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Equilibrium ratio of hydrocarbons and non-hydrocarbons at reservoir conditions: Experimental and modeling study



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ABSTRACT

Determination of equilibrium composition for various multi-phase systems is important in the context of thermodynamics. Three methods are generally employed to calculate the gas/liquid equilibrium compositions; namely, empirical graphs, correlations, and equations of state (EOSs). Empirical graphs and correlations are simple and fast in terms of calculation procedure. Furthermore, using an EOS requires an initial guess, which is usually obtained via empirical correlations. In this study, the gas-oil composition of 10 different crude oils (20–40 °API) are experimentally determined by a gas chromatography (GC) apparatus within a temperature range of 600–1212 °R and a pressure range of 14.7–7000 psi. A robust predictive model is then proposed to estimate the equilibrium ratios (K_i) of hydrocarbons and non-hydrocarbons. This model is generated by utilizing the least squares support vector machine (LSSVM), while genetic algorithm (GA) is used for selection and optimization of hyper parameters (γ and σ^2) that are embedded in the LSSVM model. The coefficient of determination (R^2) for the introduced model is 0.9991 and 0.9979 and the mean squared error (MSE) is 0.00074 and 0.044 for the hydrocarbons and non-hydrocarbons, respectively. The proposed model is simple to use and exhibits high accuracy and reliability, which can have various applications in chemical and petroleum industries where the thermodynamic equilibrium is maintained.

1. Introduction

Accurate knowledge of phase equilibria is vital in several engineering processes. The empirical graphs, correlations, and equations of state (EOSs) are three common techniques to obtain mixture characteristics at equilibrium conditions [1–3].

An important parameter in gas-oil equilibrium predictions is the equilibrium ratio. The equilibrium ratio of i^{th} component in a mixture (K_i) is defined as the ratio of the fraction of i^{th} component in the gas phase to that in the liquid phase, at vapor-liquid equilibrium, as shown below.

$$K_i = \frac{y_i}{x_i} \quad (1)$$

where y_i and x_i stand for the mole fraction of component i in the vapor phase and the liquid phase, respectively.

Equilibrium ratios may reach unity at high pressures for some multi-component mixtures, meaning that the concentration of i^{th} component is equal in both liquid and vapor phases [4].

The most common empirical graphs used in the phase equilibrium calculations are Katz and Cox charts. In both charts, the K_i values of

each component are independent of the composition mixture. These charts, which were presented by Gas Processors Society in 1957, are available for paraffins (C_1 – C_{10}), ethylene, propylene, nitrogen, and carbon dioxide [4,5].

According to the Raoult's law for hydrocarbons, a plot of K_i values versus pressure yields a straight line with a slope of unity at low pressures (10–500 psi). The intercept of the line is dependent on the molecular weight of the constituent. Katz et al. presented a series of revised graphs for various hydrocarbons for a convergence pressure of 5000 psi [5]. They also showed that K_i value of CO_2 can be estimated as the square root of the product of K_i values of methane and ethane [5].

Empirical correlations are the mathematical forms of the empirical graphs. These correlations generally include convergence pressure and a parameter representing the component as the variables [6]. For example, Standing et al. proposed an equation for estimating K_i value of Oklahoma oil/gas mixtures [7]. The K -value in Standing et al.'s Equation is assumed independent of the mixture composition. The correlation is only accurate at low pressures (below 1000 psi) [7]. There is another empirical correlation which is called the Wilson correlation. This equation is commonly used for calculating K_i values of paraffins. The correlation is applicable over the pressure range of 14.7–500 psi as

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Nomenclature		Variables	
<i>Abbreviations</i>			
AARD	average absolute relative deviation	P_{ci}	critical pressure of i^{th} component (psi)
EOS	Equation of State	ω_i	acentric factor i^{th} component
FID	flame ionization detector	T_{ci}	critical temperature i^{th} component ($^{\circ}\text{R}$)
GA	Genetic algorithm	e_k	the regression error
GC	gas chromatography	x_k	k^{th} input data in the input space
GOR	Gas to oil ratio (SCF/STB)	α_k	Lagrange multipliers
LSSVM	least squares support vector machine	n	space's dimension
MSE	mean squared error	P	Pressure (psia)
QP	Quadratic programming	T	Temperature ($^{\circ}\text{R}$)
RBF	Radial basis function	y_k	output value for a specified input variable (i.e. x_k)
SVM	Support vector machine	b	a term of bias
TCD	thermal conductivity detector	ω	the vector of weight
		γ	the regularization parameter
		σ^2	kernel sample variance

listed below. This relationship results in accurate estimations where the target pressure is below the critical pressures of components. The modified Wilson equation is an extension of Wilson equation which can be utilized at higher pressures up to sub-critical condition [8].

Support vector machine (SVM), which was first introduced by Vapnik in 1998, is a type of machine learning approach [9]. SVM is an efficient method that has been widely employed for solving different complex cases in various engineering disciplines [10]. The main aim of SVM is to convert the nonlinear input space into a high-dimensional characteristic space and to obtain a hyper-plane through nonlinear mapping [11]. This new methodology is based on the different statistical concepts [12]. Quadratic programming (QP) is rather than returning many local solutions like other regression methodologies, the solution returned by SVM is global or even unique. This is because the QP puzzle is a convex function [13]. This method might be time-consuming and difficult to be used as it should find a solution for a set of nonlinear equations. Suykens and Vandewalle proposed the least square support vector machine (LSSVM) method as an alternative form of the SVM method [14–16]. LSSVM's advantage over SVM is that it only requires a group of linear calculations. This makes LSVVM computationally straightforward and easier.

This study uses the LSSVM model, as a generalization of traditional SVM, to estimate the equilibrium ratios (K_i) of hydrocarbons and non-hydrocarbons. Genetic algorithm (GA) is implemented as an optimizer scheme for adjustment of LSSVM variables. This work contains the novelty of using the SVM approach to forecast the equilibrium ratios (K_i) of hydrocarbons and non-hydrocarbons. No records of such a mathematical approach are found in the literature.

2. Experimental methodology

10 different oil samples from different Iranian oil reservoirs were employed in our experiments. As a result, the values of gas to oil ratio (GOR), bubble point pressure, and reservoir temperature were different. To analyze the components of each live oil sample, 100 cm³ of each oil sample were flashed from the reservoir condition to the atmospheric condition. The number of flashing steps strongly depends on the bubble point pressure and GOR. As each oil sample has a unique GOR and bubble point pressure, the starting pressure in the flash tests is different for various oil samples. Hence, the flash steps are different for various samples. After the flash process of the live oil sample, the compositional analysis of produced gas phase and residual hydrocarbon liquid was carried out via Agilent 7890 A gas chromatograph (GC). The range of temperature of the stationary phase at operating conditions was 600–1212 $^{\circ}\text{R}$. Using the flame ionization detector (FID), the relative concentration of each component can be determined. In this work, the thermal conductivity detector (TCD) was used to analyze the

components up to C₄ and the FID detector was employed to measure the concentrations of heavier components, particularly C₅₊.

3. Theory

3.1. LSSVM methodology

The methodology of LSSVM for nonlinear function approximation is as below. A training data set is defined for generating the model. The data set is defined as: $\{x_k, y_k\}$, $k = 1, 2, \dots, N$, where $x_k \in \mathbb{R}^n$ is the k^{th} input data in the input space, $y_k \in \mathbb{R}$ is the output value for a specified input variable (e.g., x_k) and N represents the number of the training data points. We consider the given inputs x_k such as critical pressure (P_c , psia), critical temperature (T_c , $^{\circ}\text{R}$), acentric factor, gas oil ratio (GOR, SCF/STB), temperature, and pressure. The output y is the equilibrium ratio. Using the nonlinear function, $\varphi(x)$, that maps the training set in the input space to the high dimensional space, the regression paradigm of Eq. (2) is created [17,18].

$$y = \omega^T \cdot \varphi(x) + b \text{ with } \omega \in \mathbb{R}^n, b \in \mathbb{R}, \varphi(\cdot) \in \mathbb{R}^n \rightarrow \mathbb{R}^{n_h, n_h} \rightarrow \infty \quad (2)$$

where ω is the vector of weight and b represents a term of bias. The superscript “ n ” stands for the data space's dimension, and “ n_h ” denotes the unidentified characteristic space's dimension [13]. When the LSSVM modeling is performed, a new optimization problem is obtained. The developed model deals with the optimization problem as presented by Eq. (3) [17,18].

$$\frac{\min}{\omega, b, e} \mathcal{J}(\omega, e) = \frac{1}{2} \omega^T \omega + \frac{1}{2} \gamma \sum_{k=1}^N e_k^2 \quad (3)$$

Eq. (4) is subject to the equality constraint shown by the following expression:

$$y_k = \omega^T \phi(x_k) + b + e_k \quad k = 1, 2, \dots, N \quad (4)$$

in which, γ is the regularization parameter, which balances the complexity of the model and the training error, and e_k represents the regression error [12].

To specify the solution to the restricted optimization puzzle, the Lagrangian is constructed as illustrated below.

$$\mathcal{L}(\omega, b, e, \alpha) = \mathcal{J}(\omega, e) - \sum_{k=1}^N \alpha_k \{ \omega^T \phi(x_k) + b + e_k - y_k \} \quad (5)$$

where α_k are the Lagrange multipliers or support values. Solving this equation requires differentiating Eq. (5).

Eqs. (6)–(9) show the differentiated forms of Eq. (5) with respect to ω, b, e_k , and α_k , respectively [17,18].

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