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MODELING OF PAFO SYSTEM WITH NEURAL NETWORK IN SEAWATER DESALINATION FOR AGRICULTURAL APPLICATIONS

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ABSTRACT

Brackish water, municipal and industrial wastewater is considered as a valuable source to increase agricultural production. PAFO system with the use of agricultural fertilizers as a new solution with the aim of creating hydraulic pressure less than 5 times to increase flux and water permeability compared to the system RO, FO in seawater desalination. The efficiency and performance of the system was determined by analyzing the parameters of water flux (jw), water permeability (A), permeability of dissolved matter (B), B/A ratio and finally modeling was done using MATLAB software with effective parameters in water flux based on chi model of neural network. According to the results of the model, appropriate performance of the model was determined based on the R coefficient and the distribution of the predicted points against the real data.

Introduction

Lack of water, food and increasing population has caused the use of unconventional waters such as brackish water - municipal and industrial wastewater as a valuable resource to increase agricultural production. Unconventional water refers to those waters which cannot be used normally and requires the application of special management and protection systems. In most arid countries, water resources are becoming increasingly scarce. Therefore, the use of unconventional waters seems necessary. Challenges of using unconventional water in agriculture include pollution, consumers and farmers, and the accumulation of heavy elements in soil, plants, and eventually soil sodium. At present, the productivity of the country's water resources has been somewhat improved by the following measures for agricultural application:

- Development of new irrigation resources such as micro and sprinkler systems
- Laser leveling
- Development of sub-networks with closed ducts to prevent leakage and evaporation
- Use of low pressure system
- Development of greenhouse cultivation
- Drainage of saline soils
- Development of conservation agriculture
- Intelligence of irrigation system

The philosophy behind the use of reverse osmosis (Ro) desalination system is derived from the US motto (Green the Desert). Recently, there have been countries that have used the product water of reverse osmosis desalination as agricultural water. Spain, for example, produces 1,400,000 m³/day of fresh water by Ro, 22% of which is devoted to agriculture. Kuwait's 13% m³/day 1,000,000, Italy 1.5% m³/day 64,700 and Bahrain 0.4% m³/day 62,000 are used for agricultural applications.

In recent years, the use of desalination system has become common on the northern and southern coasts of Iran. The use of these desalination system during peak hours will cause severe damage to the country's electricity network. High-pressure pumps are used in desalination system to produce pressures above 40 bar. In a study conducted in 2011 by Abdolbaidi *et al.*, the cost of desalination of Caspian Sea water with reverse osmosis system was investigated with DEEP4 desalination economic evaluation model, the cost of producing one cubic meter of fresh water at a site with a capacity of 280,000 cubic meters and a salinity of 12000 mg/l was estimated at about \$ 0.77.

Unfortunately, in the discussion of agriculture in the country, most of the agriculture is small ownership and in practice, the application of current methods is high due to the small scale of most lands; On the other hand, most of the agricultural water is obtained from groundwater sources, so it

is necessary to complete studies on reducing the cost of desalination methods according to the potential of the country so that the methods can be used in agriculture. Many researchers have pointed out the importance and necessity of processes to improve agricultural water productivity.

Zamani *et al.* (2014) also studied the productivity of different products and suggested to commensurate method or type of product in order to improve the productivity of agricultural water. Therefore, the necessity of studying the processes of improving agricultural water productivity, which provides a dynamic, continuous and complete knowledge of the agricultural water productivity cycle, becomes clearer by determining the extent of the impact of each process. (Alon Bengal Telaviv, 2008)

A study in Ashkelon, Israel, estimated that the cost of desalination of 1 m³ of seawater was about \$ 0.55 in 2006, including the boron removal, the addition of SO⁴ and Ca²⁺, and the alkalinity of the system, which is achieved with an advanced treatment stage. Irrigation with desalinated water in Israel, although associated with the use of other sources, is unreliable because of its low buffering capacity, which increases the risk of corrosion. Therefore, agricultural water supply requires a balance between economics and agricultural benefits.

Recently, in these areas, the study of agricultural water standards is a priority. Desalination of water not only removes salt, but also ions necessary for plant growth are removed, so feeds for the plant including Mg²⁺ and SO₄ should be prepared by adding fertilizer. This type of plan is to add limestone to increase Ca²⁺, which reaches a concentration of 46-40 mg / lit. During the process, SO₄ is completely removed, which is compensated by the addition of sulfuric acid, its final concentration reaches 20-25 mg / lit. (Vallandares, 2016).

In Spain, 60 designs have been reported for water treatment and storage. Studies have been conducted in this area. In these areas, standards for water quality are presented depending on the type of irrigation, which basically determines the relationship between EC and conductivity and sodium concentration and other parameters. These standards are effective on soil and soil structure modification. (Elena co, pose, 2008)

In recent years, the Fo system has not been compared in terms of economic benefits compared to conventional methods. According to the results of the study, 21% more investment cost and 56% lower operating cost due to energy storage and reduction of filling in FO forward osmosis systems were announced. The price per cubic meter of water produced is a 16% reduction in the total cost of the Fo system compared to compression systems (Rajesh Kamar, 2017).

The results are presented according to Figure 1-1

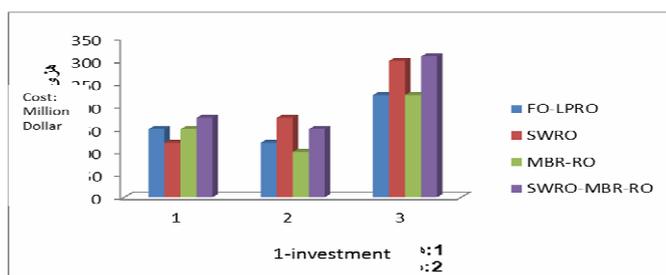


Fig. 1-1 : Comparison of cost of membrane desalination systems

Andrea Chili *et al.* In 2010 conducted studies on tensile solutions in the forward osmosis system. The most suitable tensile solution was introduced for the use of Fo. The title of the most suitable tensile solutions was introduced and it was found that water flux and return salt dispersion decreased with decreasing the concentration of tensile solution. The best tensile solutions were CaCl₂, Ca (NO₃) and NaCl (Andrea Chili *et al.*, 2010).

Ashrup Fantshu *et al.* (2011), Fo system and agricultural fertilizers were used for desalination of seawater and agricultural application. Instead of removing the tensile solution, dilution of the tensile solution was used. About 9 fertilizers were selected as tensile solution from the relevant list and their efficiency was studied by determining the pure water flux and return tensile solution. According to the results, fertilizers that have the highest solubility in water produce high osmotic pressure compared to seawater. Tensile solutions KCl – NaNO₃ and KNO₃ have the best water flux. It was estimated that one kilogram of fertilizer separates about 11-29 liters of water from the sea (Ashrup Fantshu *et al.*, 2011).

Sangmin *et al.* (2013) according to this study predicted the efficiency of Fo numerically with a one-dimensional mass balance equation for the ratio of feed and tensile solution with the water flux model. According to the results, the use of high concentration tensile solution improves water flux. Water flux in the form of series and sequence feed solution and tensile solution in a row is effective in increasing water flux.

Sangmin *et al.* (2013) forward osmosis process is a process in which water passes through semi-permeable membranes with osmotic pressure, so it is a good alternative to low-energy processes. PAFO pilot can increase the output flux by increasing the hydraulic pressure 5 times at a low cost. One of the key components in these systems is the selection of an optimal tensile solution, which is the criterion for selecting high osmotic pressure for traction. It is actually a fertilizer system that does not require final purification of the tensile solution (Sangmin *et al.* 2013).

The purpose of this project is to use water resources with renewable potential, increase the efficiency of desalination technologies in Iran, remove solids from seawater by PAFO system, use on a commercial scale for agricultural purposes.

Materials and Method

Experimental studies were performed in the HSE laboratory of the National Iranian Oil Company of Pars Assaluyeh Special Economic Zone from 2017 to 2019 on a pilot. To determine the efficiency of FO pilot in this project, 11 fertilizer solutions with a concentration of 50 mg/l were used as a tensile solution and seawater with EC = 48000 as a feed solution was used. Graphene nanotube membranes were fabricated and at the same time the effects of fabricated nanomembranes on the efficiency of PAFO system were investigated using auxiliary pressure. In the final stage of the project, effluent flux, water permeability and solubility of the dissolved material were analyzed and the system was calculated and the results were compared and modeled with similar systems.

Figure 1 shows a diagram of the Fo system and the actual order in the laboratory. Fo was investigated using a closed system.

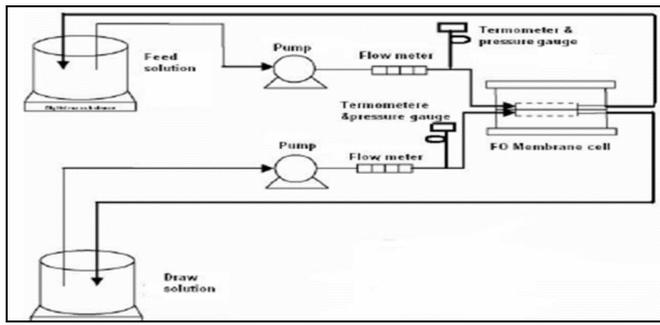


Fig. 2-1 : Forward osmosis system diagram

- Plexiglas cell with a surface of 3.75 m²
- Graphene nanotube membranes cm15 * 25
- Tensile and feed solution flow diaphragm pump (maximum flow 100 l / min and maximum pressure 7 bar)
- 200 liter tanks

To perform the osmotic pressure calculations, the theory and the diffusion coefficients of fertilizer solutions were measured with a tensiometer. Water flux was continuously recorded from the difference between the initial and final weight by the laboratory scale as the amount of water flux in time and RO was compared. The amount of B or the permeability coefficient of the dissolved material (tensile material) similar to water permeability was estimated as average. Return of salt and tensile solution was performed by EC measurement.

1-2 Osmosis:

Osmosis is the spontaneous transfer of molecules from a dilute solution to a solution with a higher concentration than a semipermeable membrane. A semipermeable membrane allows solvent molecules to pass through but does not allow the dissolved matter to pass. The volume of the solvent (V), the temperature T and the ideal constant of the gases are R.

$$\pi = \frac{n}{V} . R T \tag{1-2}$$

2-2 General equation of water flux of FO system

The general equation of water flux in forward osmosis is presented by Lee *et al.*, and Mick Chen presents 44 simplified equations for predicting water flux FO.

$$J_w = A \left[(\pi_D \exp(-J_w K_a) - \pi_F \exp(J_w / k_b)) \right] \text{Type equation here.} \tag{2-2}$$

Sangmin *et al.*, 2013)

J_w = water flux

A = Pure water permeability of membranes

π_D = osmotic pressure of tensile solution

π_F = osmotic pressure of the feed solution

k_a = specific resistance coefficient of the solution (resistance of the dissolved material to diffusion in the holes)

k_b = mass transfer coefficient

Calculation of k_a (solution specific resistance coefficient)

$$k_a = \frac{t\tau}{D\varepsilon} s = \frac{t\tau}{\varepsilon}$$

t = Membrane layer thickness

τ = curvature of membranes

ε = pores

D = tensile solution diffusion coefficient

s = membrane structure parameter

As a result, according to the placement of the structural parameter of the membrane in the Equation k_a:

$$k_a = \frac{s}{D} \tag{4-2}$$

D The diffusion coefficient of tensile solutions measured with a tachometer and s is a membrane structure parameter that in FO systems s can be estimated for the system. The s parameter is constant for each membrane in different positions.

Structure parameter calculations

$$s = \left(\frac{D}{J_w} \right) \times \ln \left(\frac{(B + A \times \pi_D)}{(\beta + J_w + A \times \pi_F)} \right) \tag{5-2}$$

D = tensile solution diffusion coefficient

π_D = osmotic pressure of tensile solution

π_F = osmotic pressure of the feed solution

A = water permeability coefficient

β = salt permeability coefficient

π_F = 0 is assumed to be an estimate in the equation and calculation of s.

The membrane structure parameter (s) indicates the resistance of the membrane support layer to the dissolved material. According to research, FO membrane developers have found that lower s levels facilitate the diffusion of dissolved matter into holes in the support layer, thereby increasing water flux.

Calculation of k_b (mass transfer coefficient)

$$k_b = \frac{shD}{d_h} \tag{6-2}$$

Sh = Sherwood number

D = tensile solution diffusion coefficient

d_h = hydraulic diameter

Sherwood number, which is called mass transfer Nusslet number is a dimensionless number that in mass transfer science indicates the amount of mass transfer from convective to mass permeability.

$$\frac{\text{Mass Transfer Coefficient}}{\text{Diffusion Transfer Coefficient}}$$

Calculating Sherwood number

$$sh = 1.85 \left[Re \times Sc \times \frac{d_h}{L} \right]^{0.33} \rightarrow Re \leq 2100 \tag{7-2}$$

(Inger Liss *et al.*, 2013)

$$sh = 1.85 [Re^{0.75} \times Sc^{0.33}] \rightarrow Re \geq 2100 \tag{8-2}$$

(Inger Liss *et al.*, 2013)

$$Re = \frac{d_h V \rho}{\mu} \tag{9-2}$$

(Inger Liss *et al.*, 2013)

Sc = Schmidt number

Re = Reynolds number

ρ / μ = kinematic viscosity

Dh = hydraulic diameter

$$d_h = \frac{4 \times \text{wettered area}}{\text{Wettered Perimeter}} \tag{10-2}$$

(Inger Liss *et al.*, 2013)

Calculating the Schmidt number. Wilhelm Schmidt

The dimensionless number indicates the ratio of momentum penetration (viscosity) to mass penetration (diffusion coefficient).

$$\frac{\mu}{D} = \frac{\text{Dynamic Viscosity}}{\text{Diffusion Coefficient}} = \frac{\left(\frac{\text{Pa.s or N.s}}{\text{m}^2}\right)}{\left(\frac{\text{m}^2}{\text{s}}\right)} \tag{11-2}$$

(Inger Liss *et al.*, 2013)

3-2 - Water flux model in PAFO system

Chi *et al.* have proposed a new equation for PAFO (a combined system of FO and RO).

$$J_w = A \left(\Delta p + \left(\pi_D \exp\left(-\frac{J_w}{k_d}\right) - \pi_F \exp\left(\frac{J_w}{k_F}\right) \right) \right) \tag{12-2}$$

(Inger Liss *et al.*, 2013)

$$J_w = A(\pi - \pi) + \Delta p \tag{20-3}$$

(Inger Liss *et al.*, 2013)

A = membrane water permeability coefficient

Δp = hydraulic pressure of the system

π_D = osmotic pressure of tensile solution

π_F = osmotic pressure of feed

k_F and k_d , which are equal to or equal to k or $1 / k$ in Equation F, respectively.

Results and Discussion

1-3- Initial evaluation of system flux

This test showed that the system needs a maximum of 2 hours to increase flux. In all tests, the flux decreases after a 2-hour period. This is due to the dilution of the tensile solution and the thickening of the feed solution over time. Or the osmotic potential of the tensile solution is higher than that of the feed solution. It occurs until we reach the osmotic equilibrium (zero osmotic gradient).

In fact, the flux decreases slowly as the tensile and feed solution becomes thinner. Flux may not be economical, so continued engineering and initialization of the process can play an important role in desalination with a forward osmosis system. The flux changes over time according to the 3-1 curve.

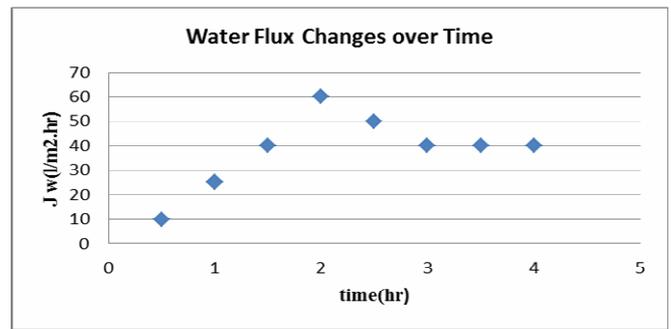


Fig. 3-1: Changes in water flux over time FO system

The results of water flux changes and flux reduction after 2 hours from the start of operation of the system are similar to the results of Verinson *et al.* In 2012 in the project Factors affecting the efficiency of forward osmosis.

2-3- Results of PAFO system modeling

First, the output flux of PAFO system was predicted using two methods of modeling with Chi equation and modeling with fitting of 50 curve with neural network for PAFO system with matlab software. Chi and modeling were compared by fitting the neural network curve. Finally, by comparing these two models, the best selected model was proposed.

The results of the real values against the values predicted by the Chi equation are presented in Figure 2-3.

3-3 Modeling the output water flux with Chi equation of PAFO system

In order to determine the relationship between the model and the real value, in many cases it is necessary to test the accuracy of the models produced. For example, using regression or artificial intelligence to model a phenomenon and now you want to examine the efficiency of the model. You should put the values simulated by the model next to the real values and evaluate the performance of the model. In addition to using model evaluation indicators such as Rsquare and RMSE by preparing a point or distribution chart, you can also be aware of the performance of the developed model by placing the predicted data in front of the real data.

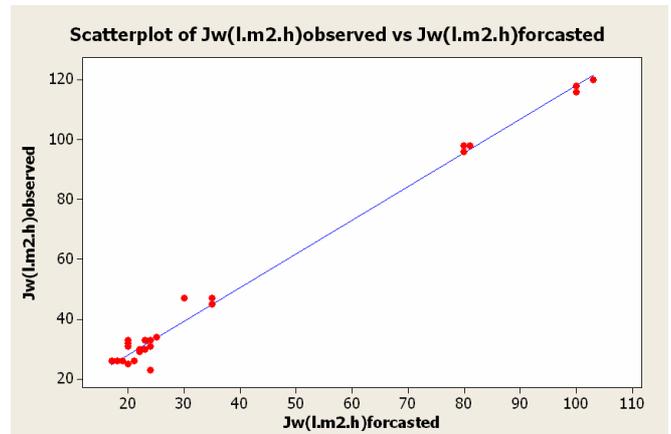


Fig. 2-3 : Distribution of observed values versus predicted values of Chi equation

According to the presented diagram and the distribution of points, it is possible to see to some extent the agreement of the chi model with the real results.

The measured flux is somewhat consistent with the prediction based on the developed water flux model in the process.

Among the things that are important in the efficiency and modeling of osmotic systems is the type of membranes; Orientation of membrane tendency and deformation of membranes and changing the parameter of membrane structure. According to Ion Knack 2014, PAFO modeling with Chi model was rejected by determining AB parameters in comparison with laboratory observations, and this was due to the use of TFC membranes in the project, so the test results Pilot and theoretical modeling are very different. It is suggested that the membrane structure for FO systems be defined and analyzed with equations before modeling.

Many studies have shown that S values are variable structure parameters. But here, because the membranes have not changed and the hydraulic pressure is constant, S values do not change much and about 450 μm is estimated based on the structure parameter calculation equation.

3-4-Modeling output water flux by fitting the curve using neural network

The function of artificial neural networks is in four classes of curve fitting, or data fitting, pattern recognition

and classification, clustering, time series prediction that can use graphical user interfaces or coding

There are four basic steps you can take to begin the process of preparation for mediation.

- Initial data preprocessing
- Determining the structure of the neural network
- Education
- Simulation and determination of model accuracy
- Modeling with curve fitting using neural network in MATLAB software

- When the goal is to communicate and estimate an output set from an input set, the curve fitting approach is considered, which is possible to perform this type of modeling both through the graphical interface and through programming.

- Normalization of output data from PAFO system

The conversion of abnormal data to normal was performed using the Cox box method in Minitab. Table 4-6 shows the values of the effective variables in the output water flux for normalization.

Table 1-3 : Values of effective variables in the output water of PAFO system

Row	Water flux	Water permeability coefficient	Osmotic pressure of tensile π (solution)	Diffusion coefficient	Hydraulic pressure(bar)	Osmotic pressure of feed solution (bar)
1	120	8.6	55	1.1	5	40
2	118	7	55	1.1	5	40
3	116	6	55	1	5	40
4	47	1.56	70	1.31	5	40
5	47	1.5	70	1.20	5	40
6	45	1.5	70	1.18	5	40
7	25	2	35	1.04	5	40
8	25	1.8	35	1.03	5	40
9	26	2	35	1.04	5	40
10	30	1.43	34	1.91	5	40
11	29	1	34	1.8	5	40
12	30	1.3	34	1.90	5	40
13	33	1.36	58	1.06	5	40
14	32	1.34	58	1.06	5	40
15	31	1.30	58	1.04	5	40
16	34	13	47	1.04	5	40
17	33	12	47	1.04	5	40
18	30	10	47	1.03	5	40
19	98	2.30	67	1	5	40
20	98	2.20	67	1	5	40
21	96	2	67	0.9	5	40
22	23	0.9	54	1.38	5	40
23	33	0.9	54	1.37	5	40
24	31	0.8	54	1.30	5	40
25	26	2.9	39	1.04	5	40
26	26	2	39	1.03	5	40
27	26	2	39	1.04	5	40

Normalization of numbers related to the parameters of water flow, water permeability coefficient, osmotic pressure, diffusion coefficient. In the following diagrams, the probability diagram after normalization is presented separately.

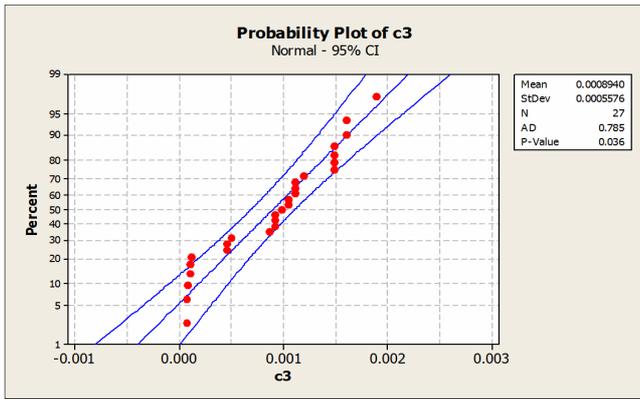


Fig. 3.3 : Normal probability after data normalization

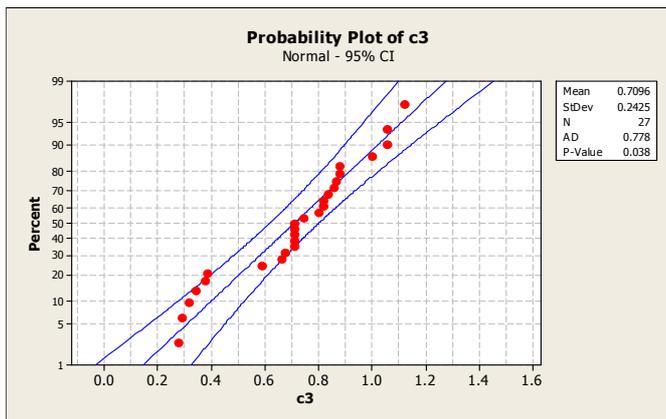


Fig. 4.3 : Normal probability of water permeability after data normalization

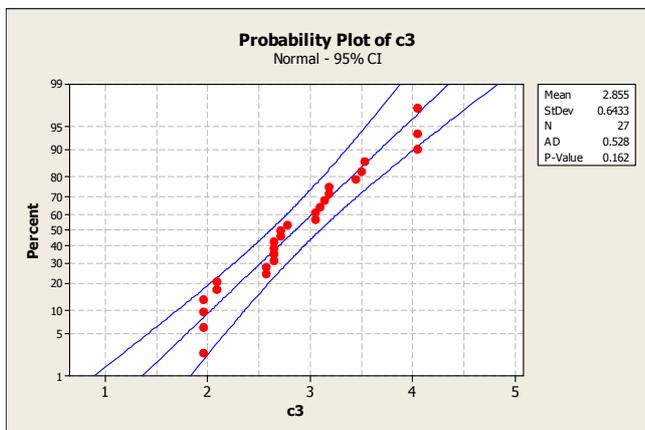


Fig. 5.3 : Normal probability of osmotic pressure of tensile solution after data normalization

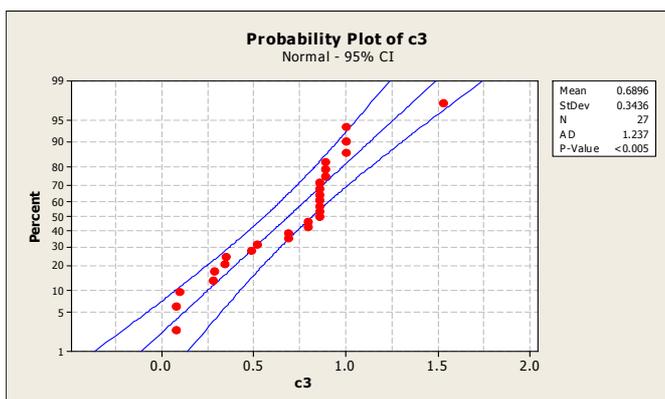


Fig. 6-3 : Normal probability of diffusion coefficient after data normalization

3-5 Modeling the output of water of PAFO system by fitting the curve using neural network in MATLAB software

Here and to estimate the amount of water flux, the number of neuron in the hidden layer equal to 10 neurons and 7 variables presented in the table (water permeability, osmotic pressure of feed solution and tensile solution, diffusion coefficient, hydraulic pressure, viscosity, membrane structure parameter) were selected. It also has an outer layer with a neuron.

The Levenberg back propagation model training algorithm was used. After selecting the algorithm, it entered the training stage. The repetition continued until we reached the least verification error equal to 2.

6-3-Model verification

Here, the performance evaluation index of the model are the two indices of mean square error of MSE and correlation coefficient or R.

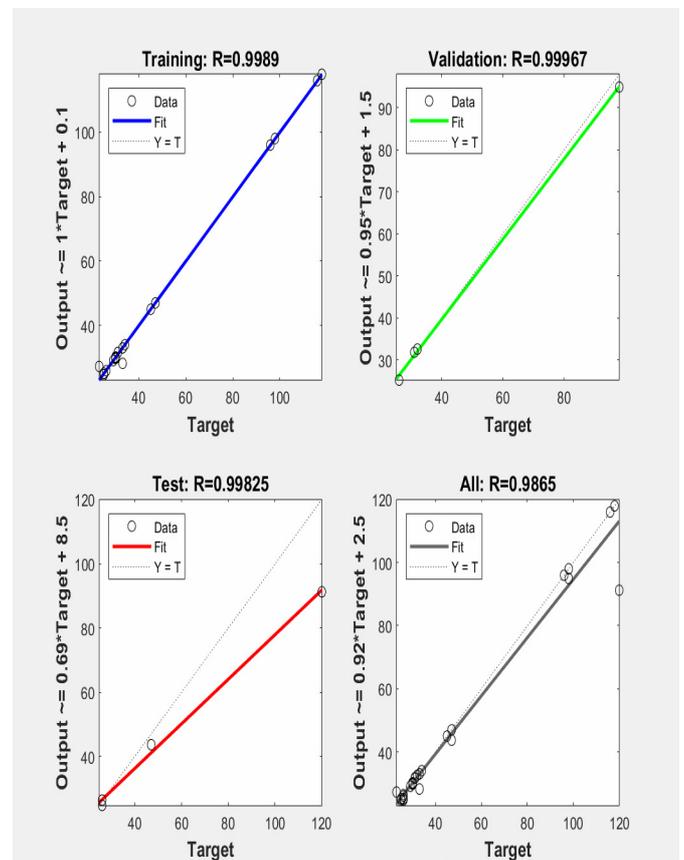


Fig. 7-3 : Fitting line and correlation coefficient value for training and verification process, test and whole process

The results of this training along with the verification and testing of the model show the remarkable efficiency of the model, because the correlation coefficient, especially in the test phase, is close to one.

If the model performance evaluation index is not appropriate, the model evaluation process can be performed again with changes in the model training algorithm.

According to Figure 7.3, the estimated values are displayed as output on the y-axis and the actual values as the target on the x-axis are displayed for each of the processes. The relationship between linear regression, fitting line and correlation coefficient for each process is shown in the graph.

As the R coefficient as well as the distribution of the predicted points against the actual flux data in the diagrams show, here we see the proper performance of the developed model. In order to determine the relationship between the model and the real value, in many cases it is necessary to test the accuracy of the produced models. For example, using regression or artificial intelligence to model a phenomenon and now you want to examine the efficiency of the model. You should put the values simulated by the model next to the real values and evaluate the performance of the model. In the face of real data, be aware of the performance of the developed model.

If the accuracy of the model is not sufficient, the model training can be performed again, or the number of neurons can be increased or more data volume can be used.

Using the nftool graphical interface, although it provides a suitable path for the modeling, it has limited configuration conditions. However, the process of training and evaluating the model and finally modeling can be followed more accurately and efficiently.

Conclusion

This study is a key framework for evaluating the PAFO system, the factors affecting the flow of water produced by this system. Efficiency of agricultural fertilizer system as tensile solution and use of graphene nanotube membranes by parameters of water flux, water permeability A) and permeability of dissolved matter (B), as well as various effects of tensile solution type, osmotic pressure values and tensile strength of zinc Output flux was checked.

High flux is the most important proof parameter of FO technology for practical application. The output flux results of fertilizers are different due to different dissolution properties and osmotic pressure. According to this study, KOH fertilizer has an osmotic pressure of 55 bar and a high diffusion coefficient of 1.31. Fulling and concentration polarization in membranes is the proper choice of a suitable tensile solution with high osmotic pressure relative to seawater osmotic pressure and hydraulic auxiliary pressure.

A constant flux is generated during the test, which is mainly due to the properties of the graphene nanotube membranes. According to the results, the maximum amount of permeability coefficient with graphene nanotube membranes has increased by almost 50% compared to the maximum amount of permeability coefficient with RO membranes. Also, the minimum amount of permeability coefficient of dissolved matter B) with graphene nanotube membranes has been reduced by almost 50% compared to the minimum amount of permeability coefficient of dissolved matter with RO membranes. Which indicates the proper performance of graphene nanotube membranes.

-Reducing the thickness of the support layer and the properties of nanotubes in the active layer of membranes cause a significant increase in the output of water. Accurate increase of water flux requires complete understanding and modeling of the size, shape and efficiency of nanocanals. High permeability of water (A) and low permeability of dissolved material (B) and water transfer coefficient in the results indicate improvement of the system. Membrane friendliness, molecular weight of ions and charge factor of nanotubes and particles are among the important parameters

in the proper efficiency of material return in graphene nanomembranes.

The percentage return of the material synthesized by the membranes in the project seems reasonable. For example, the highest percentage of return according to the table is 65% with graphene nanotube membranes, which indicates higher values compared to PA membranes with a percentage of return of 47%. They also have a high rejection compared to high molecular weight molecules. The inner nanotubes and inner holes of the nanotube are the passageway for the solvent, acting as nanochannels on the membrane surface that pass water without pressure.

Various types of membranes are made with high flux and high permeability, but due to high cost, the fabrication of these membranes is limited, while the production of graphene membranes is economical. The most important strategies for improving graphene membranes include space engineering and fabrication of membrane layers and nanopores, surface functional groups, membrane thickness. Graphene membranes may be useful in scenarios that require limiting the type and concentration of tensile solution.

-When 5 times pressure is applied on the feed solution, permeability and flux are multiplied compared to FO system. Therefore, the use of PAFO is more appropriate against common FO constraints. In osmotic membrane processes, water flux is generally dependent on membrane pressure and properties. Therefore, water flux has been increased by combining high osmotic pressure tensile solution (agricultural fertilizer) and hydraulic pressure and changing the membrane structure (reducing the support layer and increasing the permeability of membrane water with graphene nanotube in the active layer). And low pressure is needed 2-6 times, which is balanced by increasing efficiency and water flux, which has a clear effect on flux against the pressure of RO system with a pressure of 50 bar

-According to the results of modeling with chi equation and fitting of neural network curve, there is a good correlation between the measured values and the modeled flux with fitting of neural network curve. The water defined varies according to the type of membrane and is not general. It is also possible that compaction and change in the membranes due to hydraulic pressure lead to a change in the values of AB, which in turn has a significant effect on the prediction of values.

The effect of hydraulic pressure on the efficiency of forward osmosis depends on the type of membrane and its structure and the efficiency of the PAFO system depends to a large extent depending on the parameter A, B. We are faced with multiple variables. Therefore, with the neural network curve fitting approach, it is easy to simulate by changing the input and output data and changing the network settings. Using the nftool graphical interface used in this project to predict the output flux of the PAFO system. Although it provides a simple way to model, it has limited configuration conditions, while increasing the configuration with programming can follow the process of training, model evaluation and modeling more accurately and efficiently.

In this study, the PAFO system was systematically investigated. The PAFO system has overcome the FO system and compensated for the limitations of this system, including low flux. The water flux increased with increasing hydraulic

pressure and changing the structure of the membranes without increasing the concentration of tensile solution. Which is specially designed for high recovery

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