Establishment of a neural network model for ethylene production from naphtha feedstock

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Abstract

In this paper, the steam cracking process with naphtha feedstock is modeled by a multilayer, feed forward, fully connected neural network. Feed and steam residence times and coil outlet temperature were the input variables to the network. These input variables will help to generalize the model. The output variables of the network were hydrogen, methane, acetylene, ethylene and ethane yields. The cracked gas compositions were the output variables of the network. The optimum topology of network was a three layers network with fifteen neurons in hidden layer. The network outputs were in agreement with the experimental values.

Keywords: modelling, artificial neural network, thermal cracking, naphtha

1. Introduction

Thermal cracking or steam pyrolysis of hydrocarbons could convert them into valuable raw materials, which can be used in the petrochemical industry for polymer production. The reaction mechanisms of naphtha cracking are generally accepted as free-radical chain reactions. Unfortunately, the absence of a simple predictive applied model of pyrolysis is an obstacle to the development of practical methods of conversion.

Neural networks have been used as a promising opportunity, when complex reaction systems can not be well identified, or in the case of lack of basic knowledge of reaction mechanisms. It has been claimed that Artificial Neural Networks (ANN) are 120-5000 times faster than phenomenological models [1], and can therefore lead to significant reductions in computation times. Various aspects of kinetic modelling of chemical reactors with multilayer feed forward networks have been studied [2-6]. Most published works on ethylene synthesis and kinetics are based on mechanistic models. No attempts have been made to incorporate the use of neural networks in modelling such process.

In this paper, the steam cracking process with naphtha feedstock is modelled by a multi-layer feed-forward (MLP) neural network. The reactor effluent qualities, mainly the yields of light olefins are the outputs of the neural network. Coil outlet temperature, steam to hydrocarbon ratio and feed flow rate. A rigorous mathematical model is used to generate the training data. All ANN calculations were carried out using MATLAB7 mathematical software with ANN toolbox for windows.

2. Artificial Neural Networks

The feed forward neural networks, based on application of artificial neurons with a sigmoid activation function, are usually employed for modeling and prediction [7-10]. A schematic diagram of a multi-layer feed forward neural network, composed of neurons arranged in layers, is shown in Figure 1. A model equation for a single neuron can be written as follows:

$$y = \sigma\left(\sum_{j=1}^{N} W_j x_j + b\right) = \sigma\left(\sum_{j=0}^{N} W_j x_j\right) \tag{1}$$

where each input signal, x_j, is multi-plied by an appropriate weight, W_j, and the weighted sum is compared to the threshold value b. If this threshold value is treated as the weight, $b = W_0$, which is appropriate for the input signal $x_0 \equiv 1$, then the notation of the model equation can be simplified as it is shown in Equation (1). The so-called activity function is usually defined as the uni-polar sigmoid function:

$$\sigma(Z) = \frac{1}{1+e^{-z}} \tag{2}$$

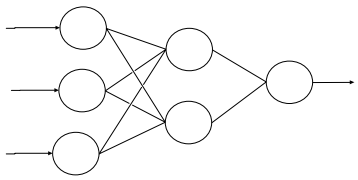

Fig. 1. Schematic of a multi-layer feed forward neural network model

Taking into account the model equation of a single neuron (Eq. (2)) as well as the schematic diagram of the feed forward neural network (Fig. 1), which explains transmission of signals thorough this net, the model equation for a whole network can be written as follows:

$$v_k = \sigma\left(\sum_{i=0}^{K} W_{ki}^{(o)} \sigma\left(\sum_{j=0}^{N} W_{ij}^{(h)} x_j\right)\right) \tag{3}$$

Eq. (3) has been formulated for the simplest feed forward net consisting of one hidden layer. The feed forward neural nets are universal approximators – cf. [11]. A solution

to the approximation problem is a set of optimal network weights. This set is determined during a learning procedure performed as follows: for each set of the input signals, X = (x1, x2, ..., xN), the output signals predicted with the ANN, Y = (y1, y2, ..., yM), are compared to the experimental learning data set, D = (d1, d2, ..., dM). The unknown network parameters are adjusted in order to minimize the sum of squared residuals defined as follows:

$$E(W) = \frac{1}{2}\sum_{j=1}^{P}\sum_{k=1}^{M}\left(y_k^{(j)} - d_k^{(j)}\right)^2 \tag{4}$$

where k=1, 2, ..., M is the current number of the output neuron, j=1, 2, ..., P is the current number of the learning data set. Plenty of learning algorithms are commonly employed to determine the optimal set of weights. In calculations performed for the purposes of this paper the Levenberg-Marquardt learning method has been used.

3. Results and Discussion

The topology of an artificial neural network (ANN) is determined by the number of layers in the ANN, the number of neurons in each layer and the transfer functions. Optimization of ANN topology is probably the most important step in the model development. According to Cybenko [12], a network that has only one hidden layer is able to approximate almost any type of nonlinear mapping. However, determination of the appropriate number of nodes for the hidden layer is difficult, and is often done by trial and error. Too few neurons in the hidden layer impair the network and prevent the network to get trained correctly. On the other hand, too many nodes allow the network to memorize the pattern (i.e., develop a correlation) presented without capturing the underlying relationship between input and output variables.

The most suitable neural network topology turned out to be a multi-layer perceptron with three nodes in the input layer (reaction conditions), fifteen nodes in the hidden layer (with sigmoid activation functions) and five nodes in the output layer (reaction results). The input variables are chosen in a way to help generalize the neural network model, so that it can be used for a similar reactor of different geometry.

Since the used transfer function in the hidden layer was sigmoid, all output data were scaled into the proper range. Figure 2 shows the optimized ANN structure. Training of the ANN was performed with data produced by numerical simulation of a detailed first principles model of the reactor [13]. Figures 3-7 show the comparison of the experimental and calculated values for different neural network outputs, trained with an incremental number of samples and backpropagation algorithm.

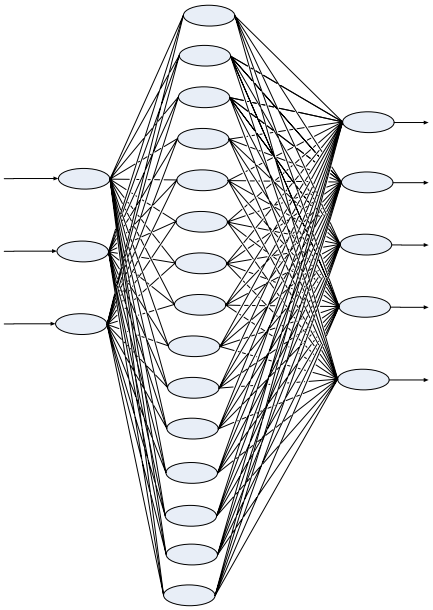

Fig.2. Optimum structure of ANN model for the reactor

The root mean squared error (RMS) is utilized as a measure to estimate the accuracy of the calculations:

$$RMS = \sqrt{\frac{\sum_{i=1}^{m}\left(Y_{PE,i} - Y_{EX,i}\right)^2}{m}} \tag{5}$$

Where YPE and YEX are the predicted value by ANN and experimental value respectively, for the object i, and m is the number of objects [14]. By calculation of RMS and as it is shown in the figures below, the difference between the experimental and calculated data is in the acceptable range.

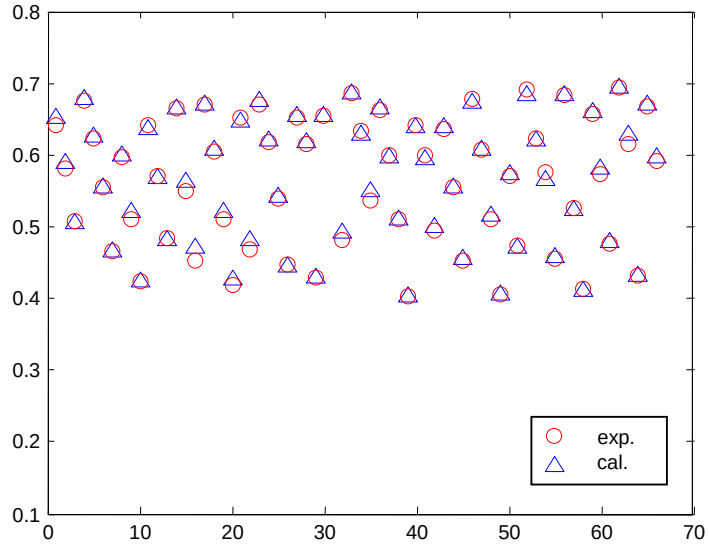

Fig.3: comparison of experimental and predicted values for H2 yield

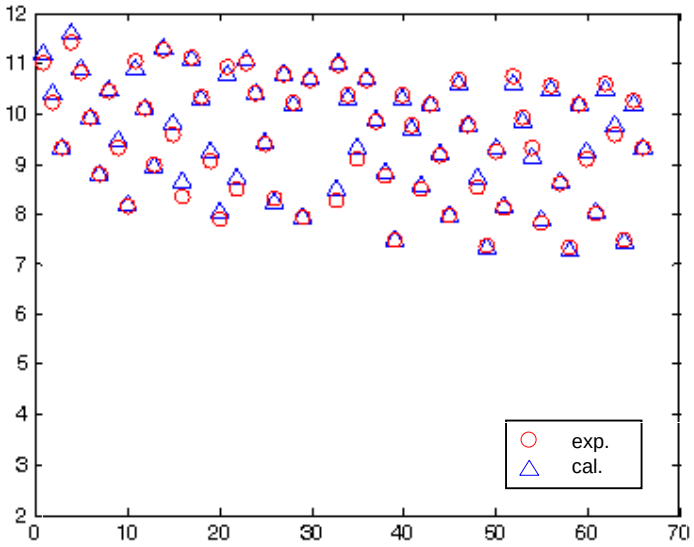

Fig.4: comparison of experimental and predicted values for CH4 yield

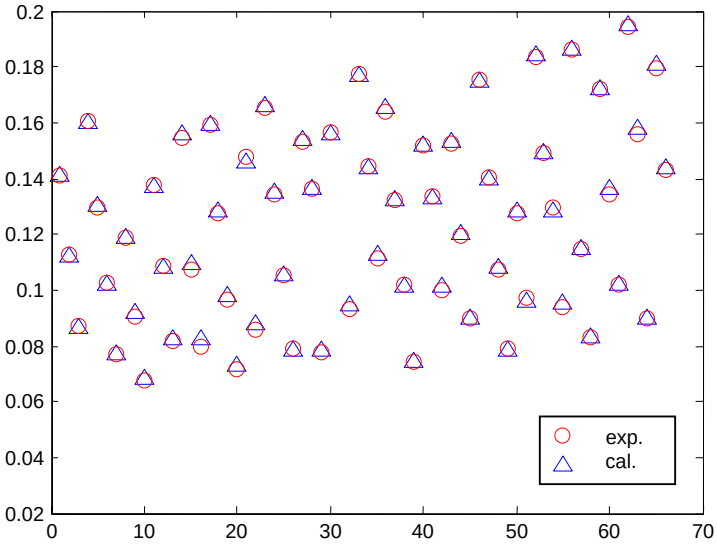

Fig.5: comparison of experimental and predicted values for C2H2 yield

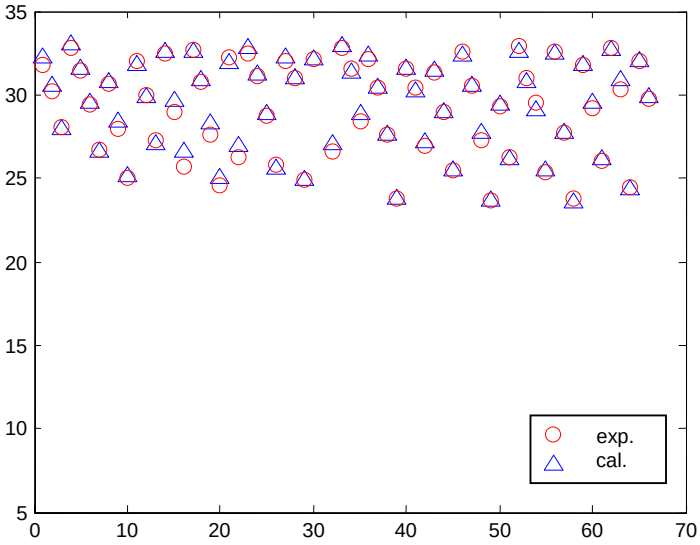

Fig.6: comparison of experimental and predicted values for C2H4 yield

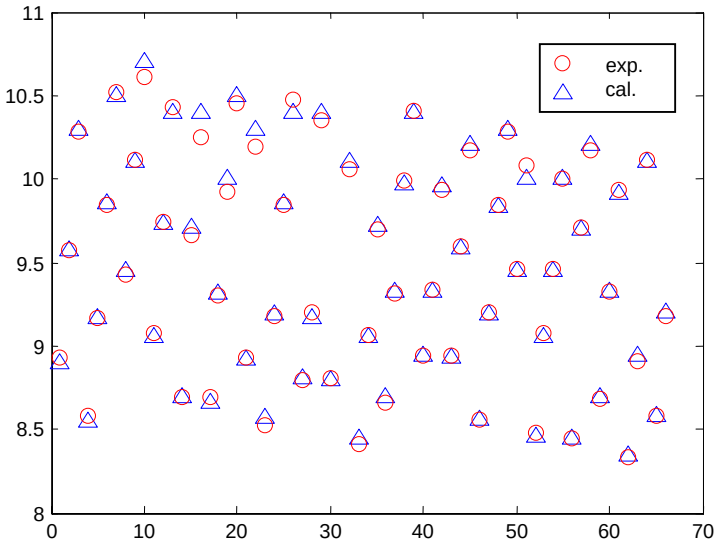

Fig.7: comparison of experimental and predicted values for C2H6 yield

4. Conclusions

An artificial neural network trained by Levenberg-Marquardt training algorithm has been implemented to model the steam cracking reaction of naphtha feedstock. The optimum structure of ANN was determined by trial and error. It was found that the structure of ANN with fifteen neurons in the hidden layer had the best performance. The best epoch of the ANN was 346 and the RMS of test was around 10^{-3} .The predicted output of the ANN approximately agreed with the experimental values.

5. References

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