Fuel 222 (2018) 779–791

Contents lists available at ScienceDirect

Fuel

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

Full Length Article

Modeling interfacial tension in N_2/n-alkane systems using corresponding state theory: Application to gas injection processes

Forough Ameli[a], Abdolhossein Hemmati-Sarapardeh[b,c], Mahin Schaffie[b], Maen M. Husein[c], Shahaboddin Shamshirband[d,e,*]

[a] School of Chemical Engineering, Iran University of Science and Technology, 16846 Tehran, Iran
[b] Department of Petroleum Engineering, Shahid Bahonar University of Kerman, Kerman, Iran
[c] Department of Chemical & Petroleum Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada
[d] Department for Management of Science and Technology Development, Ton Duc Thang University, Ho Chi Minh City, Vietnam
[e] Faculty of Information Technology, Ton Duc Thang University, Ho Chi Minh City, Vietnam

ARTICLE INFO

Keywords:
Interfacial tension
Corresponding state theory
Intelligent model
Nitrogen injection

ABSTRACT

Nitrogen is of paramount importance for many processes in chemical and petroleum engineering; including enhanced oil recovery, gas injection for pressure maintenance, and gas recycling. Precise estimation of interfacial tension (IFT) between N_2 and the reservoir hydrocarbons is, therefore indispensable. However, experimental measurement of IFT is expensive and time consuming. Therefore, reliable model for estimating IFT is vital. In this communication, the IFT between N_2 and n-alkanes was modeled over a wide range of pressure (0.1–69 MPa) and temperature (295–442 K) based on the principle of corresponding state theory using dimensionless pressure and dimensionless temperature. Three well-known models; namely, Multilayer Perceptron (MLP) Neural Networks (*optimized by Levenberg-Marquardt* (*LM*), Scaled Conjugate Gradient (SCG), or Bayesian Regularization (BR)), two Radial Basis Function (RBF) Neural Networks (*optimized by Particle Swarm optimization* (*PSO*) *technique or Genetic Algorithm* (*GA*)) and one Least Square Support Vector Machine (LSSVM) (*optimized by coupled simulated annealing*) were used to develop robust and accurate models for predicting IFT based on the proposed dimensionless parameters. Results suggested that the developed MLP-LM was the most accurate model of all with an average absolute relative error of 1.38%. MLP-LM model was compared with three well-known models in the literature; namely Density Gradient Theory (DGT), Linear Gradient Theory (LGT), and Parachor approaches combined with the Volume Translated Predictive Peng Robinson Equation of State (VT-PPR EOS) and the recently developed model by Hemmati-Sarapardeh and Mohagheghian. In addition to the advantage of being normal alkane-independent, results showed that the proposed MLP-LM model is superior to published models. Lastly, the quality of the literature IFT data and the applicability domain of MLP-LM model were evaluated using the Leverage approach.

1. Introduction

Primary and secondary oil recovery processes leave behind large amounts of residual oil, which mandates the use of more effective enhanced oil recovery techniques (EOR) [1–3]. Various EOR techniques are currently used; including miscible and immiscible gas injection, which utilize natural gas, flue gas, nitrogen, and carbon dioxide [1,4–7]. For example, CO_2 increases oil recovery by swelling, reduction of viscosity and interfacial tension (IFT) as well as oil vaporization [8–11]. In particular, CO_2 injection contributes to creating markets for greenhouse gases (GHG) usage, which in turn motivates CO_2 sequestering [12–22]. Typically, gas injection for EOR has a narrow economic operational window and, hence, must be precisely predicted. Also, it is critical to minimize corrosion and asphaltene precipitation problems in order to achieve a profit [6,7,23–27]. The injection of CO_2 sometimes would lead to formation damage, wettability modification, reduction in relative permeability, corrosion, and freezing of wellbore annular [24,26,28]. Subsequently, use of a nonhydrocarbon gas could be a good alternative.

Nitrogen is available in large volumes from air and does not lead to the corrosion problem encountered with CO_2. Moreover, it is less likely to cause asphaltene precipitation [29,30]. Nitrogen could be supplied from various nitrogen gas supplies or by direct separation from air. Cryogenic separation of nitrogen from air is the most economic

* Corresponding author at: Department for Management of Science and Technology Development, Ton Duc Thang University, Ho Chi Minh City, Vietnam.
E-mail address: shahaboddin.shamshirband@tdt.edu.vn (S. Shamshirband).

https://doi.org/10.1016/j.fuel.2018.02.067
Received 23 July 2017; Received in revised form 12 January 2018; Accepted 8 February 2018

technique for nitrogen production to be applied for gas injection processes. The mechanism included in nitrogen injection processes include reservoir pressure maintenance, immiscible and miscible displacement and miscible slug [31]. Since the minimum miscibility pressure (MMP) for a mixture of nitrogen and crude oil is high, this process typically falls under immiscible displacement [30]. Miscibility condition refers to a case in which two fluids are mixed at any ratio. MMP is the minimum operating pressure at which the crude oil and the injected gas mix at the corresponding reservoir temperature. There are various computational and experimental techniques for determining MMP. The most commonly used experimental technique is the slim tube. Other techniques include pressure-composition diagram, vanishing interfacial tension technique, and rising bubble apparatus [30].

IFT relates to the energy required to pull molecules from the bulk liquid phase to the surface of contact with another immiscible phase [32]. Similarities between the nature of molecules constituting the two immiscible phases typically lowers IFT [33]. IFT plays a key role in all the aforementioned processes in gas injection and should be accurately determined. IFT is a function of pressure, temperature and the composition of the two phases. This parameter could be determined experimentally and/or theoretically using various models and correlations [32]. Conventional experimental procedures include drop weight, capillary rise, and wilhelmy plate [34]. Other modern techniques include spinning drop, pendent drop, and sessile drop [35]. The most accurate results are obtained using pendent drop method [36]. It is worth noting that few studies have focused on determining the effect of various parameters, e.g. temperature and pressure, on IFT value of nitrogen/crude oil.

Various techniques for estimating IFT have been developed; including corresponding state theory [37], gradient theory [38], Parachor model [39,40], and Thermodynamic correlations [41]. Macleud–Sudgen [39,40] developed a model in which surface tension is proportional to the molar density of pure compounds. The Parachor model of Weinaug and Katz [42] is also used for binary mixtures interfacial tension.

In the present study, the IFT between a mixture of normal alkanes (as representative of crude oil) and nitrogen was modeled using the corresponding state theory through defining two input parameters; namely dimensionless pressure (P_D) and dimensionless temperature (T_D). This means that IFT of normal alkanes and nitrogen at the same dimensionless temperature and pressure is the same for different normal alkanes. Actually, regardless of the type of normal alkane, if different normal alkanes and nitrogen have the same P_D and T_D, IFT of the systems would be the same. To this end, a large data bank in a wide range of pressure and temperature was collected from experimental IFT values of pendent drop approach, between normal alkanes of n-C_5 [43], C_6 [43,44],C_7 [45,46], C_8 [43], C_{10} [47,48] and C_{16} [45] and nitrogen.

Application of various intelligent techniques has expanded to many chemical processes in the recent years [49–52]. In this study, Multilayer Perceptron (MLP), Neural Networks optimized by Levenberg-Marquardt (LM), Scaled Conjugate Gradient (SCG), and Bayesian Regularization (BR), Radial Basis Function (RBF) Neural Networks optimized by Particle Swarm Optimization (PSO) technique and Genetic Algorithm (GA), and Least square support vector machine (LSSVM) optimized by coupled simulated annealing, were applied for predicting IFT values of nitrogen and normal alkanes using two dimensionless properties. Moreover, to compare the accuracy of the developed models and pre-existing models (including Density Gradient Theory, Linear Gradient Theory, and Parachor approaches combined with Volume Translated Predictive Peng Robinson Equation of State (VT-PPR EOS) and Hemmati-Sarapardeh and Mohagheghian model [53]), graphical and statistical error analyses were applied simultaneously. In addition, in order to deepen the understanding of each parameter on IFT value, the relevancy factor (r) was determined. Lastly, the applicability domain of the best proposed model was reported.

2. Theoretical and empirical models for IFT estimation

The theoretical approaches for IFT determination are based on linear gradient theory (LGT), Parachor, and Density Gradient Theory (DGT), which are briefly summarized in this section.

2.1. Parachor method

Parachor model is widely used in industry [39,40] and is considered the most successful technique in petroleum industry. In this method, IFT of simple and complex systems could be determined at high temperatures and pressures. Macleod [40] and Sugden [39] model was introduced to estimate IFT between a liquid and a vapor phase of a pure substance. Models for estimating IFT between a liquid and a vapor phase of a pure substance were later extended by Weinaug and Katz [42] to represent IFT of mixtures using molar averaging as follows.

$$IFT = \left[\sum_{i=1}^{N} P_{ch,i}(x_i\rho^l - y_i\rho^v)\right]^E, \tag{1}$$

where, $P_{ch,i}$expresses the Parachor of component i, N is the number of components in the mixture, x_i and y_i are the equilibrium values for the mole fraction of the components in the liquid and the vapor phases, respectively, E is the scaling exponent that varies between 3.45 and 4, and ρ^l and ρ^v are the molar densities of the liquid and vapor phases, respectively [54,55]. Many studies have been conducted on scaling the exponent. Values ranging from 3.45 to 4 were proposed. Other researches attempted modeling Parachor values as a function of specific gravity, critical pressure, critical temperature, and molecular weight. Ali [56] proposed E equal to 4, while Parachor value was proposed by Fanchi [57].

2.2. Density Gradient Theory method

Density Gradient Theory (DTG) is a more rigorous theoretical model which has been widely used for IFT calculation in different systems. This method became popular after Chan and Hilliard [58]. In this technique, density of the pure components is determined by phase equilibrium properties of the components at the interface [59,60]. The origin of this technique was developed from the work of van der Walls [61] in nonhomogeneous solutions. It was then reformulated by Cahn & Hilliard [58] and its usage became widespread. The IFT value between two phases of multi-component system is calculated using the following equations:

$$IFT = \int_{-\infty}^{+\infty} \sum_i \sum_j c_{ij}\frac{d\rho_i}{dz}\frac{d\rho_j}{dz}dz = \int_{-\infty}^{+\infty} 2\Delta\Omega(\rho)dz, \tag{2}$$

$$\Delta\Omega(\rho) = f_0(\rho) - \sum_i \rho_i\mu_i + p, \tag{3}$$

where, $c_{ij}$is the parameter of cross influence, $\Delta\Omega$ expresses the changes in grand thermodynamic potential, μ_i is the chemical potential for the pure components at the equilibrium temperature and pressure, f_0 is the Helmholtz free energy density of the homogeneous fluid at the local density ρ,and P expresses the equilibrium pressure. To determine the cross influence parameter, the following equation is introduced which is a mixing rule forc_i and c_j, as the influence parameters for the individual components.

$$c_{ij} = (1-\beta_{ij})\sqrt{c_i c_j}, \tag{4}$$

where, β_{ij} denotes the value of binary interaction coefficient. In this method, the values of c_i and c_j are determined using radial density distribution function of pure substances [62,63]. These parameters are usually determined using surface tension values. There are various semi-empirical and equation of state dependent correlations [64–66]. The following equations are applied for calculating the influence