



Prediction of Surface Tension of Heteroatom-Rich Fuel Fractions from Pyrolysis of Oil Shale

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Abstract

In this work, a brief overview of the methods for calculating surface tension and analyze various methods for calculating Parachor and surface tension for Kukersite shale oil fractions. Using experimentally measured data on the surface tensions, densities and average boiling points of the industrial gasoline and middle oil fractions of oil shale, a proposed correlations for calculating both the surface tension at 20°C and for calculating the temperature dependence of the surface tension (in the temperature range from 10 to 180°C). These correlations enable the calculation of surface tension at 20°C and the temperature dependence of the surface tension with a relative accuracy of $\pm 5.5\%$. The resulting correlation also makes it possible to find temperature dependencies of the surface tension of alkanes and oil fractions, for example, with an error generally below 10%.

Paper type: Research paper

Keywords: shale oil, surface tension, temperature dependence, correlations.

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Introduction

The surface tension of a liquid is its fundamental property. The knowledge of the value of surface tension is important in many fields. In engineering it is needed to estimate liquid transport in capillary systems (for example in drying), surface tension determines the excess temperature in case of boiling (Morgan *et al.*, 1949; Roll and Myers, 1964), the knowledge of precise surface tension values is also needed in the design of separation processes (absorption, distillation, extraction), vessels, and to estimate spreading in water (for example during a spill) (Gjøsteen, 2004). As surface tension is also one input parameter in process simulators an accurate method for its calculation at different temperatures is important. Recently there has been an interest to correlate surface tension and viscosity, as both properties are related to the molecular structure of the fluids (Tian and Mulero, 2014; Aleem and Mellon, 2017).

To calculate the surface tension σ (mN m^{-1}), the Macleod-Sugden correlation is most commonly used:

$$\sigma^{1/n} = P \frac{\Delta\rho}{M} \quad (1)$$

In this equation P is parachor, $\Delta\rho$ is the difference in liquid and vapor phase densities (g/cm^3), M is molecular weight (g/mol), and n is a parameter whose value, as given in the literature, usually for pure compounds ranges from 3.67 to 4 (with a theoretical value of 3.88), and for petroleum mixtures from 1.5 to 4.43 (Miqueu *et al.*, 2001). The surface tension of a compound depends on both pressure and temperature. Parachor on the other hand can be considered to be only compound specific and its values calculated from surface tension data can be found in literature for many pure compounds (Quayle, 1953). There are different correlations for estimation of the surface tension of pure compounds or defined mixtures which rely on measurable critical properties or pseudocritical properties, acentric factors etc. Undefined petroleum fractions (or cuts) can also be treated as defined mixtures containing three pseudo components (Paraffinic, Naphthenic, and Aromatic compounds) for which surface tension can be estimated using a group contribution-based method (Darwish *et al.*, 1995b).

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For undefined liquid mixtures, also correlations for surface tension calculation have been proposed where pseudocritical temperature, pseudocritical pressure, acentric factor, and Watson characterization factor (American Petroleum Institute, 1997; Zuo and Stenby, 1997) are used as input parameters. From the practical point of view, correlation based on directly measurable properties, like boiling point, density (or specific gravity), or molecular weight is often preferred. As a result, several simple empirical correlations for estimating the value of parachor have been developed. The application of these for estimating the surface tension of petroleum fractions has been reviewed by Ali (Ali, 1994). The correlation not covered in (Ali, 1994) for estimating Parachor of undefined mixtures of petroleum origin is as follows (Fawcett, 1994):

$$P = 2.448 M + 81.2, n=11/3, \text{ crude oil fractions, } M \text{ up to } 500 \text{ g/mol} \quad (2)$$

Correlations developed using surface tension data of pure hydrocarbons or petroleum fractions have been consequently estimated to be relatively accurate for estimating the surface tension of hydrocarbons, hydrocarbon mixtures, and petroleum fractions. However, errors could be very large for nonhydrocarbons (Riazi, 2005), heavy fractions containing asphaltenes or surface active materials or fractions of non-conventional pyrolysis oils, as is also shown below. For that purpose also the correlation suggested by API (American Petroleum Institute, 1997) for the calculation of surface tension of petroleum fractions is not recommended for example for coal liquids. For coal liquids, parachor can be estimated using the equation proposed by Tsoupoloulos (Tsoupoloulos *et al.*, 1986):

$$P = 1.7237 T_b^{0.05873} SG^{-0.64972} M, n=4 \text{ for coal liquids} \quad (3)$$

Where T_b is the normal boiling point, and SG is specific gravity at 15.5°C. The inaccuracy of proposed correlations is also faced when trying to predict the surface tension of oil shale pyrolysis liquids, as shale oils are known to contain relatively large amounts of heteroatoms. Depending on the origin, shale oil could be rich in oxygen (phenolic) compounds (Kukersite shale oil) (Baird *et al.*, 2015), nitrogen compounds (Green River shale oil) (Baird *et al.*, 2023), or sulphur compounds (Jordan shale oil) (Baird *et al.*, 2023). The main aim of the current study was to develop a correlation for estimating the surface tension of pyrolysis liquids rich in phenolic compounds. As a consequence also the surface tension data along with other properties that can be used in the future to develop a comprehensive correlation are given. Additionally, several correlations originally developed for conventional petroleum fractions were tested for their accuracy.

1 Materials and Methods

1.1 Samples

The study was performed using shale oil technical fractions (middle oil and gasoline) produced from Kukersite oil shale by the Galoter process as a starting liquid. Additional information about Kukersite shale oil can be found for example from Baird (Baird *et al.*, 2023) and the references therein. Generally, the middle oil fraction can be characterized as a liquid having a low pour point, high OH content (around 5wt%), and viscosity usually less than 100m.Pa.s (at 25°C). Compared to middle oil, gasoline has lower OH content (below 1wt%), much lower pour point and viscosity. Samples used in the study were fractions obtained by laboratory distillation of these technical fractions. Additionally, to reduce the content of phenolic compounds in shale oil (or to make it more similar to petroleum fractions), deadenylation of original technical middle oil fractions was carried out and obtained dephenolated oil was separated into fractions with narrower boiling point distributions. Technical shale gasoline fraction was separated into narrower fractions using both fractional distillation (in accordance to ASTM D2892 ('Standard Test Method for Distillation of Crude Petroleum (15-Theoretical Plate Column)', 2013)) and simple laboratory distillation (similar to Engler distillation; ASTM D86 ('Standard Test Method for Distillation of Petroleum Products at Atmospheric Pressure', 2016)). A simple laboratory distillation was used for the separation of middle oil and dephenolated middle oil into fractions. The details about distillation and dephenolation can be found in (Järvik *et al.*, 2021). The total number of used fractions was 94, including 30 gasoline fractions, 33 dephenolated middle oil fractions, and 31 middle oil fractions. The average densities of the technical shale gasoline and middle oil at 20°C were 786.7kg/m³ and 1022.2kg/m³, respectively, number average molecular weights of 132g/mol and 228g/mol, hydrogen-to-carbon ratios of 1.78 and 1.35, and OH contents of 0.2wt% and 5.0wt%, respectively. The main average properties of the fractions were as follows: boiling point ranged from 66 to 450°C, density at 20°C from 707 to 1070kg/m³, number average molecular weight from 87 to 410g/mol, hydrogen to carbon ratio from 1.26 to 1.98, and OH content from 0 to 8.2wt%.

1.2 Measurement methods

Surface tension was measured using Rame-Hart goniometer Model 260 (Ramé-hart instrument Co., Succasunna, USA) with a high-temperature chamber. Surface tension values were calculated by processing the pendant drop image in DROPimage Advanced program to obtain drop shape parameters (β -drop shape parameter, and R_0 -drop radius of curvature at the apex). These parameters together with the density data were used to calculate surface tension values at respective temperatures. Average boiling points were

measured using TGA based method developed in our laboratory (Rannaveski *et al.*, 2016). OH content of shale oil fractions was determined using FTIR based method developed in our laboratory (Baird *et al.*, 2015). Density was measured using Anton Paar DMA 5000M density meter (Anton Paar GmbH, Austria). Number average molecular weights were measured using cryoscopic/freezing point depression technique (built in-house) using benzene as the solvent or/and vapor pressure osmometry using Kanuer K-7000 vapor pressure osmometer (Wissenschaftliche Gerätebau Dr. Ing. Herbert KNAUER GmbH, Germany) using benzene as the solvent.

2 Results and Discussion

2.1 Surface tension values estimated by correlations including molecular weight, specific gravity and normal boiling point

Generally, as shown in **Figure 1**, the surface tension values for shale oil fractions (at 20°C) are an average of 15% higher than those of petroleum fractions with similar molecular weight/boiling point. This kind of behaviour can be explained by the increased cohesive forces caused by the hydrogen bonding as Kukersite shale oil has a high content of phenols (Baird *et al.*, 2015). Surface tension data for coal liquids as presented by Gray (Gray *et al.*, 1983) mostly do show similar behaviour as shale oil fractions. The reader should be aware that in the case of coal liquids, the results were obtained by extrapolating using available data points. The surface tension of mixtures with undefined composition can be estimated through *Eq. 1* using several correlations available in the literature for estimating parachor (for example *Eq. 2* or 3). However, as for practical calculations, surface tension value is needed, and there should be no need to develop a correlation for the estimation of parachor value, as parachor is itself calculated with the aid of *Eq. 1* using measured molecular weight, density, and surface tension values.

The correlations based only on directly measurable properties can be combined with *Eq. 1* to obtain surface tension values. As expected, correlations developed based on pure hydrocarbons and petroleum fractions (for example *Eq. 2*) do not predict parachor values accurately. The parachor values calculated using *Eq. 2* and *Eq. 3* are shown in **Figure 2**, using equations given for example in reference (Ali, 1994) yields for most of the shale oil fractions errors similar to *Eq. 2*, which had an average absolute deviation (AAD) of 14.4%. Parachors calculated using *Eq. 3* developed for coal liquids have AAD of 2.0%. As a result, the calculated surface tension values (**Figure 3**) have in the best case AAD of 9.0% (*Eq. 3*), while using *Eq. 2* yields AAD of surface tension value close to 30%. As will be discussed later, it is also evident by looking at Fig. 2 and Fig. 3 that the simple correlations that do not account for the OH content of oil (*Eqs. 2*, and 6) fail especially when the OH content of the original shale oil is higher than 4wt%. For similar reasons also the correlation (*Eq. 4*) developed by Kawai *et al.*, (1990) to calculate the surface tensions of brown coal liquids fails in the case of shale oil fractions.

$$\sigma [N m^{-1}] = 9.05 \times 10^{-5} M + 1.59 \times 10^{-6} \quad (4)$$

This simple correlation underestimates shale oil surface tension values by as much as almost 62%. Therefore, simple one-parameter correlations like this can only be considered to be useful for liquids with compositions corresponding to those that were used to obtain the correlation.

2.2 Surface tension values estimated using predicted pseudocritical properties

If a fraction has a relatively narrow boiling point distribution, it can be represented as a pseudo component. In this case, it is possible to estimate both critical properties and acentric factors from appropriate correlations which are presented by Riazi (Riazi, 2005). The problem here again is that most of these correlations are developed for petroleum fractions. Nevertheless, in some cases surface

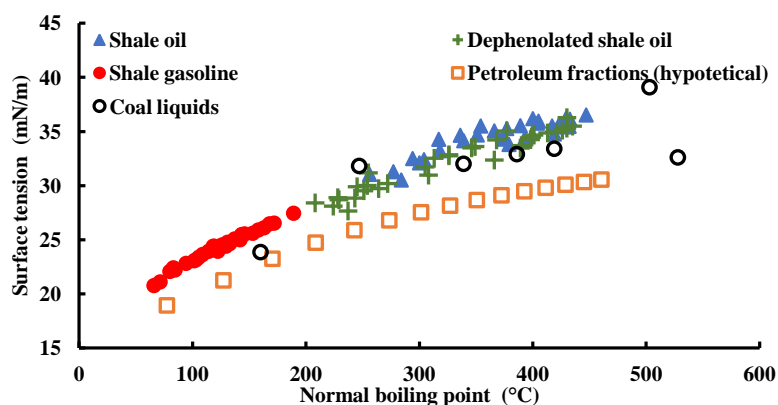


Fig. 1 Surface tension as a function of boiling point for shale oil fractions, narrow boiling point distribution coal liquid fractions (from (Gray *et al.*, 1983)) and hypothetical petroleum fractions (calculated using the equation for undefined petroleum fractions (Daubert and Danner, 1997)).

tension of shale oil fractions at 20°C can be predicted relatively accurately. **Table 1** shows the combinations of correlations that gives the most accurate results. It should be noted that in all cases predicted values are higher compared to measured values. Additionally, the Block and Bird correlation (as given in (Poling *et. al.*, 2000)) together with Riazi-Daubert correlation for hydrocarbons in the molecular weight range of 70 to 300g/mol (also adopted by API (American Petroleum Institute, 1997)) predicts surface tension within 3% error for those fractions that have OH content lower than 2wt% (shale gasoline). Therefore, the corresponding-state models that rely on the accuracy of the estimation of critical properties is mostly superior over the presented correlations (Eqs. 2 to 4) for the estimation of parachor or surface tension in the case of shale oil fractions.

Of course, none of these correlations can be considered adequate for high OH content oil (larger than approximately 4wt%), as in that case errors were on average greater than 8% and it generally increases as OH content increases. Also, the deviation between measured and calculated values are slightly increased as the temperature is increased (by 0.002 to 0.03%/°C depending on the correlation).

2.3 Correlations for oils with high phenols content

Kukersite shale oil is a shale oil with high content of phenolic compounds, which are usually quantified by measuring the OH content (Baird *et al.*, 2015). As can be seen from the results obtained using different correlations presented in the literature, the error of estimated surface tension values increases as the OH content of a fraction increases (**Figure 4**). To overcome this problem one of the two possibilities may be used. The simplest possibility is to adjust the parameters of the available correlations (for example Eq. 2). In that case, the parachor can be calculated using the following equation:

$$P = 67.9 + 2.13 \times M \tag{5}$$

Eq. 5 is similar to the one developed by Fanchi (Fanchi, 1990) for petroleum fractions:

$$P = 69.9 + 2.30 \times M \tag{6}$$

However, as can be seen in **Figure 4**, errors in calculated parachor and surface tension values behave similarly and are comparable to those obtained using correlations based on petroleum fractions. Namely, compared to the measured surface tension values, calculated values for fractions with OH content below approximately 4wt% are usually lower and for fractions with OH content above 5wt% are higher. Therefore, considering the dependence of surface tension and parachor on OH content, a better fit could be obtained if this is taken into account. It can be done directly by measuring OH content, however this data is mostly unavailable. Another possibility is to use, instead of OH content, a two-parameter correlation as proposed for complex mixtures by Riazi and Daubert (Riazi and Daubert, 1987). In this correlation the estimated parameter, for example, parachor or surface tension, is dependent on the size and the

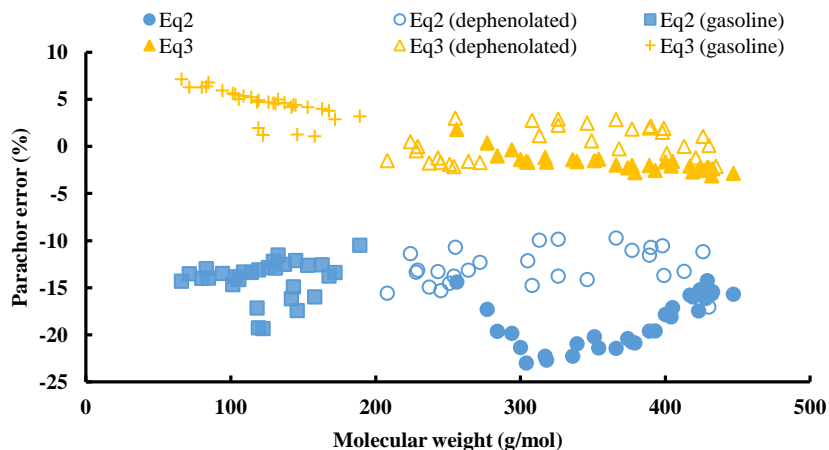


Fig. 2 The dependence of error of calculated parachor values (using Eqs. 2 and 3) on the molecular weight of shale oil fractions. $Error [\%] = (P_{measured} - P_{calculated})/P_{measured} \times 100$.

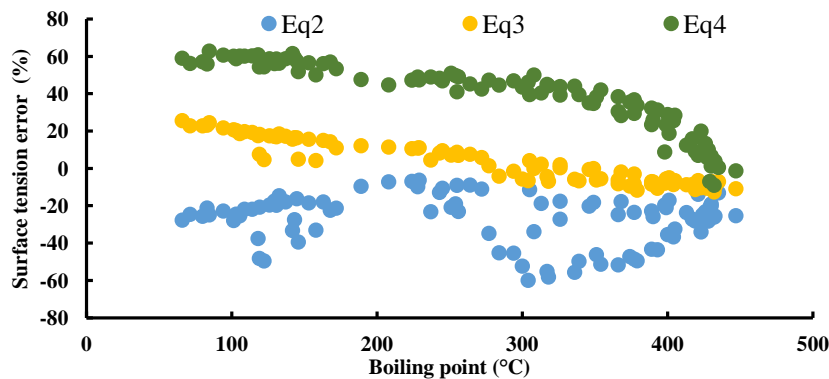


Fig. 3 The dependence of error of calculated surface tension values on boiling point of shale oil fractions. $Error [\%] = (\sigma_{measured} - \sigma_{calculated})/\sigma_{measured} \times 100$.

energy of the molecules in the mixture. For example, specific gravity could be taken as the parameter describing the size of an average molecule, while average boiling point describes the energy of an average molecule. This approach is an attempt to describe the average sample composition by using average parameters. The obtained general empirical correlation for estimating surface tension (mNm^{-1}) at 20°C is the following:

$$\sigma_{20} = aSG^bT_b^c \tag{7}$$

Table 1 The accuracy of the correlations for prediction of surface tension of shale oil fractions at 20 °C. In the table, only the results of the methods that gave the most accurate predictions (including the method of estimating the critical properties), are shown.

Correlation for surface tension	Properties needed for correlation	AAD, %	Max deviation ^a	Min deviation ^a
API-TBD (American Petroleum Institute, 1997)	T_c using Riazi-Daubert method (M range $>300 \text{ g mol}^{-1}$), T_b, SG	13.6	1.1	-24.4
Block and Bird (Poling, Prausnitz and O'Connell, 2000)	T_c, P_c using Lee-Kesler method (M range 70 to 700 g mol^{-1}), T_b	5.7	3.6	-20.1
Gray (Gray <i>et al.</i> , 1983)	T_c, P_c using Riazi-Daubert method (M range $>300 \text{ g mol}^{-1}$)	11.5	21.7	-28.3
Tsonopoulos <i>et al.</i> (Tsonopoulos, Heidman and Hwang, 1986) (Eq 3 combined with Eq 1)	T_b, SG, ρ^L, ρ^V	10.1	25.6	-12.5

^a deviation = $\frac{\sigma - \sigma_{\text{calculated}}}{\sigma} \times 100$, where σ is the experimental surface tension value.

where T_b is the normal boiling point of the sample (in °C) and SG is specific gravity at 20°C, and coefficients $a=8.486$, $b=0.462$, and $c=0.234$ were obtained using least squares regression (standard errors of coefficients are 1.091, 0.061, and 0.015, respectively, which allow estimation of the surface tension values with the accuracy of $\pm 1 \text{ N/m}$ at the 95% confidence level). For the studied oils it results in AAD of 1.7% (highest 5.4 %, lowest -4.2%). Surface tensions of paraffin and olefines (surface tension data taken from (Jasper, 1972), SG and T_b from (Riazi, 2005)) in the molecular weight range of 70 to 280g/mol is predicted using Eq. 7 with the AAD of

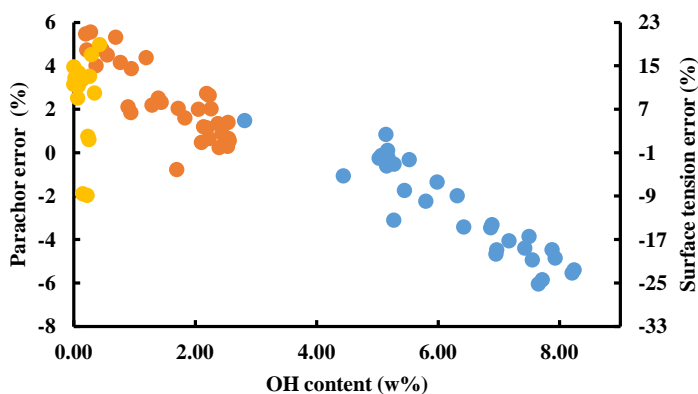


Fig. 4 Errors in estimated (Eq. 5) parachor and surface tension values as a function of OH content of shale oil fractions.

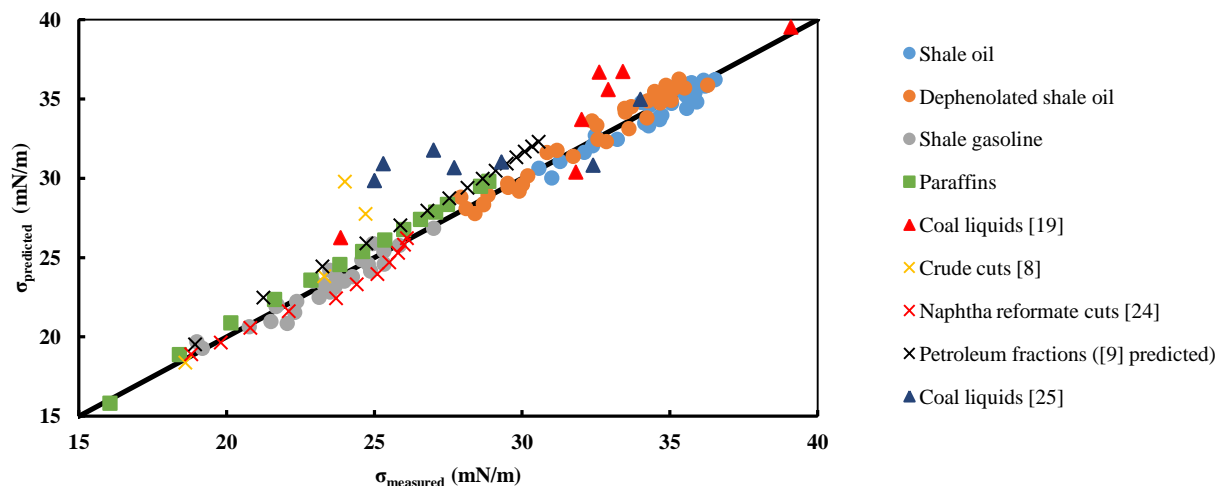


Fig. 5 Comparison of calculated surface tension values to those predicted using Eq. 7. ● – shale oil fractions from current study (blue – initial oil fractions, orange – dephenolated fractions, grey – gasoline fractions); × – petroleum fractions (red – (Darwish *et al.*, 1995a), black – predicted using the method recommended by API-TBD (American Petroleum Institute, 1997), yellow – (Darwish *et al.*, 1995b)); ■ – alkanes; ▲ – coal liquids (dark blue – extrapolated to 20°C and 1 atm from data in (Hwang *et al.*, 1982); red – extrapolated to 20°C from data in (Gray *et al.*, 1983)).

2.7% (minimum -3.6%, maximum 4.2%). As a result, also surface tension values of petroleum fractions are predicted relatively accurately (**Figure 5**). It should be noted that in some cases the SG values given in the references at 15.6°C, were used, which however has only a small effect (less than 0.3%) on the predicted surface tension value. The coefficients in the correlation were obtained using shale oil fractions with the SG (20/20) in the range of 0.71 to 1.07 and boiling points in the range of 70 to 445°C.

The developed correlation (Eq. 7) allows estimation of surface tension at 20°C. In practical situations (for example in the case of oil spills) the temperatures could vary from below 0°C (during winter) to well above room temperature (in the industry). A common way of developing a correlation for a temperature dependent property have been through the use of temperature dependent constants as it is done by Riazi (Riazi, 2005). In the case of surface tension, however, the temperature-independent paracore described above is used, and the temperature dependence of the surface tension value is taken into account by the change in density. However, the temperature dependence of the surface tension as a temperature-dependent quantity at a temperature much lower than the critical point can be represented with the following equation:

$$\sigma_T = \sigma_{20} + k(T - 20) \quad (8)$$

Where σ_{20} (mN/m) is surface tension at 20°C (Eq. 7) and $k = \frac{\Delta\sigma}{\Delta T}$ is the change in surface tension value with the temperature change of 1°C. The value of the quantity k can be calculated as follows:

$$k = \frac{\Delta\sigma}{\Delta T} = a_1 SG^{b_1} T_b^{c_1} \quad (9)$$

Where a_1 , b_1 and c_1 are empirical coefficients with values of -0.417, 0.173 and -0.296. Using these coefficients, AAD for k was found to be 5.1%, with relative differences between calculated and measured k values ranging from -19 to 17%. Despite the relatively large error in the k , the differences between the calculated and experimental surface tensions in the presented temperature range were generally within $\pm 5\%$ (**Figure 6**).

The obtained correlation (Eq. 8) was also tested for different pure substances and mixtures. In the case of short-chain alkanes (up to nonane), the relative differences in the predicted surface tension values to the values given in the literature are within 10% up to the boiling point of the substance (**Figure 7**). In the case of narrow boiling crude oil fractions, the presented correlation also enables the temperature dependence of the approximate surface tension of the fraction to be calculated. In this case, the errors were generally less than 10% (**Figure 7**) which is equivalent to or smaller than those calculated with correlations considered by Darwish et al. (Darwish et al., 1995a). It should be emphasized that in the case of correlations studied by Darwish (Darwish et al., 1995b) the error is increasing as the boiling point increases. On the other hand, the correlation given in the present work gives more accurate results especially for fractions with a higher boiling temperature while the modified UNIFAC group contribution method (Darwish et al., 1995b) gives large errors (up to 37%) for fractions boiling at high temperature.

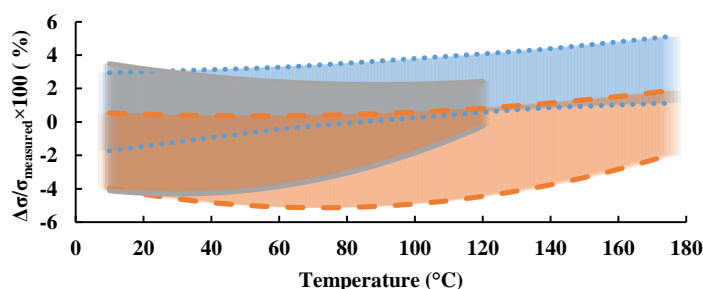


Fig. 6 Temperature dependence of the limits of the relative differences of the experimental and predicted (Eq. 8) surface tensions of shale oil gasoline, middle oil and dephenolized middle oil fractions and correlation (Eq. 8) calculated. $\Delta\sigma = \sigma_{measured} - \sigma_T$, where σ is experimental value and σ_T is predicted value.

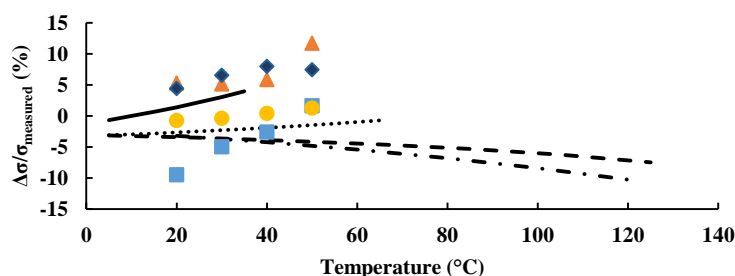


Fig. 7 The temperature dependences of relative differences of the experimental surface tensions of crude oil cuts presented by Darwish et al (Darwish, Al-Sahhaf and Fahim, 1995a) (average boiling points of fractions: ■ – 85 °C, ▲ – 105 °C, ◆ – 115 °C, ● – 165 °C) and some alkanes given in the literature (Jasper, 1972) to those calculated with the correlation presented in this work (solid line – pentane, dotted line – hexane, dashed line – octane, dash dot line – hexadecane).

Conclusions

There has always been a need for a better fit between predicted and actual values. However, as different liquid fuels may have very different compositions, hence also different properties, there are currently no universal correlations that could fit them all. It is well known that correlations obtained from oil fraction data do not give accurate results for coal tars, however, by applying the combinations of corresponding state methods, it is possible to obtain relatively accurate results for non-conventional oils as well. The same result was reached in the present work in the case of shale oil fractions. The correlation found in this work based on shale oil fractions makes it possible to relatively accurately determine surface tensions for oils of different compositions/origins at 20°C, provided that the boiling point and specific gravity of the fraction are known. Here, there is no significant difference in whether the relative density is determined at 20 or 15°C. Due to the fact that the temperature of the environment, where it may be necessary to estimate the surface tension value, can vary within relatively wide limits, this work proposed a correlation for estimating the temperature dependence of the surface tension. The proposed correlation enables to predict the surface tension value of shale oil fractions (density range of 700 to 1070 kg/m³, normal boiling point range of 66 to 450°C, OH content range of 0 to 8.2 wt%, molecular weight range of 87 to 410 g/mol) with an accuracy of about ±5%. Although the proposed correlation also seems to enable to accurately predict the surface tension of petroleum fractions, it is difficult to assess its general prediction power as there is very little reliable data on the temperature dependence of the surface tension at atmospheric pressure with necessary descriptive properties for surface tension prediction.

Nomenclature

σ	=surface tension	[mN/m] or [N/m]
σ_T	=surface tension at temperature T	[mN/m]
σ_{20}	=surface tension at 20°C	[mN/m]
P	=parachor	[-]
$\Delta\rho$	=difference in liquid and vapor phase densities	[g/cm ³]
M	=molecular weight	[g/mol]
n	=experimental parameter	[-]
T_b	=normal boiling point	[K] or [°C]
SG	=specific gravity	[-]
T_c	=critical temperature	[K]
P_c	=critical pressure	[bar]
ρ^L	=density of liquid phase	[g/cm ³]
ρ^V	=density of vapor phase	[g/cm ³]

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