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Estimation of temperature distribution along an annular fixed bed reactor in the oxidative coupling of methane (OCM) process by using artificial neural network

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ABSTRACT

In this research an expert model based on artificial neural network was used to estimate temperature distribution along an annular fixed bed reactor which has been used in the Oxidative Coupling of Methane (OCM) Process. Experiments was done by using the Li/MgO Catalyst with different percentage of Li content in range of 1.6-6.6 %. In order to find the best efficiency estimator of sieve tray, different training schemes for the back-propagation learning algorithm, such as; Scaled Conjugate Gradient (SCG), Levenberg-Marquardt (LM), Gradient Descent with Momentum (GDM), variable learning rate BP(GDA) and Resilient BP(RP) methods were examined. Finally among those trained networks, the LM algorithm with ten neurons in the hidden layer shows the best suitable algorithm with the minimum average absolute relative error 0.005226.

KEYWORDS

Artificial neural network (ANN);
Annular fixed bed reactor;
Oxidative coupling of methane (OCM);
Catalyst;
Natural gas.

INTRODUCTION

Due to importance of natural gas production in the world, the various methods and processes of have been established. So widespread research about the mechanical processes in the natural gas conversion such as Compressed Natural Gas (CNG), Natural Gas Liquefaction (NGL) and conversion to hydrocarbon products i.e. the Oxidative Coupling of Methane (OCM) process have been done. The main product of the OCM process is Ethylene which has a higher added-value compared to the other products with the highest volumetric consumption demand in the market among the other petrochemical products. Ethylene is directly or indirectly feed for most petrochemical units. Ethylene occupies the highest rank among thermoplastic polymers in global production. The OCM process is a new and developed method that directly converts a significant amount of the natural gas to C_2^+. The method uses a specific catalyst in the conversion process[1].

The Methane and oxygen are the main reactants that are fed along with a nitrogen carrier to an annular fixed bed reactor in the OCM process. The furnace temperature is fixed at 775°C to maintain the reaction temperature in the range of 750°C -850°C. This rage of temperature has been obtained using an annular reactor with passing cooled air from the outer and inner layers. ANN as a new method and good predictor

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has been recently applied in many fields especially in chemical engineering processes[2]. ANN is a model that attempts to mimic simple biological learning processes and simulate specific functions of human nervous system[3]. This model creates a connection between input and output variables and keeps the underlying complexity of the process inside the system. The ability to learn the behavior of the data generated by a system is the neural network's versatility and privilege. Fast response, simplicity, and capacity to learn are the advantages of ANN compared to classical methods. In this work, an expert model based on ANN by using some experimental results of OCM process is proposed to predict the temperature along the annular fixed bed reactor.

ARTIFICIAL NEURAL NETWORK

In order to find relationship between the input and output data derived from experimental work, a more powerful method than the traditional methods are necessary. ANN is an efficient algorithm to approximate any function with finite number of discontinuities by learning the relationships between input and output vectors[4]. These algorithms can learn from the experiments, and also are fault tolerant in the sense that they are able to handle noisy and incomplete data. The ANNs are able to deal with non-linear problems, and once trained can perform prediction and generalization rapidly. They have been used to solve complex problems in control, optimization, pattern recognition, and classification[5]. ANNs are biological inspirations based on the various brain functionality characteristics. They are composed of many simple elements called neurons that are interconnected by links and act like axons to determine an empirical relationship between the inputs and outputs of a given system. Multiple layers arrangement of a typical interconnected neural network is shown in Figure 1. It consists of an input layer, an output layer and one hidden layer with different roles. Each connecting line has an associated weight. An ANN is trained by adjusting these input weights (connection weights), so that the calculated outputs may be approximated by the desired values. The output from a given neuron is calculated by applying a transfer function to a weighted summation of its input to a give output, which can serve as input to other neurons, as follows[6]:

$$\alpha_{jk} = F_k\left(\sum_{i=1}^{N_{k-1}} w_{ijk}\alpha_{i(k-1)} + \beta_{jk}\right) \quad (1)$$

Where a_{jk} is neuron j's output from k's layer β_{jk} is the bias weight for neuron j in layer k. The neurons in the hidden layer perform two tasks: summing the weighted inputs connected to them and passing the result through a non linear activation function to the output or adjacent neurons of the corresponding hidden layer.

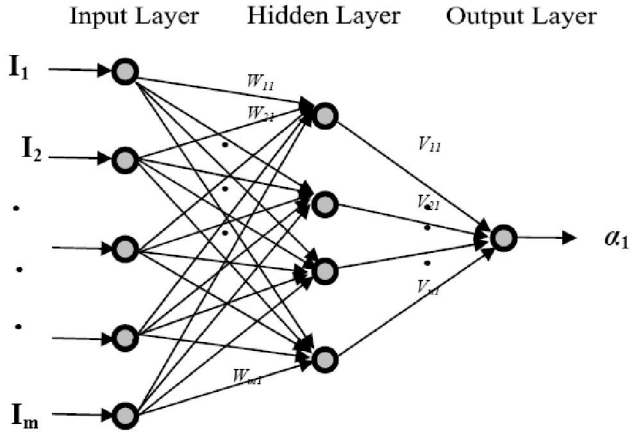

Figure 1 : Schematic of typical multi-layer neural network model

The model fitting parameters w_{ijk} are the connection weights. The nonlinear activation transfer functions F_k may have many different forms[7,8].

The training process requires a proper set of data i.e. input (I_i) and target output (t_i). During training the weights and biases of the network are iteratively adjusted to minimize the network error function[9]. The typical error function that is used is the Average of Absolute Relative Errors (AARE) Eq. 2.

$$AARE = \frac{1}{N}\sum_{i=1}^{N} ABS\left(\frac{t_i - \alpha_i}{t_i}\right) \quad (2)$$

There are many different types of neural networks, differing by their network topology and/or learning algorithm. In this paper the Back Propagation (BP) learning algorithm, which is one of the most commonly used algorithms is applied to predict the sieve tray efficiency. BP is a multilayer feed-forward network with hidden layers between the input and output[3]. The simplest implementation of BP learning is the network weights and biases updates in the direction of the negative gradient that the performance

function decreases most rapidly. An iteration of this algorithm can be written as follows[5]:

$$x_{k+1} = x_k - l_k g_k \quad (3)$$

There are various BP algorithms such as Scaled Conjugate Gradient (SCG), Levenberg-Marquardt (LM), Gradient Descent with Momentum (GDM), variable learning rate BP (GDA) and Resilient BP (RP). LM is the fastest training algorithm for networks of moderate size and it has the memory reduction feature to be used when the training set is large. One of the most important general purpose BP training algorithms is SCG[3,7].

The neural nets learn to recognize the patterns of the data sets during the training process. Neural nets teach themselves the patterns of the data set letting the analyst to perform more interesting flexible work in a changing environment[7]. Although neural network may take some time to learn a sudden drastic change, but it is excellent to adapt constantly changing information. However the programmed systems are constrained by the designed situation and they are not valid otherwise. The neural networks can easily model data even with very complex interactions, which are too difficult to model with traditional methods like nonlinear regressions[10]. Performance of neural networks is at least as good as classical statistical modeling, and even better in most cases[9]. The neural networks built models are more reflective of the data structure and are significantly faster.

EXPERIMENTAL SETUP

The general schematic diagram of the OCM process components are shown in the Figure 2. A minimum of 30 gr of the Li/MgO catalyst was used in each step of the catalyst testing procedure in the reactor. The used catalysts have been fabricated with different Li content of 1.6, 2.5, 3.3 and 6.6 %. The procedure of catalyst fabrication has been mentioned in our previous work[11]. An annular reactor with passing cooled air from the outer and inner layers was used for performing OCM process reactions. Four thermometers were put at inlet, outlet of reactor and height of 5cm and 20 cm along the reactor for temperatures measuring. Experimental data sets were collected for ANN training. TABLE 1 lists the range of experimental data that are used to predict the temperature along the reactor.

TABLE 1 : Minimum and maximum rage of experimental data.

	Minimum	Maximum
Temperature (C)	43.35024	342.3387
%Li content	1.6	6.6
Height (cm)	0	40

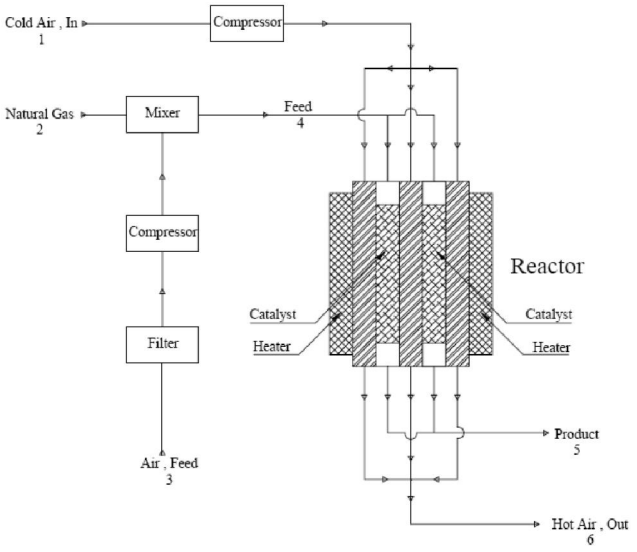

Figure 2 : OCM process catalyst test components

MODEL DEVELOPMENT

The BP method with SCG, LM, RP and GDA learning algorithms has been used in feed forward, single hidden layer network (such as figure 1). Input layer neurons have no transfer functions. Inputs are the Li content percentage and height while output is the temperature. The computer program in MATLAB was developed. Two thirds of data set was used in ANN

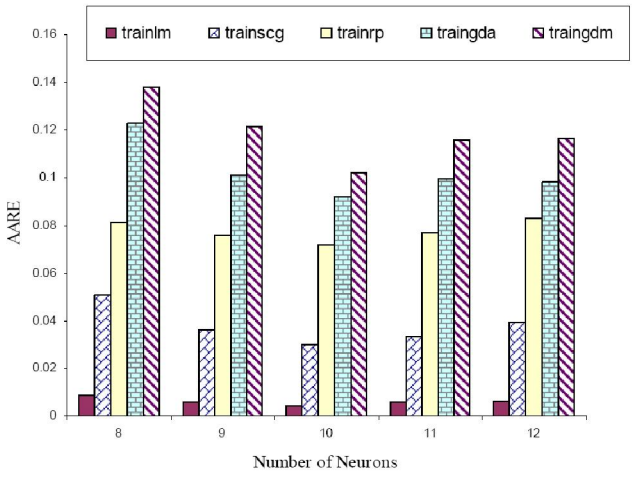

Figure 3 : Determining the optimum number of hidden layer neurons.

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training and the remaining data were employed to evaluate the best obtained network generalization capacity. The number of the hidden layer neurons is systematically varied to obtain a good estimate of the trained data. The selection criterion is the error function. The AAREs of various number of hidden layer neurons are shown in Figure 3. According to the figure the optimum number of hidden layer neurons is ten.

Similarly the AARE of various training algorithms were calculated and listed in TABLE 2 for the obtained ten hidden layer neurons. As TABLE 2 shows the LM algorithm has the minimum AARE.

TABLE 2 : AARE comparison between different algorithms to train ANN

algorithm	AARE of network training
trainlm	0.005226
trainscg	0.030817
trainrp	0.081500
traingda	0.112004
traingdm	0.132157

RESULTS AND DISCUSSION

The results show that the ANN predicts temperature along the reactor very close to the experimentally measurements. Figure 4 shows the scatter diagrams that compare the experimental data versus the computed neural network data. This indicates an excellent agreement between the experimental and the calculated data. Figure 5 illustrates the ANN estimation and experimental data of temperature variations along the annular fixed bed reactor for different Li content. This model can be useful for OCM or other process development and temperature control in such reactors.

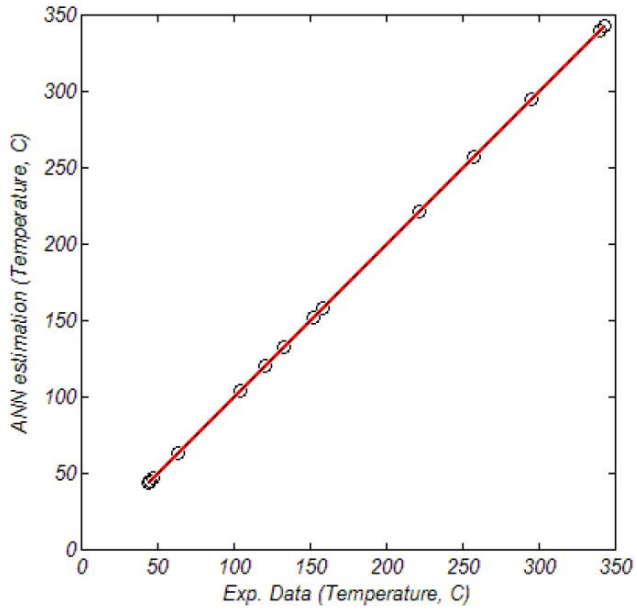

Figure 4 : Evaluation of ANN performance; a scatter plot of typically measured experimental data against the ANN model

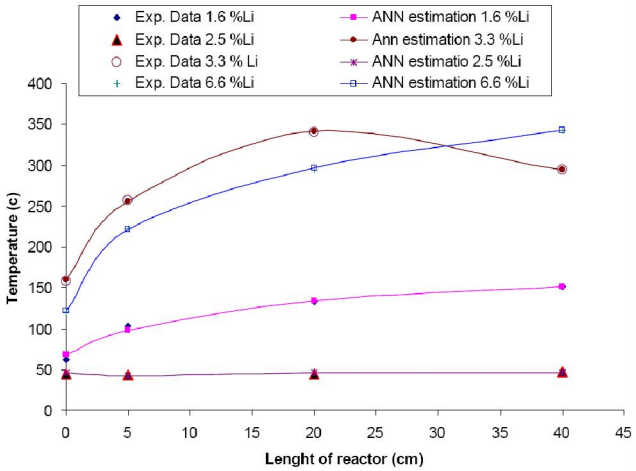

Figure 5 : Temperature distribution along the reactor

CONCLUSION

The ability of ANN to model and predict temperature distribution along an annular fixed bed reactor which is used in OCM process has been investigated in this work.

The results show a good agreement between experimental data and those predicted by ANN. An important feature of the model is that it doesn't require any theoretical knowledge or human experience during the training process. It has been clearly shown that of the ANN calculates the temperature distribution based on the experimental data only, instead of using empirical models. Therefore it is not necessary to use approximate and complex analytical equations to calculate temperature.

REFERENCES

[1] Shenyfu Ji, Tianeun Kiao, Shube Li, Lingjum Chou, Bing Zhang, Chuan Zhi Xu, Ruiling Heu, Andrew, Andrew P.E.York, Malcolm L.H.Green; Journal of Catalysts, **220**, 47-56 **(2003)**.

[2] R.B.Bozorgmehry, F.Abdolahi, M.A.Moosavian; Fluid Phase Equilibr., **231**, 188 **(2005)**.

[3] A.R.Moghadassi, F.Parvizian, S.M.Hosseini, A.R.Fazlali; Brazilian Journal of Chemical Engineering, **26**, 199-206 **(2009)**.
[4] M.T.Hagan, H.B.Demuth, M.Beal; Neural Network Design, PWS Publishing Company, Boston, **(1996)**.
[5] A.R.Moghadassi, F.Parvizian, S.M.Hosseini, Amir Sharifi; Journal of Engineering and Applied Sciences, **3**, 18-27 **(2008)**.
[6] A.R.Moghadassi, F.Parvizian, S.M.Hosseini; Australian Journal of Basic and Applied Sciences, **3(3)**, 1851-1862 **(2009)**.
[7] R.I.W.Lang; A Future for Dynamic Neural Networks, Dept. Cybernetics, University of Reading, UK, **(2000)**.
[8] A.B.Bulsari; Neural Networks for Chemical Engineers, Amsterdam, Elsevier Science Press, **(1995)**.
[9] H.Demuth, M.Beale; Neural Network Toolbox User's Guide, **(2002)**.
[10] M.R.Nikkholgh, A.R.Moghadassi, F.Parvizian, S.M.Hosseini; The Canadian Journal of Chemical Engineering, **88**, 200-207 **(2010)**.
[11] M.Torangi, A.Vatani, M.Yousefi, A.R.Abbasnejad; Journal of Applied Sciences Research, **72**, 2085-2088, December **(2010)**.