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Estimating of CO_2 Conversion in Falling Film Reactor Using Artificial Neural Network

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ABSTRACT - This paper presents the development of Artificial Neural Network (ANN) model for absorption process of CO_2 gas using monoethanolamine (MEA) as a solvent in a falling film reactor. Although studies on ANN applications in chemical engineering in the literature are more concentrated on utilizing dynamic models, there has been an increasing trend for diverse application of ANN to model steady state systems. The feed-forward artificial neural network was adopted and trained by back-propagation algorithm. In this paper 216 sets of data are used to train and test the network. This study shows that ANN model with one hidden layer and nine neurons in the hidden layer gives a very close estimation of the CO_2 conversion and there is high potential for absorption application of ANN model.

Keywords: Artificial Neural Network, Back-propagation algorithm, Falling film reactor.

1. INTRODUCTION

Falling film reactors are generally used in processes where it is essential that temperature is maintained below certain limits – for example, removal of carbon dioxide, sulfonation, and concentration of syrups or the manufacture of cosmetics. Removal of carbon dioxide has been practiced industrially for several decades [(1)]. CO_2 capture is typically done by absorption with alkanolamine-water solution. The alkanolamines are bases, and they react with the acid species CO_2 to form different reaction products [(2)]. In the heart of successful process analysis is the step of mathematical modeling. The objective of modeling is to construct, from theoretical and empirical knowledge of a process, a mathematical formulation which can be used to predict CO_2 conversion of this process [(3)]. A simulation model for the prediction of the conversion of CO_2 in the falling film reactor involved complex non-linear problem of

simultaneous diffusion and chemical reaction in the liquid phase. The Artificial neural network (ANN), is not fully studied and explored in the field of chemical engineering, provides an alternative method for modeling complex systems. Neural Networks are computer algorithms inspired by the way information is processed in the nervous system. An ANN is a massively parallel distributed processor that has a natural propensity for storing experimental knowledge and making it available [4,5]. An important difference between neural networks and standard Information Technology (IT) solutions is their ability to learn. This learning property has yielded a new generation of algorithms that can:

- learn from the past to predict the future;
- extract rules for reasoning in complex environments;
- offer solutions when explicit algorithms and models are unavailable or too cumbersome [4].

Due to the complexity of falling film reactor, an alternative ANN approach was employed to model and predict the conversion of CO_2 in the (CO_2-MEA) system in falling film reactor. Artificial neural network (ANN) does not require a prior fundamental understanding of the process or phenomena being modeled, thus, eliminating the need for numerous mathematical relationships. The architecture of the network used in this research was Feed Forward Artificial Network (FFAN) and the training of the network was done using Back Propagation Neural Network (BPNN) algorithm. This research developed ANN model using adequate number of training points obtained from the experimental study [6].

2. ARTIFICIAL NEURAL NETWORK (ANN)

Over the past few years, Artificial neural network (ANN) has received a great deal of attention and is now being proposed as a powerful computational tool. The structures of ANN are nervous system. The potential benefits of ANN extend beyond the high computation rates provided by massive parallelism. The application phase of ANN takes relatively little time compared to its training phase and therefore offers potentially faster solutions for problem solving. ANNs can be used to map linear as well as non – linear relations. These consist of a number of very simple and highly interconnected processors called "neurons" or processing Elements (PEs). The PEs are interconnected by connection weights. The neural net can be made to map input patterns to output patterns by adjusting or altering the connection weights. This process is called "learning" during the training phase. The ANNs program develops a model during the training, form repetitive exposures to data and readjustment of the weights. A subgroup of PEs is called a layer in the network. The first layer is the input layer and the

last layer is the output layer. The layers that are placed between the input and the output layer are called hidden layers. Each PE typically receives many signals over its incoming connections. These signals may arise from other PEs or from the external environment. A PE in a neural network receives input stimuli along its input connections and translates those stimuli into a single output response, which is then transmitted along the PEs output connections. The mathematical expression that describes the translation of the input stimulus pattern to the output response signal is called the transfer function of the PE [7].The network was training by Back Propagation Neural Network (BPNN) algorithm. The architecture of the BPNN is a hierarchical design consisting of fully interconnected layers of rows of processing units as shown in Fig.(1). Each unit is itself comprised of several individual PEs. This architecture does not have feedback connections, but errors are back propagated during training. In here, BPNN has forward flowing information in the prediction mode and back propagation error correction in the learning mode. Errors in the output determine measures of hidden layer output errors, which are used as a basis for adjusting the two sets of weights between the pairs of layers and recalculating the outputs is an iterative process that is carried on until the errors fall below a tolerance. The ANN program develops a model during training, from repetitive exposures to data (data could be noisy, highly nonlinear and complex) and readjustment of the weights. In BPNN, the network takes a set of inputs and produces predicted outputs, which are then compared to the actual outputs. An error signal alters the weights of all interconnections, so that subsequent predictions are closer to the actual value. Initial weights can be set randomly. Eventually, after a sufficient number of training iterations, the net learns to recognize pattern in the data or a set of weights for all interconnections. Then the trained network, with the corresponding good weights, can use the internal model to make predictions on the outputs from sets of inputs previously unknown to it.It important to note that this internal model is not based on any specification of the underlying mechanism for process, the net itself generates this model (8).

3. METHODOLOGY

The following steps were carried out in the development of ANN-based model used for the prediction of the CO_2 conversion in the falling film reactor.

3.1 . Database Generation

The network is trained by the database based on the results obtained from experimental measurements (6). 216 sets of data adapted to train and test the ANN model. Further quantities

such as mole fraction of carbon dioxide in gaseous mixture (Y), molar concentration of the absorbent (monoethanolamine) (CMEA), volumetric flow rate of liquor MEA (QMEA) and its temperature (T) effects the conversion of CO_2 and they are used as input parameters to predict the conversion of CO_2 (the only output parameter).

3.2. Normalizing the Raw Data Collected

Generally, majority of the effort in developing a neural network model into collecting data and preprocessing them appropriately. The standard process is to normalize the raw data. Here, the requirement is that the inputs to each input PEs should be in the between -1.0 to 1.0, inclusive and the output to each output PEs should be between 0.0 to 1.0. Normalizing the raw data avoids numerical overflows due to very or small weights [(9)]. The approach adopted for normalizing the raw data is:

Normalized value of a variable = Raw value of a variable divided by the largest absolute value.

3.3. Selection of The Number of Hidden Layer

The hidden layer abstracts the characters of the input information. Increasing the number of hidden layers, the performance of the treatment ability of a feed-forward artificial neural network will be promoted. But it may cause the complexity of training procedure, the increase of training samples and training time. Generally speaking, we should start with a system with one hidden layer and increase the number of hidden layer by requirement. For a continuous output or even a discontinuous output in some cases, a very close prediction can be obtained via a feed-forward artificial neural network with only two hidden layers [[9]]. In most cases, even a feed-forward artificial neural network with one hidden layer, can reach a considerable good prediction [(9,10)].

3.4. Selection of the Number of Hidden Layer Neuron

The selection of the number of the hidden layer neuron is very important and troublesome. If the number of the hidden layer neuron is fewer, the ANN cannot receive all necessary information of the modeling system and less tolerance on faults, so that it gives wrong outputs. On the contrary, the ANN may cause a phenomenon called overfitting. The overfitting is that the ANN can even recognize the noise during the training procedure. Under this circumstance, the outputs of ANN are ideal when the training samples are applied, while the outputs are not satisfied when the test samples are adopted. At the same time, ANN needs a long time for training and running. In some cases, it may even make it hard to determine the weights [(9)]. There are some theories to determine the optimum number of hidden neuron

depends mostly on experience, one of them are assume that the number of hidden layer neuron should be 2N+1 to obtain reasonable output for any inputs. Here N is the number of input neuron [11].

3.5. ANN Design and Training

A Feed Forward Artificial Neural Network (FFNN) trained by back propagation, is widely used based on the complexity of the problem and the size of the database, the number of hidden layer and the neurons within each hidden layer, can be varied, Fig. (1) shows a three-layer ANN structure with four inputs, one hidden layer with nine neurons, and one output. The input layer that distributes the inputs to the hidden layer does not have any activation function. Mathematically the network computers; see the ANN structure shown in Fig.(1),

1. The output of the hidden layer (treating the bias as another input, but being counted as a real input of our ANN structure).

$$h_1(j) = \text{sum}\,(w_1(i,j) * U(i)\ ,\ i = 1\ ,\ 5)$$

$$H(j) = f(h_1(j))$$

2. For the output layer calculation.

$$h_2(k) = \text{sum}\,(w_2(j,k) * H(j)\ ,\ j = 1\ ,\ 9)$$

$$S(k) = f(h_2(k))$$

where, U(i) is the network input, S(k) is the network output, $w_1(i,j)$ represents the weight connection neuron i in the input later to neuron j in the hidden layer , $w_2(j,k)$ represents the weight connecting neuron j in the hidden layer to neuron k in the output layer , and f(x) is the neuron transfer function, for example a sigmoid $f(x) = 1 / (1 + \exp(-x))$, which is adapted in this research[4,5].

4 - RESULTS AND DISCUSSION

ANN of BPNN learning algorithm was used in the prediction of the conversion of CO_2 in the falling film reactor in terms of mole fraction of carbon dioxide in gaseous mixture (Y), molar concentration of the absorbent (monoethanolamine) (CMEA), volumetric flow rate of liquor MEA (QMEA) and its temperature (T). During the training process, four inputs and one output variables were used. The training data, which were concretely selected, consisted of 190 patterns as shown in Table(1). Sufficient data (26 patterns) were used as test sets as shown in Table(2) which shows that the values of CO_2 conversion predicted by ANN model were found to be very close to the values obtained from experimental study and the error between them were very small about 0.6% .It is essential to have enough data as training and

testing sets to train and evaluated the performance of the network effectively. In the application of the backpropagation algorithm by matlab program [12], a number of different layers and processing elements were tried. It should be noted that the number of hidden layers and number of processing elements in each layer are problem dependent and are empirically selected. The time of convergence depended on the number of PEs in the hidden layer. Moreover, the addition of momentum parameter and noise factor also helped the simulation to converge. It is necessary to vary the parameters used in the neural network such as the learning rate, error tolerance, momentum parameter, and noise factor in order to get the fastest convergence. In this research, the best result was obtained using the following input parameters:

(A) Error tolerance = 0.001

(B) Learning parameter = 0.05

(C) Total number of layers = 3

(D) Total number of processing elements for every layer

(Input hidden output = 4 9 1)

(E) Momentum parameter = 0.0005

(F) Noise factor = 0.0005

4.1- Effect of Liquid Temperature on ANN Model Behavior

Figures (2) and (3) show the effect of liquid temperature on the conversion of carbon dioxide in monoethanolamine solution for different flow rates at constant mole fraction of CO_2 (Y=0.1), (Y=0.075) and constant absorbent concentration (Molarity = 3M). The temperature increase has a positive effect on CO_2 conversion, since increasing temperature will also increase the rate of chemical reaction and decreases the viscosity of the solution, which leads to an increase in absorption rate and consequently CO_2 conversion. These results are in agreement with Abid [13]. Figures (4) and (5) also show the effect of liquor temperature on CO_2 conversion. But for different liquid concentration and at constant mole fraction of carbon dioxide (Y=0.1) and (Y=0.075) and constant liquid flow rate (Q =20 L/hr) .A highest conversion is noticed at a solution of (3M) and 20 L/hr of monoethanolamine. Training data in Fig.s (2 - 5) at monoethanolamine solution flow rates (10, 15, and 20 L/hr) and monoethanolamine concentrations (1, 2, and 3 M) respectively are in solid symbols in three curves. Testing points at the intermediate conditions were on the three curves (same curves with that of the training data). While ANN predictions at additional conditions were made at flow rates 7, 12, and 18 L/hr .It is observed that ANN testing and prediction are almost similar

with that of the experimental results. It can be seen on these figures that the ANN is able to predict accurately the values of CO_2 conversion at other testing conditions (Q=7, 12, and 18 L/hr) and (CMEA=1.5 and 2.5 M).

4.2- Effect of Mole Fraction of CO_2 in Gaseous Mixture on ANN Model Behavior

Experimental and ANN results show a proportional relation between mole fraction of carbon dioxide in gas phase and conversion of carbon dioxide, starting from 0.05 to 0.1, this behavior is shown in Fig.s (6) and (7) and are in agreement with the results of Tontiwachwuthinkul et al [14] and Abid [13] . ANN mode was able to predict the CO_2 conversion at different liquid flow rates (Q=7, 12, and 18 L/hr) which are not found in the experimental data. It is noted that ANN testing (at intermediate conditions) and predication are almost as the same with that of experimental results.

4.3- Effect of Absorbent Concentration on ANN Model Behavior

Figures (8) and (9) show a comparison between the predictions obtained using the ANN model and experimental data for (CO_2 – MEA) system at different MEA solution flow rates at constant mole fraction of CO_2 (Y=0.1) and (Y=0.075) and constant liquid temperature at (T=55°C). The trend shown by the ANN model is in agreement with the recent studies which show that using of highly concentrated amine exhibit a high conversion of CO_2 but stopping at 3M which is more economic since it shows an acceptable conversion [13,15].

5 . CONCLUTIONS

The ANN model developed to apply on the absorption process of CO_2 gas by MEA solution in falling film reactor to predict the CO_2 conversion in a wide range of operating conditions. The values predicted by ANN model were found to be very close to the values obtained from experimental results. The average error as predicted by ANN was 0.6% which are within the acceptable level. It has demonstrated that the optimal model is a network with one hidden layer and nine neurons. Further work (experimental and CFD simulation) is required to provide a more completed database to train the network and validate its usefulness. From the results obtained the ANN models were found to give at least satisfactory, if not excellent predictions.

REFERENCES

1. Bishnoi, S., Ph.D, Thesis ,Texas University at Austin , 2000.
2. Al-Baghli, N.A., Pruess, S.A.,Yesavage, V.F., Selim, M.S., Fluid Phase Equilibria. 185, P.31-43, 2001.

3. Himmeblau, D.M., "Progress analysis of statistical method" Wily, 1984.
4. Ashfaq S., Al-Dahhan M.,Chemical Engineering and Processing , 42, P.599-600, 2003.
5. Ripley, B.D" Pattern Recognition and Neural Network," Cambridge University Press, Cambridge, 1996.
6. Saba A., Ph.D., Thesis "Mathematical Modeling and Experimental Measurements of CO2-MEA System in a falling Film Contactor" , University of Technology, 2006.
٧. الشبكات العصبية، البنية الهندسية، الخوارزميات، التطبيقات " ترجمة م.علام زكي عيسى , ومراجعة د.م.عماد عزوا لمحمد , ٢٠٠٠ .
8. Ben KrÖse , Patrick Van der Smaget "An introduction to neuralNetworks " 8th edition, 1996.
9. You , X .Y and Yang , Z .S., Chen.Biochem.Eng.Q., 17(2),153-158,2003
10. Hornik K ., Stinchcombe M.,White H., Multilayer Feedforward Neural Networks and Universal Approximates, Neural Networks 2,P.359, 1989.
11. Kung, S.H., Hwang, J.N., IEEE , I:363. , (1991)
12. Howard, D., Mark, B." Neural Network Toolbook for use with Matlab" 2001.
13. Abid, M.F. Ph.D. Thesis, University of Technology, 2002.
14. Tontiwachwuthinkul, P., Meisen, A. and C.J.Lim,Chem.Eng.Sci.47, P.381, 1992
15. Weibin, C.,Yujun, W. and Shenlin, Z.,Chemical Eng. Journal, 108,P.161-168, 2005.

NOMENCLUTURE

Symbol	Definition	Unit (SI System)
Y	Mole fraction of CO_2 in gaseous mixture	-
CMEA	Molar concentration of monoethanolamine	$kmol/m^3$
QMEA	Volumetric flow rate of liquor monoethanolamine	L/hr
T	Liquid temperature	°C
SM	Simulation	-

Table (1): Sample training data for prediction of the CO_2 conversion in the falling film reactor before normalized. (Note: only 15 out of 190 patterns are shown)

Input variables					Output variables
No.	Y	CMEA (M)	QMEA (L/hr)	T(°C)	CO_2 Conversion (%)
1	0.05	1	5	30	14.37
2	0.05	1	5	35	15.86
3	0.05	1	5	40	17.06
4	0.05	1	5	45	18.93
10	0.075	2	10	45	26.34
11	0.075	2	10	50	29.74
12	0.075	2	10	55	32.86
13	0.1	3	15	30	53.42
14	0.1	3	15	35	57.42
15	0.1	3	15	40	59.14

Table (2): Sample testing data for prediction of the CO_2 conversion in the falling film reactor after normalized. (Note: only 6 out of 26 patterns are shown)

Input variables					Output variables of ANN model	Experimental data	Correlation
No.	Y	CMEA (M)	QMEA (L/hr)	T (°C)	CO_2 Conversion (%)	CO_2 Conversion (%)	
1	0.075	3	20	30	61.5207	62.35	0.987
2	0.075	3	20	35	65.3862	66.08	0.989
3	0.075	3	20	40	69.7303	70.13	0.994
4	0.1	3	20	45	83.4812	84.35	0.990
5	0.1	3	20	50	86.7331	87.68	0.989
6	0.1	3	20	55	92.6915	92.84	0.998

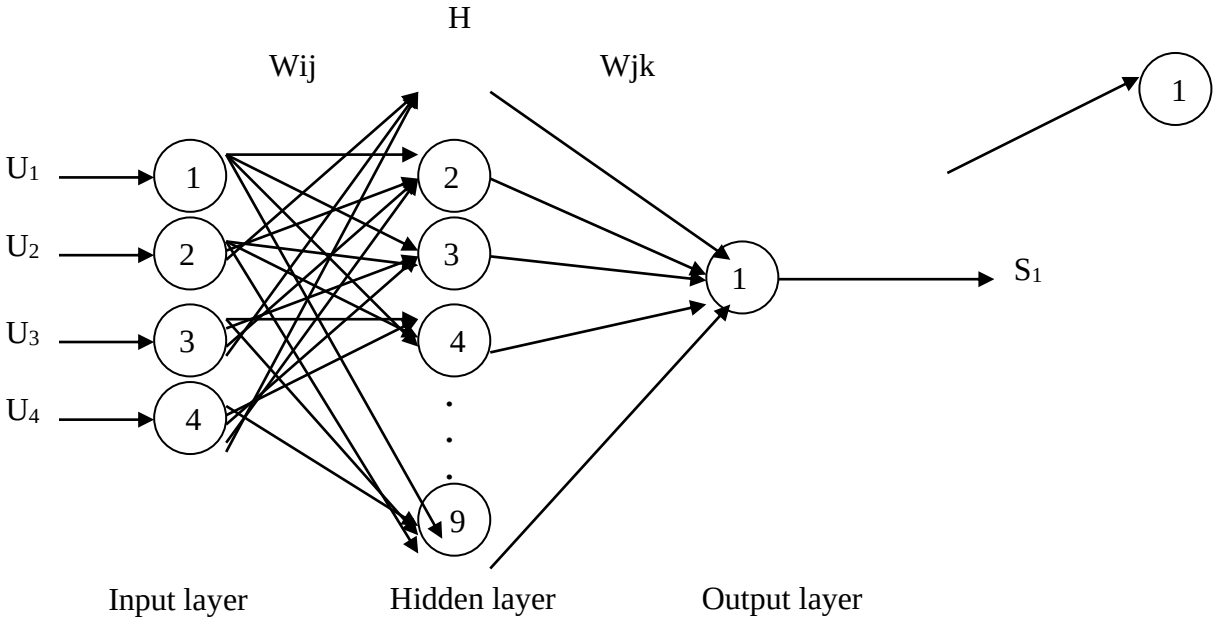

Fig. (1): Architecture of the three – layered feed forward neural network with a single hidden layer.

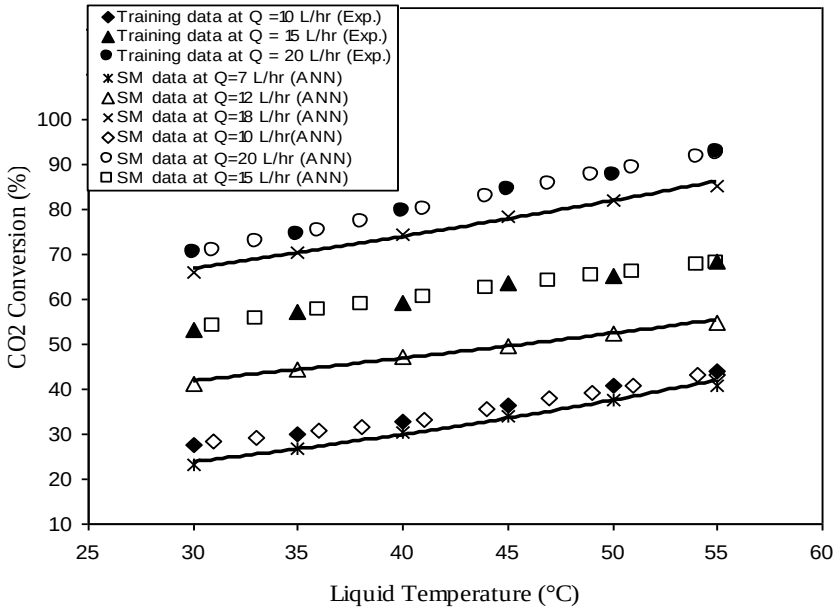

Figure (2): CO2 conversion vs. liquid temperature for different liquid flow rates at constant mole fraction of CO2 (Y=0.1) and absorbent concentration (Molarity=3M)

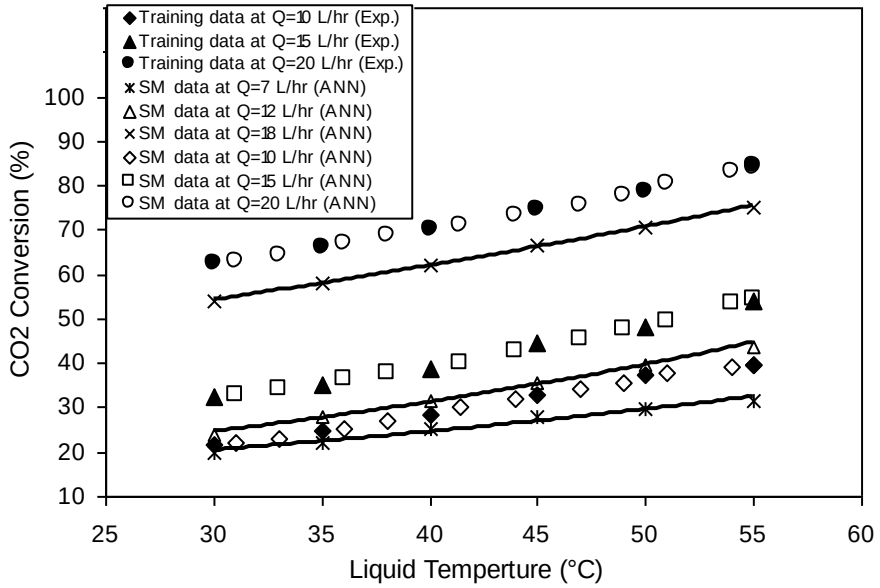

Figure (3): CO2 conversion vs. liquid temperature for different liquid flow rates at constant mole fraction of CO2 (Y=0.075) and absorbent concentration (Molarity=3M)

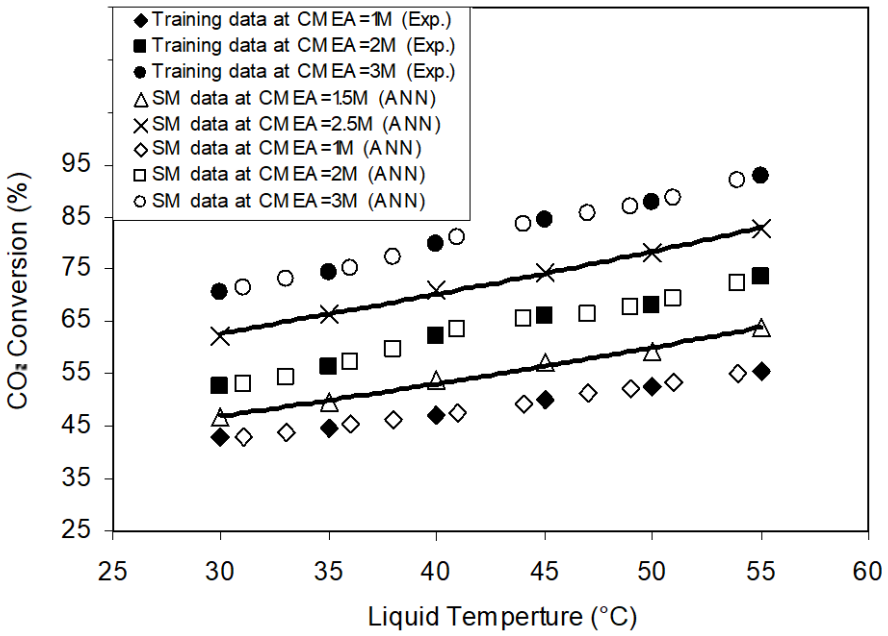

Figure (4): CO_2 conversion vs. liquid temperature for different liquid concentration at constant liquid flow rate (Q=20 L/hr) and CO_2 mole fraction (Y=0.1)

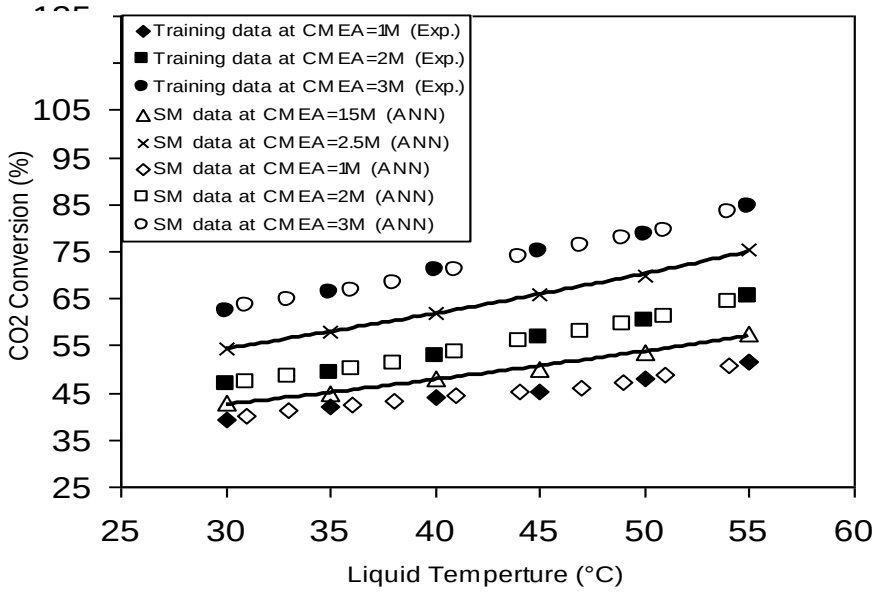

Figure (5): CO2 conversion vs. liquid temperature for different liquid concentration at constant liquid flow rate (Q=20 L/hr) and CO2 mole fraction (Y=0.075)

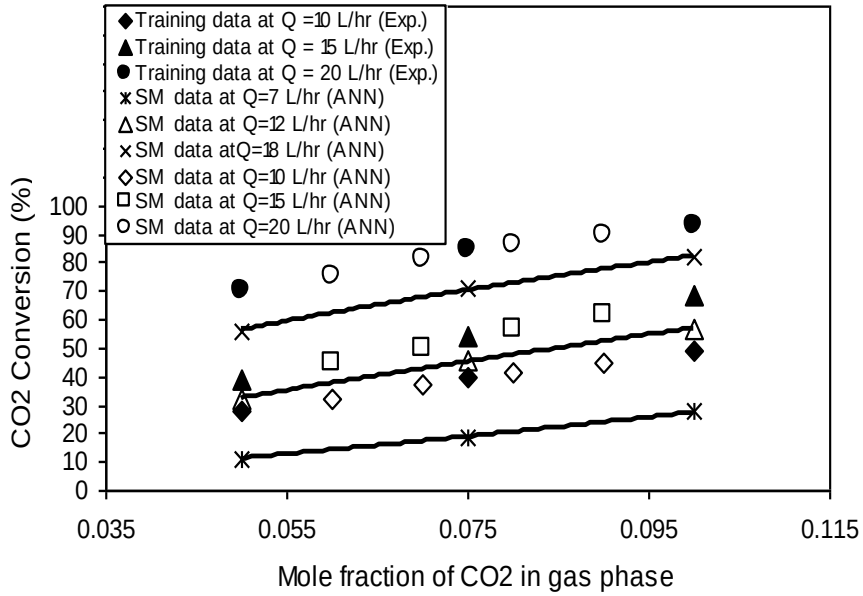

Figure (6): CO2 conversion vs. mole fraction of CO2 in gas phase for different liquid flow rates at constant liquid concentration (3M) and liquid temperature(T=55°C)

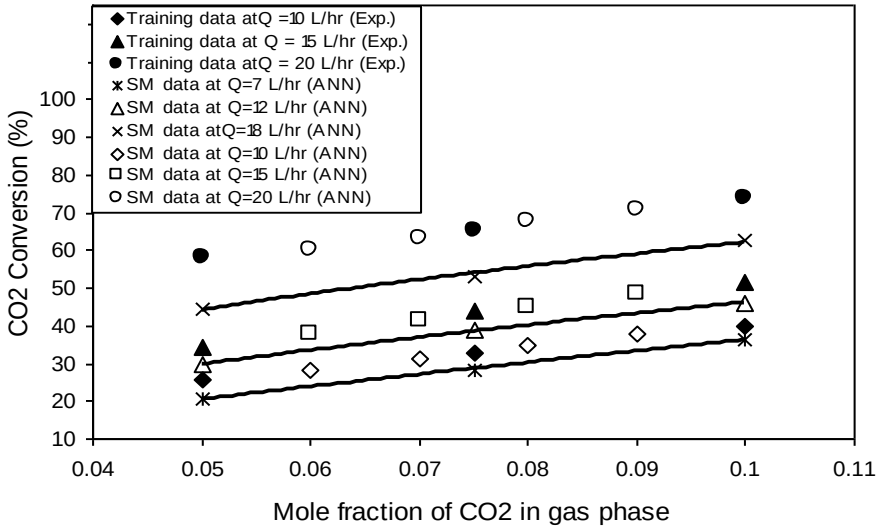

Figure (7): CO2 conversion vs. mole fraction of CO2 in gas phase for different liquid flow rates at constant liquid concentration (2M) and liquid temperature(T=55°C)

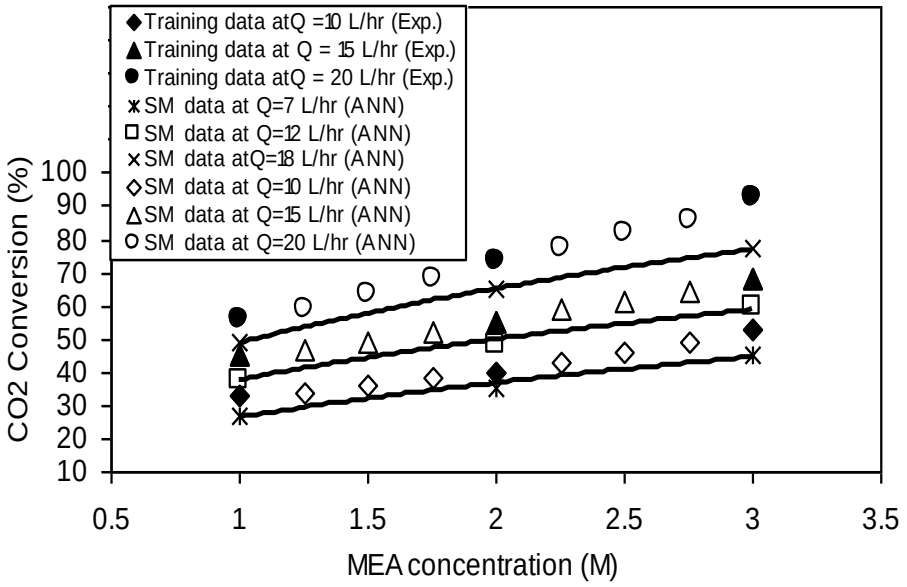

Figure (8): CO2 conversion vs. liquid concentration for different liquid flow rates at constant liquid temperature (T=55°C) and CO2 mole fraction (Y=0.1)

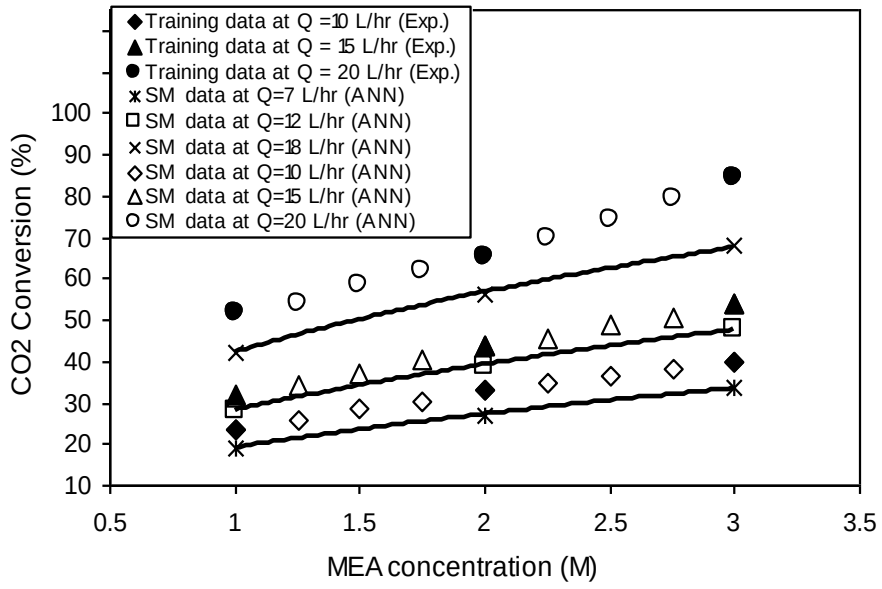

Figure (9): CO2 conversion vs. liquid concentration for different liquid flow rates at constant liquid temperature (T=55°C) and CO2 mole fraction (Y=0.075)

تحديد نسبة تحول غاز CO_2 في مفاعل الطبقة المتساقطة بتطبيق شبكة الذكاء الصناعي

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الخلاصة

يُقدّم هذا البحث موديل مطور لشبكة الذكاء الصناعي لعملية امتصاص غاز ثاني أوكسيد الكاربون باستخدام أحادي أيثانول أمين كمذيب في مفاعل الطبقة الساقطة. بالرغم من أن الدراسات على تطبيقات شبكة الذكاء الصناعي في الهندسة الكيمياوية أكثر تركيزا على استعمال الموديلات المتحركة ، فقد كان هنالك اتجاه متزايد للتطبيق المتنوع لشبكة الذكاء الصناعي لتشكيل الأنظمة المستقرة .شبكة الذكاء الصناعي ذات الانتشار الأمامي تبنَّت وتدربت بخوارزمية الانتشار العكسي . في هذا البحث تم استخدام ٢١٦ من مجموعة البيانات لتدريب واختبار الشبكة وقد بينت هذه الدراسة بأن موديل شبكة الذكاء الصناعي بطبقة مخفية واحدة وتسع خلايا عصبية في تلك الطبقة يعطي تقدير قريب جدا من نسبة تحول غاز ثاني أوكسيد الكاربون وهنالك إمكانية عالية لتطبيق عمليات الامتصاص بموديل شبكة الذكاء الصناعي.

الكلمات الدالة: شبكة الذكاء الصناعي ، خوارزمية الانتشار العكسي ، مفاعل الطبقة الساقطة.