PREDICTION OF PHASE BEHAVIOR OF MIXED REFRIGERANTS HFC125-HFC134a
BY USING RADIAL BASIS FUNCTION ARTIFICIAL NEURAL NETWORK
Bahman ZareNezhad

Faculty of Chemical, Petroleum and Gas Engineering
Semnan University, P.O. Box: 35195-363
Semnan, Iran
E-mail: bzarenezhad@semnan.ac.ir

ABSTRACT

A Normalized Radial Basis Function (NRBF) neural network has been presented for accurate prediction of the vapor-liquid equilibrium (VLE) of pentafluoroethane (HFC125) and 1,1,2-tetrafluoroethane (HFC134a) mixed refrigerants. According to the network's training, validation and testing results, a network with sixteen hidden nodes is selected as the best architecture. The presented model is very accurate over wide ranges of experimental pressure and temperature values. The predicted VLE of the refrigerant mixture is accurate enough to be employed in the design of refrigeration cycles.

Keywords: RBF, neural network, VLE, HFC refrigerants, prediction.

INTRODUCTION

Hydrocarbons (HCs) are excellent refrigerants, both for their energetic efficiency and their environmental compatibility. Unfortunately, they are highly flammable and for this reason, they are not widely applied. On the other hand, hydrochlorofluorocarbons (HCFCs) are important refrigerants in vapor compression refrigeration systems. However, the concern about the depletion of the stratospheric ozone layer by chlorine derived from HCFCs has led to the Montreal Protocol and international agreements [1, 2]. Hydrofluorocarbons (HFCs) are a new family of substances which might substitute HCFCs and HCs. Indeed, they are harmless towards the ozone layer, because they do not contain chlorine.

The most promising alternatives are mixtures which offer the possibility of matching several key thermodynamic properties of conventional HCFCs and HCs. Therefore, there is a great deal of interest in binary and ternary refrigerant blends based on the hydrofluorocarbon refrigerants due to their excellent thermodynamic performances and environmental characteristics [3]. The refrigerant mixing allows us to reach the desired thermodynamic properties by changing the mole percents of the constituents [4]. In order to use these new refrigerants properly, their thermodynamic, thermo-physical, transport and heat transfer properties must be known.

The experimental data on the thermodynamic properties of binary mixtures of HFCs is still limited and the evaluation of the vapor-liquid equilibrium (VLE) behavior is crucial, especially at near critical points. Furthermore, the experimental studies are expensive and time consuming, especially when there are different influencing parameters.

Therefore, accurate prediction of VLE of new blended refrigerants is the key to design and develop energy-efficient, cost-effective and environment-friendly refrigeration cycles. In order to predict the behavior of the binary mixture of HFCs, accurate thermodynamic models are required in terms of VLE data. However, the thermodynamic models need very many parameters and in many cases especially near the critical region, the predicted results are not accurate enough. In order to increase the prediction accuracy, an artificial neural network according to the radial based function (RBF) technique for determination of the VLE of HFC125-HFC134a mixtures in refrigeration systems has been presented in this work.
NRBF NEURAL NETWORK MODELING

Radial Basis Functions (RBF) are three-layer feed-forward neural networks with radial basis functions being the activation function of the hidden units (Fig. 1). RBF networks have established themselves as a choice of neural model for approximation and pattern recognition tasks [5]. RBF are a special class of functions whose characteristic feature is that their value decreases (or increases) monotonically with the distance from a central point, called a center of RBF. One of the most important activation functions is the Gaussian activation function which can be written as follows:

\[
\theta(x_i) = \exp \left( -\frac{\|x - u_i\|^2}{2\sigma_i^2} \right)
\]

(1)

where \(x\) is the input vector, \(u_i\) is the center vector of \(i\)-th hidden node, \(\theta(x)\) is the radial basis activation function of the hidden layer, and \(\sigma\) is the width of the basis function. Here, \(\|\|\) denotes the Euclidean norm.

RBF networks have feed-forward architecture with just one hidden layer composed of \(m\) units computing non-linear radial basis functions and fully connected to the input nodes. In this work, the softmax activation function is used for the hidden nodes such that the activations of all hidden nodes are normalized. This type of network is often called “normalized RBF” or NRBF network. Once the parameters of the hidden layer, using K-means or C-means algorithms are defined, the output weights \(w_i\) may be determined by iterative methods.

An RBF network can be modeled by the following equation:

\[
f(x) = \sum_{i=1}^{m} w_i \theta_i(x) + b_0
\]

(2)

where \(b_0\) is the bias value, while \(f\) is the RBF network output. When designing an RBF network, the most critical task is certainly the determination of the hidden layer. A straightforward approach is to fix the topology and use the GA, C-means, or K-means algorithms to compute the centers and the widths of the hidden nodes.

In this work, the K-means algorithm is used to determine the network topology through an iterative procedure, while the weights in the output layer are computed by LMS method.

Each NRBF network is the ratio of a bell-shaped Gaussian surface to sum of Gaussian surfaces known as the softmax activation function. In mathematical terms, this can be expressed as follows:

\[
\theta(x_i) = \frac{e^{h_i}}{\sum_{i=1}^{N} e^{h_i}}
\]

(3)

\[
h_i = \left( -\sum_{j=1}^{m} \left( \frac{x_j - u_{ij}}{2\sigma_i^2} \right)^2 \right)
\]

(4)

where \(x\) are the input vectors, \(u_{ij}\) is the center of the \(i\)-th hidden node that is associated with the \(j\)-th input vector, \(\sigma\) is a common width of the \(i\)-th hidden node in the layer, while the softmax \((h_i)\) is the output vector of the \(i\)-th hidden node.

Training involves the determination of the centers and the widths of the basis functions for each hidden node. The output layer weights are determined by minimizing the quadratic error between the predicted values and the desired values. In this work, the required mean square errors (MSEs) in prediction of the equilibrium pressure and the vapor phase composition are defined as follows:

\[
MSE = \frac{1}{N} \sum_{k=1}^{N} \left( P_{k, pred}^{P} - P_{k, exp}^{P} \right)^2
\]

(5)

\[
MSE = \frac{1}{N} \sum_{k=1}^{N} \left( y_{k, pred}^{y} - y_{k, exp}^{y} \right)^2
\]

(6)

RESULTS AND DISCUSSION

In order to predict the VLE of HFC125-HFC134a system, the required input/target data are taken from refs. [6, 7] that are used for the training and testing the NRBF network. The temperature and the liquid-phase

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Fig. 1. Topology of the proposed NRBF neural network.
mole fraction of HFC125 have been selected as input variables, while the pressure and the vapor-phase mole fraction are selected as output variables. Prior to the training the network with input/output data, the input and output data sets are normalized. The widths and the centers of the hidden layer nodes associated with each input vector and the weights between the hidden and output layer are shown in Table 1.

The proposed NRBF network has been trained, validated and tested by using 70 %, 15 % and 15 % of all measured VLE data points, respectively. The best performance is obtained when a network comprising of three layers, with two and sixteen neurons in the input layer and the hidden layer, respectively and two neurons in the output layer is used.

Figs. 2 and 3 show the comparison between the experimental data and the NRBF neural network predicted results for the training process. Figs. 2 and 3 show that the deviation found is quite low. The MSEs of the optimal NRBF network architecture for training, validation, and testing data are ca 0.0018, 0.0024, and 0.0042, respectively.

The comparison between the experimental measurements and the outputs predicted on the ground of the proposed NRBF neural network regarding validation and testing data sets are shown in Figs. 4 and 5. It should be noted that these data sets are not used during the training of the NRBF neural network [8, 9]. The correlation coefficient ($R^2$-value) of 0.9978 and 0.9932 are obtained for the equilibrium pressure and vapor mole fraction.
validation. The $R^2$-value of testing process regarding the equilibrium pressure and the vapor mole fraction are ca. 0.993 and 0.9983 in this work verifying the excellent performance of the proposed neural network.

The experimental data sets were chosen within the temperature range from 268.15 K to 353.13 K and the pressure range from 0.249 MPa to 3.925 MPa, respectively. Fig. 6 shows the P-x-y predictions of the proposed NRBF model in comparison with the experimental data. As shown in this figure the predicted results are in good agreement with the measured data for all experimental systems considered in this study.

Fig. 4. Comparison between experimental and predicted outputs by NRBF for validation data, a) Predictions of bubble pressure, b) Predictions of vapor mole fraction.

Fig. 5. Comparison between experimental and predicted outputs by NRBF for testing data, a) Predictions of bubble pressure, b) Predictions of vapor mole fraction.

Fig. 6. Comparison of the proposed NRBF model predictions with the experimental data at different temperatures.

Fig. 7. Comparison between proposed NRBF model predictions and experimental equilibrium pressures.
The proposed NRBF model predictions are compared with all experimental data in Figs. 7 and 8. The correlation coefficients ($R^2$-value) for the equilibrium pressure and the vapor phase mole fraction predictions are 0.9918 and 0.9976, respectively, indicating a very good agreement between the experimental and predicted values.

**CONCLUSIONS**

The main objective of this work is to prepare an accurate neural network model for predicting vapor-liquid equilibrium (VLE) pressure and compositions of HFC refrigerant mixtures. According to the network’s training, validation and testing results, a network with sixteen hidden nodes is selected as the best architecture. Comparison of the developed NRBF model with the experimental data shows that the model proposed can be used for accurate prediction of the VLE of refrigerant mixtures especially at high-pressure operating conditions where most thermodynamic models give poor results. The presented model can be used for accurate design of advanced refrigeration systems using the environmental friendly refrigerant mixtures.

**REFERENCES**