A model to predict physical properties for light lubricating oils and its application to the extraction process by furfural

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Abstract

In the lubricating oil manufacturing process, the aromatic content of vacuum distillates is reduced by solvent extraction, frequently with furfural. In this work, a method based on average pseudo-components properties is developed to calculate physical properties (density, refractive index and sulfur content) of hydrocarbon mixtures. Obtained values were compared to those calculated by other methods reported in the literature, obtaining similar results. In order to simulate the extraction operation, a model based on a reduced number of pseudo-components and the NRTL model is reported for the system furfural+SPD lubricating oil. Thereafter, the extraction operation was simulated by using such model and Aspen Plus$^{®}$ commercial software. Good agreement was found between predicted and experimental values of yield, furfural content, composition and physical properties for raffinates and extracts.

Keywords: Extraction, liquid-phase equilibria, separation, simulation, light lubricating oil, furfural.

1. Introduction

In the process of manufacturing lubricating mineral oil, the removal of aromatic hydrocarbons from vacuum distillates is required to improve several lubricating properties (Sequeira, 1994; Singh et al., 1978). The residue from the crude oil atmospheric distillation (long residue) is transferred to a vacuum distillation column and separated into different lube oil cuts, characterized by their boiling range and viscosity. Five raw cuts are commonly obtained, called SPD (spindle distillate), LND (light neutral distillate), MND (medium neutral distillate), HND (heavy neutral distillate) and BSD (bright stock distillate).

For many years, several works have been focused on looking for selective solvents for aromatics extraction from hydrocarbon mixtures (Vakili-Nezhaad et al., 1999). A good solvent has to maximize differences in properties between the liquid phases to reduce the loss of oil (Sequeira, 1994). Furfural is one of the most widely used solvents because its selectivity towards aromatic compounds is high enough and decreases slowly with increasing temperature. In addition, such selectivity is acceptable for both light and heavy vacuum distillates as reported by different authors (De Lucas et al., 1993).

The design and simulation of solvent extraction processes have been performed mostly by fully empirical methods (Rahman et al., 1984), requiring experimental information usually not available. Such approach is usually expensive because large experimental determination is needed. Rigorous modeling of the extraction process would be a suitable tool to simulate changes in operating conditions or feed quality, and thus to properly describe the liquid-liquid equilibrium (LLE) established in the extraction operation, a consistent thermodynamic model is needed.

Complex mixtures such as petroleum fractions must have their composition defined by empirical methods because it is not possible to identify all the individual compounds present (Hariu and Sage, 1969). The pseudo-components approach based on distillation curves is widely used to represent the complex composition of petroleum fractions (Briesen et al., 2004), although it is not effective in LLE modeling because chemical structure has much bigger effect than boiling temperature. For that reason, the "molecules-type" approach should be more convenient since it makes difference according to chemical nature of compounds (Vakili-Nezhaad et al., 1999). In order to determine the composition of complex mixtures, standard test methods, such as ASTM D2007, are frequently used. However, these methods are time and money consuming and, therefore, composition data are not usually available. For that reason, the characterization of petroleum mixtures is frequently carried out by their physical properties. Such properties can be experimentally determined, but usually are calculated by correlating with other ones. Many relations between properties have been reported in the literature. In this study, only a few ones concerning with density, refractive index and sulphur content will be considered, since these properties are commonly used to characterize lubricant mixtures. Gomez (1989) developed a method to calculate the liquid density for petroleum mixtures, using as experimental information temperature, specific gravity and Watson factor. Reported results show the suitability of such correlation to calculate density for petroleum mixtures within the range 313-923K. Riazi and Roomi (2001) have reported correlations to calculate both liquid density and refractive index using as experimental information specific gravity, molecular weight and mean average boiling point of the mixtures. Good results are reported for pure compounds and for petroleum mixtures with boiling point up to 575K. However, results for heavier fractions were not reported. In order to calculate density, the American

Petroleum Institute has reported different relations for petroleum fractions with molecular weight ranging from 70 to 700 and boiling point up to 840K. Riazi et al., (1999) have proposed a method to calculate the sulfur content for petroleum mixtures with molecular weight ranging from 75 to 1500 and sulfur contents up to 6%. These authors found a good agreement between calculated and experimental values for a wide range of petroleum mixtures. Therefore, the correlation between physical properties and composition appears as the key point for the characterization of complex hydrocarbon mixtures. According to that, different authors as Riazi and Daubert (1986) have proposed correlations between the composition (in paraffins, naphtenes and aromatics) and the physical properties (such as the refractive index and the viscosity) for the petroleum mixtures, obtaining good results.

Thermodynamic models, such as NRTL (Renon and Prausnitz, 1968) and group contribution methods have been used to describe LLE in the system solvent+lubricating oils. Different authors (Letcher et al., 2003; Morawski et al., 2003) have recently correlated LLE data for the system furfural+hydrocarbon by means of NRTL and UNIQUAC thermodynamic model. Likewise, De Lucas et al. (1993) have shown that the system furfural+heavy lubricating oils presents type I isotherms and therefore, NRTL model is the most appropriate model to describe LLE in such systems.

Recently, we have reported a method to correlate average pseudo-components properties with composition (in saturates, aromatics and polars) for calculating physical properties (such as the refractive index) of the involved mixtures (feed, raffinates and extracts) (van Grieken et al., 2005). In addition, a model based on such pseudo-components and the NRTL model was developed to simulate the extraction operation for the system furfural+heavy neutral distillates, obtaining good results.

In this work, a model was developed to describe the LLE established in the system furfural+light lubricating oil (SPD). The liquid phases (feed, raffinates and extracts) were considered formed by three groups of pseudo-components: saturates (S), aromatics (A) and polars (P). In order to calculate pseudo-component properties (specific gravity, density, refractive index and sulfur content) the method reported was followed. NRTL parameters were calculated by correlating compositions of the different extraction experiments for the considered system at different temperatures and furfural/feed ratios. Consequently, the LLE can be described by means of a thermodynamic model with a reduced number of parameters.

The accuracy of the pseudo-component method and the thermodynamic model was checked by performing eight extraction runs with other SPD lubricating oil, modifying the extraction temperature or the furfural/feed ratio in each experiment. The composition of the different hydrocarbon mixtures (feed, raffinates and extracts) lumped in saturates, aromatics and polars was determined following the ASTM D2007 standard test method. In addition, specific gravity, liquid density and refractive index at 343K and 293K, sulfur content and distillation curves of these mixtures (feed, raffinates and extracts) were experimentally determined by means of ASTM D1298, ASTM D1747, ASTM D4249 and ASTM D2887, respectively (Annual book of standards, 2003). Values for density, refractive index and sulfur content were calculated and compared to those ones obtained by the different methods reported in the literature, obtaining similar results. Finally, these extraction experiments were simulated with a commercial process simulator (Aspen Plus®) including the developed model, and a good agreement was obtained between predicted and experimental results.

In order to summarize all the parameters needed for the description of the LLE in the extraction operation, a scheme of calculations is shown in Figure 1.

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2. Experimental Section

Spindle Distillate (SPD) was provided by REPSOL-YPF from its refinery in Puertollano (Spain). Furfural was also supplied by REPSOL-YPF and distilled before use to remove the oxidation products formed due to air contact.

The experimental results for a first set of extraction experiments were supplied by REPSOL-YPF. A 2L cylindrical stirred glass reactor was used which temperature was set by recirculating silicone oil from a thermostatic bath, and controlled within $\pm0.1°C$. A gentle stream of nitrogen was passed to prevent furfural decomposition. Different conditions for extractions with furfural can be found in the literature. Singh and Kishore (1978) reported thirty minutes for agitation and two hours for settling; De Lucas et al. (1993) used two hours for agitation at 280 rpm and fifteen minutes for settling. In this work, the procedure optimised by REPSOL-YPF (Moreno, 1992) was used. Agitation was maintained at 430 rpm for one hour, followed by settling for another hour to achieve a good separation of the two phases. Furfural was removed from extracts and raffinates by vacuum distillation. Table 1 shows composition (in saturates, aromatics and polars), specific gravity (SG), liquid density at 343K (D_{343}), refractive index at 343K (RI_{343}) and sulfur content ($S\%$) of feed, raffinates and extracts determined by means of ASTM D2007, ASTM D1298, ASTM D1747 and ASTM D4294, respectively (Annual book of standards, 2003). Each mixture is denoted by a letter (R, raffinate; E, extract), followed by the corresponding number of the experiment.

In addition, a second set of eight extraction experiments for a different SPD cut was carried out following the same procedure mentioned above, but in a 0.5L cylindrical stirred glass reactor. Table 2 shows experimental conditions (temperature and furfural/feed ratio), extraction yields, and furfural content. The characterization of the

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involved mixtures (feed, raffinates and extracts) was the same as the mentioned above. Composition (in saturates, aromatics and polars), SG, D_{343}, RI_{343}, and $S\%$ of feed, raffinates and extracts are also listed in Table 2. For such mixtures, the simulated distillation curves were obtained by means of ASTM D2887 (Annual book of standards, 2003) and they are shown in Table 3.

The quality of experimental data obtained in the second set of extraction experiments was checked by mass balance. The feed composition was calculated from the composition and yield of raffinates and extracts of each experiment, and compared with the experimental value as it is shown in Figure 2. Average absolute deviations between experimental and calculated composition values for saturates, aromatics and polars were 1.2%, 1.9% and 0.9%, respectively. Such values are all within the limits of reproducibility indicated by the ASTM D2007 standard test method. Therefore, the quality of such experiments can be considered satisfactorily.

As it is shown in Tables 1 and 2, for experiments at the same temperature, lower yields of extract were obtained when decreasing the furfural/feed ratio: species undergo less dissolution in furfural, and therefore, the efficiency of the extraction is lower. Consequently, the yield of raffinate is higher. When experiments with the same furfural/feed ratio and different temperature are compared, higher temperatures increase not only aromatic, but also other compounds extraction, reducing the selectivity of the process.

The experimental compositions show that furfural dissolves preferently aromatic compounds, which is the main compound in the extract: 84.2% (T=323K, furfural/feed=1), 73.5% (T=323K, furfural/feed=9), 73.3% (T=353K, furfural/feed=1) and 57.8% (T=353K, furfural/feed=8). On the opposite, in the raffinates are present mainly saturates. Such experimental results confirm the suitability of furfural for

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extracting aromatic compounds from light distillates. An additional benefit is the extraction of polars (<2.5% in all raffinates), which are usually sulfur containing compounds, undesirable in lubricating oils, as reported before (van Grieken et al., 2005).

Extraction experiments carried out at lower furfural/feed ratios yield raffinates with higher content of aromatics, showing that extraction of aromatic species decreases when furfural/feed ratio becomes lower. As it is shown in Tables 1 and 2, raffinates of experiments carried out at the same furfural/feed ratio and different temperature do not exhibit important differences regarding aromatics content. However, the content of saturates in extracts increases with the temperature, showing that furfural selectivity towards aromatic compounds decreases.

3. Model description

A model was developed to predict both the physical properties of the mixtures and the LLE in the system furfural+SPD lubricating oil. Such model is based on a reduced number of pseudo-components, following that reported elsewhere (van Grieken et al., 2005).

3.1 Pseudo-components properties. The involved mixtures (feed, raffinates and extracts) present very complex composition and pseudo-component definition is needed. In this work, the properties considered for characterizing the pseudo-components were $T_{50\%}$, SG, D_{343}, RI_{343} and $S\%$. The first one was obtained from ASTM D1160 distillation curve and defined as the temperature at which 50 v% of the vacuum distillate used as feed is distilled. It was assumed the same value for the three pseudo-components considered: saturates, aromatics and polars. The following mixing rule was proposed to calculate hydrocarbon mixture properties:

$$P_{calc} = \left[\frac{X_S}{100} \overline{P}_S + \frac{X_A}{100} \overline{P}_A + \frac{X_P}{100} \overline{P}_P \right] \qquad (1)$$

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where P is the considered physical property and P_{calc} is the value calculated for each mixture; X_S, X_A and X_P are the compositions (in weight percent) in saturates, aromatics and polars, presented in Table 1; and finally, $\overline{P}_S, \overline{P}_A, \overline{P}_P$ are the average property for saturates, aromatics and polars. Optimum values of $\overline{P}_S, \overline{P}_A, \overline{P}_P$ are obtained by minimizing the objective function defined as the sum of deviations between experimental and calculated values for each property of the studied lubricating oil:

$$F = \sum \left| P_{\exp} - P_{calc} \right| \qquad (2)$$

The pseudo-component properties corresponding to SPD lubricating oil were calculated from experimental data reported in Table 1. Based on the experimental data for pure hydrocarbons (Riazi, 2005) and the average pseudo-component properties reported for HND (van Grieken et al., 2005) and other lubricating oil cuts (Peña, 2000), the following constrains were imposed to the values of pseudo-components properties:

- o SG, D_{343} and RI_{343} for saturates has to increase from SPD to HND.

- o SG, D_{343}, and RI_{343} for aromatics and polars have to decrease from SPD to HND (Altgelt and Boduszynski, 1994).

- o $S\%$ has to decrease when increasing the carbon number (from SPD to HND), and it has to be higher in polar compounds.

Having in mind these considerations, the minimization of equation (2) leads to average values of SG, D_{343}, RI_{343} and $S\%$ for each pseudo-component listed in Table 4. To check the accuracy of this method, the deviation of the prediction through equation (1) was calculated by means of the absolute average deviation ($\overline{\varepsilon}$) as follows:

$$\overline{\varepsilon} = \frac{\sum \varepsilon_i}{N} \qquad (3)$$

where N represents the number of mixtures considered (in this case all the mixtures reported in Table 1) and ε_i represents the absolute deviation for each mixture (i), calculated according to the following expression:

$$\varepsilon_i = \left| P_{\exp} - P_{calc} \right| \tag{4}$$

Absolute average deviation of 0.003 for the specific gravity, 0.004 for the liquid density, 0.005 for the refractive index and 0.4 for the sulfur content were obtained.

3.2 NRTL parameters. In the description of the extraction experiments, each mixture was considered formed by the solvent and three pseudo-components (Furfural+S+A+P). NRTL was the thermodynamic model used to describe the LLE established in the extraction process. The NRTL equation is based on the local composition concept and considers only binary interactions. The NRTL expression for activity coefficient is given by (Poiling et al., 2001; Prausnitz et al., 2000; Raal and Mühlbauer, 1998):

$$\ln \gamma_i = \frac{\sum\limits_{j=1}^{c} x_j \tau_{ji} G_{ji}}{\sum\limits_{k=1}^{c} x_k G_{ki}} + \sum\limits_{j=1}^{c} \left[\frac{x_j G_{ij}}{\sum\limits_{k=1}^{c} x_k G_{kj}} \left(\tau_{ij} - \frac{\sum\limits_{m=1}^{c} x_m \tau_{mj} G_{mj}}{\sum\limits_{k=1}^{c} x_k G_{kj}} \right) \right] \tag{5}$$

$$G_{ij} = \exp \left(\alpha_{ij} \tau_{ij} \right) \tag{6}$$

$$\tau_{ij} = a_{ij} + \frac{b_{ij}}{T_{ext}} \tag{7}$$

where x_i is the molar fraction of component i; α_{ij} is the tendency of species i and j to be randomly distributed, and τ_{ij} is the parameter of interaction between pairs of molecules i and j. τ_{ij} depends on the temperature of extraction (T_{ext}) according to (7) in terms of binary parameters (a_{ij} and b_{ij}) as proposed by Demirel and Gecegörmez (1991). As $\tau_{ii}=0$, $a_{ij} \neq a_{ji}$, $b_{ij} \neq b_{ji}$ and $\alpha_{ij}=\alpha_{ji}$, five binary parameters should be considered as adjustable parameters to characterize each binary interaction.

The SPD NRTL binary interaction parameters were calculated from the SPD extraction experiments shown in Table 1. Liquid-liquid equilibrium data from the SPD experiments in Table 1, $T_{50\%}$ and the pseudo-component average specific gravity from Table 4, were used to determine the NRTL adjustable parameters by means of a suitable algorithm provided in Aspen Plus$^®$, based on the generalized least squares method (Britt and Luecke, 1973). The values obtained for the NRTL parameters for SPD are shown in Table 5.

4. Results and discussion

4.1 Physical properties. Once the pseudo-component properties were estimated from the first set of experiments (Table 1), the properties of each mixture involved in the second set of extraction experiments (SG, D_{343}, RI_{343} and $S\%$) were estimated through equation (1), using the composition of each mixture from Table 2 and the pseudo-components properties from Table 4. Experimental and calculated values are compared in Figure 3 and no important deviations were found. Absolute average deviations between experimental and predicted values were 0.005 for SG, 0.004 for D_{343}, 0.007 for RI_{343} and 0.4 for $S\%$. According to such results, the pseudo-component description is accurate enough. Therefore, it is possible to predict such properties for the experiments presented in Table 2, by using the pseudo-components properties calculated from experiments carried out with a similar lubricating oil but not the same (Table 1).

In order to check the quality of pseudo-component method, the obtained results were compared to those calculated by other methods reported in the literature. The methods reported by Riazi and Daubert (1986), Riazi and Roomi (2001), API (1987) and Gomez (1992) were used to calculate the liquid density at 293K for the involved mixtures. In addition, Riazi and Daubert (1986), and Riazi and Roomi (2001) reported a method used to calculate the refractive index at 293K. The method proposed by Riazi et al.

(1999) allowed the estimation of the sulfur content in similar mixtures to the ones here reported. All these methods require the average boiling point of the mixture obtained from the ASTM D86 distillation curve. In this study, the distillation curve for each fraction was experimentally determined following the ASTM D2887 standard test method and presented in Table 3. Such curves were converted to ASTM D86 by using the method proposed by Daubert (1994) and the average boiling point for each fraction was calculated following the procedure 2B1.1 proposed by API (API, 1987). Table 6 shows the average boiling point ($\bar{T}$), the liquid density and the refractive index at 293K (D_{293} and RI_{293}, respectively) and the sulfur content ($S\%$) for each mixture calculated by the methods mentioned before. Such results and those ones obtained by the pseudo-component method were compared to the experimental values as shown in Figure 4. D_{293} values for the method reported here were obtained from D_{343} calculated ones by using a relation between densities at different temperatures (Peña, 2000). RI_{293} calculated values for the pseudo-component method were obtained according to the following expression (Altgelt and Boduszynski, 1994):

$$RI_{T_1} = RI_{T_2} + 0.0004 \cdot \Delta T \qquad (T_1 < T_2) \qquad (8)$$

where $T_1 = 293K$ and $T_2 = 343K$.

The predictions for D_{293} by the methods proposed by Riazi-Daubert, Riazi-Roomi, and API give very similar values, underestimating slightly such property for the mixtures. On the contrary, the method proposed by Gomez and the one reported here based on the pseudo-component properties provide accurate predictions, showing no systematic deviations. Such methods consider the nature of the mixture by using the Watson factor (Gomez) or the composition in saturates, aromatics and polars (pseudo-component method). Therefore, the nature of the mixture must be considered to improve the prediction of the density for petroleum fractions as reported by Gomez (1992).

Similar results were obtained for the predictions of RI_{293} as it can be seen in Figure 4. The methods proposed by Riazi-Daubert and Riazi-Roomi underestimate the experimental values. However, no systematic deviations were found by using the method based on pseudo-components. The sulfur content can be estimated by both the method proposed by Riazi et al. and the one here reported, obtaining in all cases a good agreement with the experimental values.

To check the accuracy of the methods considered in this work, the absolute average deviation was calculated and shown in Table 7 for the prediction of the studied properties. According to such results, both the method proposed by Gomez ($\bar{\varepsilon} = 0.003$) and that based on pseudo-components ($\bar{\varepsilon} = 0.004$) can be used to properly calculate the D_{293} for the involved mixtures. The obtained deviations for the RI_{293} values reveal that all methods provide similar deviations, although those proposed by Riazi-Daubert and Riazi-Roomi underestimate the true values. On the contrary, the pseudo-component method shows a some higher deviation (0.007), but no systematic deviations are observed. Finally, the sulfur content of the involved mixtures could be similarly predicted by both the method proposed by Riazi et al. ($\bar{\varepsilon} = 0.4$) and that one based on the pseudo-component properties ($\bar{\varepsilon} = 0.4$). Obtained results confirm the suitability of the pseudo-component method to predict properties (density, refractive index and sulfur content) not only for heavy lubricating oils (van Grieken et al., 2005), but also for light ones. In addition, the method reported here is more flexible than the other ones, since it allows to predict not only one property, but several ones. The pseudo-component method is easier to apply than the others checked in this study, because fewer calculations and correlations are needed.

4.2 Extraction model. To check the quality of the application of NRTL model for SPD+furfural mixtures, the experimental conditions presented in Table 2 were

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simulated by a single stage decanter. The simulation was performed with a commercial simulator, Aspen Plus[®], using the average boiling temperature ($T_{50\%}$), the specific gravity of each pseudo-component presented in Table 4 and the NRTL parameters previously obtained and shown in Table 5. The simulation results for SPD extraction experiments (extraction yields, furfural content, composition and physical properties for each mixture) are presented in Table 8. Experimental and predicted values for SPD extraction yields and furfural content are compared in Figure 5. Predicted yields are in good agreement to experimental values obtained in this work, confirming the expected distribution of phases. Thus, at lowest temperature and solvent/feed ratio, a raffinate yield of 85.4% was predicted, which compares favorably with the 80.9% experimentally obtained. At higher temperature and furfural/feed ratio, species undergo larger dissolution, which makes the yield of raffinate decrease. Thus, a yield of 24.7% was predicted, which again shows a good concordance with the 25.3% experimentally obtained. In order to determine the accuracy of the predictions of the extraction yields, absolute average deviation was calculated, obtaining a value of 2.2%. The content of furfural in raffinates and extracts is an important information and a good agreement was found between experimental and predicted values as it is shown in Figure 5. Absolute average deviations of 1.3% and 2.2% were obtained for raffinates and extracts, respectively. Figure 6 shows the comparison between experimental and predicted compositions of the involved mixtures (feed, raffinates and extracts). As it is shown, no important deviations were found, obtaining absolute average deviations of 3.1% for saturates, 2.9% for aromatics and 0.4% for polars. Such values are all within the limits of reproducibility established by the ASTM D2007 standard test method.

The studied properties (SG, D_{343}, RI_{343} and $S\%$) were calculated by using expression (1), taking into account the average properties of each pseudo-component from Table 4

and the predicted compositions listed in Table 8. Experimental and predicted properties of each mixture (feed, raffinates and extracts) are compared in Figure 7. A good agreement between experimental and predicted values was found in all cases. Absolute average deviations were calculated, obtaining 0.007 for SG, 0.005 for D_{343}, 0.004 for RI_{343} and 0.5 for $S\%$. According to these results, the model accurately predicts the selected properties for the studied mixtures.

There is a limitation in the application of the model as indicated previously (van Grieken et al., 2005) for the system furfural+HND lubricating oils. Such limitation was also found for the system furfural+SPD lubricating oil. Thus, the experiment carried out at highest temperature and furfural/feed ratio could not be simulated because the system is near the miscibility region. For that reason, no accurate predictions are obtained in these conditions. However, this limitation is not a big model lack because in the practice these severe conditions are not very usual.

5. Conclusions

The experimental results obtained in this work confirm that aromatics extraction could be enhanced by increasing the furfural/feed ratio, although it is limited in the practice. Similarly, temperature must be a compromise between solubility of species and solvent selectivity.

A method based on pseudo-component properties, can be successfully used to predict properties of different mixtures (feed, raffinates and extracts) from light vacuum distillates (SPD). In this work, good description of specific gravity, liquid density and refractive index at 343K and sulfur content was obtained. Such method exhibits similar or even higher accuracy than other reported in the literature. Obtained results confirm the suitability of the proposed method to predict not only one property (as the other methods checked) but several ones, which makes the calculations easier.

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The extraction operation can be described using Aspen Plus$^{®}$ with the pseudo-components properties and NRTL parameters calculated from experimental data. Thus, in this work, no important deviations were found when predicting extraction yields ($\bar{\varepsilon} = 2.2\%$), furfural content ($\bar{\varepsilon} = 1.3\%$ and 2.2% for raffinates and extracts, respectively) and compositions ($\bar{\varepsilon} = 3.1\%$, 2.9% and 0.4% for saturates, aromatics and polars, respectively). In addition, properties such as specific gravity, liquid density and refractive index at 343K and sulfur content of involved mixtures can be calculated, obtaining no remarkable deviations (0.007, 0.005, 0.004 and 0.5, respectively).

Acknowledgements

Nomenclature

Symbols

D_{293}: Liquid density at 293K, g/ml

D_{343}: Liquid density at 343K, g/ml

E: Extract

f: Furfural

F: Objective function

G: NRTL interaction parameter given by eq. 6

P: Studied property such as density, specific gravity or refractive index

$\bar{P}$: Average property.

R: Raffinate

RI_{293}: Refractive index at 293K

RI_{343}: Refractive index at 343K

SG: Specific gravity at 288K

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S%: Sulphur content, w%

T_{ext}: Temperature of extraction, K

$\bar{T}$: Average boiling point, K.

$T_{50\%}$: Average boiling point of the feed lubricating oil, K

v/v: volume/volume

w/w: weight/weight

X: Composition, w%

x: Molar fraction.

γ_i: Activity coefficient of component i

α, a, b: NRTL interaction parameters

τ: NRTL interaction parameter given by eq. 8

Subscripts

A: Aromatics

i, j, k, m: Component i, j k or m.

P: Polars

S: Saturates

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Table captions

Table 1. Experimental results for the first set of SPD extractions.

Table 2.Experimental results for the second set of extractions of SPD.

Table 3.Simulated distillation for the second set of SPD extractions.

Table 4.SPD pseudo-components properties.

Table 5.NRTL binary interaction parameters for furfural+SPD system.

Table 6.Calculated values for properties obtained by different methods.

Table 7. Obtained deviations for the different methods.

Table 8.Simulation results of SPD extraction experiments.

Figure captions

Figure 1. Scheme of calculations.

Figure 2. Material balance for SPD extraction experiments.

Line: True feed composition

Symbols: Calculated feed composition in: ▫ , Saturates; ▽ , Aromatics; △ , Polars.

Figure 3. Comparison between experimental and calculated properties for SPD mixtures (feed, raffinates and extracts).

Figure 4. Comparison between predicted values for properties obtained by different methods: ▽ Riazi-Daubert; △ API; ▫ Riazi-Roomi;

◇ Gomez; ○ Riazi et al.; ■ This report.

Figure 5. Comparison between experimental and predicted values for extraction yields and furfural content for SPD extraction experiments:○ Raffinates; ● Extracts

Figure 6. Comparison between experimental and predicted compositions for SPD mixtures (feed, raffinates and extracts).

Raffinates: ▫ , Saturates; ▽ , Aromatics; △ , Polars.

Extracts: ■ , Saturates; ▼ , Aromatics; ▲ , Polars.

Figure 7. Comparison between experimental and predicted properties for SPD mixtures (feed, raffinates and extracts).