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Prediction and extension of curves of distillation of vacuum residue using probability functions

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Prediction and extension of curves of distillation of vacuum residue using probability functions

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Abstract. The use of the probability functions for the prediction of crude distillation curves has been implemented in different characterization studies for refining processes. The study of four functions of probability (Weibull extreme, Weibull, Kumaraswamy and Riazi), was analyzed in this work for the fitting of curves of distillation of vacuum residue. After analysing the experimental data was selected the Weibull extreme function as the best prediction function, the fitting capability of the best function was validated considering as criterions of estimation the AIC (Akaike Information Criterion), BIC (Bayesian information Criterion), and correlation coefficient R2. To cover a wide range of composition were selected fifty-five (55) vacuum residue derived from different hydrocarbon mixture. The parameters of the probability function Weibull Extreme were adjusted from simple measure properties such as Conradson Carbon Residue (CCR), and compositional analysis SARA (saturates, aromatics, resins and asphaltenes). The proposed method is an appropriate tool to describe the tendency of distillation curves and offers a practical approach in terms of classification of vacuum residues.

1. Introduction

Global trends show an increase in the production of heavy crude oil, with which high yields are projected in the production of atmospheric residues and vacuum residues. In order to take advantage of the products obtained from the new diets refining on fuel demand, it has been showing great interest in the study of the characterization of the vacuum residues, to expand their knowledge about the behaviour new refining schemes. The vacuum residues have atmospheric points higher than 525 ° C and operational are classified as the non-distillable fraction of petroleum vacuum distillation conditions [1, 2]. These charges are considered as a complex mixture of many components and their processing is related to the chemical structure of their species [3, 4].

The characterization of the crudes and vacuum residues plays an important role on predicting yields products obtained in refining processes. One method of characterization is the distillation curve TBP (True Boiling Point); it provides information on the composition of raw materials and performance. For heavier hydrocarbon fractions TBP curve is obtained from the ASTM D1160 and ASTM D7169. However, the vacuum residues with high concentrations of asphaltenes and resins have the limitation on the distillate yield, because their end boiling point is about 50% of the distillate volume. For reasons of operation it is important extend the curves of distillation of the vacuum residues, from the available data. To this end, it is possible to use probability functions that help to predict such points from the known properties.

Several authors have used probability functions to classify and study the trend of the crude distillation curves of different nature. For example, Behrenbruch et al. [5], they developed a methodology for ranking of the crude, based on the form of the distillation curve parameters using the probability function Gamma. Sanchez et al. [6] determined that the adjustment of the curves of distillation for oil fractions, from probability functions with four parameters, shown best fit compared with experimental data. Haitham et al [7] estimated the prediction of the curves of distillation of distillates obtained in the hydrotreating of vacuum gas oil, using the probability function of Riazi and adjusting the parameters with the density of the products.

The main objective of this work is to develop a methodology for predicting and extension distillation curves TBP of the vacuum residues, using probability functions. For this purpose, four probability functions were evaluated in order to find the function with greater adjustment capacity for data TBP of the vacuum residues. For the evaluation of these functions the statistical criteria AIC (Akaike Information Criterion) and BIC (Bayesian Information Criterion) were used.

2. Experimental methodology

For the development of this work, fifty-five (55) vacuum residues were selected. The characterization was carried out using the ASTM methods for the following properties: Conradson Carbon (CCR) D-4530, D-7169 simulated distillation and compositional analysis SARA D-2007.

2.1. 2.1 Evaluation of probability functions

50 samples were selected to evaluate the adjustment of the probability functions Weibull extreme, Weibull, Kumaraswamy and Riazi. Subsequently, 5 samples for validation of the selected probability function were taken. For this purpose, temperatures were normalized so that all temperature values were between values of zero and one, using the following equation:

$$\theta_i = \frac{T_i - T_0}{T_l - T_0} \tag{1}$$

Where θ_i is the dimensionless temperature, T_i is the average temperature current boil, and T_0 and T_l are reference temperatures, that for the development of this study were 150 and 750, respectively. The parameters of probability functions were calculated with the optimization of the residual sum of squares (RSS), from the difference between the experimental weight fractions and calculated for each point of temperature. The predictive ability of the probability functions; it was evaluated from the statistical criteria AIC (Akaike Information Criterion) and BIC (Bayesian Information Criterion) [8]. The parameters AIC and BIC are indicators that take into account the complexity of a model and the good fit of the data with a minimal number of parameters. These statistical criteria are determined by the following expression:

$$AIC = 2k + n\ln\left(\frac{RSS}{n}\right) \tag{2}$$

$$BIC = k\ln(n) + n\ln\left(\frac{RSS}{n}\right) \tag{3}$$

Where k represent the number of parameters, n the number of observations and RSS the residual sum of squares. To evaluate the extent of the curves of distillation, from the functions of probability were selected the points T_5, T_{10}, T_{20}, T_{30}, T_{40} y T_{50}. To adjust the maximum point of distillation for the extension of the distillation curves was chosen as a reference the percentage of total distillate maltenes (saturates aromatics and resins). For this purpose, the TBP curves of vacuum residues were compared with the TBP curves reconstructed from the data TBP fractions of saturates, aromatics and resins.

To extend the study of predicting the TBP curve was divided into three study areas. The first region corresponds to the region between the T_5 and $T_{50.}$ The region 2 corresponds to the region between the T_{50} and the final boiling point FBP of the vacuum residues validation. The last region is the extension of the distillation curve from the final boiling point FBP to the point where the maximum proportion corresponding to maltenes distillable fraction is obtained.

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3. Results and discussion

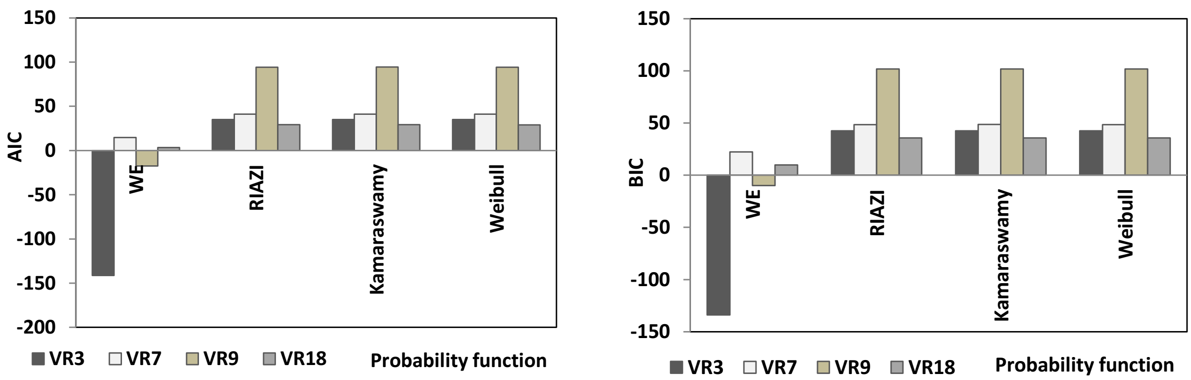
The Table 1 shows that data from the selected vacuum residues differ significantly in their properties. The content of saturates, aromatics, resins and asphaltenes vary by a factor of 4, 1.5, 2.5 y 6, respectively.

Table 1. Characterization of vacuum residues.

Property	Method	Min.	Max.
CCR (%wt)	ASTM D-4530	15	30
Saturated (%wt)	ASTM D-2007	6	23
Aromatic (%wt)	ASTM D-2007	36	55
Resins (%wt)	ASTM D-2007	15	37
Asphaltenes (%wt)	ASTM D-2007	5	30
T50, °C	ASTM D- 7169	638	747

3.1. Selecting of the probability function

The Figure 1 shows the results of AIC and BIC for different randomly selected samples and evaluated with the four (4) probability functions. Considering the results of the statistical criteria AIC and BIC it is noted that the probability function Weibull Extreme presents the best adjustability for the data of TBP curves of vacuum residues. The analysis of the remaining 46 samples presented a similar behaviour.



(a) (b)

Figure 1. Statistical parameters: (a) AIC and (b) BIC.

3.2. Extension of distillation curves

In Figure 2 an insignificant difference was observed in Zone 1 between the temperatures T5 to T50 experimental and calculated with the probability function Extreme Weibull (WE), for the vacuum residue 2. In general, it was determined that the average deviation for validation vacuum residues in zone 1 was 1.23°C. Meanwhile, the extension of the distillation curve in zone 2 with the probability function, from the T50 until the end boiling point corresponding to 61% in weight of distilled of the vacuum residue 2, has an average deviation of 1.15°C. The results indicate that the probability function evaluated has a satisfactory performance in the prediction and extension of distillation curves until the end boiling point FBP of the vacuum residues.

Figure 2 shows that the boiling temperature for validation vacuum residue is available to 61% by weight of distillate, so it is necessary a greater extent considering as reference the percentage of total maltenes distillates. The TBP curve of the vacuum residues depends of the nature of his components, for this reason the TBP curve of validation samples was reconstructed from the TBP curve of fractions SAR, for the purpose of comparing their behaviour with extended curve with the proposed methodology. The results indicate that the boiling points of the curve extended with the probability function Extreme Weibull are close to the values obtained with the distillation curve recombined.

Therefore, at the time of the extension through the proposed methodology, this have a behaviour similar to the nature of the sample trends.

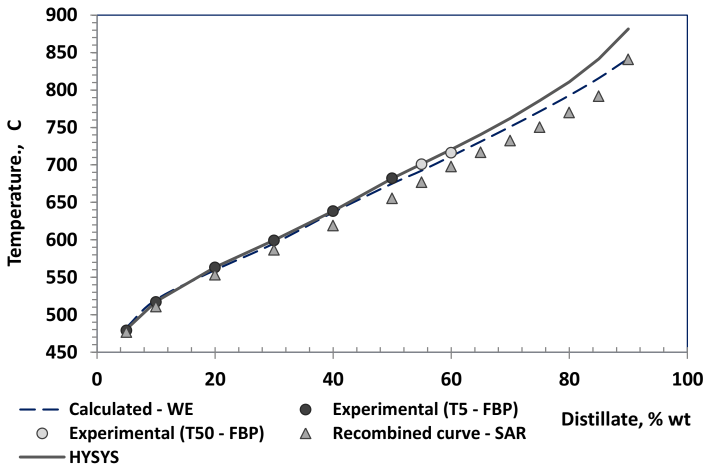


Figure 2. Extension of the distillation curve of vacuum residue 2.

Comparing the curve extension with the proposed methodology and the extended curve with the program ASPEN HYSYS V8.0, it is observed that the prediction curve program ASPEN HYSYS has a greater deviation from the end boiling point of the total percentage of distillate curve reconstructed from the SAR fractions.

4. Conclusion

The probability function with greater ability to fit the data of the curve of distillation of the vacuum residues was the Weibull Extreme, and as second option is the three parameters Riazi.

The recombined curve of the vacuum residue from total percentage of the fraction of maltenes is a criterion of reference to evaluate the methodology of extension from the probability functions.

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