-based pharmaceutical contaminants and we studied some of the material properties using six contaminants and

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Nano-graphene at various lengths with Artificial Neural Network (ANN) and Adaptive Neural Fuzzy Inference System (ANFIS) and calculated the most impact in the absence and presence of Nano-graphene.

2.1. Pharmaceutical contaminants in this study

2.1.1. Phenobarbital

Phenobarbital reduces brain and nervous system activity and is used to treat or prevent epileptic seizures. The most common side effects of phenobarbital use are drowsiness and fatigue, depression, increased activity in children (hyperactivity), attention deficit disorder, Confusion, memory problems, decreased libido, stuttering, stomach upset, anemia, folic acid deficiency, rash, fever, decreased calcium levels and bone marrow weakness. [6]

2.1.2. Diazepam

Diazepam is a Painkiller and sedative drug. Diazepam is prescribed to relieve anxiety, sleep disorders, and panic disorder. It is also used as a muscle relaxant and anti-skeletal muscle, to treat muscle contraction and seizures (epileptic seizures in children or epileptic seizures). The most common side effects are mental retardation, severe drowsiness, inappropriate speech, slow heart rate, shortness of breath, dysfunction, rash, sore throat, Memory loss, insomnia, anxiety, or irritation, and diazepam can also be addicted. [6]

2.1.3. Theophylline

Theophylline is a type of bronchodilator and is used in the treatment of asthma, emphysema, and bronchitis. Essentially, theophylline facilitates air circulation by loosening and opening the bronchial muscles and improving breathing in cases of reverse airway obstruction. Side effects of theophylline use include headache, insomnia, irritability, sleep problems, stomach discomfort, diarrhea, vomiting, arrhythmia, rash and seizures, esophageal reflux. [6]

2.1.4. Phenytoin

Phenytoin is a drug to treat epilepsy, epileptic seizures, seizures, trigeminal neuralgia, and cardiac arrhythmias. It is used topically to accelerate deep wound healing. The harmful effects of phenytoin are the cardiovascular, neurological, and fetal effects during pregnancy (teratogenic and fetal syndrome), carcinogenesis, gingivitis, skin complications and autoimmune complications of phenytoin. [6]

2.1.5. Lindane

Lindane or gamma benzene hexachloride is used to treat lice and gall. Lindane is absorbed through the skin and can cause toxicity to the central nervous system, liver and kidneys, especially in infants and children. Side effects are caused by and rashes, as well as symptoms of poisoning (dizziness, lightheadedness, seizures, muscle cramps, anger, Abnormal restlessness and irritability, rapid beating, vomiting.) [6]

2.1.6. Diuron

Diuron is one of the most commonly used pollutants that has no medicinal use for humans and is used in agriculture. Diuron dust is harmful when working with it and appropriate clothing and masks should be used when working with it. [6]

2.1.7. Graphene

Graphene is one of the most well-known materials in nanotechnology. The chemical and physical properties of graphene make it unpredictable, and when carbon is covalently bound to the other three carbon atoms, a two-dimensional sheet called graphene is created. [7]

Graphene has a carbon nanotube-like structure. The only difference between graphene and nanotubes is that they are flat, while nanotubes are cylindrical. [8] Because of the covalent association between graphene atoms, graphene has a very high tensile strength. Besides, unlike carbon nanotubes, graphene is accessible from both sides and can interact more with the molecules while in nanotubes, each carbon atom on the surface, can only interact and react with the molecules that surround it. [9]

Graphene is very light due to its very small thickness (only one atom). The electrical properties of graphene are extremely useful and effective because in graphene each carbon atom is bound to only three atoms and one atom is free.

Due to its electrical properties, graphene can absorb 2 to 3 percent of white light, and the very high surface area of graphene volume has led to extensive research on its use as a potential water-absorbent. Graphene has unique features such as high surface area, high mechanical strength and flexibility, optical permeability, excellent electrical and thermal conductivity, gas permeability and many other properties. [10]

In this study, we investigated the effect of graphene levels on pollutants using the smart neural network system, the Fuzzy inference system, based on matching and application software (ChemOffice software, Open Babel software, Gaussian & GaussView software, Multiwfn software, and MATLAB software). We first mapped the compounds in 2D and 3D space using ChemOffice software. We then modified the format of the stored files with Open Babel software and prepared them for analysis and logging into Gaussian software.

We used Multiwfn software to calculate the main bipolar parameters, total surface area, and volume and completed the parameter tables by adding the log parameter which was constant and its value was calculated experimentally. Next, we designed the desired nano-graphenes with modeler nanotube software and put the same nano-graphenes into the mix. We based these three-dimensional states on our work and re-calculated the molecular parameters. To compare and analyze the tables, we used the Neuro-Fuzzy Inference System and ANFIS algorithm in MATLAB software and we studied test error and calculated control error values for the compounds.

2.1.8. ChemOffice Software

This software is one of the most useful application software for students and professors of chemistry, that is widely used. It has three parts;

2.1.9. ChemDraw section

This section contains many applications such as reaction design, spectrum mapping, drawing the shapes of organic and inorganic chemical compounds, chemical nomenclature of compounds, and providing information such as melting point and boiling point, molecular mass and chemical formula.

2.1.10. Chem3D section

This section also has many uses, including the representation of organic and inorganic chemical forms in three-dimensional form, the representation of atoms and molecules in a 3D space, the molecular volume, the chemical state of the species, and many related computations, Bandenic calculations of energy, bond length, normal angle, and Dihedral Angle, computing the spectra of chemical structure.

2.1.11. Chemfinder section

This section is used to search for research resources. We use ChemOffice software to design and store our compounds in 2D and 3D modes.

2.1.12. Open Babel Software

This software is used by many researchers today and enables the conversion, search, analysis, and storage of various molecular modeling data, chemistry, solid-state structures, and biochemistry. Creating and converting more than one hundred different formats of structure and molecular information files, searching and filtering chemical files in different ways, and changing data formats. The ability to read, build and convert over 100 different file formats of molecular structure and information, search and filter chemical files in different ways, and modify data formats are unique features of this software.

2.1.13. Gaussian & GaussView software

Key features of GaussView software include the Calculation of molecular energies and structures. Energy and structure Transient modes of vibrational frequencies, Thermo-chemical properties, reaction energy of reaction path orbitals of electrostatic potential molecules and electron densities of electrons and ionization potentials. GaussView is not associated with Gaussian arithmetic units but it is a pre-arithmetic / post-arithmetic processor that helps in using Gaussian.

2.1.14. Multiwfn software

Powerful software for wave function analysis that except NBO, is capable of performing almost all-important wave function analyzes.

2.1.15. Nanotube Modeler

This program designed to map carbon nanotubes with XYZ chemistry coordinates.

2.1.16. Artificial Neural Network (ANN)

Artificial Neural Networks are patterns of information processing that are manufactured by simulating biological neural networks such as the human brain. The main component of this model is the new structure of its information processing system, and it consists of a large number of elements (neurons) with strong internal connections that work together to solve specific problems. [11] Artificial neural networks transfer the knowledge or law behind the data by processing over experimental data into the network structure, which is called learning.

Learning ability is the most important feature of an intelligent system. A system that can learn is more flexible and easier to program, and thus it can respond better to new problems and equations. [12]

2.1.17. ANFIS

The Adaptive Neuro-Fuzzy Interface System based on network adaptation was first introduced by Jang in 1993. [13]

It has been successfully applied to solve various problems. The Neuro-Fuzzy system uses a neural network learning algorithm combined with fuzzy logic to estimate the output distribution with the help of input distribution. The Adaptive Neuro-Fuzzy Interface System is usually trained using a monitored learning algorithm to optimize linear and nonlinear parameters. [14]

3. RESULTS

1. According to Table 10 and Fig. 1, in the absence of Nano-carbon graphene, it is observed that the test error for generally available surface parameters is lower than other parameters. Therefore, we conclude that the pollution of materials studied by these parameters is more important than other parameters.

2. According to the values observed in Table 11 and Figure 2, it is deduced that in the presence of 10 x 10 Nano-graphene with 20 angstroms length (middle contaminant of Nano-graphene) the test error value for the main dipole parameter is less than the other parameters. This indicates that the pollutants studied by this parameter are more important than other parameters.

3. According to the values observed in Table 12 and Figure 3, it is deduced that in the presence of 10 x 10 Nano-graphene with 30-angstrom length (middle contaminant of Nano-graphene) the test error value for the volume parameter is lower than the other parameters. This indicates that the pollutants studied by this parameter are more important than other parameters.

4. According to the values observed in Table 13 and Figure 4, it is deduced that in the presence of 10 x 10 Nano-graphene with 40-angstroms (middle contaminants of Nano-graphene) the test error value for the main dipole parameter is lower than the other parameters. This indicates that the pollutants studied by this parameter are more important than other parameters.

5. According to the values observed in Table 14 and Figure 5, it can be seen that in the presence of 10 x 10 Nano-graphene with 50 angstroms length (middle

contaminant of Nano-graphene) the test error value for the main dipole parameter is lower than the other parameters. This indicates that the pollutants studied by this parameter are more important than other parameters.

Table 1. The compounds without the presence of carbon nanotubes

Name	log z	Total Dipole	Overall Surface Area	Volume	Lumo	Homo
Diazepam	-1.92	2.0548436	288.37.41	308.33515	-2.838	-0.19201
Diuron	-2.02	2.7734482	196.25699	193.55259	-0.30034	-0.24233
Landane	-3.21	1.1044038	123.49207	115.45419	-0.27466	-0.2378
Phenobarbital	-1.67	2.9846577	277.68863	240.73944	-0.30663	-0.16431
Phenytoin	-2.12	1.7173734	255.62977	271.27786	-0.30941	-0.17543
Theophylline	-0.68	2.2881954	191.43228	184.30928	-0.28057	-0.15579

Table 2. Placing the compound close to (center of) the Nano-graphene with these Specifications: Nano-graphene 10-10, 2 nm length

Homo	Lumo	Volume	Overall Surface Area	Total Dipole	log z	Name
-0.21907	-0.27912	327.39233	289.9244	2.7865353	-1.92	Diazepam
-0.22762	-0.28046	205.90888	205.54187	1.5168839	-2.02	Diuron
-0.23807	-0.26991	115.66318	123.99048	1.0323713	-3.21	Landane
-0.25121	-0.27798	258.90107	238.7947	2.5398992	-1.67	Phenobarbital
-0.20825	-0.31221	292.15424	264.46035	3.008972	-2.12	Phenytoin
-0.21727	-0.26491	190.58553	191.0342	2.23978	-0.68	Theophylline

Table 3. Placing the compound close to (center of) the Nano-graphene with these Specifications: nao graphene 10-10, 3 nm length

Homo	Lumo	Volume	Overall Surface Area	Total Dipole	log z	Name
-0.228	-0.28064	327.71998	290.27558	2.7244954	-1.92	Diazepam
-0.21875	-0.28003	205.6219	203.81053	5.0391927	-2.02	Diuron
-0.23778	-0.27037	115.56675	123.92603	1.1138759	-3.21	Landane
-0.25412	-0.27495	259.70887	237.38559	2.2815127	-1.67	Phenobarbital
-0.20828	-0.31282	292.37586	264.81112	2.869562	-2.12	Phenytoin
-0.21788	-0.26599	190.3646	190.92093	2.3253592	-0.68	Theophylline

Table 4. Placing the compound close to (center of) the Nano-graphene with these Specifications: Nano-graphene 10-10, 4 nm length

Homo	Lumo	Volume	Overall Surface Area	Total Dipole	log z	Name
-0.21847	-0.2791	327.42089	290.33062	2.7727927	-1.92	Diazepam
-0.22797	-0.28064	206.02403	205.90667	1.5038905	-2.02	Diuron
-0.2372	-0.27093	115.46715	123.85575	1.082344	-3.21	Landane
-0.24929	-0.27973	259.34938	238.9279	2.242278	-1.67	Phenobarbital
-0.20814	-0.31108	292.62721	265.07859	2.998309	-2.12	Phenytoin
-0.21805	-0.26473	190.66628	191.20855	2.142784	-0.68	Theophylline

Table 5. Placing the compound close to (center of) the Nano-graphene with these Specifications: Nano-graphene 10-10, 4 nm length

Homo	Lumo	Volume	Overall Surface Area	Total Dipole	log z	Name
-0.21838	-0.27924	327.18155	290.29819	2.7383771	-1.92	Diazepam
-0.22604	-0.27793	206.05916	205.93575	1.5821424	-2.02	Diuron
-0.23849	-0.26797	115.3254	123.72304	1.1628061	-3.21	Landane
-0.25212	-0.27724	259.24623	239.15922	2.5517131	-1.67	Phenobarbital
-0.21021	-0.3123	291.79111	263.99383	2.993838	-2.12	Phenytoin
-0.2171	-0.26635	190.18526	190.72262	1.9988354	-0.68	Theophylline

Table 6. Placing the compound close to (edge of) the Nano-graphene with these Specifications: Nano-graphene 10-10, 2 nm length

Homo	Lumo	Volume	Overall Surface Area	Total Dipole	log z	Name

-0.21828	-0.27963	327.57659	290.06691	2.7661188	-1.92	Diazepam
-0.22797	-0.27931	205.91062	205.56507	1.4445196	-2.02	Diuron
-0.23693	-0.26922	115.39093	123.80023	1.1379927	-3.21	Landane
-0.25156	-0.27926	259.16351	238.80765	2.1842164	-1.67	Phenobarbital
-0.20838	-0.21189	292.52793	256.12266	2.9690266	-2.12	Phenytoin
-0.21823	-0.26479	190.72283	191.06988	2.1830462	-0.68	Theophylline

Table 7. Placing the compound close to (edge of) the Nano-graphene with these Specifications: Nano-graphene 10-10, 3 nm length

Homo	Lumo	Volume	Overall Surface Area	Total Dipole	log z	Name
-0.21862	-0.27936	372.19781	290.20322	2.7569319	-1.92	Diazepam
-0.22599	-0.27994	205.81669	205.52707	1.5103491	-2.02	Diuron
-0.23555	-0.26794	115.4552	123.75535	1.0790553	-3.21	Landane
-0.21284	-0.31415	259.09174	238.96494	2.6414897	-1.67	Phenobarbital
-0.20957	-0.31138	292.65269	265.14959	2.913673	-2.12	Phenytoin
-0.21633	-0.26577	190.67386	191.0488	2.2164864	-0.68	Theophylline

Table 8. Placing the compound close to (edge of) the Nano-graphene with these Specifications: Nano-graphene 10-10, 4 nm length

Homo	Lumo	Volume	Overall Surface Area	Totall Dipole	log z	Name
-0.21969	-0.27933	327.12748	289.84592	2.7757839	-1.92	Diazepam
-0.22687	-0.27953	205.9641	205.94984	1.3500249	-2.02	Diuron
-0.2383	-0.2702	115.43336	123.74065	1.0506251	-3.21	Landane
-0.25316	-0.27484	259.38095	239.05639	2.6505966	-1.67	Phenobarbital
-0.20865	-0.31286	291.72573	264.00252	2.794308	-2.12	Phenytoin
-0.21669	-0.26618	190.61917	191.18701	2.0682495	-0.68	Theophylline

Table 9. Placing the compound close to (edge of) the Nano-graphene with these Specifications: Nano-graphene 10-10, 5 nm length

Homo	Lumo	Volume	Overall Surface Area	Total Dipole	log z	Name
-0.21901	-0.27977	327.19645	290.19062	2.8093254	-1.92	Diazepam
-0.2291	-0.28021	205.97648	205.80119	1.4568903	-2.02	Diuron
-0.23692	-0.26892	115.41943	123.79426	1.1591905	-3.21	Landane
-0.25527	-0.27659	259.46774	239.03366	1.9929556	-1.67	Phenobarbital
-0.20911	-0.31351	292.48768	264.79069	2.880297	-2.12	Phenytoin
-0.21725	-0.26454	190.62896	191.01244	2.2877643	-0.68	Theophylline

The calculated test and control error values for drugs in the absence of Nano-graphene with single parameter

Table 10. The Diagram of calculated test error and control error values for compounds in the absence of Nano-graphene

trn test error	Chk control error	The selected parameter
0.0002	0.8526	Homo
0.0007	0.8963	Lumo
0.0000	2.4842	Volume
0.0000	2.1057	Surface Area
0.0000	0.7461	Total Dipole

The selected parameter: td

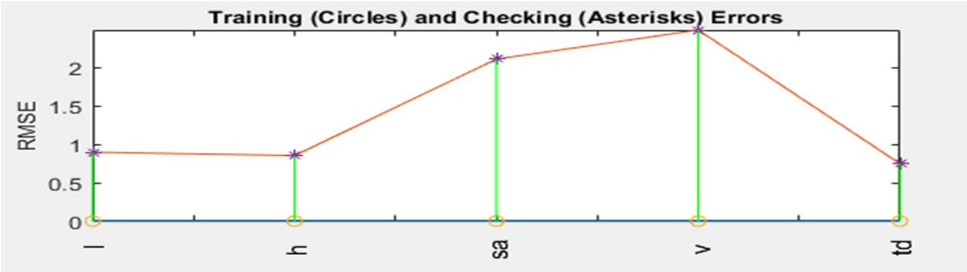

Figure 1. Training and checking errors

Calculated test and control error values for drugs in the presence of 10 x 10 10 nm carbon Nano-graphene with a single parameter

Table 11. The Calculated test and control error values for drugs in the presence of 10 x 10 10 nm carbon Graphene with a single parameter

trn test error	Chk control error	The selected parameter
0.0015	1.3856	Homo
0.0004	1.1900	Lumo
0.0000	2.5369	Volume
0.0000	2.0573	Surface Area
0.0000	0.4337	Totall Dipole

The selected parameter: td

Diagram of Calculated Test Error and control Error Values for Compounds in the Presence of 10-10 Graphene Nanotube with 20 Angstroms

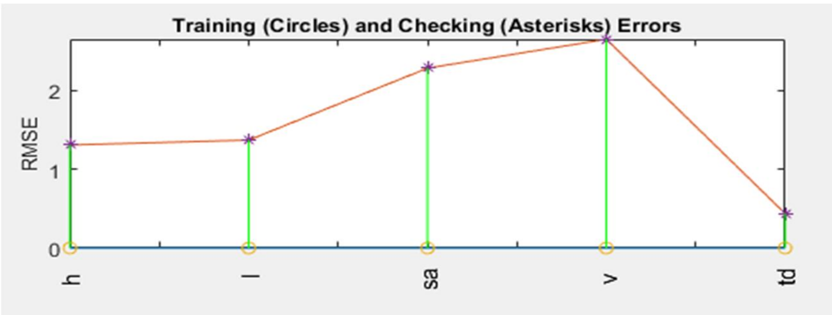

Figure 2. Calculated Test Error and control Error Values for Compounds in the Presence of 10-10 Graphene Nanotube

Calculated test and control error values for drugs in the presence of 10 x 10 10 nm carbon Nano-graphene with a length of 30 angstroms with one parameter

Table 12. test and control error values for drugs in the presence of 10 x 10 10 nm carbon Nano-graphene with a length of 30 angstroms with one parameter

trn test error	Chk control error	The selected parameter
0.0013	1.2393	Homo
0.0002	1.8040	Lumo
0.0000	2.5169	Volume
0.0000	2.2896	Surface Area
0.0000	0.6980	Total Dipole

The selected parameter: td

Diagram of Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 30 angstroms

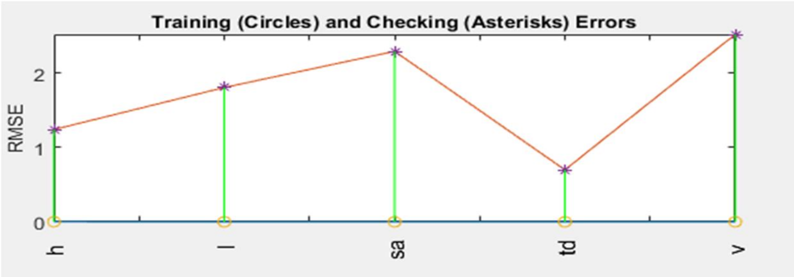

Figure 3. Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 30 angstroms

Diagram of Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 40 angstroms

Table 13. Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 40 angstroms

trn test error	Chk control error	The selected parameter
0.0014	1.3634	Homo
0.0009	1.3628	Lumo
0.0000	2.4646	Volume
0.0000	2.2923	Surface Area
0.0000	0.4240	Total Dipole

The selected parameter: td

Diagram of Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 40 angstroms

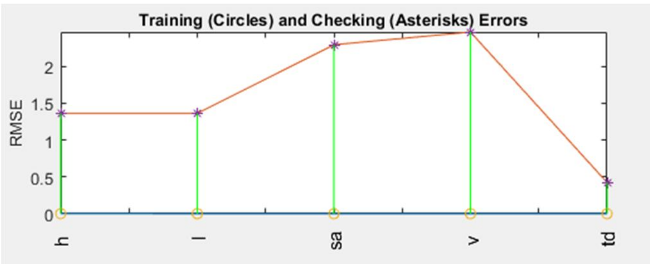

Figure 4. Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 40 angstroms

Calculated test and control error values for drugs in the presence of 10 x 10 nm carbon Nano-graphene with a length of 50 angstroms with one parameter

Table 14. Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 40 angstroms

trn test error	Chk control error	The selected parameter
0.0017	1.1719	Homo
0.0001	1.3554	Lumo
0.0000	2.6694	Volume
0.0000	2.2716	Surface Area
0.0000	0.5286	Total Dipole

The selected parameter: td

Diagram of Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 50 angstroms

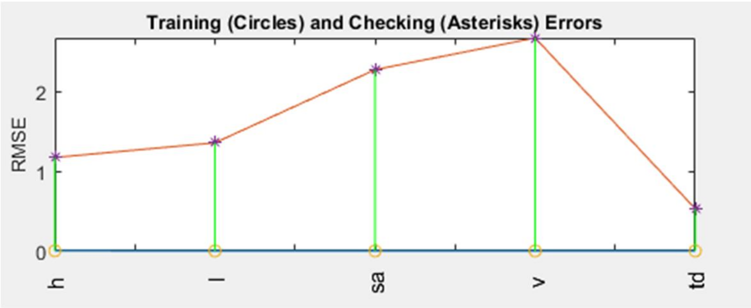

Figure 5. Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 50 angstroms

Calculated test and control error values for drugs in the presence of 10 x 10 Nano-graphene (graphene edge) with a length of 50 angstroms with one parameter

Table 15. Calculated test and control error values for drugs in the presence of 10 x 10 Nano-graphene (graphene edge) with a length of 50 angstroms with one parameter

trn test error	Chk control error	The selected parameter
0.0015	1.3856	Homo
0.0004	1.1900	Lumo
0.0000	2.2369	Volume
0.0000	2.0573	Surface Area
0.0000	0.4337	Total Dipole

The selected parameter: td

Diagram of Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 20 angstroms

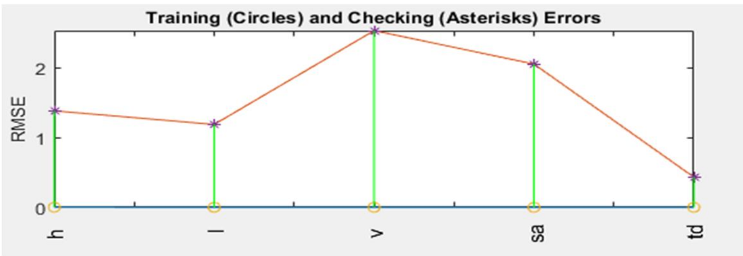

Figure 6. Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 20 angstroms

Calculated test and control error values for drugs in the presence of 10 x 10 nm carbon Nano-graphene with a length of 30 angstroms with one parameter

Table 16. Calculated test and control error values for drugs in the presence of 10 x 10 nm carbon Nano-graphene with a length of 30 angstroms with one parameter

trn test error	Chk control error	The selected parameter
0.0006	0.7088	Homo
0.0004	1.3240	Lumo
0.0000	2.2543	Volume
0.0000	2.0685	Surface Area
0.0000	0.3277	Totall Dipole

Diagram of Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 30 angstroms

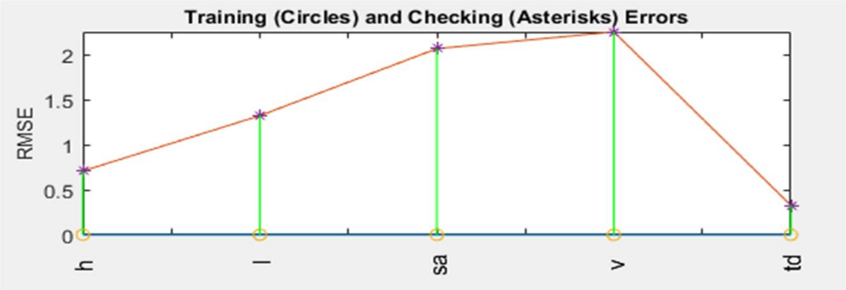

Figure 7. Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 30 angstroms

Calculated test and control error values for drugs in the presence of 10 x 10 nm carbon Nano-graphene with a length of 40 angstroms with one parameter

Table 17. Calculated test and control error values for drugs in the presence of 10 x 10 nm carbon Nano-graphene with a length of 40 angstroms with one parameter

trn test error	Chk control error	The selected parameter
0.0009	1.3512	Homo
0.0006	1.3682	Lumo
0.0000	2.1705	Volume
0.0000	2.2220	Surface Area
0.0000	0.6246	Totall Dipole

The selected parameter: td

Diagram of Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 40 angstroms.

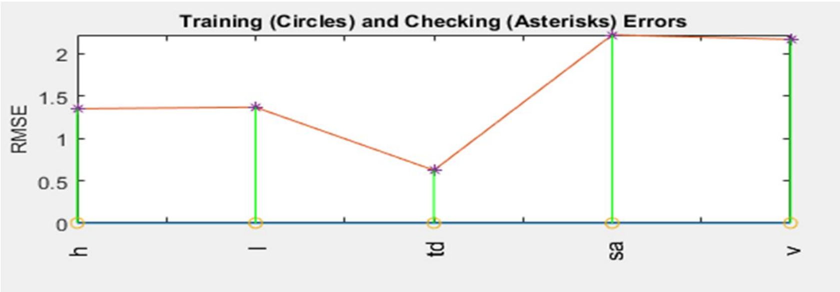

Figure 8. Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 40 angstroms

Calculated test and control error values for drugs in the presence of 10 x 10 nm carbon Nano-graphene with a length of 50 angstroms with one parameter

Table 18. Calculated test and control error values for drugs in the presence of 10 x 10 nm carbon Nano-graphene with a length of 50 angstroms with one parameter

trn test error	Chk control error	The selected parameter
0.0002	1.3014	Homo
0.0002	1.3755	Lumo
0.0000	2.6658	Volume
0.0000	2.1871	Surface Area
0.0000	0.5254	Totall Dipole

The selected parameter: td

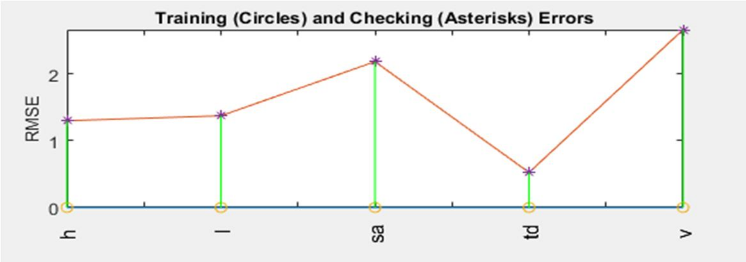

Figure 9. Test and control error values for drugs in the presence of 10 x 10 nm carbon Nano-graphene with a length of 50 angstroms with one parameter

Diagram of Calculated Test Error and control Error Values for Compounds in the Presence of Graphene Nanotube 10-10 with a length of 50 angstroms

4. CONCLUSION

In this study, pharmaceuticals were modeled in the presence and absence of carbon Nano-graphene using the prediction capability of artificial neural network methods and adaptive fuzzy-neural inference system, and also the changes in molecular properties of the materials were studied. It can be seen from the results that the main volume and dipole of the other studied parameters in the presence and absence of carbon Nano-graphene have more influence on water pollution considering different conditions. So it can be stated that if the empirical experiments in this field are to be targeted, we should focus on the two major volume and dipole parameters to obtain better results.

It should be noted that in the case of Nano-graphene with different levels, when the drug location was in the middle of the Nano-graphene surface, the dipole parameter had the greatest impact on the contamination, but when the drug was modeled on the Nano-graphene edge, the volume parameter and the original dipole were equally effective.

5. SUGGESTIONS

1. Further study on different surfaces of Nano-graphene and comparing them with the results of this research
2. Investigation of multilayer Nano-graphs and comparing them with the results of this study
3. Investigation of other pollutants with modeling conditions in this research and comparing them with the results of this research.
4. Study and research using other artificial neural network algorithms and comparing them with the results of this research
5. Evaluation of Neural Network Performance and Adaptive Fuzzy-Neural Inference System using more data sets and evaluating more parameters

REFERENCES

[1] Ahmad Reza Sayyadi Anari, Mohammad Asadpour, Ziba Sheibani, Mohammad Hossein Sayyadi Anari “Interaction of Drugs in the Environment and its Impact on Human Health” (2012)
[2] Arezoo Najai “Application of Nanotechnology in Urban and Industrial Wastewater Treatment” (2013)
[3] Mehdi Farahani, Ebrahim Ali Nia Ahandani, Masoumeh Biranvand, Abazar Khalaji Zavajeri, Hamid Dzhakam, Reza Ebrahim Talem Khan “Investigation of Water Pollution and Application of Nanotechnology in Water and Wastewater Treatment” (2011)
[4] Kumar S, Nair RR, Pillai PB, Gupta SN, Iyengar M, Sood AK. Graphene Oxide−MnFe2O4 Magnetic Nanohybrids
[5] for Efficient Removal of Lead and Arsenic from Water. ACS Appl Mater Interfaces. 2014; 6(20): 17
[6] wikipedia.org 426-36.
[7] Mahvi AH, Maleki A, Eslami A. Potential of rice husk and rice husk ash for phenol removal in aqueous systems. Am J Appl Sci. 2004;1(4):321-6.
[8] Sheshmani SH, Arab Fashapoyeh M, Amini R. Iron (iii) hydroxide/graphene oxide nano composite and investigation of lead adsorption. Quarterly Journal of Applied Researches in Chemistry (JARC). 2013;6(4):17-23. [Russian]
[9] Novoselov, K. S., A. K. Geim, S. V. Morozov, et al. 2005. Two-dimensional gas of massless Dirac fermions in graphene. Nature 438 (7065):197–200
[10] Behnam & Shahrokh Rahbari, 2014, Study of the Methods of Preparation and Investigation of Graphene Based Super Adsorbents for Removal of Organic Petroleum Pollutants, National Conference on Environment and Green Industry, Isfahan, Environmental Research Institute of Isfahan University
[13] Menhaj M.B, "Fundamentals of Computational Neural Networks", Volume I, Fifth Edition, Amir Kabir University of Technology Publications, Tehran, Iran, (2008)
[14] Farkhondeh S., "Application of Fuzzy Logic and Neural Networks in Predicting Clay Soil Density Index", M.Sc. Thesis, Ferdowsi University, Mashhad, (2010)