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THE DETERMINATION OF EQUILIBRIUM RATIOS OF HYDROCARBONS AT RESERVOIR CONDITION

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Abstract

Equilibrium ratios play a fundamental role in understanding the phase behavior of hydrocarbon mixtures. They are important in predicting compositional changes under varying temperatures and pressures in the reservoirs, surface separators, and production and transportation facilities. In particular, they are critical for reliable and successful compositional reservoir simulation. Empirical correlations up to now are based on oil samples of other countries. Some parameters such as oil density and gas-oil ratio are not considered in these correlations. In this study has tried to focus on equilibrium ratios of hydrocarbons in the Iranian oils, for a wide range of Iranian oils pressure from 14.7 psi to 6000 psi and tempeature from 70°F to 300°F by presenting an experimental correlation. Using the mass balance on the different stages of Differential Liberation (DL) test for multiple samples from the Iranian reservoir oil, K-values calculated for these reservoirs fluids. Then by Using experimental K-values and genetic algorithm, an empirical correlation obtained between equilibrium ratio and dependent para-meters. In the end, the efficiency of correlation attained from genetic algorithm was compared to previously presented correlations.

Keywords: Equilibrium Ratio; Non-Hydrocarbons; Hydrocarbons; Prediction; Nonlinear Regression; Genetic Algorithm (GA).

1. Introduction

An important issue in thermodynamics is the determination of phase compositions at equilibrium. Three methods are generally employed for calculating gas-oil equilibrium compositions: empirical graphs, correlations, and equations of states (EOS). Empirical graphs and correlations are simple and fast to use. Furthermore, using an EOS requires an initial guess (i.e. a rough estimate of the solution), which is usually obtained via empirical correlations [1-3].

An important parameter in gas-oil equilibrium predictions is the equilibrium ratio. The equilibrium ratio of the i^{th} component in a mixture is defined as the ratio of the fraction of the i^{th} component in the gas phase to that in the liquid phase, at vapor-liquid equilibrium (Eq.1).

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

It's been shown that in a multi-component mixture, K_i values reach unity at high pressures. This means that compositions of vapor and liquid become identical at elevated pressures [4].

This study uses the genetic algorithm and nonlinear regression approach to estimate the equilibrium ratios (K_i) of hydrocarbons. Genetic algorithm (GA) is used as an optimizer scheme for adjusting the coefficients and exponents of the non-linear regression model. This work contains the novelty of using the GA-nonlinear regression approach for modeling equilibrium

ratios (K_i) of hydrocarbons and non-hydrocarbons, and no record of such approach has been found in the literature by the authors of this study.

2. Data Gathering

To develop easy-to-use and simple correlation based on GA-regression method, 576 data points from the open literature were employed. Table 1 reports the ranges of the data points used in this paper.

Table 1. Range of experimental data points employed in this study

Parameter	Range	Parameter	Range
API	1.01-3.41	C_2	20-40
GOR	0.66-1.62	C_3	292.9-1217.2
Bo	0.40-1.3	iC_4	1.25-2.09
P	0.44-1.08	nC_4	3000-7600
T	0.15-1.01	iC_5	663-740
Pb	0.14-1.04	nC_5	1615-4080
C_1	0.02-0.31	C_6	1.59-8.80

3. Theory

3.1. Non-Linear Regression

In many processes (or phenomena) in engineering and science disciplines, multiple linear regression models can be employed to find correlations to describe the objective functions in terms of independent variables. In chemical and petroleum engineering, it is common to transform all variables into dimensionless parameters as the developed correlation is applicable for other experimental and field conditions, resulting in the effective implementation of process scale-up. Considering interactions between input variables, the multivariable nonlinear regression model is written as follows:

$$y = \beta_o + \beta_1 x_1^{a1} + \beta_2 x_1^{a2} x_2^{a3} + \beta_3 x_1^{a4} x_3^{a5} x_2^{a6} + \beta_4 x_1^{a7} x_2^{a8} x_3^{a9} x_4^{a10} + \beta_5 x_1^{a11} x_2^{a12} x_3^{a13} x_4^{a14} x_5^{a15} \quad (2)$$

The above equation 2 stands for a regression model with 5 regression variables (x_1-x_5) and 15 exponents. β_0 - β_5 are the regression coefficients and y is the predicted response.

It should be noted here that the dependent or/and independent variables may appear in logarithmic, exponential, or other mathematical functions within the regression correlation, depending on the physics of process involved.

3.2. Genetic Algorithm (GA)

GA is a stochastic method for solving optimization problems. It's based on performing the Darwinian evolution theorem and various genetic operators. These genetic operators include mutation and crossover [12-14]. A favorable feature of GAs is that they do not require the differentiating of complex functions. The stochastic nature of the GA with dynamic evaluation of the fitness function makes it an efficient random search engine. This algorithm is a superior alternative to derivative-based algorithms because the fitness function can be non-differentiable, stochastic and potentially highly nonlinear [16-18].

4. Methodology

Equilibrium ratio (K_i) for hydrocarbons, as output, was estimated via the proposed regression method. The model consists of five inputs including critical pressure, critical temperature, acentric factor, reservoir temperature, and pressure. GA algorithm was applied to determine the optimum values of the coefficients and exponents in the proposed nonlinear regression method. The fitness function in the GA was the root mean squared error (RMSE) of testing data.

5. Results and Discussion

The criteria for evaluating the proposed model's performance are the root mean squared error (RMSE) and correlation coefficient (R^2). The value of RMSE reaches zero and R^2 reach unity in an ideal model. The proposed correlation based on the GA and nonlinear regression is as following as:

$$K_i = a_1 \times \left(\frac{P_{ci}}{P}\right)^{(a_2 \times \omega_i^2 + a_3 \times \omega_i + a_4)} \times \exp\left(a_5 \times \omega_i + a_6 \times \left(\frac{T_{ci}}{T}\right)\right) \quad (3)$$

Table 2 reports the coefficients and exponents of the proposed GA-regression method.

Table 2. Coefficients of the proposed correlation

a1	a2	a3	a4	a5	a6
0.424	-12.785	0.962	0.470	-29.103	5.072

The correlation coefficient of the best-fitted line for the results of the Wilson correlation is about 0.5138. Moreover, the values of RMSE and SD for the Wilson correlation are 3.6724 and 4.4925, respectively. This means that the Wilson correlation was unable to predict equilibrium ratio accurately.

The correlation coefficient of the best-fitted line for the results of the Standing correlation is about 0.4074. Furthermore, the values of RMSE and SD for the Standing correlation are 1.9907 and 2.3102, correspondingly. It means that the Standing correlation was unable to predict equilibrium ratio accurately.

The correlation coefficient of the best-fitted line for the results of the Whitson and Torp correlation is about 0.6214. Furthermore, the values of RMSE and SD for the Wilson correlation are 3.7551 and 4.4659, correspondingly. It means that the Whitson and Torp correlation predicted the equilibrium ratio much better than two previous models; however, the accuracy not enough yet.

The correlation coefficient of the best-fitted line for the results of the Almehaideb correlation is about 0.2880. Furthermore, the values of RMSE and SD for the Almehaideb are 4.1127 and 4.8757, respectively. It means that the accuracy of the Almehaideb correlation in the prediction of the equilibrium ratio was poorly in comparison with other employed correlations.

The correlation coefficient of the best-fitted line for the results of the McWiliam correlation is about 0.5776. Furthermore, the values of RMSE and SD for the McWiliam are 2.2259 and 3.1350, correspondingly. It means that the accuracy of the McWiliam correlation in the prediction of the equilibrium ratio as the same as Wilson correlation.

Figure 1 is a plot of real hydrocarbon K_i values vs. estimated K_i values by GA-regression method. This figure shows that the plot of experimental K_i values of hydrocarbons versus the model's predictions falls in a straight line with a slope of unity, and there is a very little scattering of actual data points in the vicinity of the line.

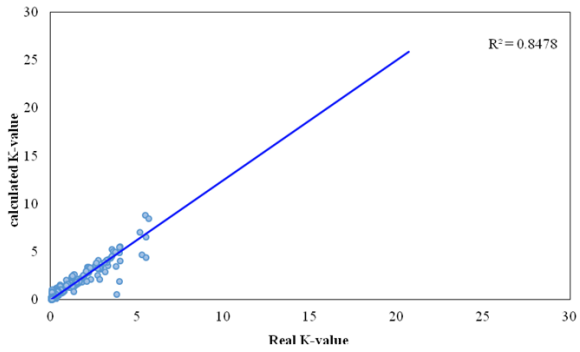

Figure 1. Scatterplot of measured and estimated equilibrium ratio (K_i) for hydrocarbons by GA-Regression method

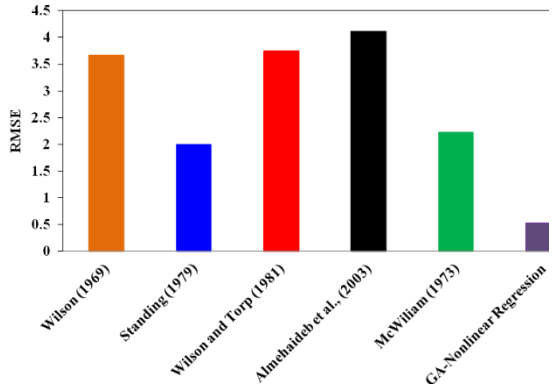

Figure 2. Comparison between root mean squared errors of used models for prediction of equilibrium ratio (K_i) for hydrocarbons

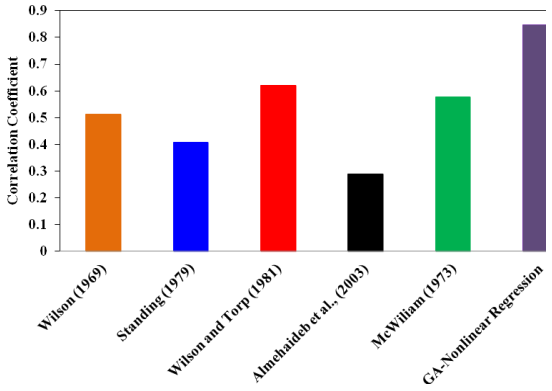

Figure 3. Comparison between correlation coefficient of used models for prediction of equilibrium ratio (K_i) for hydrocarbons

The model's excellent performance is better seen in Figure 2 in terms of root mean squared (RMSE). As clear be seen from Figure 2, the lowest value of RMSE is for GA-regression method proposed in this study. Moreover, the highest value of RMSE is for Almehaideb correlation. This means that the outputs of GA-regression method have the lowest deviation from experimental ones. Conversely, the outputs of Almehaideb correlation have the highest deviation from experimental ones.

Finally, Figure 3 shows the correlation coefficient of the five conventional approaches alongside the correlation coefficient of the proposed model of this study. As yet again shown in this figure, the proposed model is by far more accurate in predicting equilibrium ratios of hydrocarbons in comparison with the conventional methods. Table 3 shows the calculated values of RMSE, Standard deviation (SD), R and R^2 for all methods employed in this study. According to this table, the R^2 values are close to unity, and the RMSE is very low (close to zero) for the hydrocarbons. This shows that the model has satisfactory performance.

Table 3. Comparison between performances of GA-Regression method with optimized coefficients and other conventional methods for prediction of equilibrium ratio (K_i) of hydrocarbons in terms of statistical parameters

	RMSE	SD	R	*R2*
Wilson (1969) [8]	3.6724	4.4925	0.8697	0.5138
Standing (1979) [7]	1.9907	2.3102	0.6841	0.4074
Whitson and Torp (1981) [2]	3.7551	4.4659	0.8819	0.6214
Almehaideb *et al.*(2003) [10]	4.1127	4.8757	0.7918	0.2880
McWiliams (1973) [9]	2.2259	3.1350	0.8911	0.5776
GA-Nonlinear Regression	0.5247	0.9458	0.9415	0.8478

6. Conclusions:

According to the findings of this study the following conclusions can be made:

1- The viability and ability of the GA-Regression method to estimate equilibrium ratio of hydrocarbons were successfully proven based on accurate experimental database extracted from the open literature.

2- A hybrid of a nonlinear regression method and GA is shown to have promising outcomes for estimating the equilibrium ratio of hydrocarbons. The results of the proposed method have a good agreement with the experimental data. The correlation coefficients and root mean squared errors of the model are 0.8478 and 0.5247 for equilibrium ratios of hydrocarbons, respectively.

3- The proposed modeling technique is found to have favorable characteristics including generalization and efficiency and it is also simple to perform.

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