INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2017) 1–19

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he

Toward generalized models for estimating molecular weights and acentric factors of pure chemical compounds

Abdolhossein Hemmati-Sarapardeh [a,b], *Forough Ameli* [c], *Amir Varamesh* [i], *Shahaboddin Shamshirband* [d,e,*], *Amir H. Mohammadi* [f,g], *Bahram Dabir* [h]

[a] *Department of Petroleum Engineering, Shahid Bahonar University of Kerman, Kerman, Iran*
[b] *Department of Chemical & Petroleum Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada*
[c] *School of Chemical Engineering, Oil and Gas, Iran University of Science and Technology, Tehran, 16846, Iran*
[d] *Department for Management of Science and Technology Development, Ton Duc Thang University, Ho Chi Minh City, Viet Nam*
[e] *Faculty of Information Technology, Ton Duc Thang University, Ho Chi Minh City, Viet Nam*
[f] *Institut de Recherche en Génie Chimique et Pétrolier (IRGCP), Paris Cedex, France*
[g] *Thermodynamics Research Unit, School of Engineering, University of KwaZulu-Natal, Howard College Campus, King George V Avenue, Durban, 4041, South Africa*
[h] *Department of Chemical Engineering, Amirkabir University of Technology, Tehran, Iran*
[i] *Institute of Petroleum Engineering, School of Chemical Engineering, College of Engineering, University of Tehran, Tehran, Iran*

ARTICLE INFO

Article history:
Received 29 August 2017
Received in revised form
9 November 2017
Accepted 4 December 2017
Available online xxx

Keywords:
Molecular weight
Acentric factor
MLP
RBF
LSSVM
GMDH

ABSTRACT

In this work, four prompt and robust techniques have been used to introduce new generalized models for estimation of the physical properties of pure substances, including molecular weight and acentric factor. These methods were developed based on radial basis function (RBF) neural networks, group method of data handling (GMDH), multilayer perceptron (MLP), and least square support vector machine (LSSVM) techniques. Models were introduced based on a set of experimental data including 563 pure compounds that were collected from available literature. Input parameters for estimation of molecular weight were considered as specific gravity and normal boiling point. Critical temperature, critical pressure and normal boiling point were selected as inputs for estimation of the acentric factor. Statistical and graphical error analyses normal boiling point revealed that all of the developed models are accurate. The designed RBF models give the most accurate results with an AAPRE of 5.98% and 1.92% for molecular weight and acentric factor, respectively. The developed GMDH models are in the form of simple correlations, which can be used easily in hand calculation problems without any need to computers. Comparison of the developed models with the available methods showed that all of the developed models are more accurate than the existing methods. Using the relevancy factor, the impact of each input parameter on the output results was determined. Additionally, to find out the applicability region of the developed models, and to demonstrate the reliability of the models, the Leverage method has been used. There are few data out of the applicability domain of the proposed models. All the statistical and graphical resolutions, demonstrate

* *Corresponding author*. Department for Management of Science and Technology Development, Ton Duc Thang University, Ho Chi Minh City, Viet Nam.
E-mail address: shahaboddin.shamshirband@tdt.edu.vn (S. Shamshirband).
https://doi.org/10.1016/j.ijhydene.2017.12.029

the reliability of the developed models in estimating the molecular weight and acentric factor.

Introduction

The behavior of each fluid is determined by the behavior of its constituents. Studying this behavior is of paramount importance in managing the various systems such as chemical and petroleum industries. Hence, fully understanding the molecular behavior of various compounds is very important. In order to design many chemical and petrochemical processes, developing new techniques for determination of the physical properties of these constituents is highly important [1]. These properties could be applied in the following applications:

(1) To specify the constants of equations of state to model the phase behavior of various systems including refineries and petrochemical processes [2,3].
(2) To model the fluid transport properties in different systems such as oil and gas production and distribution [2,3].
(3) To specify the thermal properties of various compounds, including heat of combustion, enthalpy, and viscosity [4].

Determining such properties, might be very challenging and also costly, or in some situations, impossible, since the components may degrade prior to reaching the desired conditions. This limitation leads to application of predicting techniques for supplying these properties in the lack of experimental data [1]. The precision of thermodynamic models highly depends on the estimation of pure compounds' properties. Molecular weight and acentric factor are the most important correlating parameters for the transport properties [5]. Over the past years, various models were introduced for estimation of these parameters. Lee and Kesler [6] developed two correlations with regard to reduced boiling point range, to estimate the acentric factor as a function of the critical temperature, critical pressure, and boiling point based. The developed Lee and Kesler [6] correlations have the following formula:

For $T_{br} \leq 0.8$:

$$\omega = \frac{-\ln P_c/1.01325 - 5.92714 + 6.09648/T_{br} + 1.28862 \ln T_{br} - 0.169347T_{br}^6}{15.2518 - 15.6875/T_{br} - 13.4721 \ln T_{br} + 0.43577T_{br}^6} \quad (1)$$

For $T_{br} \leq 0.8$:

$$\omega = -7.904 + 0.1352K_w - 0.007465K_w^2 + 8.359T_{br} + (1.408 - 0.01063K_w)/T_{br} \quad (2)$$

In the above equations, ω stands for the acentric factor, P_c denotes the critical pressure, T_{br} is the reduced boiling point which is defined as the ratio of normal boiling point to critical temperature and K_w is the Watson characterization factor defined by Eq. (3) [7].

$$K_w = \frac{(1.8T_b)^{1/3}}{SG} \quad (3)$$

where T_b represents the normal boiling point and SG is the specific gravity.

Edmister [8] developed a simple equation for estimating acentric factor with the same input parameters as considered by Lee and Kesler [6] method:

$$\omega = \left(\frac{3}{7}\right) \times \left(\frac{T_{br}}{1 - T_{br}}\right) \times \left[\log_{10}\left(\frac{P_c}{1.01325}\right)\right] - 1 \quad (4)$$

Korsten [9] modified Edmister methods and proposed the following equation:

$$\omega = 05899\left(\frac{T_{br}^{1.3}}{1 - T_{br}^{1.3}}\right) \times \left[\log\left(\frac{P_c}{1.01325}\right)\right] - 1 \quad (5)$$

More recently, Hosseinifar and Jamshidi [10] proposed a simple correlation for estimation of some thermophysical properties of pure compounds including, acentric factor and molecular weight. In their proposed method, acentric factor is considered as a function of two input parameters, which can be either of specific gravity and molecular weight or specific gravity and normal boiling point. Moreover, molecular weight is considered as function of specific gravity and normal boiling point. Hosseinifar and Jamshidi method [10], which was developed based on a data set of 255 pure compounds, has the following formulation:

$$\phi(f(SG), \xi) = \left(a \cdot f(SG)^b \xi^c + d \cdot f(SG)^e \xi^f\right)^g \quad (6)$$

where:

$$f(SG) = \sqrt{\frac{3 + 2 \times SG}{3 - SG}} \quad (7)$$

In the above equations, ϕ is the property which can be molecular weight or acentric factor, ξ is an input parameter which can be substituted by molecular weight or normal boiling point and a, b, c, d, e, f and g are adjustable parameters.

There are also other methods and equations available for estimation of acentric factor. For instance, Lin and Chao [11]

Please cite this article in press as: Hemmati-Sarapardeh A, et al., Toward generalized models for estimating molecular weights and acentric factors of pure chemical compounds, International Journal of Hydrogen Energy (2017), https://doi.org/10.1016/j.ijhydene.2017.12.029