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Modelling Interfacial Tension of Crude Oil-Brine-Anionic Surfactant Using a Genetic Programming Approach

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Abstract

Surface active agents (surfactants) as the most important chemicals to enhance oil recovery (EOR) can reduce interfacial tension between the injected aqueous solution and the oil in a reservoir. Moreover, they change wettability of the porous media to release and move the remaining oil trapped in the pores and throats towards the well. According to the important roles of the surfactants, it is necessary to predict their performance for EOR process. In this research, two data-based mathematical models were developed to estimate interfacial tension of the oil, salty water and anionic surfactant system using 598 experimental data. To obtain the correlations between the independent variables and the objective function, genetic programing has been applied. Squared correlation coefficient (R^2) of the models is 0.946 and 0.9387; moreover, root-mean-square deviation (RMSD) of the models is 3.4439 mN/m and 3.3261 mN/m respectively. Simplicity and acceptable estimation are particular features of the models.

Keywords: Interfacial Tension, Anionic Surfactant, Crude Oil, Salty Water, Mathematical Model, Genetic Programing.

Introduction

Surface active agents (surfactants) are known as the main materials in chemical enhance oil recovery (EOR), and their key role is to reduce the amount of the trapped residual oil in the pore volumes by reducing the interfacial tension (IFT) between injected aqueous solution and the reservoir crude oil which leads to microscopic displacement of oil to the wells [1]. This process is also known as surfactant flooding in which a certain concentration of surfactant and some soluble salts (such as NaCl, $CaCl_2$, etc.) are dissolved in water and injected to the reservoir. Residual oil saturation decreases due to increasing viscose forces and/or reduction of capillary forces on oil droplets. To investigate these two important forces, there is a dimensionless quantity called "capillary number" that is defined as the ratio of viscous forces to capillary forces [1]:

$$N_c = \frac{v\mu}{\sigma \cos\theta} \quad (1)$$

v, μ and σ are velocity of the injected fluid in the pores, viscosity of the displacing phase (injection flood) and the IFT between displacing and displaced phases (oil reservoir) respectively. ϑ is the angle between the higher-density fluid (aqueous solution) and the rock surface and N_c is the capillary number. By increasing the capillary number, more oil can be produced. The capillary number increases with lowering the IFT which is implemented by adding surfactant to the injected fluid [1].

Surfactants are highly diverse due to their molecular structure and consequently, have different functions in the process of chemical flooding. Hence, it is necessary to evaluate the surfactant parameters for selection of the suitable surfactants. The modeling techniques are usable to estimate and select the best conditions for implementing the process.

Several researches and different laboratory experiments [2-4] have examined the effects of different factors on IFT. Briefly, the variables affecting the interfacial tension of the aqueous solution-crude-surfactant system can be classified as follows (based on the Table 1).

The most famous method for estimating IFT was presented by Gibbs [1] which is used highly in thermodynamics:

$$\Gamma_i = -\frac{1}{nRT}\left(\frac{\partial\sigma}{\partial Ln(C_i)}\right)_T \quad (2)$$

Γ_i, T and Ci are surfactant surface concentration, temperature and surfactant concentration in the aqueous solution, respectively. n is surfactant number which is 2 or more. By plotting the IFT data vs. surfactant concentration, it is observed that the IFT value is almost constant at the critical micelle concentration (CMC) and larger concentrations. An example of this diagram is shown in Figure 1. According to Eq. 6, the surfactant surface concentration is calculated from the slope of such diagram.

Table 1: Variables affecting intermediate level elasticity of aqueous solution - Crude oil - surfactant.

Environmental parameters	Aqueous solution parameters	Crude oil parameters
Temperature	pH	Specific gravity
Pressure	Salinity	Acid number
	Surfactant concentration	Oil composition
	Surfactant structure	

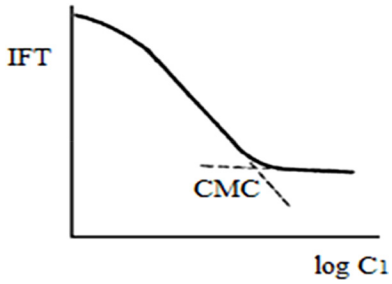

Figure 1: IFT vs. logarithm of surfactant concentration.

In the present study, a new method is proposed for estimating IFT for a number of anionic surfactants based on genetic programming.

Materials and methods

Collecting dataset

598 experimental data were collected from various experimental studies for modelling the IFT between crude oil and aqueous solution in the presence of anionic surfactants. In order to achieve higher accuracy, total dataset were divided into two general categories including critical concentration data (CMC) less than 1 mmol/L and the data with CMC greater than 1 mmol/L and each category was used to generate a model. In each category, 70% of the data was randomly considered as "training data" to construct the model. moreover, the remaining data (30% of the total data) were randomly divided into two groups with equal number including "external validation data" and "test data". The external validation data was used to improve the model accuracy and test data was applied to evaluate the model estimating ability.

Genetic Programming Method

Genetic programing (GP) is a well-known powerful mathematical-statistical tool which has been introduced in the early 1990s and has been developed mostly by John Koza. GP is a machine learning algorithmic methodology evolving evolutionary computer programs to execute tasks. In this method, a preliminary population of random mathematical functions is generated in the form of chromosome-like syntactic tree structures to be operated on input data. These tree structures are known as "genes" [5].

After producing the first population known as "parents", a number of parent functions are randomly chosen to form some genes and subsequently, primary model will be specified by weighted summation of all the genes with a bias term.

Then, modification of tree structures will be implemented by crossing over the best performing trees (cutting some parts of trees and replacing the cut parts between themselves). This modification is to create a new population (children) of functions and this process is often known as "generation". Generation will be repeated several times until the last population contains functions having enough ability to solve the problem, successfully.

Evaluation of Produced Models

For evaluation of new developed models, the statistical parameters including the correlation coefficient (R^2), root mean square error (RMSD) and mean absolute error (AAD) were used. These parameters are defined as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i^{exp.} - y_i^{cal.})^2}{\sum_{i=1}^{n}(y_i^{exp.} - y^{exp.ave})^2} \quad (3)$$

$$RMSD = \sqrt{(1/n)\sum_{i=1}^{n}(y_i^{exp.} - y_i^{cal.})^2} \quad (3)$$

$$AAD = \left(\frac{1}{n}\right)\sum_{i=1}^{n}\left|y_i^{exp.} - y_i^{cal.}\right| \quad (5)$$

$y^{exp.}$, $y^{cal.}$, $y^{exp.ave}$, and n are the actual values, the calculated values, mean of actual values and the number of data in the dataset, respectively. Smaller values of RMSD and AAD represent greater accuracy and the R^2 value should be near to unity.

Results and Discussion

By implementing genetic programming on input data, two relationships were found for the IFT between crude oil and saline water containing anionic surfactant. The models are as follows:

For CMC less than 1 mmol/L:

$$IFT_{O\text{-}B\text{-}AnionSurf\,(1)} = IFT_{O\text{-}B}|\ln(1.652\exp(-2\,C_S(M_W + IFT_{O\text{-}B})) - 0.7378\exp(-2\,C_S(S_{eq} + IFT_{O\text{-}B})) + 1.79\exp(\tilde{n}(-TC_S) + 29.4\,pH\,\frac{\exp(-2C_S)}{M_W} - 2.001\exp(-M_W C_S - \frac{\tilde{a}_O}{IFT_{O\text{-}B}}) - 8082\,pH\,\frac{\exp(-\frac{C_S}{\tilde{a}_O})}{(M_W(M_W + C_S))} + 0.7842\exp(-TM_W C_S) + 1.018| \quad (6)$$

For CMC more than 1 mmol/L:

$$IFT_{O\text{-}B\text{-}AnionSurf\,(2)} = IFT_{O\text{-}B}|\ln(0.7419\exp(-0.0008981\,S_{eq}C_S) - 0.6618\exp(-S_{eq} - \exp(-C_S)) + 0.1031\exp(pH - IFT_{O\text{-}B} - TC_S) + 0.2943\exp(-S_{eq} - C_S) - 0.6116\tanh(TC_S) - 0.0005594(pH - \exp(-C_S))(T - pH + M_W) - 3.002\exp(-IFT_{O\text{-}B} - C_S)(IFT_{O\text{-}B} + C_S) + 3.859)| \quad (7)$$

The Eq. 6 was developed for 6 alkanes and 9 anionic surfactants. The statistical parameters of this model are presented in Table 2. The variables of Eq. 6 are shown in Table 3.

Table 2: The statistical parameters of Eq. 6.

n_{train} = 162 R^2_{train} = 0.9559 AAD_{train} = 2.197 $RMSD_{train}$ = 3.211 mN/m	n_{test} = 35 R^2_{test} = 0.9106 AAD_{test} = 2.701 $RMSD_{test}$ = 3.7354 mN/m
$n_{ext\text{-}val}$ = 35 $R^2_{ext\text{-}val}$ = 0.9228 $AAD_{ext\text{-}val}$ =2.846 $RMSD_{ext\text{-}val}$ = 4.1161 mN/m	n_{total} = 232 R^2_{total} = 0.946 AAD_{total} =2.371 $RMSD_{total}$ =3.4439 mN/m

Table 3: The variables of Eq. 6.

variable		Range
$IFT_{O\text{-}B\text{-}AnionSurf\,(1)}$	IFT	52.980.0006 -
$IFT_{O\text{-}B}$	IFT without surfactant	52.9839.492 -
γ_o	Oil specific gravity	- 0.8743 0.6882
T	Temperature (K)	333.15293.15 -
pH	pH	7 – 11.133
S_{eq}	NaCl equivalent salinity (ppm)	0 - 5405
C_s	Surfactant concentration (mmol/L)	0 – 147.58
M_w	Surfactant mol. weight (g/mol)	761.3 - 321.56

The Eq. 7 has been produced for 3 anionic surfactants and 12 types of oleic phase. The statistical parameters and the variables of Eq. 7 are presented in Table 4 and Table 5, respectively. In the current project, by implementing genetic programming method, two new models were developed to estimate the IFT between oleic phase and and saline water in the presence of some anionic surfactants. These models have high estimation ability and simplicity compared to the Gibbs method and are applicable to industries and processes associated with IFT of the crude oil/ brine/ anionic surfactant systems. Particularly, in the process of surfactant flooding, they can be used extensively in the chemical EOR. The efficiency of these models can save the cost of various laboratory operations.

Table 4: The statistical parameters of Eq. 7.

n_{train} = 256	n_{test} = 55
R^2_{train} = 0.9489	R^2_{test} = 0.9143
AAD_{train} = 2.202	AAD_{test} = 2.680
$RMSD_{train}$ = 3.0754 mN/m	$RMSD_{test}$ = 3.9764 mN/m
$n_{ext-val}$ = 55	n_{total} = 366
$R^2_{ext-val}$ = 0.9101	R^2_{total} = 0.9387
$AAD_{ext-val}$ =2.825	AAD_{total} =2.368
$RMSD_{ext-val}$ = 3.7163 mN/m	$RMSD_{total}$ =3.3261 mN/m

Table 5: The variables of Eq. 7.

variable		Range
$IFT_{O-B-AnionSurf (2)}$	IFT	0.033 to 52.49
IFT_{O-B}	IFT without surfactant	52.49 - 3.235
T	Temperature (K)	292.65333.15-
pH	pH	7 - 6.65
S_{eq}	NaCl equivalent salinity (ppm)	0 - 80000
C_s	Surfactant concentration (mmol/L)	79.984 – 0
M_w	Surfactant mol. weight (g/mol)	309.5 - 265.44

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