Modeling Of Adsorption Process In Wastewater Treatment Using Artificial Neural Network

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Abstract: Activated carbon is a common and popular adsorbent that has been extensively used in separation and purification processes due to its high adsorption capacity and high active levels. Also, due to the unique properties of activated carbon adsorbent, this type of adsorbent has been used for this research. Adsorption is a surface phenomenon; therefore, the total surface area with respect to pore size and volume might be a criterion in determining its effectiveness in a particular application. Porous carbons can be manufactured from many carbonaceous starting materials such as wool, coconut shell, peat, bone char, petroleum, or rayon cloth. These materials in different forms play an important role in several industries. Fundamental adsorption data is useful for characterizing different adsorbent surfaces and investigating the nature of their interactions with the adsorbed molecules [1-3]. The sorption of pollutants on adsorbents is receiving increasing attention in view of removal and recovery of pollutants from liquid or gas mixtures. Activated carbon is also a common and popular adsorbent that has been used extensively in separation and purification processes due to its high adsorption capacity, high surface area and adequate pore size distribution. Effective for collection of suspended solids, odors, organic matter, and oils. Powder or granular activated carbon is the most widely used adsorbent for this purpose also it has high adsorption capacity [4]. Adsorption process involves the selective transfer of solute onto the surface or onto the bulk of the solid material. This solute transfer process is found to occur through varied mechanisms such as external mass transfer, intraparticle diffusion and adsorption at sites [5]. In this study, it will be possible to absorb an amine organic compound from its solution using active carbon. In addition, the results of this study by use of ANN reflected a suitable accuracy.

Keywords: activated carbon, adsorption, organic solvent, wastewater treatment, Artificial Neural Network

1. Introduction
Activated carbon is a common and ideal organic adsorbent that is widely used in separation and purification processes due to its high adsorption capacity and high active levels. Also, due to the unique properties of activated carbon adsorbent, this type of adsorbent has been used for this research. Adsorption is a surface phenomenon; therefore, the total surface area with respect to pore size and volume might be a criterion in determining its effectiveness in a particular application. Porous carbons can be manufactured from many carbonaceous starting materials such as wool, coconut shell, peat, bone char, petroleum, or rayon cloth. These materials in different forms play an important role in several industries. Fundamental adsorption data is useful for characterizing different adsorbent surfaces and investigating the nature of their interactions with the adsorbed molecules [1-3]. The sorption of pollutants on adsorbents is receiving increasing attention in view of removal and recovery of pollutants from liquid or gas mixtures. Activated carbon is also a common and popular adsorbent that has been used extensively in separation and purification processes due to its high adsorption capacity, high surface area and adequate pore size distribution. Effective for collection of suspended solids, odors, organic matter, and oils. Powder or granular activated carbon is the most widely used adsorbent for this purpose also it has high adsorption capacity [4]. Adsorption process involves the selective transfer of solute onto the surface or onto the bulk of the solid material. This solute transfer process is found to occur through varied mechanisms such as external mass transfer, intraparticle diffusion and adsorption at sites [5]. In this study, it will be possible to absorb an amine organic compound from its solution using active carbon. In addition, the results of this study by use of ANN reflected a suitable accuracy.

2. Activated carbon adsorbent
Activated carbon is a completely amphiratic solid with very high porosity and considerable internal volume and volume. It has a high absorption property and also provides excellent resilience. The above properties of activated carbon have led to the use of this material as a very common in the processes of gas and liquid treatment in large and small industries. Activated carbon is a carbon-based layer that has cross-linked aliphatic groups. X-ray experiments indicate that activated carbon does not have a graphite structure. In figure 1, a visualization structure of activated carbon porosity is given [6].

The active activated carbon level according to the raw material, activation method, density and other parameters can increase up to 3000 m²/g. Its shapes include beads, pills, pellets and powder. Some of its important applications include water and wastewater treatment for the removal of organic pollutants, cleaning up of gas streams, including volatile organic compounds (especially solvents that need to be recovered), raising the quality of methane from wells, decontamination of compounds and purification of compounds Medication. Placing activated carbon into the cleaning masks to absorb organic compounds is another of its applications. Activated carbon introduces a number of other uses, such as the removal of mercaptans and hydrogen sulfide, by introducing some materials such as iron oxide [7, 8]. Granular activated carbon can be used to eliminate the majority of liquid phase pollutants. This type of activated carbon is used in continuous systems and is renewable. For the following reasons, the use of granular activated carbon is preferable to powdered activated carbon [9]:
- There is a possibility of a stable use of granular activated carbon.
- Reduction of granular activated carbon is as common as possible.
- Due to the stability of the system used in granular activated carbon, it is possible to use optimum absorption capacity using cross-flows or cross-linking systems, but the active activated carbon can only be used discontinuously. Due to the fact that the powdered...
carbon cannot be used as a fixed bed, it can only be used as a droplet that requires the recovery of activated carbon.

Activated carbon adsorption is mainly carried out in the form of physical absorption, but if the absorption temperature increases, chemical absorption also occurs. Activated carbon mainly tends to absorb non-polar materials [10]. In the activation phase, the functional groups are produced by oxygen and nitrogen on the activated carbon surface, giving them specific chemical properties. The activated carbon level is generally water-repellent and has a slight negative charge, but by performing the acidification and dilution process, the surface load and its hydrophobic properties can be greatly changed [11].

3. Artificial Neural Network (ANN)

Recently, there have been a number of researches conducted on data processing for problems for which there is no solution, or problems that are not easily solvable. The ANN pattern is inspired by the neural system of living organisms that includes some constituent units called ‘Neuron’. Most of the neurons are composed of the three main parts including cell body (that includes nucleus and other protective parts), dendrites, and axon. The last two parts are the communicative parts of the neuron. Figure 2 displays the structure of a neuron.

![Figure 2. Major parts of a biological cell](image)

Dendrites, as electric signal receiving areas, are composed of cell fibers with unsmooth surface and many splitted extensions. That is why they are called tree-like receiving networks. The dendrites transfer the electrical signals into cell nucleus. The cell body provides the required energy for neuron activity that can be easily modeled through an addition and comparison with threshold level. Unlike Dendrites, axon has a smoother surface and fewer extensions. Axon is longer and transfers the received electro-chemical signal from the cell nucleus to other neurons. The influence of a cell’s axon and dendrites is called synapse. Synapses are small functional structural units that enable the communication among neurons. Synapses have different types, from which one of the most important ones is the chemical synapase. Artificial neural cell is a mathematical equation in which \( p \) represents an input signal. After strengthening or weakening as much as a parameter \( w \) (in mathematical terms, it is called weight parameter), an electric signal with a value of \( pw \) will enter the neuron. In order to simplify the mathematical equation, it is assumed that the input signal is added to another signal with \( b \) value in the nucleus. Before getting out of the cell, the final signal with a value of \( pw + b \) will undergo another process that is called “Transfer function” in technical terms. This operation is displayed as a box in Figure 3 on which \( f \) is written. The input of this box is the \( pw + b \) signal and the output is displayed by a. mathematically, we will have:

\[
a = f(pw + b)
\]

Putting together a great number of the above-mentioned cells brings about a big neural network. As a result, the network developer must assign values for a huge number of \( w \) and \( b \) parameters; this process is called learning process.

![Figure 3. Mathematical model of a neuron](image)

Within the structure of neural networks, sometimes it is needed to stack up a number of neurons in a layer. Moreover, it is possible to take advantage of neuron crowds in different layers to increase the system efficiency. In this situation, the network will be designed with a certain number of inputs and outputs too; while the difference is that there would be more than one layer (instead of having only one layer). In this manner (multi-layer network), the input layer is the layer through which the inputs are given to the system, the output layer is the layer in which the desired the results are delivered, and the other layers are called hidden layer. Figure 4 displays a neural network with three layers. Input layer, output layer, and hidden layer (that is only one layer in this figure). Through changing the number of hidden layers, and changing the number of present neurons in each layer, it is possible to enhance the network capabilities [8].

![Figure 4. A schematic view of Neural Network and its constituent layers](image)

3.1. Modeling dehydration of organic compounds by use of Neural Network

In this research, the influence of ANN input parameters (volumetric flow, pressure and temperature) as well as the flux characteristics (the fluxes are the network output) on the efficiency of dehydration process. One ANN was designed for analysis of the flux parameter. Feed-forward multilayer
perceptron ANN and Levenberg-Marquardt function with two inputs and two outputs were used. The Tanhig transfer function was used for the hidden layer, and Purelin was utilized for the output layer. Five neurons were determined for the hidden layer. After data processing, 70 percent was dedicated for learning, 30 percent was dedicated for testing. Such organic compounds as ethanol was selected in this research; and, Matlab version R2014b was used. Figure 5 displays a schematic view of a two-layer ANN with only one hidden and output layer. The inputs are multiplied by a \( w \) value, and there is a bias factor \( b \) that is added to the input (bias is a fixed value that is added to the input in order to increase the accuracy). Afterward, the result will undergo a function and the resulted value will be multiplied by a weight and added with a bias. The final result will pass another function (with different form and functionality) and output is made. There are five neurons and two inputs on the first layer; however, the number of neurons in the output layer is the same as the number of outputs.

**Figure 5. A schematic view of the ANN**

The following points about the algorithms must be considered: The Data Division compartment totally scrambles the defined data for the system. This compartment randomly defines the Train, Validation, and Test data, so that there will be samples from everywhere of the environment. Levenberg-Marquardt function was used in Training phase. The Mean Squared Error (MSE) functions for performance measurement. The default settings were used for derivative issue. Epoch is accepted from iteration 0 to 1000. It means the weights consecutively changed for 1000 times based on the Levenberg-Marquardt function, and the training procedure was done. If the iteration number reaches 1000, the procedure stops (here it stopped at 24). There was no limit for time (but it could be set for training to stop after 30 seconds for example). Validation check is the maximum number of times that network failure can be tolerated.

### 3.2 Activated carbon adsorbent

The activated carbon adsorbent used in this research is commercial and cylindrical (extruded) to make the country of China available on the market. The dimensions of active activated carbon beams are 5 mm in diameter and 3 mm in diameter. The cylindrical activated carbon used in this study has a specific surface area of 952 m\(^2\)/g, a density of 0.48 g / m\(^3\) and an ash of 9.5%, as measured by the Petroleum Research Institute.

### 3.3. Test equipment

The instruments used in this design include laboratory dishes, digital scales, shakers, heater magnet, sampling dishes, oven, Armani year, pipette, sucker, buccaneer funnel, filter paper and vacuum pump. To perform different absorption tests, an organic compound of 99.5% purity was used which was prepared according to the need and by adding different amounts of distilled water twice distilled, appropriate feeds were prepared. The exact specification of the final specimens was performed by the quality control laboratory using the Varian 3400 GC (Gas Chromatography) apparatus, which carries the hydrogen gas, its column Polyethylene glycol, 5 micron in size, 120 °C column temperature, TCD (150 °C), flow rate of the detector ml / min 15, the gas flow rate is 5 ml / min, the column pressure is 1.5 kPa and the input pressure is 20 kPa.

### 3.4 Procedure

To do this research, a laboratory shaker was used. To perform any shaking test, sample containers containing the test solution and activated carbon adsorbent on the shaker are placed in places that are embedded in the device. The machine moves back and forth at different speeds. The following conditions were observed for performing activated carbon shaking tests [12].

1. Due to the fact that activated carbon is in the form of a granule, it is impossible to weigh accurately and equal the active activated carbon weight in all dishes, so some granules are crushed to smaller sizes so that even the active activated carbon weight of the dishes is almost identical.
2. Before using activated carbon for 6 hours, it was rinsed in boiling water and then dried at 100 °C for 12 hours, so that in the presence of dust particles or other possible materials, the material would be exposed to carbon monoxide Evacuated.
3. The activated carbon was stored in a closed container.
4. Due to the fact that the experiments are time consuming, several experiments were carried out in parallel.
5. The containers used in these experiments had the power to withstand high temperatures.
6. The proper percentage of wastewater was prepared and placed in suitable containers.
7. We added the weighted activated carbon to the sample vessels.
8. Sample containers are placed inside the shaker and mixed for a long time.
9. After the work was completed, the samples were evaluated by gas chromatography.

A certain amount of adsorbent is mixed with a certain amount of amenc waste (with a specific amount of amine) in a container and cooled down for a certain length of time. After that, the mixture passes through the filter paper and the remaining liquid is obtained from the absorption action (absorption residue). Using the liquid chromatography of the remaining filtration analysis, the effect of the adsorbent on the wastewater and thus the amount of absorbance of the organic amine by the adsorbent is obtained, and these results are presented below.

### 4. Discussion and Conclusion

#### 4.1 Effect of Adsorption on Absorption from organic Waste

In the first organic solvent drainage experiments on granular activated carbon, the same solutions were prepared in Jemm 200 cc wastewater containing 1000 ppm organic compounds and these solutions were adjacent to different amounts of activated carbon. These solutions and the activated carbon contained in the intra-shaker laboratory conditions were vigorously stirred for 60 minutes until the relative equilibrium was reached. Samples were then taken from the
containers and the samples were analyzed by gas chromatography. Figure 6 shows the results of this test. As shown in the figure, the amount of amine absorption is increased by increasing the amount of active carbon, and in the amount of carbon 11 grams of amine in the wastewater is absorbed almost entirely on the activated carbon surface. It should be noted that the results presented are based on the accuracy of the GC device used up to 4-10, and it is obvious that the amount of organic matter remaining in the test solution does not reach zero.

At this stage, activated granular activated carbon was contacted at ambient temperature with wastewater samples with various amines and contact times (10 minutes to 210 minutes). As shown in Fig. 9, the absorption rate is lower for the initial values of the effluent, and the increase in the initial amount of amine in the wastewater has reduced the absorption ratio. The reason for this is due to the fact that in the first case there is a higher carbon content than the amount of amine and the rate of absorption is higher, but in the second case, the amount of amine is higher, although the final absorption value is slightly higher, but the arrival speed Balance and balance are less. It shows that the ratio of amine in the wastewater to the active carbon is less than the efficiency and absorption rate. Also, the rate of absorption is a function of the initial amount of amine in the wastewater.

4.2. Effect of time on absorption of organic amine solvent from effluent
Other tests were performed to determine the amount of amine adsorption at lesser times and with different levels of amine in the wastewater. In these tests, the amount of active carbon contained in the environment was constant (10 g) and the initial amine levels were different in the wastewater (up to 2000 ppm). The different sampling times for these tests were lower than those previously tested to determine the capability and amine capability at low rates for this activated carbon type. The results of this section of the study are shown in Figures 7 and 8.

4.3. Comparison of ANN output and experimental Data
The comparison of the performance of the neural network with the experimental results is shown in the figs 10 and 11. As can be seen, the neural network model has been able to predict the results of the experimental data well and the resulting error is less than 1%.
Figure 11: Comparison of Experimental Data and Network Model for Amine adsorbed on activated carbon relative to the equilibrium amine

5. Conclusion
According to the study, granular activated carbon is well absorbed by organic compounds from wastewater and the amount of active carbon contained in the effluent has a direct effect on the absorption of amine from the wastewater. Also, with increasing contact time under the same conditions, the adsorption rate rises and the amount of adsorption on activated carbon is directly proportional to the initial amount of amine in the wastewater. In this study, it was found that the higher the ratio of amine to the activated carbon would be less, the higher the absorption rate and intensity. This study showed that activated carbon has potential for use as a good adsorbent in adsorption processes, and can be used in processes such as treatment of wastewater containing organic compounds. Adsorption of water-organic solvent by use of Activated carbon adsorbent was modeled in ANN. the ANN in this study reflected the error suitably.

Reference