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An accurate model for predictions of vaporization enthalpies of hydrocarbons and petroleum fractions

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ABSTRACT

Vaporization enthalpy is an essential property in various areas of science and engineering applications such as optimizing the transportation processes, designing the oil and gas production and processing facilities, and heat flux calculations. This work aims to develop an intelligent technique, namely Radial Basis Function (RBF) approach to predict the vaporization enthalpy of petroleum fractions and pure hydrocarbons. The model was coupled with an optimization algorithm namely Genetic Algorithm (GA) to determine the tuning parameters of RBF model. The model performance was evaluated through various graphical and statistical approaches. Results of the developed GA-RBF model were also compared with other literature correlations and intelligent models. It was found that the proposed GA-RBF model exhibits reliable results with acceptable accuracy for the prediction of experimental vaporization enthalpy data. In addition, results show that the model outperforms other literature models and correlations and exhibits better performance for prediction of experimental data.

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1. Introduction

Vaporization enthalpy is defined as the difference between enthalpies of vapor and liquid phases at the same temperature and pressure. Vaporization enthalpy (ΔH^{vap}) is the amount of energy, which is required to transform a liquid phase material into the vapor phase at the boiling temperature [1]. Consequently, the vaporization enthalpy is utilized in many chemical disciplines and in oil and gas industries as well. From a thermodynamic standpoint, vaporization enthalpies can be utilized in processing and transportation facilities, which are aimed to optimize and design oil and gas production in addition to heat flux calculations. Moreover, they can be applied in order to predict some physical phenomena such as the solubility parameters of hydrocarbons [2]. The vaporization enthalpy of pure components, especially hydrocarbons, is a significant thermodynamic property that depends upon specific gravity (SG), normal boiling point temperature (T_b), and molecular weight (Mw) amongst thermodynamic relationships [3].

From both experimental and theoretical points of view, the vaporization enthalpy is of great importance due to its use in engineering optimization and design. Therefore, experimental techniques, correlations, and estimation models have been developed to be helpful for petroleum and chemical engineers in thermodynamic calculations [4]. In this regard, Vetere [5,6] introduced two empirical correlations to calculate vaporization enthalpy by two variables, which are molecular weight and normal boiling temperature. An empirical correlation to predict the vaporization enthalpy as a function of T_b and SG was consequence of Riazi and Daubert [7] work. Correlations of Vetere [5,6] and Riazi and Daubert [7] illustrate a rough error of 7%.

A simple correlation was developed by Mohammadi and Richon [2] in order to calculate vaporization enthalpy. It is just a function of T_b and SG. Additionally, it is able to calculate the vaporization enthalpies of pure hydrocarbon components and petroleum fractions. Moreover, they developed a classical Artificial Neural Network (ANN) tool to compare the results obtained by their empirical correlation. The results were indicative of the fact that empirical correlations and the ANN model are in compliance with experimental values. Other correlations such as Gopinathan and Saraf [8], Trouton's rule [4], Kistiakowsky rule [4] are also reported for prediction of vaporization enthalpy. The Gopinathan and Saraf [8] correlation is based on M_w, T_b and SG while the Trouton's and Kistiakowsky rules [4] are just based on T_b. Parhizgar et al. [1]

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proposed an empirical approach to determine vaporization enthalpies of pure hydrocarbon components and petroleum fractions by genetic programming that is a function of T_b and SG. Their results illustrate that their correlation is able to calculate the vaporization enthalpy of pure hydrocarbon components and petroleum fractions that has an average absolute relative deviation (AARD%) of almost 1.35%. Kamari et al. [3] proposed an intelligent model based on CSA-LSSVM for prediction of vaporization enthalpy. They also compared their results with the models and correlations developed by Mohammadi and Richon [2], Fang et al. [4], and Parhizgar et al. [1]. The CSA-LSSVM model was superior to other literature models and correlations.

Majority of methods available to calculate vaporization enthalpy have been based on laboratory obtained data in the case of hydrocarbon components. Therefore, they may not be precise in the case of petroleum fluids [2]. Additionally, in order to calculate vaporization enthalpy by conventional thermodynamic methods, many adjustable parameters are normally required. On the other hand, there are many weaknesses in existing thermodynamic models to calculate thermo-physical properties. These weaknesses include their lack for generalization of results because most of these models are applicable in specific domains and are not universal models and also the fact that the results of thermodynamic models are limited to mixtures and systems which they have been designed and adjusted for. In other words these models require several tuning and adjustable variables which their values should be optimized according to experimental data within limited and narrow range of thermodynamic conditions. These thermodynamic approaches need accurate and precise characterization of reservoir fluids and petroleum fractions as well. Moreover, thermodynamic models need dependable multiphase-multicomponent flash calculation algorithms and accurate properties (enthalpy, saturation temperature, etc). Some of these models may also result in convergence problems. Thus, there is a need for rapid, yet robust, and predictive approaches for determining the vaporization enthalpy for both petroleum fractions and hydrocarbon components. To achieve this objective, some smart approaches such as Least Square Support Vector Machine (LSSVM), Artificial Neural Network (ANN), Genetic Algorithms (GA), Particle Swarm Optimization (PSO), etc., have been utilized in recent years for solving regression, and classification problems [3,9–13].

This study highlights the application of a dependable intelligent model namely Radial Basis Function Neural Network (RBF-NN) to determine the vaporization enthalpy of pure hydrocarbon components and petroleum fractions as a function of Mw, SG and T_b using experimental data.

2. Radial Basis Function Neural Networks (RBF-NN)

Artificial Neural Networks (ANNs) are intelligent approaches, which own various advantages including their learning ability, which are capable to learn from previous processing operations to enhance their accuracy and high adaption capability, which easily adjust their performance with the environmental changes [14]. The main advantage of ANNs is that they can handle and control large scale problems, which require processing of complex and large amount of data points. ANNs have special structures comprising of various interconnected processing units called neurons. The units are distributed in their structure in a manner that they are located in specific layers with linking connections [9,14]. Two known types of ANNs which are similar in their performance but different in data processing are Multilayer Perceptron Neural Networks (MLP-NN) and Radial Basis Function Neural Networks (RBF-NNs) [14]. The structure of both RBF-NNs and MLP-ANNs consists of three layers named input, hidden, and output layers. The difference is that the MLP-ANN can have more than one hidden layer but the RBF-NN just holds one fixed hidden layer in its structure, which is one of the superiorities of RBF-NN over MLP-NN [15]. Owing to their simpler structure, it is easier to design and construct RBF-NNs. In addition the RBF-NN usually provides higher generalization ability and more efficient instant learning capability compared to MLP-NN. Moreover, RBF-NNs exhibit better responses to unseen testing patterns, which are used for general verification of model [16]. The simpler structure of RFB-NNs leads to faster training process of them [17]. These advantages of RBF-NNs position them as popular alternatives over MLP-NNs to be used in modeling purposes. The concept of RBF-NNs originates from the problem of efficient interpolation of a number of data points in a multidimensional domain [17]. RBF-NNs have a structure identical to structure of regularization networks. Three main characteristics of these networks are as follows [18,19]:

1. If sufficient number of data points available, the network will be capable to predict any multi-variable continuous function on a desired domain.
2. It provides the best possible solutions for the problem under consideration because it uses a cost function to control the level of smoothness of the problem.
3. The un-known parameters have linear nature, which brings the network to provide the best approximation feature.

The hidden layer of RBF-NNs contains various nodes in which each node holds a specific function named Radial Basis Function (RBF) denoted by $\phi(r)$. The input layer is responsible to deliver the input parameters as an input vector to hidden layer. The hidden layer performs a nonlinear transformation on this vector. The input of RBF is the vector distance between the weights terms of RBF and the product of input vector and its related biases. The output layer linearly maps the nonlinearity into a new domain. The values of weight terms can be optimized by utilizing the linear optimization approaches in the light of minimizing a predefined cost function, which is normally the Mean Square Error (MSE) between target values and model predictions [19,20]. The most important differences between MLP and RBF-NNs are as follows [16]:

1. The structure of MLP-NNs has more complexities compared to structure of RBF-NNs.
2. Due to the fact that RBF-NNs have just one fixed hidden layer the learning and training of them is simpler than MLP-NNs.
3. RBF-NNs are localized based networks in which the network output is a result of certain units in specific local receptive areas, however, MLP-NNs are general predictive tools such that the output is determined by contribution of all neurons.

Further details about the performance of RBF-NNs are found in open literature [9,15].

3. Results and discussion

3.1. Data acquisition

There are basically two empirical approaches to determine the value of vaporization enthalpy. The first approach correlates the vaporization enthalpy with the normal boiling point and critical properties of substance [21]. Another approach uses molecular weight, specific gravity, and normal boiling point temperature to correlate the

Table 1
Input and output parameters utilized in this work.

Parameter	Maximum	Minimum	Average	Standard deviation
ΔH^{vap} (kJ/mol)	80.1	19.0	42.1	14.46
T_b (K)	722.8	231.1	451.9	111.25
Mw (g/mol)	422.8	44.1	160.2	84.5
SG	0.8	0.8	0.7	0.07

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