PREDICTION OF HYDRATE FORMATION TEMPERATURE FOR NATURAL GAS USING ARTIFICIAL NEURAL NETWORK

Amir Heydari[1], Keivan Shayesteh[1,2], Ladan Kamalzadeh[1]

1.Department of Chemical Engineering , Mohaghegh-e-Ardebily University , Ardebil, I.R.Iran tel+989143512924 ,e-mail: Heydari.amir@gmail.com , www.uma.ac.ir
2.Ardebil Gas Company,Baseej SQ,Ardebil,I.R.Iran , tel+984517719828, www.gas-ar.ir

Abstract

A great number of petroleum engineering calculations require knowledge of natural gas hydrate formation conditions. Ideally, natural gas hydrate formation conditions are determined experimentally in the laboratory, but these data are not always available. Correlations are consequently used to determine values for natural gas hydrate formation conditions. In this paper, an alternate tool, i.e. the artificial neural network (ANN) technique has been applied for estimation of temperature for gas hydrate formation.

ANN was applied to the 167 raw data in the range of 32-74 $^{\circ}F$, 50-4200 psia and 0.554-1 for temperature, pressure and specific gravity, respectively. To check the ANN model, the samples were divided into two groups. One of them contained 149 samples and was used to train the network and the remaining 18 samples were used as the test sets. For the training of the different networks, the standard feed forward back propagation algorithm was used and several types of structures were tested to obtain the most suitable network for the prediction of solubility. To check the reproducibility of the results, each of the networks studied was trained three times. Finally the best ANN structure was determined as 7-5-1.

In comparison of performance analysis of ANN, the relative error (RE) was studied and maximum error found 3.035 percent and R^2 value was equal to 0.9941. To ensure, the results of ANN was compared with the results of Sloan model. To sum up ANN shows the better results in comparison with it. So it can be concluded that ANN provides a good method in predicting temperature at witch hydrates formation occurs.

Keywords: Artificial neural network, hydrate, natural gas

1. Introduction

Gas hydrate are ice-like crystalline compounds, inclusions with get their stability through occupation of suitable size gas components (guest molecules) into cavities form by water molecules (host molecules) [1]. Hydrates were discovered in 1810 by Sir Humphry Davy. During the first 100 years after the discovery of gas hydrates, the interest in these compounds was academic. It was concerned with the identification of (a) the species that can form hydrates and (b) the pressure and temperature conditions at which the formation occurs. Today, naturally occurring clathrate hydrates in the earth, containing mostly methane, are regarded as a future energy resource [2]. Clathrate components from mainly two structures, structure I and II, although structure H has also been known [1]. Most studies of gas hydrates have concentrated upon measuring the three-phase dissociation pressure. However, few data are available for *H–L*W phase equilibria [3]. The use of hydrates as a means of storing natural gases and desalination of seawater has been suggested [1]. In 1934, it was recognized that the plugging of natural gas pipelines was due to formation of clothrate hydrates of natural gas (Hammerschmidt). Typical operating problems include the fouling of heat exchangers and other vessels, erosion of expanders, in addition to plug gage of transmission lines with the solid hydrate [1]. The best method for determining conditions of hydrate formation is to experimentally measure the formation at the temperature, pressure and composition of interest. Because it is impossible to satisfy the infinite number of conditions for which measurements are needed, hydrate formation prediction methods are needed to interpolate between measurements. However, such experimental endeavors are both time consuming and expensive relative to industrial needs for a number of hydrate formation conditions. Therefore some means of interpolation between the experimental results are needed, and ideally one would be able to extrapolate beyond the condition of the data. The petroleum industry spends millions US dollars to combat the formation of hydrates. So, the accuracy of estimating the natural gas hydrates is extremely important for optimizing the cost of piping systems and processing units. Understanding how, when, and where gas hydrate form provides the engineer the method to predict the occurrences of hydrates. Therefore, an accurate and simplified model for predicting the calculations of natural gas hydrate is desirable [4]. Parrish and Prausnitz developed an algorithm based on statistic model of van der Waals and Platteeuw that can predict the incipient of

hydrate formation for pure water. Later this model was improved by Ng and Robinson and Holder et al [1]. The gas gravity method is very simple for predicting the gas hydrate conditions. The gas gravity method was conceived by Katz of the GPSA Data Book. Also, the gas gravity method has served the gas processing industry well, as an initial estimate for a long period of time. Based on the GPSA data book, hydrate equations were developed for gases where specific gravity was known. The available correlations for a specific gravity method to calculate the hydrate formation conditions are Sloan, Berge, Motiee, and Hammerschmidt correlations [4]. The use of artificial neural networks (ANNs) in chemical and pharmaceutical areas has been increased recently. The wide applicability of ANNs stems from their flexibility and ability to model linear and non-linear systems without prior knowledge of an empirical model. This gives ANNs an advantage over traditional fitting methods for some chemical applications [5]. ANN eliminates the limitations of the classical approaches by extracting the desired information using the input data. Applying ANN to a system needs sufficient input and output data instead of a mathematical equation. ANN can be trained using input and output data to adapt to the system. Also, ANN can be used to deal with the problems with incomplete and imprecise input data [6].

In this work, an artificial neural network (ANN) is used for prediction of the temperatures at witch the hydrates formation occurs. The results of this study include the calculation of relative error and R^2 values between the experimental data and ANN predictions. Finally the results compared with Sloan model for prediction of temperature for hydrates formation.

3. Artificial neural networks theory

In the last decade, ANN has been widely used for many different industrial areas such as control, prediction, pattern recognition, classification, speech and vision. ANN has been trained to solve nonlinear and complex problems that are not exactly modeled mathematically [6]. The ANNs are able to acquire information and provide models even when the information and data are complex, noise contaminated, non-linear or incomplete. The goal of ANN is to map a set of input patterns onto a corresponding set of output patterns. The network accomplishes this mapping by learning from a series of past examples and defining the input and output sets for a given system. The network then

applies what it has been learned to a new input pattern to predict the appropriate output [7]. Artificial neural networks consist of large numbers of computational units connected in a massively parallel structure. The processing units (neurons) from each layer “n” are linked to all of the other processing units appearing in layer “n+1” by weighted connections. Collectively, these connections (as well as the transfer functions of the processing units) form more or less good distributed representations of relationships between input and output data. ANN has so far mainly been used in process modeling, process control, fault diagnosis, error detection, data reconciliation and process analysis [8]. ANN was first introduced as a mathematical aid by McCulloch and Pitts (1943). More ANNs history and a comprehensive review for their industrial applications can be found in the papers by Patterson (1996) and Meireles et al. (2003), respectively [9]. Many different types of ANNs have been developed. The multilayer feed-forward network with back propagation (BP) learning method is the most popular network chemical applications and is used in this work [10]. The back-propagation neural network (BPN) developed by Rumelhart et al. (1986) is the most representative learning model for the ANN [9]. Neural networks do not need an explicit formulation of the mathematical or physical relationships of the handled problem. The input layer of the network (see Fig. 1) does not perform any processing, but acts as a means to introduce scaled data to the network. The data from the input neurons are propagated through the network via the interconnections [8]. In a configuration of a neural network model one of the most important factors is to determine the number of hidden layers to be used and the number of neurons in the hidden layer. Although Hecht-Nielsen (1987) suggested that an upper limit for the number of hidden layer neurons should be smaller than $2N_1+1$, where N_1 is the number of input neurons, in order to insure that ANNs are able to approximate any continuous function [9]. Every neuron in a layer is connected to every neuron in adjacent layers. A scalar weight is associated to each connection. The neurons within the hidden layer perform two tasks: they sum the weighted inputs connected to them and then pass the resulting summations through a non-linear activation function to the output neuron or adjacent neurons of the corresponding hidden layer (in case of more than one hidden neuron layer). In this work, the sigmoid function: $f(x) = 1/(1+e^{(-x)})$ is used in the interval (0, +1). A bias term is associated with each interconnection in order to introduce

a supplementary degree of freedom. The expression of the weighted sum to the kth neurone in the jth layer (j ≥ 2) is given by

$$S_{j,k} = \sum_{i=1}^{N_{j-1}} (w_{j-1,i,k} I_{j-1,i}) + b_{j,k}$$

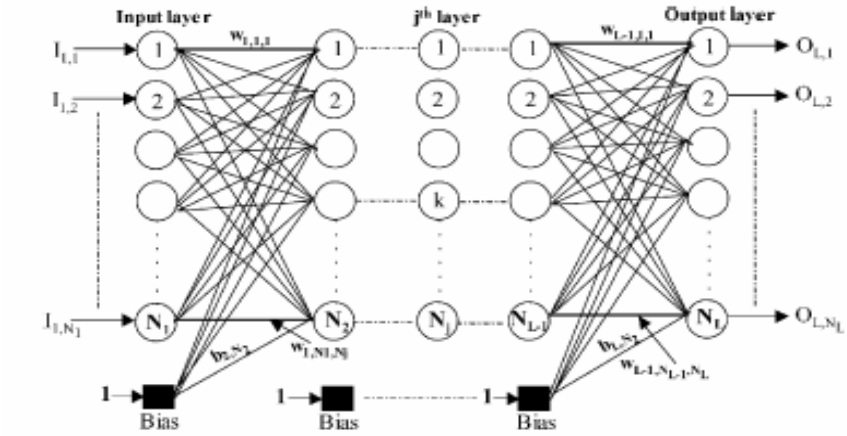


Fig 1. Feed-forward artificial neural network architecture

Where $I_{J-1,i}$ is the information from the ith neuron in the (j-1)th layer, $b_{j,k}$ the bias term andN_{j-1} is the number of neurons in the layer j-1. The output of the kth neuron in the layer j (j ≥ 2) is

$$O_{j,k} = \frac{1}{1+\exp(-S_{j,k})}$$

An important aspect of a neural network is the learning step, based on a set of measured numerical values (the learning database). Representative examples are presented to the network so that it can integrate this knowledge within its structure. The accuracy of model representation depends directly on the topology of the neural network. Numerous papers have shown that a feed-forward network is potentially able to approximate any non-linear function. The learning process consists of identifying the weights $W_{i,j,k}$ and $b_{j,k}$ that produce the best fit of the output data over the entire training data set. At the beginning of the learning step, random values are chosen to initialize weight data. During the learning step, the weights of the network are continuously adjusted, based on the error signal generated by the deviation between the output data computed through the network (O_L) and the data from the database used in the training

examples (target vector T_v). This is accomplished by means of learning algorithms (Matlab toolbox) designed to minimize the least square total output error given by the objective function

$$F = \frac{1}{2}\sum_{i=1}^{N_d}\sum_{s=1}^{N_L}(T_{V,s}(i) - O_{l,s}(i))^2$$

N_d is the number of examples in the data set, N_L corresponds to the number of outputs of the neural network, $T_{v,s}$ represents the target value or responding to the sth neuron of the output layer and $O_{L,s}$ the calculated value corresponding to the sth neuron of the output layer. The deviations between network outputs and targets are summed over the entire data set and updating of the weights is performed after every presentation of the complete data set [8].

Because network models are not based on physical theory and contain nonlinearities, the predictions are suspect when extrapolating beyond the range of the original training data. Furthermore, due to non-uniform distribution of the training examples and noise over the domain, the network may have local areas of poor fit even when not extrapolating [11].

3. Design of artificial neural network model

The most common type of hydrate data taken are the formation temperature, pressure and specific gravity. This type of data is most important to natural gas applications [4].In this research 149 data gathered carefully as far as possible from gas gravity diagram(D. L. Katz, R. L. Lee, Natural Gas Engineering Producing and Storage)[12]. Also 18 experimental data supplied for testing the artificial neural network [4].

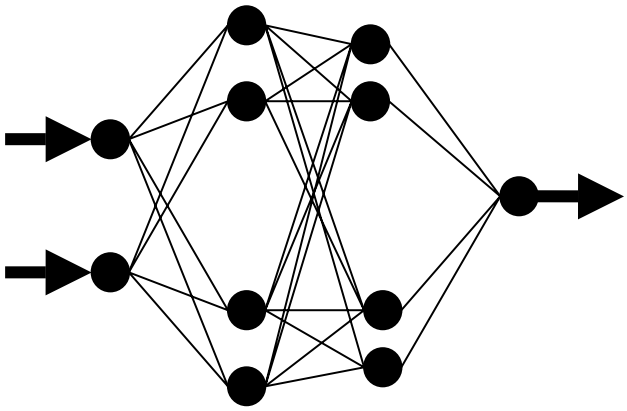
All of these point are consist of temperature, pressure and specific gravity of hydrate formation conditions of natural gas.

The ANN used here is a four-layer feed-forward network (see fig. 2) with BP learning as its teaching algorithm. Training the neural network was performed with 149 data.18 data were used for testing the neural network. two hidden layers consist of 7, 5 neurons in each layer respectively, an input layer consists of two neurons (pressure and

specific gravity) and an output layer consists of one neuron (temperature), was designed for prediction of hydrate formation in natural gas. It is understood generally that an improper set-up for the hidden neurons may be difficult for the ANN to converge to the best state in application [13]. There are no rigorously heretical principles for choosing the proper network topology, so different structures were tested in order to obtain the optimal hidden neurons and training cycles. Log-sigmoid is the transfer function that used here. One of the reasons for using these transformation functions is the ease of evaluating the derivatives that is required for minimization of the error function [14]. By this function, output values have the range from 0 to 1 and therefore output data have been normalized in the range of [0, 1] by following equation:

$$T_{new} = \frac{T_{old} - T_{\min}}{T_{\max} - T_{\min}}$$

Trainrp that is used in this study is a network training function that updates weight and bias values according to Resilient back-propagation (RPROP). All the ANNs calculations were carried out using Matlab mathematical software with artificial neural network toolbox.



Inputs (P, SpGr) **7** **5** **output (T)**

Fig. 2. Topology of the used neural network model

4. Results and discussion

As well as known, analysts can evaluate whether an analytical result is satisfactory by comparing the tested result (y_i) with the ideal one (f (x_i)), an analytical calculation can be drawn according to the value of RE

$$RE = \frac{y_i - f(x_i)}{y_i}$$

In this work, the statistical error analyses were used to check the performance, as well as the accuracy, of the hydrate formation correlations. Fig. 3 shows the relative error percent between experimental values and calculated solubility by ANN.

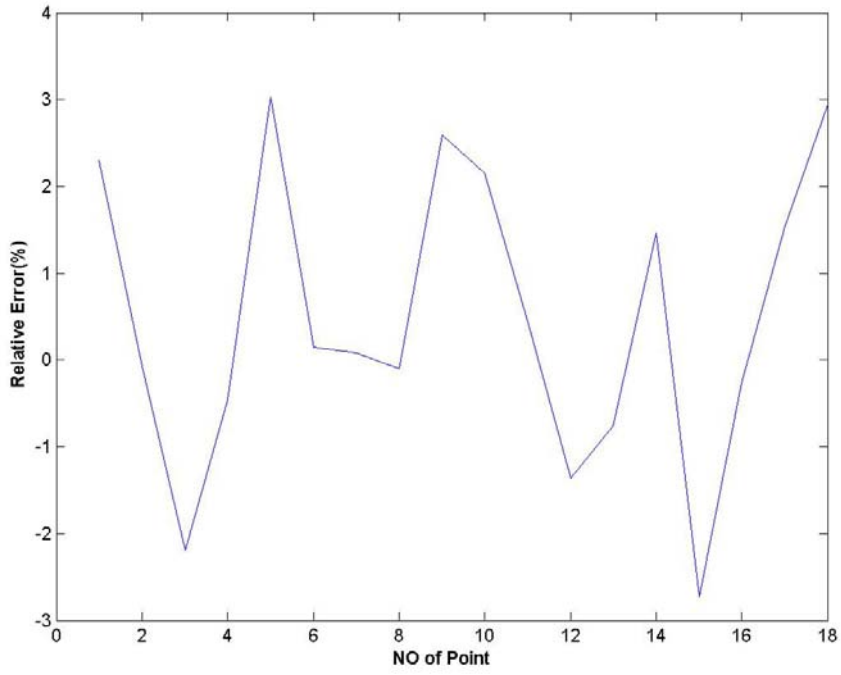


Fig. 3. Plot of relative error vs. training and experimental hydrate formation temperature.

The R^2 value for both the training and experimental data sets for the gas hydrate formation is 0.9941 that shows the model has captured the features accurately. Also the results of experimental study are compared with the results of Sloan model. In this case R^2 value is obtained 0.9263 that say ANN shows more successful results as compared with it. Figs. 5, 6 show a plot between experimental and computed data by ANN and computed data by Sloan model for the formation of gas hydrate.

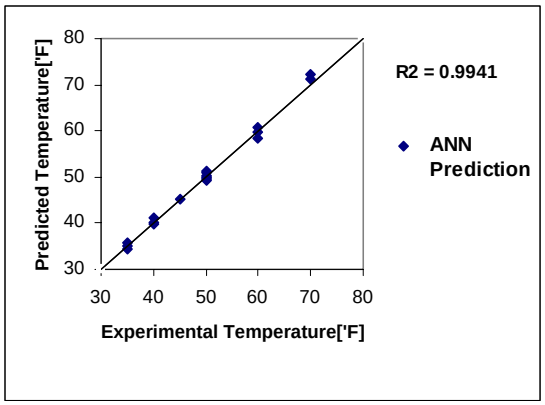


Fig. 5. Comparison of experimental data and estimated hydrate formation by ANN

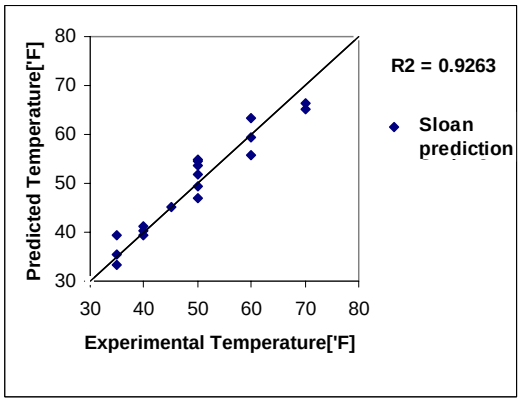


Fig. 6. Comparison of experimental data and estimated hydrate formation by Sloan model

These results prove that the proposed ANN can be used successfully for the prediction of hydrate formation in natural gas.

5. Conclusions

In this work, artificial neural network model have been developed for the prediction of hydrate formation in natural gas, in the pressure range, 50–4200 psia, the temperature range of 32-74 $^{\circ}F$ and the specific gravity range, 0.554–1. The weights have been optimized so as to minimize the error between the estimated and experimental hydrate formation temperature. Once the ANN model is trained estimation of hydrate formation is a one step process. This considerably saves computational time. Hence, it may be highly suitable to use in place of conventional methods for real time process control. However, the major disadvantage of this technique is that it can be used only in the range in which it has been trained, as it is empirical in nature. The model is as good as the quality of data used for the training of the model. As no model is the best model, the model can be improved if more data are available in a wider range of temperature and pressure.

References

1. Kh.Nasrifar, M.Moshfeghian, R.N.Maddox, prediction of equilibrium conditions for gas hydrate formation in the mixtures of both electrolytes and alcohol, Fluid Phase Equilibria 146 (1998) 1-13

2. Peter Englezos, REVIEWS Clathrate Hydrates, Ind. Eng. Chem. Res. 1993, 32, 1251-1274

3. S.O. Yang, S.H. Cho, H. Leeb, C.S. Le, Measurement and prediction of phase equilibria for water + methane in hydrate forming conditions, Fluid Phase Equilibria 185 (2001) 53–63

4. Khaled Ahmed Abdel Fattah, Evaluation Of Empirical Correlations For Natural Gas Hydrate Predictions, Oil and Gas Business Journal, 2004 , http://www.ogbus.ru/eng/authors/Fatahh/Fatahh_1.pdf

5. Abolghasem Jouybana,., Mir-Reza Majidib, Farnaz Jabbaribarc, Karim Asadpour-Zeynalib, Solubility prediction of anthracene in binary and ternary solvents by artificial neural networks (ANNs), Fluid Phase Equilibria 225 (2004) 133–139

6. M. Ali Akcayol, Can Cinar, Artificial neural network based modeling of heated catalytic converter performance, Applied Thermal Engineering 25 (2005) 2341-2350.

7. J. Zupan, J. Gasteiger, Neural Networks in Chemistry and Drug Design, 2nd ed., Wiley/VCH, New York, 1999.

8. A. Chouai , S. Laugier , D. Richon , Modeling of thermodynamic properties using neural networks Application to refrigerants, Fluid Phase Equilibria 199 (2002) 53–62

9. Guleda Onkal-Engin, Ibrahim demir, Seref N. Engin, determination of the relationship between swage odour and BOD by neural networks, Environment modeling & Software 20 (2005) 843-850

10. D.Svozil, V. Kvasnicka, J. Pospichal, Chemom. Intell. Lab. Syst. 39 (1997) 43–62.

11. J. A. Leonard, M. A. Leonard, L. H. Ungar, Computers & Chemical Engineering 16 (1992) 819-835

12. D. L. Katz, R. L. Lee, Natural Gas Engineering Producing and Storage, McGraw Hill, New York, 1990

13. Yu Lu, Liping Bian, Pengyuan Yang, Quantitive artificial neural network for electronic noses, Analitica Chimica Acta 417 (2000) 101-110

14. Swati Mohanty, Estimation of vapour liquid equilibria of binary systems, carbon dioxide–ethyl caproate, ethyl caprylate and ethyl caprate using artificial neural networks, Fluid Phase Equilibria 235 (2005) 92–98