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DEVELOPMENT OF AN ARTIFICIAL NEURAL NETWORK ALGORITHM FOR PREDICTION OF ASPHALTENE PRECIPITATION

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Abstract

The Precipitation and deposition of crude oil polar fractions such as asphaltenes in petroleum reservoirs reduces considerably the rock permeability and the oil recovery. Therefore, it is of great importance to determine "how" and "how much" the asphaltenes precipitate as a function of pressure, temperature and liquid phase composition. In present work, an Artificial Neural Network (ANN) model was designed and applied to predict the amount of asphaltene precipitation at a given operating condition. Among this training the back-propagation learning algorithm with different training methods were used. The most suitable algorithm with appropriate number of neurons in the hidden layer which provides the minimum error was found to be the Levenberg-Marguardt (LM) algorithm. An extensive experimental data for the amount of asphaltene precipitation at various temperatures (293-343 K) was used to create the input and target data for generating the ANN model. The predicted results of asphaltene precipitation from ANN model was also compared with the results of proposed scaling equations in the literature. The results revealed that scaling equations cannot predict the amount of asphaltene precipitation adequately. While an acceptable quantitative and qualitative agreement between experimental data and predicted amount of asphaltene precipitation for all ranges of dilution ratio, solvent molecular weight and temperature was obtained through using ANN model.

Keywords: Asphaltene Precipitation; Scaling Equation; Artificial Neural Network; Dilution Ratio; Molecular Weight; Temperature.

1. Introduction

Crude oils have complex composition; hence characterization by the individual molecular types is not possible. Instead, hydrocarbon group type analysis is commonly employed ^[1, 2]. The SARA separation is an example of such group type analysis, separating the crude oils in four main classes based on differences in solubility and polarity. Instead of molecules or atoms, certain structures are here considered as the components of the crude oil. The four SARA fractions are saturates, aromatics, resins and asphaltenes. Asphaltenes are high-molecular weight solids which are soluble in aromatic solvents such as benzene and toluene and insoluble in paraffinic solvents ^[3-5]. Asphaltene precipitation is one of the most common problems in both oil recovery and refinery processes. In oil recovery, especially in gas injection, formation of asphaltene aggregation, following their deposition causes blocking in the reservoir. This makes the remedial process costly and sometimes uneconomical. Unfortunately, there is no predictive model for asphaltene problem treatment. Hence it is necessary to predict the amount of asphaltene precipitation, as a pre-emptive measure. The major questions in facing such problems are "How" and "How much" heavy organic compounds will precipitate in operational condition. Over the years, many researchers have tried to find the answer. They introduced experimental procedures or even analytical models, but a fully satisfactory interpretation is still lacking. The problem is very difficult mainly because of the fuzzy nature of asphaltene and the large number of parameters affecting precipitation. The existing models fall into three categories:

(I) Molecular thermo-dynamic models in which asphaltenes are dissolved in crude oil and crude oil forms a real solution ^[6-10]. The validity of such models depends on the

reversibility of asphaltene precipitation. Reversibility experiments strongly support this type of models ^[8, 11-13].

(II) Colloidal models in which, asphaltene is suspended in crude oil and peptized by resins. The asphaltene precipitation is irreversible in such models ^[14-16]. Reversibility experiments are strongly against this type of models.

(III) Models based on scaling equation, in which the properties of complex asphaltenes are not involved ^[17-20]. Analytically, an EOS used for calculating thermodynamic parameters assuming asphaltene precipitation is completely reversible. The calculation process is often found to be a difficult task because of the complexity of asphaltene. Nevertheless, neither using EOS nor assuming asphaltene reversibility brings enough accuracy and trustable results.

2. Scaling Equation

Rassamdana et al. ^[17] gathered extensive experimental data for the amount of precipitated asphaltene formed with crude oil and various solvents ($n-C_5$ to $n-C_{10}$). All experiments were performed at atmospheric pressure and room temperature. They employed a thermodynamic model that uses Flory-Huggins theory of polymer solutions and an equation of state was also used for predicting the experimental data, and its predictions were found in disagreement with the data. As an alternative, they proposed a simple scaling equation that appears to be capable of providing accurate prediction for the data. They assumed that formation of asphaltene structure is to some extent similar to aggregation and gelation phenomena. These phenomena are associated with universal properties independent of many microscopic properties of their structure.

To develop such scaling equation, they manipulated three main variables: W, amount of asphaltene precipitated (wt %), R_v , solvent to oil dilution ratio (mL/g), M_w , molecular weight of solvent, and combined them into two new variable X and Y in which:

$$X = R_v / M_w^{Z}$$

$$Y = W / R_v^{Z'}$$
(1)
(2)

Z and Z^{\sim} are two adjustable parameters and must be carefully tuned to obtain the best scaling fit of the experimental data. They suggested Z^{\sim} is a universal constant of -2 and Z = 0.25 regardless of oil and precipitant used. The proposed scaling equation is expressed in terms of X and Y through a third-order polynomial function

$$Y = A_1 + A_2 X + A_3 X^2 + A_4 X^3 \quad (X > X_c)$$
(3)

where X_c is the value of X at the onset of asphaltene precipitation.

Yu-Feng Hu et al. ^[19] performed a detailed study on the application of scaling equation proposed by Rassamdana et al. ^[17] for asphaltene precipitation. They checked the predictive capability of the scaling equation in comparison with literature precipitation data and reported that the scaling equation is an attractive tool for modeling asphaltene precipitation. They examined the universality of exponents *Z* and *Z* and found that *Z* is a universal constant (*Z* =-2) while exponent *Z* depends on the oil composition and independent of specific precipitant (n-alkane) used. For the experimental data used, they found also that the optimum value of *Z* is generally within the range of $0.1 \le Z \le 0.5$.

Despite the simplicity and accuracy of the scaling equation mentioned above, it is restricted to use at a constant temperature and since temperature is not involved in the scaling equation as a variable, it is not adequate for correlating and predicting the asphaltene precipitation data measured at different temperatures. Due to this issue, Rasamdana et al. ^[18] modified their scaling equation by implanting temperature parameter in the scaling equation. Based on the previous equation, they defined two new variables *x* and *y*:

$$x = X / T^{CT}$$

$$(4)$$

$$y = Y / X^{C2}$$

$$(5)$$

in which X and Y are variables defined as in equations (1) & (2) and constant C1 and C2 are adjustable parameters. They reported that the good fit of their experimental data can be achieved by setting C1 = 0.25 and C2 = 1.6.

Again the new scaling equation is a 3rd order polynomial in general form of:

$$l = b_1 + b_2 x + b_3 x^2 + b_4 x^3 \quad (x > x_c)$$
(6)

Fig. 1 shows the collapse of all data onto scaling curve using above equation.

Yu-Feng Hu et al. ^[20] studied the effect of temperature, molecular weight of n-alkane precipitants and dilution ratio on asphaltene precipitation in a Chinese crude oil experimentally. The amounts of asphaltene precipitation at four temperatures in the range of 293-338 K were measured using seven n-alkanes as precipitants. They found that their experimental data could not be well correlated by setting C1 = 0.25 and C2 = 1.6 recommended by Rassamdana et al. ^[18]. They reported that their experimental data could be correlated successfully by choosing C1 = 0.5 and C2 = 1.6. They showed that the proposed new scaling equation is adequate for correlating and predicting the asphaltene precipitation data measured at different temperatures using various n-alkane precipitants. Fig. 2 depicts the collapse of all data onto a single curve using their equations.





Fig. 1 Collapse of data onto a single curve by Rasamdana et al. scaling equation. (x = X / T C1 & y = Y / X C2)^[18]

Fig. 2 Collapse of data onto a single curve Yu-Feng Hu et al. scaling equation^[20]. $(X=R_v / M_w^{0.5}T^{0.25}) \& Y = W / (M_w R_v)^{-0.4})^{-0.4}$

Ashoori et al. ^[21] also studied the amount of asphaltene precipitated at various temperatures and atmospheric pressure. At each temperature some n-alkanes were used as precipitants at various dilution ratios. Their proposed scaling model includes the following two equations:

$$X = R_v / (T^n . M_w^Z)$$
(7)
$$Y = W / R_v^{Z'}$$
(8)

In this equation, X altered by implementing temperature parameter but Y had no change. The exponent n is a constant chosen between 0.10 and 0.25. Two other constants, Z and Z', are the same as the first scaling equation, i.e. Z = 0.25 and Z' = -2. For this scaling equation introduced in Eq. (8) and Eq. (2) the best match was gotten by setting n = 0.15. Fig. 3 shows the collapse of all data onto a single curve using their equations.

3. Artificial Neural Network Model

Neural networks are composed of simple elements operating in parallel. These elements are inspired by biological nervous systems. As in nature, the network function is determined largely by the connections between elements. One can train a neural network to perform a particular function by adjusting the values of the connections (weights) between elements. Commonly neural networks are adjusted, or trained, so that a particular input leads to a specific target output. Such a situation is depicted in Fig. 4. There, the network is adjusted, based on a comparison of the output and the target, until the network output matches the target. Typically many such input/target pairs are needed to train a network.

In this network, extensive data of the amount of asphaltene precipitation as a change of dilution ratio, molecular weight of n-alkane and temperature were used to generate ANN model. Fig. 5 shows the detail of designed network. As it is shown, dilution ratio, molecular weight of n-alkane and temperature were used as a input data and the amount of asphaltene precipitation was use as a target data. The network has three layers, Layer1, 2 and 3 that has 10, 5 and 1 neurons respectively. It should be mentioned that the number of neurons for each layer was determined after several iterations. 60% of experimental data was used to train the network and the rest 40% of data was used to test the network simulation.





Fig. 3 Collapse of data onto a single curve Ashoori et al. scaling equation.

 $(X = Rv / (T n.MwZ) \& Y = W / Rv Z')^{[21]}$





Fig. 5: Schematic of the designed ANN for simulation of asphaltene precipitation

4. Results and Discussion

Figures 6 through 8 show the comparison of experimental data with simulated values for the amount of asphaltene precipitation by Rassamdana et al. ^[18], Yu-Feng Hu et al. ^[19] and Ashoori et al. ^[21] scaling equations respectively. Considering these figures reveals that the predicted results by Rassamdana et al. scaling equation is not satisfactory respect to two other scaling equations. Error analysis of these three equations shows that the Yu-Feng Hu et al. ^[19] scaling equation is more accurate to predict and simulate the amount of asphaltene precipitation at different operating conditions (molecular weight of n-alkane precipitants, dilution ratio and temperature).



Fig. 6 Comparison of experimental data with simulated values for all data by Rasamdana et al. scaling equation. (x = X / T C1 & y = Y / X C2)^[18]



Fig. 7 Comparison of experimental data with simulated values for all data by Yu-Feng Hu et al. scaling equation^[20]. (X=Rv/(Mw 0.5T 0.25) & Y=W/(MwRv)-0.4)



Fig. 8 Comparison of experimental data with simulated values for all data by Ashoori et al. scaling equation. $(X = Rv / (T n.MwZ) \& Y = W / Rv Z')^{[21]}$

Fig. 9 Comparison of experimental data with simulated values that used to train the network.

Figures 9 through 11 depict the comparison of simulated values of asphaltene precipitation by ANN model with experimental data. Fig. 6 shows the comparison between simulated and experimental data that used to train the network. In Fig. 7, the values of weights and bios (W & b) that obtained through training the network are applied to simulate some other data to test the network. The agreement between simulated and experimental values of asphaltene precipitation in this figure confirms the ability of network to simulate and predict the amount of asphaltene precipitation for other ranges of dilution ratio, molecular weight of solvent and temperature. Fig. 8 shows the simulation of all input data respect to measured value for asphaltene precipitation.

12

10

8

6

4

Wt% (Simulated)



Ω 4 б 10 12 8 Wt% (Experimental) Fig. 11 Comparison of experimental data

Fig. 10 Comparison of experimental data with simulated values that used to test the network.

with simulated values for all data that simulated by the network.

Table 1 illustrates the accuracy of each method to predict the amount of asphaltene precipitation by comparison the relative absolute deviation (σ) and average relative absolute deviation ($\bar{\sigma}$) of simulated data. σ and $\bar{\sigma}$ are defined as follows:

$$\sigma = \sum_{i=1}^{n} \left| \left(Wt_{Exp} - Wt_{Cal} \right) / Wt_{Exp} \right|$$

$$\overline{\sigma} = \sum_{i=1}^{n} \left(\left(Wt_{Exp} - Wt_{Cal} \right) / Wt_{Exp} \right) / n$$
(8)
(9)

Table 1: Relative absolute deviation (σ) and average relative absolute deviation ($\bar{\sigma}$) for simulated data

| Method | Rassamdana et al. Eq. ^[18] | Yu-Feng Hu et al. Eq. ^[19] | Ashoori et al. Eq. ^[21] | ANN Model |
|--------|--|--|---------------------------------------|-----------|
| σ | 169.31 | 137.43 | 144.87 | 64.43 |
| ā | 0.64 | 0.52 | 0.55 | 0.24 |

As it is apparent, the deviation is the less for ANN model, while it is much higher for scaling equations. This analysis shows that the ANN model is more accurate than the other methods to simulate the asphaltene precipitation.

5. Conclusion

In this work, an Artificial Neural Network (ANN) model was developed to predict and simulate the amount of asphaltene precipitation as a function of dilution ratio, molecular weight of solvent and temperature. Furthermore, the results from ANN model were compared with predicted values using some scaling equations such as Rassamdana et al. ^[18], Yu-Feng Hu et al. ^[19] and Ashoori et al. ^[21] scaling equations. Finally it was concluded that scaling equations were not capable enough to predict and simulate the amount of asphaltene precipitation for all ranges of dilution ratio, molecular weight of solvent and temperature and their results were not fully satisfactory. Conversely, the developed ANN model had better fit than the above equations and adequately predicted and simulated the asphaltene precipitation.

Nomenclature

Symbols:

| R_v | Dilution ratio |
|---------------------------|--|
| M_w | Molecular weight of the solvent |
| T | Temperature |
| W_t | Weight percent of asphaltene precipitation |
| Z, Z', c_1, c_2 and n | Constants |
| A_i | Scaling equation coefficients of Eq. (3) |
| X | Function defined by Eq. (1) |
| Y | Function defined by Eq. (2) |
| b_i | Scaling equation coefficients of Eq. (6) |
| X | Function defined by Eq. (4) |
| y | Function defined by Eq. (5) |
| ANN | Artificial Neural Network |
| W | Weight |
| W | Weight |
| B | Bias |
| - | |

Greeks:

- σ Relative absolute deviation defined by Eq. (8)
- $\bar{\sigma}$ Average relative absolute deviation defined by Eq. (9)

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