RESEARCH ARTICLE

Oxidative Desulfurization of Diesel Fuel Using Three Kinds of Carboxylic Acids Supported by Iron(III) Chloride

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ABSTRACT

Aqueous carboxylic acids (CA) are generally used as attractive catalytic extractants in the field of desulfurization of petroleum products. In the present study, a triple system consisting of CA-ferric chloride-hydrogen peroxide has been used for the removal of aromatic S-compounds from partially hydrotreated diesel by liquid – liquid oxidative-extraction. The influence of various operating parameters affecting the oxidative desulfurization was experimentally investigated. Formic acid (HCOOH), acetic acid (CH₃COOH), and propanoic acid (CH₃CH₂COOH) as aqueous solutions with hydrogen peroxide and iron(III) chloride (FeCl₃) as oxidant and catalytic agent, respectively, were used. All experiments were carried out at 55°C with different oxidant to sulfur mole ratios (nH₂O₂/nS) (15–36), CA to sulfur mole ratios (nCA/nS) (2–26), and oxidation reaction times (5–25 min). Within 25 min of the treatment, a maximum elimination of aromatic S-compounds of 65.1% was obtained when molar ratio of oxidant to sulfur (nH₂O₂/nS) was 36 and molar ratio of CA to sulfur (nCA/nS) was 26. Surface tension calculations for the CAs demonstrated that the average void radius of the acids has a pronounced effect on the fitting of S-compounds from diesel fuel into acids and is important to sulfur removal. Further, increasing the desulfurization efficiency was also energetically affected in the presence of ferric halide. The obtention of the sulfur removal ability value was noticeably higher than was achieved by employing similar reaction conditions in the absence of FeCl₃.

Keywords: Oxidation; Diesel fuel; Ferric chloride; Hydrogen peroxide; Pollution; Desulfurization

INTRODUCTION

Recently, the proportion of heavy low sulfur-containing oils in total petroleum production being treated and produced has increased drastically worldwide as the largest deposits of low and light sulfur hydrocarbons. The existence of heteroatomic molecules in petroleum feedstock not only effects the decreasing of the American Petroleum Institute (API) gravity value and poisoning catalytic convertors, but also reduces the quality of the resulting petroleum products. A significant part of the harmful materials of petroleum's components in the composition of fuels, such as sulfur and nitrogen, in which high-toxicity combustion products (SO_x and NO_x) are emitted into the atmosphere, thereby causing environmental pollution such as corrosion of construction work, harms agricultural products, impairs soil quality, and causes acid rain (Kobotaeva and Skorokhodova, 2020; Dehkordi et al., 2009). Diesel quality is of particular interest. Accordingly, removal of sulfur derivatives from petroleum has become an essential part of related industry processes. High sulfur content in Iraqi crude oil which causes environmental pollution is also the

main reason for its removal in fuel products (Dehkordi et al., 2009). To allow the transition of the Iraqi oil refining industry to the production of fuels that meet European standards, reducing aromatic S-containing compounds in oil products to a minimum (around 10–15 ppm) is vital (Kareem et al., 2019).

In the industry, hydrodesulfurization (HDS) is currently the major trend in hydrocarbons purification with regard to the removal of sulfur impurities in their hydrotreating using solid catalysts. However, this operation has a relatively low efficiency in terms of the removal of polycyclic organosulfur species such as dibenzothiophenes and their alkyl derivatives. In addition, it requires harsh operating conditions such as high temperatures (300–400°C) and high pressures (20–130 atm) which leads to very high capital and operating costs (Andevary et al., 2020; Grange, 1980).

Selecting catalysts with both good extractive ability and high catalytic activity have become vital to the super-desulfurization of petroleum products (McIntosh and Schram, 1977). Accordingly, many alternative non-

HDS technologies such as oxidation (Gao et al., 2018), extraction (Abbott et al., 2017), biodesulfurization (Gray et al., 2003), and adsorption (Tian et al., 2014) have been suggested. However, the non-HDS results imply that all these technologies are insufficient and need further work to represent practical means of oil product desulfurization (Shu et al., 2020). However, among these alternative non-HDS methods, oxidative extractive desulfurization (ODS) is one of the more promising processes for developing diesel fuel, which can typically reduce the concentration of refractory polyaromatic sulfur hydrocarbons in the fuel under moderate reaction conditions and at low cost (Campos-Martin et al., 2004). One of the advantages of ODS processes is the possibility of their implementation at atmospheric pressure and low temperature. Another significant feature of ODS is that most of the refractory aromatic sulfur molecules, which probably cannot be removed in the HDS process, investigated high chemical reactivity for oxidation in the ODS operation. Further, this method is a non-hydrogen-consuming desulfurization process (Campos-Martin et al., 2004; De Filippis and Scarsella, 2003).

Typically, ODS operation consists of two steps: Oxidation and extraction. When the oxidation reaction of S-molecules takes place in the presence of an appropriate oxidizing agent containing an appropriate catalyst, aromatic S-compounds are converted to their corresponding polar sulfone and/or sulfoxide compounds (Pawelec et al., 2011). Then, polar sulfones are easily separated from fuel using a highly polar solvent. All of the substances noted in the ODS process have a major role in the applications of the research experiments investigated (Bhutto et al., 2016; Polikarpova et al., 2018). Several types of catalytic agents and oxidants have been studied for use in the ODS method. In the presence of a catalyst like ionic liquids (Lu et al., 2007), Brønsted acids (Zhao et al., 2007), and deep eutectic solvents (DES) (Lü et al., 2015), hydrogen peroxide (H_2O_2) as an active oxidant has seen widespread use in this important area of “green chemistry” due to having a high concentration of active oxygen, a desirable influence on the reactions, it is inexpensive, easy to synthesis and produces H_2O as the only by-product (Zhao et al., 2007). H_2O_2 , for the oxidation of aromatic sulfur compounds, is energetically reactive in aqueous carboxylic acid (CA), leading to *situ* formation of peroxy acid (Khodaei et al., 2017).

In addition, to improve the extraction efficiency of S-compounds in petroleum products, many researchers have used metal in the extraction procedure in ODS such as Fe(II), Zn, Mg, Cu, Sn, and Co to enhance sulfur elimination (Zhao et al., 2014). Based on oxidative liquid-liquid extraction, separation is carried out after oxidation.

The extraction can be performed using acetonitrile as the solvent due to its low boiling point, high polarity, and high extraction effectiveness factor (Shiraishi et al., 1998; Deshpande et al., 2005).

The aim of the present work is to develop a more efficient extraction process using hydrogen peroxide-ferric chloride-CA systems to remove organosulfur compounds of partially hydrotreated diesel produced by North Oil Company (Kirkuk Refinery, Kirkuk, Iraq) with a sulfur mass content of 0.593%. The influence of different operating parameters such as H_2O_2/S , $FeCl_3$, and the CA/S molar ratios on the sulfur removal was studied. The performances of the three types of acid (i.e. formic acid, acetic acid, and propanoic acid [PA]) were also examined in this regard.

MATERIALS

The substrate utilized as the object of this investigation was a partially hydrotreated diesel with a 0.593% total sulfur content as produced by North Oil Company (Kirkuk Refinery, Iraq). Table 1 shows the physical and chemical properties of this particular diesel. All chemical materials utilized in this study, including PA (98%), acetic acid (96%), acetonitrile (99 wt.%), and hydrogen peroxide (50% w/w), were of analytical grade as purchased from Scharlau Chemie (Spain). Formic acid (>99%) was supplied by Chem-Lab NV (Belgium). Ferric chloride solution (60% w/v) was provided by BDH (England). All chemicals were employed without further purification.

METHODOLOGIES

Diesel Oxidation

Oxidation-extraction experiments were performed in 40 mL tubes, containing 20 ml of partially treated diesel. The reactor was placed in a constant temperature water bath on a hotplate coupled to a digital thermostat. For each

Table 1: Some basic physicochemical properties of diesel used in this work

Characteristic	Amount	Test methods
Initial boiling point (IBP) - °C	180	ASTM D7345
Final boiling point (FBP) - °C	346	ASTM D7345
Density @ 15°C - g/ml	0.816	ASTM 052
Sulfur content - %	0.593	ASTM D4294
Flash point - °C	68	ASTM D6450
Kinematic viscosity @ 40 °C - cSt	2.28	ASTM D7042
Cetane number	51.7	FTIR
Cetane index	52.1	ASTM D976
Water content - ppm	41	ASTM D6304
Color	0.8	ASTM D66045
Pour point - °C	-14	ASTM D97
Aromatic containing compounds - %	28.3	ASTM D1319

experiment, an appropriate amount of each of the three CA and iron halide solution was added to the tube reactor with the diesel, and the mixture was agitated vigorously at 400 rpm. During the oxidation period, an appropriate amount of oxidant was added to the mixture, where this point in time was considered to represent the beginning reaction for experimental purposes. The reactions of the samples were performed for a certain amount of time and the temperature maintained at a constant $55 \pm 1^\circ\text{C}$. After the oxidation stage, the organic and aqueous layers were separated by simple decanting. The elimination of oxidized hydrocarbon in the aqueous phase was performed by washing the oxidized diesel with an equal volume of the deionized water. Thereafter, an equal volume of acetonitrile was introduced to the treated sample in a separating funnel which was shaking manually for about 5 min to remove the oxidized sulfur products. The extraction stage was repeated in triplicate. Ultimately, a sulfur analysis was obtained. Because there can be more readily regenerated, acetonitrile was used (Aghaei et al., 2020). Based on the system, practically, the single influence of aqueous H_2O_2 on a sulfur molar ratio ($\text{H}_2\text{O}_2/\text{S}$) that was varied between 15 and 37 and a CA to sulfur mole ratio (CA/S) from 2 to 26, and oxidation time of 5 to 25 min, was examined. To obtain more accurate results each experiment was repeated 3 times, whereby the reproducibility of the replicated measurements could be seen from the error bars.

Analytical Methods

Diesel desulfurization was carried out using a triple system consisting of hydrogen peroxide (oxidant) and iron(III) chloride as a catalyst with formic acid, acetic acid, and PA as catalytic media with concentrations depending on total moles of sulfur in the feedstock. The sulfur content in the organic phase before and after oxidation has measured using X-ray fluorescence (Tanaka Scientific sulfur Meter Model RX-360SH, Japan) (Figure 1). According to ASTM D-4294, after bombarding a material (sulfur elements) in petroleum products with high-energy X-rays or gamma rays, secondary or fluorescent rays are emitted from it that has been excited. The experimental approach is based on the energy dispersive X-ray fluorescence technique.

The minimum applicable sulfur detection in this technique is at least 10 ppm. The total amounts of sulfur removed with these compounds were calculated according to the equation (1):

$$\text{Desulfurization efficiency(\%)} = \left(1 - \frac{S_i}{S_f} \right) \times 100 \quad (1)$$

where S_i and S_f are sulfur content of the initial diesel, and the sulfur content of the oxidized diesel, respectively. To

Figure 1: X-ray fluorescence device (Tanaka Scientific Sulfur Meter Model RX-360SH) that has used to measure total sulfur contents in diesel

obtain more accurate results, each experiment was repeated 3 times and the error bars for all the data were given.

A Krüss Tensiometer K9 model K9MK1 was employed to measure CA surface tensions. A glass dish containing the acid was surrounded by a water jacket connected to a thermostat to control the temperature of the acid sample. Surface tensions were recorded wherein a Pt-Ir alloy plate was immersed in the acid surface layer.

RESULTS AND DISCUSSION

Table 1 summarizes the physicochemical properties of diesel produced by Kirkuk Refinery. As can be seen, the boiling point range for the diesel used in the extraction is $180\text{--}346^\circ\text{C}$. It has been analyzed that the basic sulfur species of fuel products in the boiling range of diesel are almost alkylbenzothiophenes and alkyldibenzothiophenes (Ma et al., 1994). To investigate the effects of several operating parameters on the oxidative sulfur reduction process, various mixtures of immiscible solutions (CA-Lewis acid-Fe(III) halide) in diesel fuel were made up for oxidation with H_2O_2 and which played a triple role in the process of sulfur removal. All oxidation reactions were carried out with varying molar ratios of $\text{H}_2\text{O}_2/\text{S}$ and CA/S at a constant 55°C . Moreover, in comparison with simple extraction to reduce sulfur from diesel, ODS of diesel using ferric halides was carried out to investigate the importance of the catalyst-oxidation stage before the extraction stage in the final stage of desulfurization.

Ferric chloride has a pronounced effect on the extraction of organo S-compounds from oil products. Dharaskar et al., 2015, noted that due to the specific interaction between the Fe^{3+} cation and aromatic sulfur compounds, up to 59% of sulfur species could be extracted into the Lewis acidic FeCl_3 -based (Bmim)Cl phase. Similarly, Zhang et al., 2009, extracted around 96% of thiophenic compounds from model fuel into anhydrous ferric chloride-based (Bmim) BF_4

ionic liquid. In the current study, four different iron(III) concentrations were used under otherwise identical reaction conditions to examine the effects of the amount of cation on the oxidative reaction properties (Table 2). FeCl_3 increased the extraction ability to about 4–7% of the ODS process.

What is interesting about the data in this table is that the sulfur removal gradually increased from 14 to 21% and 15.5 to 21% in FA and AA, respectively, as $[\text{Fe}^{3+}]$ was varied from 3.7 to 11.1 mmol/L. However, the sulfur removal dropped as the Fe^{III} Lewis acid concentration was changed from 11.1 to 14.8 mmol/L with sulfur removals of 21% to 20% and 21% to 19% in FA and AA, respectively. The reason behind the decrease in desulfurization efficiency was possibly due to fact that using high concentrations of FeCl_3 enhanced the decomposition of H_2O_2 . Based on the above result, I have used 11.1 mmol/L in the ODS process.

Effect of Mole ratio Of CA/S on Reactions

As mentioned in the literature review, during the oxidation stage, various non-aliphatic sulfur compounds were oxidized to their corresponding sulfoxide and sulfones. CA might be the best solvents that act as extractants in the oxidation desulfurization through the formation of percarboxylic acids, which catalyze and give their oxygen atoms to the sulfur-containing species present in diesel (Ali et al., 2006). Percarboxylic acid is produced *in situ* from CA and the oxidant (H_2O_2). In the ODS process, it was found that an increase in extractant dosage has a pronounced effect on its extraction power, and therefore the sulfur removal efficiency will significantly increase (Lü et al., 2013).

Based on this, the ODS reaction can be improved by increasing the mass of the R-COOH in the reaction. In addition, CA is well known as a good extractant for the simultaneous extraction of the oxidized sulfur-based molecules in the reaction medium compared to aldehydes and ketones. To investigate the influence of stoichiometric of nCA/nS on the performance of oxidation reactions, the oxidation reactions for AA and FA at $55 \pm 1^\circ\text{C}$, with stoichiometries of nCA/nS = 2, 8, 14, 20, and 26, a mole ratio of $\text{H}_2\text{O}_2/\text{S} = 15$, time of reaction = 25 min were

Table 2: Influence of the concentration of FeCl_3 on the removal of S-compounds

[FeCl_3]/mmol/L	S-removal (ppm)	
	At FA	At AA
3.7	819.7±7.8	914.7±10.4
7.4	1080±8.2	1123.4±9.4
11.1	1230±4.7	1251.6±8.5
14.8	1203.3±8.4	1133.5±4.5

Experimental conditions: $T=55^\circ\text{C}$, $t=25$ min, nCA/nS=4, $\text{H}_2\text{O}_2/\text{nS}=7$, $S_0=5930$ ppm and mixing speed=400 rpm

carried out. Whereas Xu et al., 2018, used a PA-based DES for deep desulfurization, due to its complete solubility in diesel fuel, PA could not be utilized as an aqueous catalytic medium for the ODS system in this work, as shown in Figure 2. To demonstrate the miscibility of PA in choline chloride as DES, I have prepared a eutectic solvent according to their experimental method and mixed this with diesel and n-heptane; however, the PA-based DES completely dissolved in both non-polar phases.

With an increasing number of methylene groups, the hydrophobic interaction increases, as analyzed by Yamamoto and Nishi, 1990. There is a significant difference in the hydrophobicity of methyl, ethyl, and propyl groups which is probably enough once diarized to make the difference. Therefore, only AA and FA were used as aqueous extractants. The percentage sulfur removal versus nCA/nS is shown in Figure 3, where the stock weight concentration of sulfur molecules was 0.593%.

In the present experiment, it was shown that the sulfur elimination increases with increasing CA/S mole ratio. When the mole ratio of nCA/nS in FA and AA increased from 2 to 26, the sulfur removal increases from 36 to 55% and 38 to 61.8%, respectively. In the reaction medium, an increasing CA concentration is the consequence of the expected increment in percarboxylic acid concentration that leads to enhanced *in situ* extraction of oxidized S-compounds in the lower layer of the aqueous reaction medium. Extraction and catalytic oxidation in the CA/ FeCl_3 solution clearly removes the sulfur from the diesel. Moreover, the capability of ODS for S-removal in AA is higher than in FA as shown in Figure 3.

Recent evidence suggests that surface tension is an indicator and an important aspect of understanding the required energy to increase the surface area and form a

Figure 2: Forming two phases in extraction by AA and FA, and one phase by propanoic acid after adding diesel

hole in the fluid for the S-compounds to fit into (Chandler, 2005, Abbott et al., 2017). High surface tension prevents the extracted liquid from forming an emulsion due to mechanical excitation, and hence reduced extraction efficiency. Any decrease in the cohesive forces at the interface result in low surface tension, hence increasing liquid solubilization (Abbott et al., 2017). Using Krüss tensiometer, the surface tensions (γ) at 55°C were measured for AA (23.4 mN.m⁻¹) and FA (33.5 mN.m⁻¹) to calculate the average radius of the holes (r_H) of the extractants using equation 2 (Abbott et al., 2007):

$$r_H = \sqrt{(3.5KT / 4\pi\gamma)} \quad (2)$$

where T is the temperature in Kelvin and K is the Boltzmann constant.

Average void radius r_H (Å) of AA and FA extractants were 23.2 and 19.1 respectively. It is cleared that AA has lower surface tension than the FA which directly proportional with the capability of the extraction. It can be deduced that the energy required to make a hole in the AA is lower than in the FA due to the bigger average hole size, which is ultimately the controlling factor limiting the transportation of aromatic S-species from the non-polar diesel phase into the CA.

Effect of H₂O₂/S Mass Ratio on ODS

In the R-COOH-H₂O₂ extraction-oxidation sulfur elimination system with oxidant (i.e. H₂O₂), the dosage of H₂O₂ directly influences the amount of peroxy-carboxyl produced in the oxidation process, and thus has a direct effect on the desulfurization efficiency (Zhang et al., 2011). The influence of the H₂O₂ as a unique oxidizing agent to sulfur mole ratio on the ODS of the aromatic sulfur compounds present in diesel was investigated at 55°C. Based on the stoichiometry of the reaction, two moles of oxidant should be consumed per mole of sulfone product (equation 3) (Campos-Martin et al., 2004).

H₂O₂/S molar ratios of 15, 22, 29, and 36 were selected, and the removal of heterocyclic sulfur compounds over 25 min was plotted, as per Figure 4.

It can be seen in the figure that the removal of aromatic sulfur species gradually increases from 55.8% to 65% and 51% to 59.1% when using AA and FA, respectively, when the mole ratio of H₂O₂/S increased from 15 to 36. Whereas the oxidizing agent is usually employed in excess of the stoichiometric ratio in ODS, in the present findings the

Figure 3: Effect of the molar ratio of carboxylic acids/S on sulfur removal. Reaction conditions: H₂O₂-FeCl₃-carboxylic acid system; T = 55°C; Si = 0.593%; [FeCl₃] = 11.1 mmol/L, nH₂O₂/nS = 15 (i.e., for oxidation of 20 ml of diesel, 2.58 ml H₂O₂ and 0.345, 1.38, 2.42, 3.46, and 4.5 ml of acetic acid and 0.23, 0.91, 1.6, 2.3, and 2.96 ml of formic acid for nAA/nS or nFA/nS equal to 2, 8, 14, 20, and 26, were used, respectively)

Figure 4: Sulfur removal as a function of H₂O₂/S mole ratio. Reaction conditions: H₂O₂-FeCl₃-carboxylic acid system; T = 55°C; Si = 0.593%; [FeCl₃] = 11.1 mmol/L, nCA/nS = 26 (i.e., for oxidation of 20 ml diesel, 4.5 ml acetic acid, 2.96 ml formic acid, and 2.58, 3.77, 4.98, and 6.2 ml H₂O₂ and for nH₂O₂/nS ratios of 15, 22, 29, and 36, were used, respectively)

maximum removal capability appeared to be up to 65% of the sulfur compounds in diesel, which was expected and essentially unsurprising. The first possible reason for just 65% removal of S-compounds is shown in Table 1, namely, that 28.3% of diesel is made up of aromatic species, some of which will probably be polyaromatic compounds such as

phenanthrenes that prevent sulfur extraction from fuel, as highlighted by Xiao et al., 2012. Due to high concentrations of aromatic compounds in diesel, the cetane number is reduced to 51.7 and negatively impacts the fuel's quality. The second possible reason is due to the lack of efficient mass transfer between the aqueous layer and diesel phase reaction systems (Feng, 2010). While 55°C as a reaction temperature has been used in this work, oxygen and water are products of thermal decomposition has been reported by Hiroki and LaVerne, 2005.

Another problem is with the consumption of oxidant by the nitrogen-containing compounds' co-oxidation reactions in the diesel, which seriously complicate matters. These reactions are undesirable because of the consequent high oxygen consumption and because all N-compounds appear to inhibit ODS reactions of aromatic S-species, as reported by Caero et al., 2006. Another possible reason for the efficiency of the ODS of used diesel in this study is that the addition of peroxide to petroleum products results in epoxidation of olefins in tandem with the oxidation of sulfur compounds making this method ineffective, as investigated by Ali et al., 2006. In addition, finding an appropriate extractant to efficiently adsorb sulfur molecules rather than aromatic hydrocarbons and olefins is a particular challenge to the ODS process. Abro et al., reported that choosing unsuitable extractants has a pronounced effect on the undesired parallel extraction of S-free olefins or aromatics from the fuel liquid with the intended sulfones (Abro et al., 2014). A maximum excess of oxidant was 6 ml versus 20 ml diesel when nH_2O_2/nS was 36, because if a very high excess of hydrogen peroxide had been used in this study, the operation would be no longer representative of any industrial application. From the abovementioned reasons, the ODS process remains a matter of controversy.

Effect of Reaction Time on Sulfur Elimination

The efficiency of removing organic S-compounds from the partially hydrotreated diesel as a function of various reaction times (5, 10, 15, 20, and 25 min) at a 55°C reaction temperature and at 400 rpm was examined (Figure 5). According to the van't Hoff law, increasing temperature up to 70°C in extraction reactions results in a decline in sulfur removal capability. Thus, the extraction process becomes exothermic and S-compounds start to repartition from the extractant phase to the diesel phase (Rahma et al., 2017). In addition, a high reaction temperature results in catalyst deactivation and H_2O_2 decomposition (Tian et al., 2015). Lü et al. found that at room temperature, the ODS is relatively low compared to a higher temperatures due to reduced H_2O_2 reactivity (Lü et al., 2015). Therefore, 55°C was utilized as the reaction temperature.

Figure 5: Oxidative desulfurization from diesel as a function of time. Reaction conditions: H_2O_2 - $FeCl_3$ -carboxylic acid system; $T = 55^\circ C$; $Si = 0.593\%$; $[FeCl_3] = 11.1$ mmol/L, $nCA/nS = 20$ (i.e., for oxidation of 20 ml of diesel, 3.46 ml of acetic acid, 2.96 ml formic acid, and 5 ml of H_2O_2 were used, respectively)

It is shown from Figure 5 that the extractive desulfurization in both AA and FA improved from 39.4 to 50.7% and 37 to 49.5%, respectively, as the reaction time increased from 5 to 25 min. The reaction rates in AA and FA are clearly rapid, as the S-removal after 5 min had reached 39.4 and 37%, respectively. These results indicate that oxidant-supported ferric chloride is a key factor affecting S-removal. The aqueous solution of H_2O_2 - $FeCl_3$ -R- CO_2H system is mostly caught in the bottom phase of two immiscible biphasic systems. Thus, it can be operatively reutilized for sulfur removal in new feeds, which can be considered as an important feature of the ODS system.

CONCLUSIONS

In this study, the ODS of partially hydrotreated diesel using the triple system of H_2O_2 -ferric chloride-CA (formic acid, acetic acid, or PA) was studied experimentally. The influences of different operating parameters such as reaction time, $FeCl_3$ concentration, and the nH_2O_2/nS , and nCA/nS ratio on the performance of the ODS operation were examined.

Due to the difference in hydrophobicity between formic acid, acetic acid, and PA, the latter dissolved fully in diesel and thus could not be used as an aqueous extractant. There is a good correlation between the sulfur compound removal and the energy required to make a hole in the FA and AA. It was shown that AA (lower surface tension) showed better extraction performance than FA (higher surface tension),

because the average void radius in AA (23.2 Å) is bigger than that of FA (19.1 Å).

An $\text{nH}_2\text{O}_2/\text{nS}$ molar ratio of 36 gave allowed for the greatest removal of sulfur compounds at 55°C. The extraction of sulfur species in the desulfurization process of partially hydrotreated diesel in the absence of oxidation is not in any way an efficient method.

Increasing the molar ratio of nCA/nS in reaction medium results in an increase in S-removal due to the associated increase in percarboxylic acid concentration, which enhances *in situ* extraction of oxidized sulfur compounds. Maximum sulfur-based compound removal observed in the current study was 65.1%. This was due to the large amounts of aromatic-containing compounds in the diesel which negatively affected its quality and reduces its cetane number from a more normal range to 51.7.

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