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ORIGINAL ARTICLE

Modeling of deionization process of water using zeolite membranes

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Abstract

One of the types of membranes used in the industry for separation is zeolite membranes. These membranes perform the separation process by the mechanism of liquid penetration or gas penetration. The separation mechanism in zeolite membranes is based on molecular sieving, adsorption, and penetration. One of the applications of these membranes is for the deionization of different waters by the osmosis method. In this research, two types of zeolite membranes, NaA and ZSM-5, have been used for deionization. They have holes of 0.4 nm and 0.51 nm, and the water molecule can easily pass through them, but the ions are more significant than these holes and do not pass. In this research, the experimental values of these isolates are modeled, and the model results are compared with the experimental results. The modeling method used is a multilayer neural network method that includes one output and two inputs. For this modeling, 70% of the experimental data was used for the learner, about 15% for the validation, and the other 15% for the experience. The results showed that the model could predict the experimental results well

1. Introduction

Some polymer materials demonstrate the phenomenon of osmosis when used to separate a solvent from a solution. So if a solution of salt and water is placed in a chamber and an adjoining chamber has placed the solvent, water, with the osmotic membrane forming the barrier between the chambers, ions from the salt in the solution will migrate across the membrane to the solute until an equilibrium state is reached with a more dilute solution of equal salinity in both chambers. The migration of the ions is driven by a pressure called the osmotic pressure, which exists across the membrane [1-5]. Osmosis is a reversible process, so if there are two chambers with the same solution in each, applying pressure above the osmotic pressure to the solution in one of the chambers will cause ions to migrate from it, across the membrane and into the answer in the other chamber. This is the basis of the reverse osmosis process of desalination. However, the osmotic pressure of a saline solution is high, so high pressures are needed to achieve reverse osmosis, and the higher the saline concentration, the higher the osmotic pressure. Pressures are typically 15 to 100 bar or atmospheres, needing robust, high specification and relatively complex types of pumps and accounting for most of the energy used in reverse osmosis desalination [6-9]. Polymer materials such as polyamides or cellulose acetate have been used for membrane materials in reverse osmosis. However, there has been considerable research into improved membrane formulations, and now several proprietary materials have been developed for a high-performance operation to enable desalination to be undertaken faster, at higher pressures, with higher solute removal rates and lower levels of brine reject. Zeolites are among the least-known products for environmental pollution control, separation science and technology. Due to their unique porous properties, they are used in various applications. Zeolites are crystalline, porous, hydrated aluminosilicates of alkaline or

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alkaline earth metals. The frameworks are composed of $[SiO4]^{4-}$ and $[AlO4]^{5-}$ tetrahedra, which corner-share to form different open structures with an overall negative charge, balanced by the cations that move freely in and out of its framework. A representative empirical formula for a zeolite would be:

1.1 $M_{2/n}O: Al2O3:xSiO2: yH_2O$

Where M represents the charge-balance cation, n is the charge of the cation, x is generally x> 2, and y is the water contained in the voids of the zeolite. It is generally accepted that no two AlO4 can be linked directly by sharing their corner in the zeolite framework [10-15]. However, these zeolites are also used in the manufacture of zeolite membranes. These membranes have special applications due to their tiny cavities. One of these applications is the ionization of water. The size of ZSM-5 and NaA zeolite cavities is 5.1 angstroms and 4 angstroms, respectively. On the other hand, the size of the water molecule is less than 3 angstroms, and the ions associated with water are much larger than the size of the zeolite cavities. Therefore, in zeolite membranes, due to the small size of the water molecule, only this molecule can pass through the pores of the membranes, and the ions remain behind the membranes. Thus the deionization process is performed. In this research, the experimental data results of two types of zeolite membranes, ZSM-5 and NaA, were used for modeling by the neural network method. The model and experimental data results are compared and studied as parameters of flux, separation coefficient and ion repellency.

1.2 NaA and ZSM-5 Zeolite membranes

Zeolites are fine-porous crystalline aluminosilicates with a three-dimensional open frame structure. They are composed of quadrilateral alumina and silica, forming regular interconnected pores and channels. Due to the presence of mixed oxide in the composition, there is a negative charge in the framework. It produces the properties of zeolite, which is more beneficial than other amorphous porous materials. The opposing charge centers are often neutralized by cations such as Na+, K+, and Ca2+, which would be eventually exchangeable with specific heavy metal ions in solutions. Linda Type A (LTA) zeolite has the lowest silicon/aluminum (Si/Al) ratio of 1:2, leading to the highest cation exchange capacity. LTA zeolite is one of the most common zeolites used to remove heavy metal and radioactive metal ions from an aqueous solution. The pore size of this zeolite is equal to 4 angstroms. ZSM-5 Zeolite is an aluminosilicate zeolite belonging to the pentasil family of zeolites. Patented by Mobil Oil Company in 1975, it is widely used in the petroleum industry as a heterogeneous catalyst for hydrocarbon isomerization reactions [16-19]. ZSM-5 zeolite contains several pentasil units. These pentacles are connected by oxygen bridges so that they can form pentasil chains. Each of the five five-membered rings includes a pentasil unit. Inside these rings, the vertices contain Al or Si, and O is the bond between the vertices. Oxygen steps connect the pentasil chains in the zeolite structure to form corrugated sheets with 10-ring holes. Like Pentacle units, each 10-ring hole with Al or Si is assumed to be vertices with O that are connected between each vertex. Oxygen bridges connect each corrugated sheet to form a structure with "straight 10-loop channels that run parallel to the corrugated and 10-loop sinusoidal channels perpendicular to the sheets." Adjacent layers of sheets are associated with an inversion point. The estimated pore size of the channel moving parallel to the waves is 5.4–5.6 Å [20-22].

2. Theory

2.1 Artificial Neural Network (ANN)

Recently, in the field of engineering, a lot of research has been done in the field of data processing and for data that has no solution or problems that are not easily solved. These solutions use the ANN model, which is inspired by the nervous system of living organisms. In this pattern, there are units called neurons. Neurons are usually made up of three main parts: the cell body (which includes the umbilical cord and other protective factors), dendrites, and axons. In this structure, dendrites and axons are from the communication parts of neurons. Dendrites are composed of cellular fibers with uneven surfaces and many fissured extensions as areas for receiving electrical signals. This is why they are called treelike input networks. Dendrites transmit electrical signals to the cell nucleus. The cell body provides the energy needed for a neuronal activity that can be easily modeled by adding and comparing to the threshold level. Unlike dendrites, axons have a smoother surface and less elongation. The axon is longer and transmits the electrochemical signal from the nuclear cell to other neurons. The neighborhood of axons and cell dendrites is called the synapse. Synapses are small functional, structural units that enable communication between neurons. There are different synapses, one of the most important of which is chemical synapses. An artificial nerve cell can be thought of as a mathematical equation in which the mathematical equation p is denoted as an input signal. After amplifying or attenuating as much as a parameter w (in mathematical terms, it is called the weight parameter), on the other hand, an electrical signal enters the neuron with a value pw. To simplify this mathematical equation, we can assume that the input signal is added to another signal with a value of b in the kernel. Before it leaves the cell, a final signal with a value of pw+b will undergo another process called "transmission function" in technical terms. This operation is shown as a box in Fig.1, which is *f* written on it. The input of this box is the signal, and the output is displayed mathematically. We will have:

$$a = f\,(pw+b)$$

According to what has been said, putting many of these cells together can form an extensive neural network. Therefore, the network developer must specify large values w and b parameters. This process is called the learning process.

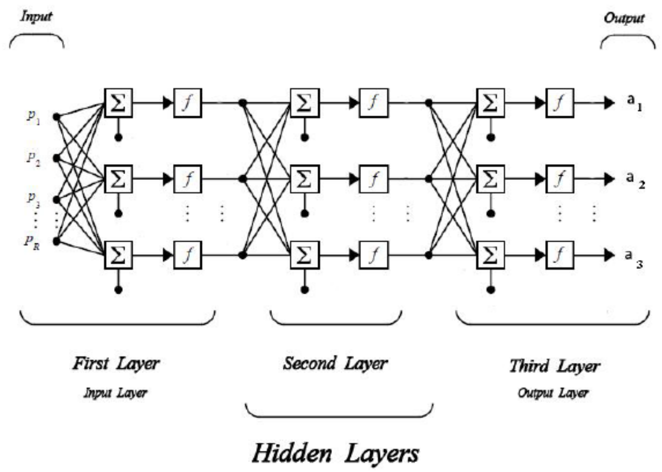

Figure 1. Image of a neural network with its constituent layers

In the structure of neural networks, it is sometimes necessary to gather several neurons in one layer. Also, many neurons can be used in different layers to increase the system's efficiency. In this case, the network will be designed with a certain number of inputs and outputs. While the difference is that there will be more than one layer (instead of having only one layer). In this method (multilayer 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 results are presented, and the other layers are called the hidden layer. A neural network has three layers: an input layer, an output layer and a hidden layer. Network capabilities can be increased by changing the number of hidden layers and the number of neurons in each layer.

2.2 Modeling of Desalination process by use of Neural Network

In this study, the effect of ANN input parameters (operating conditions) on the desalination efficiency of saline water solution. An ANN is designed for conversion parameter analysis. ANN feed multilayer perceptron and Lundberg-Marquardt function with two inputs and two outputs were used. The Tansig transfer function was used for the hidden layer and the Purelin for the output layer. Five neurons were identified for the hidden layer. After data processing, 70% was allocated to learning and 30% to testing. In this study, Matlab version R2014b was used. This is a two-layer ANN network with only one hidden layer and output. Here the inputs in the value of w must be multiplied, and then a bias coefficient (b) is added to the information (said bias is a fixed value that is added to the input value to increase accuracy). After this, the result will be a function of the function, and the resulting value is multiplied by a weight and added by bias. The result passes another process (with a different form and function), and the output is generated. There are five neurons and two inputs in the first layer. However, the number of neurons in the output layer is equal to the number of outputs. The following points about algorithms should be considered: The Data Division completely integrates the defined data for the system. This section randomly defines Train, Validation, and Test data, so there are examples from all over the environment. The Levenberg-Marquardt function was used here in the teaching phase. The mean square error (MSE) functions were also used to measure performance and the default settings for the derivative. Performance courses from 0 to 1000 repetitions are accepted. The weights were changed consecutively 1000 times based on the Lundberg-Marquardt function, and the training method was performed. If the number of iterations reaches 1000, this method stops. There was no time limit (but it can be set to stop training after 30 seconds, for example). A validation check is the maximum number of times a network failure can be tolerated.

3. Desalination test

Water-saline separation tests were carried out using an evaporative process. These experiments were performed on NaA and ZSM-5 zeolite membranes using a standard laboratory porosity system. In these experiments, the operating conditions, such as time, ion removal, flux and temperature, were evaluated [23]. The following experimental results and neural network modeling predictions are discussed below.

4. Comparison of experimental data with neural network modeling results

4.1 Variation of ion rejection and Flux vs. time

As can be seen from Figs. 2-5, the change in water flux and ion repellency versus PV operation time for different ionic solutions is shown. Obviously, ions are effectively repelled from NaA and ZSM-5 membranes, and only water molecules are allowed to pass through the membranes. For all solutions, the water flux decreases while the ion excretion increases over time. It should be noted that the diagrams mentioned show the correspondence of the modeling results with the experimental data. The results are very accurate. In the following figures, you can see Figs. 6-8, in which there is a three-dimensional diagram showing the neural network model results and the effect of different ions on water flux and membrane ion repulsion in the figures.

4.2 Changes in ion repellency and flux versus temperature

As we know, the temperature in membrane processes is one of the critical parameters that this parameter can significantly affect the performance of membranes. Figures 9-12 show the effect of process operating temperature on product flux and ion excretion from feed for different solutions. These results will show that the output fluxes depend more on temperature than ion diffusion. The results also showed that the output product flux values increase with increasing process temperature, while the rejection values decrease slowly. Therefore, it can be said that with increasing the temperature of the separation process, the mobility of water molecules in the zeolite channels increases and as a result, the product flux increases. The presented results also confirmed that increasing the process temperature increased the product water flux and ion diffusion and reduced the ion excretion rate for NaA and ZSM-5 zeolite membranes.

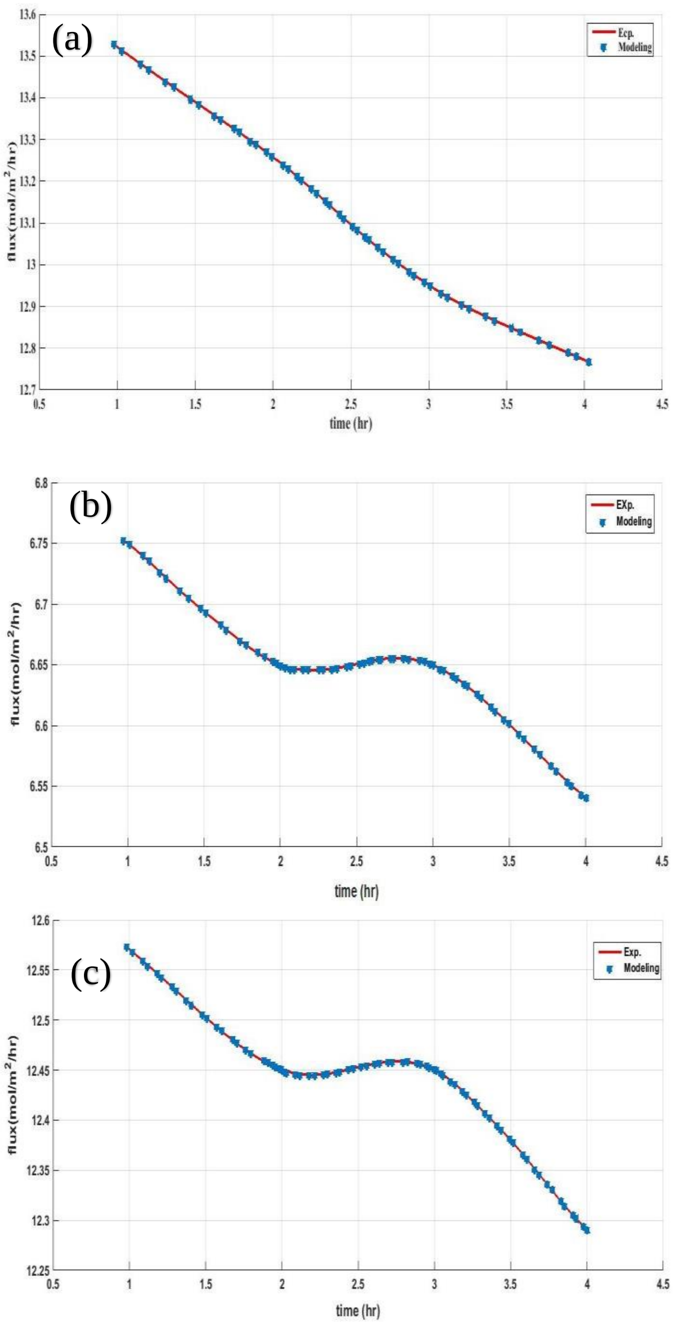

Figure 2. Flux vs. time for ionic solutions through a NaA membrane a) Cs+; b) Sr2+; c) I- (Experimental Data and Network Model Data)

Therefore, the flux increases and the reflux decrease with temperature. As seen from the graphs (Figs. 9-12), the neural network model has been able to predict the experimental results well and accurately

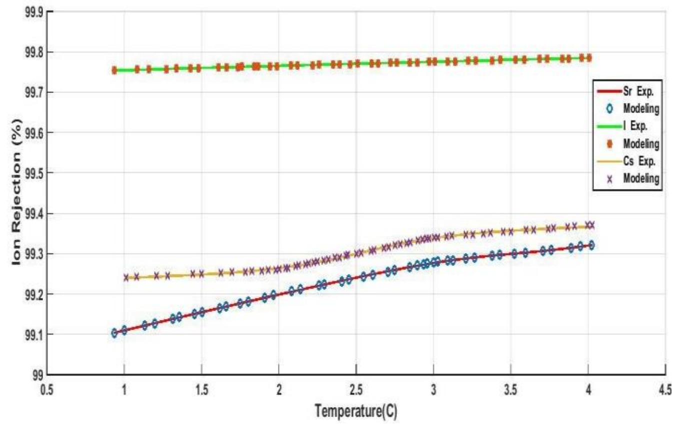

Figure 3. Ion rejection vs. time for ionic solutions through a NaA membrane Cs+; Sr2+; I- (Experimental Data and Network Model Data)

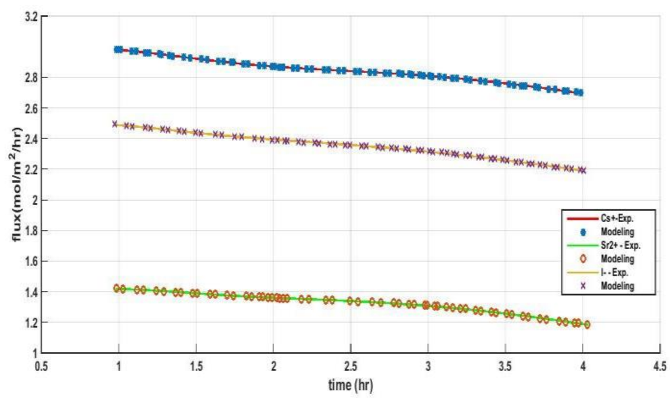

Figure 4. Flux vs. time for ionic solutions through a ZSM-5 membrane Cs+; Sr2+; I- (Experimental Data and Network Model Data)

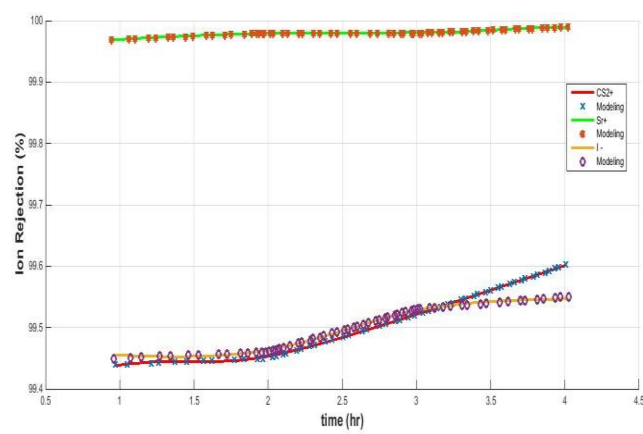

Figure 5. Ion rejection vs. time for ionic solutions through a ZSM-5 membrane Cs+; Sr2+; I- (Experimental Data and Network Model Data)

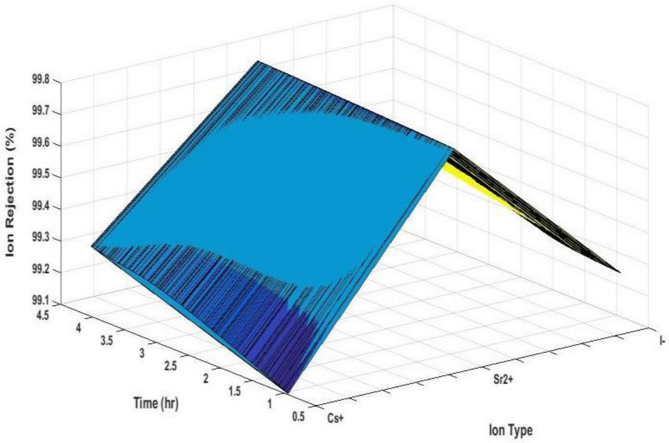

Figure 6: Network Model Prediction for Ion rejection vs. time for ionic solutions through a NaA membrane Cs+; Sr2+; I-

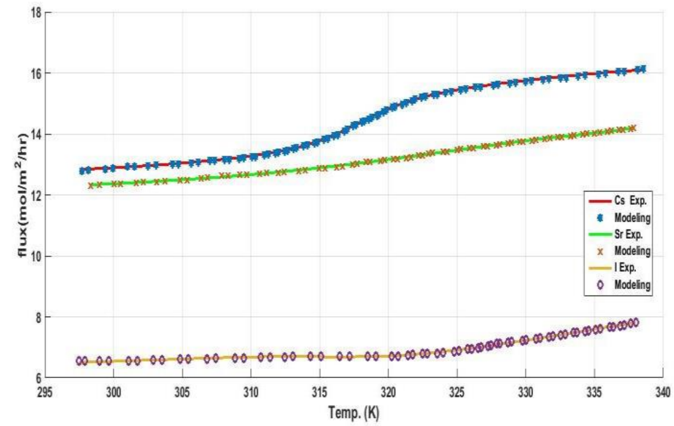

Figure 9. Variation of flux versus temperature for Cs+, Sr2+ and I- ionic solutions for a NaA membrane (Experimental Data and Network Model Data)

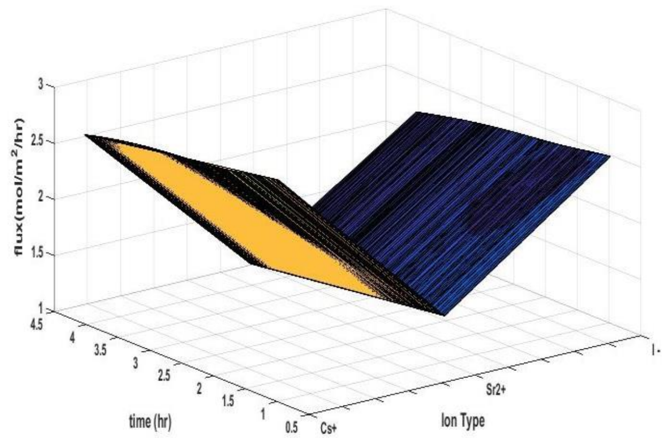

Figure 7: Network Model Prediction for Flux vs. time for ionic solutions through a ZSM-5 membrane Cs+; Sr2+; I-

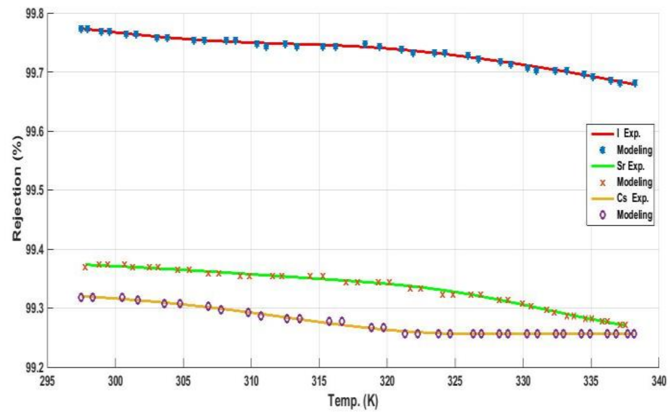

Figure 10. Variation of Ion rejection versus temperature for Cs+, Sr2+ and I- ionic solutions for a NaA membrane (Experimental Data and Network Model Data)

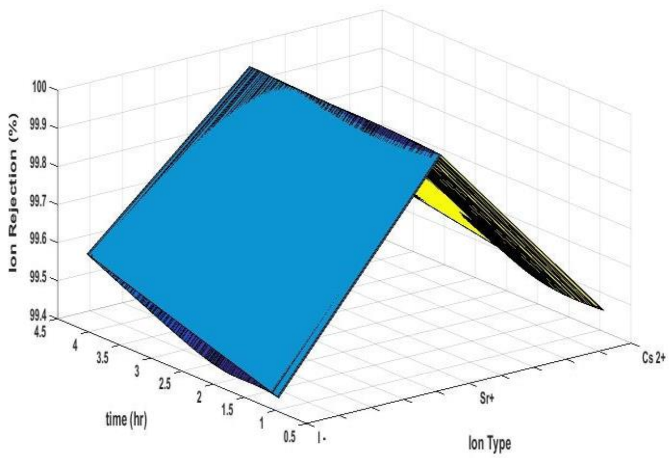

Figure 8: Network Model Prediction for Ion rejection vs. time for ionic solutions through a ZSM-5 membrane Cs+; Sr2+; I-

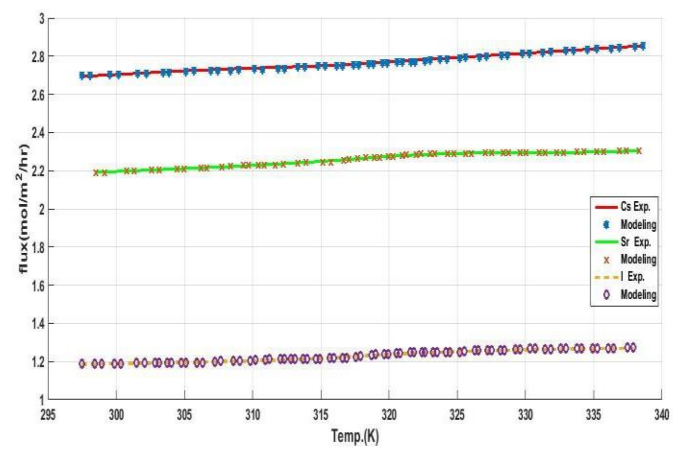

Figure 11. Variation of flux versus temperature for Cs+, Sr2+ and I- ionic solutions for a ZSM-5 membrane (Experimental Data and Network Model Data)

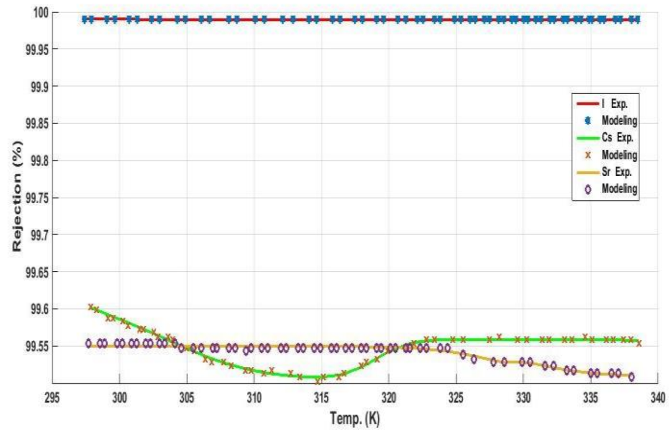

Figure 12. Variation of Ion rejection versus temperature for Cs+, Sr2+ and I- ionic solutions for a ZSM-5 membrane (Experimental Data and Network Model Data)

Also, three-dimensional graphs (Figs 13-16) of the results of the neural network model and the effect of Flux and ion rejection verses temperature.

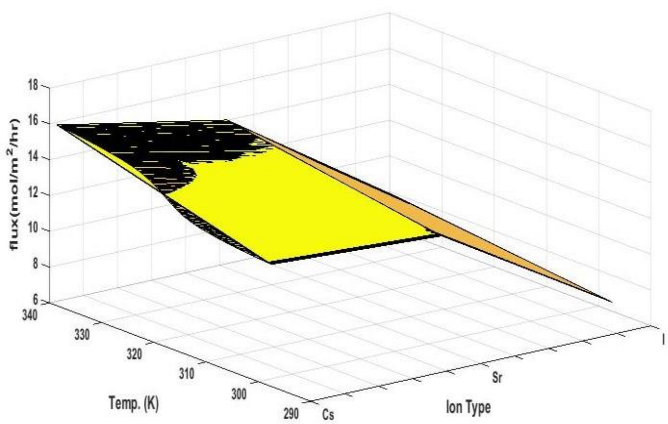

Figure 13: Network Model Prediction flux versus temperature for ionic solutions through a NaA membrane Cs+; Sr2+; I-

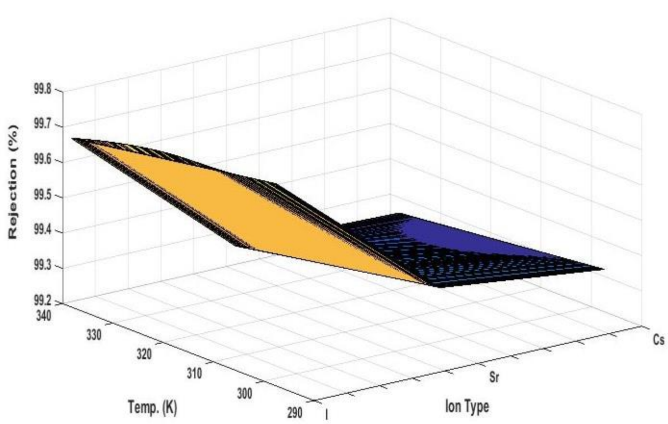

Figure 14: Network Model Prediction Ion rejection versus temperature for ionic solutions through a NaA membrane Cs+; Sr2+; I-

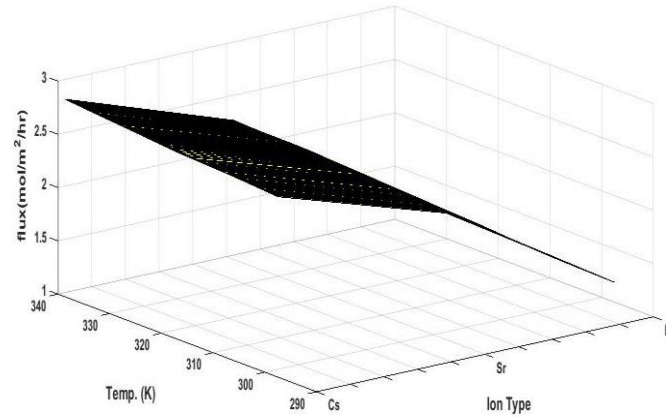

Figure 15: Network Model Prediction flux versus temperature for ionic solutions through a ZSM-5 membrane Cs+; Sr2+; I-

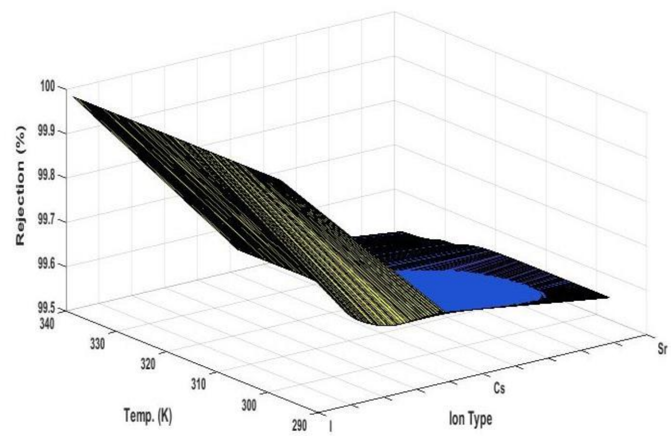

Figure 16: Network Model Prediction Ion rejection versus temperature for ionic solutions through a ZSM-5 membrane Cs+; Sr2+; I-

5. Conclusions

NaA and ZSM-5 zeolite membranes were observed that can not only separate water from organic molecules but also remove ions from aqueous solutions. Examination of desalination tests for several different types of single salt solution confirmed that this method could be used to process and concentrate saline water. High rejection values were obtained from other ions. These analyzes revealed that NaA and ZSM-5 zeolite membranes have great potential for desalination of complex mixtures. As noted, the neural network model described can be used to predict the performance of NaA and ZSM-5 zeolite membranes in the evaporation process to isolate saline solutions. The neural network model can reasonably expect the effect of operational parameters of process temperature and time and experimental results. The results of neural network modeling here also showed that this model has a minor error in predicting experimental results.

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