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Improved Kerosene Quality with the Use of a Gamma Alumina Nanoparticles Supported Zinc Oxide Catalyst in a Digital Batch Baffled Reactor: Experiments and Process Modelling

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Abstract – To create an environmentally sustainable fuel with a low sulfur concentration, requires alternative sulfur removal methods. During the course of this study, a high surface gamma alumina-supported ZnO nanocatalyst with a ZnO/-Al_2O_3 ratio of 12% was developed and tested for its ability to improve the activity of the oxidative desulfurization (ODS) process for the desulfurization of kerosene fuel. Scanning electron microscopy (SEM) and Brunauer-Emmett-Teller (BET) were used to characterize the produced nanocatalyst. In a digital batch baffled reactor (20~80 min), the effectiveness of the synthesized nanocatalyst was tested at different initial concentrations of dibenzothiophene (DBT) of 300~600 ppm, oxidation temperatures (25~70 ℃), and oxidation periods (0.5, 1, and 2 hours). The baffles included in the digital baffled batch reactor resist the swirling of the reaction mixture, thus facilitating mixing. The ODS procedure yielded the maximum DBT conversion (95.5%) at 70 ℃ with an 80-minute reaction time and an initial DBT level of 600 ppm. The most precise values of kinetic variables were subsequently determined using a mathematical modelling procedure for the ODS procedure. The average absolute error of the simulation findings was less than 5%, demonstrating a good degree of agreement with the experimental results acquired from all runs. The optimization of the operating conditions revealed that 99.1% of the DBT can be removed in 140 minutes.

Key words: Gamma alumina, Mathematical model, Optimization process, Digital baffled batch reactor Nanocatalyst, Zinc oxide

1. Introduction

It is no secret that numerous industries rely on petrochemicals and fuels derived from petroleum. While thiophenes and other organic sulfur compounds have numerous practical applications, their existence presents a significant issue due to the damage they do to the environment, the increased cost of petroleum products as a result of corrosion of refining equipment and pipelines, and the poisoning of the catalyst [1-4]. As a contaminant, sulfur is commonly present in the majority of petroleum products, including kerosene, gasoline, jet fuel, and diesel. When petroleum fractions containing sulfur compounds are burned, SO_X is released into the environment as a pollutant. This causes a number of problems, such as the spread of serious illnesses and damage to the environment [4-7]. The need for petroleum products of the highest possible quality, coupled with the emergence of increasingly stringent environmental regulations and restrictions, implies that the development of many technologies for the elimination of sulfur compounds is an issue that is both vital and urgent [8-10]. In accordance with Environmental Protection Agency (EPA) standards, the allowable sulfur compound content in highway diesel and gasoline in several nations has been reduced to 15 ppm and 30 ppm, respectively [1, 11, 12]. Hydrodesulfurization (HDS), oxidative desulfurization (ODS), adsorptive desulfurization (ADS), extractive desulfurization (EDS), and biodesulfurization (BDS) are only some of the methods that have been the focus of research to improve in order to remove sulfur from fuels. ODS is among the most promising technologies for diesel fuel sulfur removal. Sulfoxides and sulfones can be removed, adsorbed, or precipitated from fuel after reaction under atmospheric pressure and modest reaction temperatures. This approach removes sulfur compounds including thiols and benzothiophenes that are difficult to remove using HDS [13-15]. The geometry, material, and number of baffles of tank reactors with mechanical agitation are all design variables that might affect the final product. Fluids with low viscosity move tangentially when the impeller rotates in a stirred tank without baffles. Inadequate mixing occurs when fluid is moved in a circular pattern at a high circumferential velocity, and a deep vortex forms at the free surface, the depth of which is dependent on the mixing intensity. With baffles, circular fluid flows can be disrupted, preventing vortex formation and making the fluid surface practically flat. Also, axial flows become much stronger, which makes the rate of mixing go up [16]. The ODS process makes use of zinc oxide

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(ZnO) as a catalyst since it is both cheap and extremely active. Due to the large surface area of the catalyst support, zinc oxide can be evenly distributed over it. This boosts the catalyst's activity by creating more active sites[17]. Alumina is used as a refractory, an insulator, and an abrasive in numerous types of machinery and industry. In oil and petrochemical production, it is used as catalyst support because of its large surface area, efficient thermal stability, little cost, and satisfactory mechanical strength of phase [18]. In two investigations, heterogeneous ZnO was employed as an active component and γ -Al_2O_3 as a catalyst support to remove sulfur compounds from ODS. Abdulateef et al. (2018) used a batch reactor and a catalyst with a surface area of 107.429 m^2/g to remove sulfur compounds using the ODS method. This was achieved at a relatively low temperature and period (45 minutes at 190 degrees Celsius) [19]. Nawaf et al. (2019) investigated the oxidative desulfurization of kerosene with air as the oxidizing agent and a catalyst of (18% ZnO/γ-Al_2O_3, surface area of 159.267 m^2/g) in a batch reactor. The ODS process efficiency was 70.5% after 50 minutes at 190 degrees Celsius [20]. Also, Humadi et al. (2022) investigated the activity of MnO_2/SnO_2 nanocatalyst at various amounts of MnO_2 (0%, 1%, and 5%) in eliminating sulfur from kerosene using the oxidative-extractive desulfurization process (OEDS). The results proved that increasing the amount of MnO_2 was dramatically improved the performance of ODS process [6]. This study investigated how increasing the catalyst's (12% ZnO/γ-Al_2O_3) surface area with high-surface-area gamma alumina affected the catalyst's properties and the ODS's performance. The ODS method was also made more effective by the incorporation of a computer-controlled baffled batch reactor, which improved mixing. To reduce sulfur content and produce a cleaner and greener fuel, the verified process mathematical model was applied in an optimization framework to establish the optimal operating parameters.

2. Methodology and Experimental Materials

2-1. The application of materials

2-1-1. Hydro processed Kerosene

Since hydrotreated kerosene was readily available from the Daura Refinery in Iraq, it was employed as the oil feedstock in the ODS process testing. Hydrated kerosene has an API gravity of 48.8, a flash point of 52 degrees Celsius, a specific gravity of 0.784, and an initial sulfur content of 10 parts per million.

2-1-2. Dibenzothiophene (DBT)

DBT, purchased from Sigma Aldrich with a purity of 98%, is one of the refractory aromatic sulfur compounds used to study the activity of the ODS reaction in the presence of the produced catalyst.

2-1-3. Zinc acetate

The catalyst was prepared using a zinc acetate ($Zn(CH_3COO)_2 \cdot 2H_2O$) active metal purchased from Sigma.

2-1-4. Gamma alumina (γ-Al_2O_3)

Table A.1 summarizes the characteristics of gamma alumina (Al_2O_3) nanoparticles, which are employed as catalytic support (supplied by SkySpring Nanomaterials Inc).

2-1-5. Hydrogen Peroxide (H_2O_2)

Ultra-pure hydrogen peroxide from Aldrich is used as the oxidant in the ODS reaction to turn the model sulfur molecule into sulfoxides and sulfones.

2-2. Preparation of catalyst

The method of incipient wetness impregnation is employed in preparing nano-catalyst for application in reactions. The active ingredient is made by dissolving zinc acetate, $Zn(CH_3CO)_2 \cdot 2H_2O$, in 148 mL of deionized water. The generated solution is then agitated with a magnetic stirrer for an additional hour at room temperature. After the solution has been thoroughly stirred for 1.5 hours, 8.8 grams of Al_2O_3 support are added to complete the IWI process. After the solution has been impregnated, it is exposed to drying in an oven for 24 hours at 120 ℃. The produced material is calcined in a heating furnace at 550 ℃ to create the 12% ZnO/ γ-Al_2O_3 nanocatalyst. Process steps for preparing 12% ZnO/γ-Al_2O_3 using IWI are shown in Fig. B.1.

2-3. Experimental methodology

2-3-1. Batch reactor with digital baffles (DBBR)

To get a better mass transfer rate during ODS technology, a DBBR was designed, built, and run locally. This reactor was created and built at Tikrit University's College of Petroleum Processes Engineering. The DBBR has a cylinder made of stainless steel, a digital mixer, and a rotary impeller with six flat blades and a depth of 5 cm, and a length of 5 cm. Improvements in mixing channels in the DBBR and greater sulfur removal efficiency from the fuel, oxidant, and catalyst were accomplished by the use of a unique design for a flat blade turbine that incorporates circular holes that are spread in regular form in a hexagonal configuration over the metal surface. The stainless steel 200 ml DBBR was fitted with four baffles of stainless steel (width of 2.5 cm and height of 20 cm). Each of the four baffles was inserted into the DBBR at a uniform depth of 2.5 centimeters, and spaced uniformly apart from one another in the batch reactor at a distance of 38 centimeters. The DBBR operates at extremely high temperatures (over 1000 ℃) and is insulated via woolen material from the reactor's exterior perimeter. It is also supplied with electrical power with a rotating range of up to 5000 rev/min. The operation diagram is shown in Fig. B.2, and the general specifications of the DBBR are detailed in Table A.2.

2-3-2. The method of oxidative desulfurization

For this study, hydrotreated kerosene from the Daura Refinery was used as a fuel. Large-surface-area γ-Al_2O_3 was used as a catalyst support. Injecting DBT into used fuel that has an initial sulfur level of (300, 450, or 600) ppm allows for the preparation of a sample of kerosene feedstock. Kerosene was used as a feedstock for the ODS reactions that were carried out in the DBBR, and hydrogen peroxide was used as the oxidizing agent. For each run of the ODS that was carried out in this study, 100 milliliters of oil feedstock was used. In all of the tests, the oil feedstock to H_2O_2 oxidizing agent ratio was 25 (Kerosene/Oxidant = 25) at a constant pressure of 1 atm. Kerosene/Oxidant ratio was selected based on the previous literature [2,6,13]. The kerosene-filled DBBR receives a nano-catalyst ($ZnO/\gamma\text{-}Al_2O_3$) injection. ODS reactions are often carried out at relatively gentle working conditions, including the following: reaction temperatures of (25-70) ℃, reaction periods of (20-80) min, and a steady stirring speed of 600 rpm.

3. Development of a Mathematical Model for the ODS Process

The treatment of industrial issues with mathematical equations that may be solved by numerical and theoretical techniques has been one of the most important contributions that mathematical modelling operations have made to the field of engineering [21]. Mathematical modelling of the DBT removal by the ODS process was performed with the help of the General Process Modeling System software (gPROMS) [22]. The mathematical modelling for ODS processes involves a set of equations, which are summarized in Table 1.

4. Kinetic Parameter Estimation

By precisely correlating the experimental findings and the data from using the ODS model, it is possible to estimate the optimal parameters for ODS kinetic. To figure out which kinetic parameters were better, the objective function was minimized as follows:

$$OBJ = \sum_{n=1}^{Nt}(C_{DBT}^{exp} - C_{DBT}^{pred})^2 \tag{20}$$

Table 1. The equations used in the mathematical modelling of ODS

Parameter	Equations/values	Eq. no.	Ref.
Rate of reaction ($-r_{DBT}$)	$(-r_{DBT}) = \eta_0 k C_{DBT}^n$	(1)	[20]
Reaction rate constant (k) (Arrhenius equation)	$k = k_0 e^{\left(-\frac{EA}{RT}\right)}$	(2)	[23,24]
Final concentration of dibenzothiophene (C_{DBT})	$C_{DBT} = [C_{DBT.t}^{(1-n)} + (n-1).t.K_{in}\eta_0]^{\left(\frac{1}{1-n}\right)}$	(3)	[14]
The effectiveness factor (η_0)	$\eta_0 = \frac{3.0(\phi\coth\phi - 1.0)}{\phi_2}$	(4)	[14,25]
Thiele modulus (ϕ)	$\phi = \frac{V_p}{S_p}\sqrt{\left(\frac{n+1.0}{2.0}\right)\frac{k_{in}C_{DBT}^{(1-n)}\rho_p}{D_{ei}}}$	(5)	[14,25]
Effective diffusivity (D_{ei})	$D_{ei} = \frac{\varepsilon_B}{\mathcal{T}}\sqrt{\left(\frac{n+1.0}{2.0}\right)\frac{k_{in}C_{DBT}^{(1-n)}\rho_p}{D_{ei}}}$	(6)	[20]
The porosity of catalyst (ε_B)	$\varepsilon_B = V_g\rho_p$	(7)	[20]
Particle density (ρ_p)	$\rho_p = \frac{\rho_B}{1-\varepsilon_B}$	(8)	[20]
The tortuosity factor ($\mathcal{T}$)	Tortuosity factor ($\mathcal{T}$) ranged (2 to 7) for the pores network	----	[26]
Knudsen diffusivity (D_{ki})	$D_{ki} = 9700.0 r_g\left(\frac{T}{M_{wi}}\right)^{0.50}$	(9)	[20]
Mean pore radius (r_g)	$r_g = \frac{2V_g}{S_g}$	(10)	[14]
Molecular diffusivity (D_{mi})	$D_{mi} = 8.93\times 10^{-8}\left(\frac{v_l^{0.267}T}{v_{DBT}^{0.433}\mu_l}\right)$	(11)	[27,28]
Molar volume for dibenzothiophene (v_{DBT})	$v_{DBT} = 0.2850(v_{cDBT})^{1.0480}$	(12)	[25]
Kerosene molar volume (v_l)	$v_l = 0.2850(v_{cl})^{1.0480}$	(13)	[29]
Critical volume of oil (v_{cl})	$v_{cl} = (7.52140\times 10^{-3.0}(T_{meABP})^{0.28960}(\rho_{L15.6})^{-0.76660})M_{w_L}$	(14)	[29]
External volume of catalyst (V_p)	$v_p = \frac{4.0}{3.0}\pi(r_p)^{3.0}$ (sphere particle)	(15)	[30]
External surface of catalyst (Sp)	$S_p = 4.0\pi(r_p)^{2.0}$ (sphere particle	(16)	[30]
Fuel viscosity (μ_l)	$v_l = 3.1410\times 10^{10}(T-460.0)^{-3.4440}(\log API)^{\alpha}$	(17)	[29]
Dimensionless number, (α)	$\alpha = 10.3130[\log_{10}(T-460.0)] - 36.4470$	(18)	[29]
American petroleum Institute (API)	$\text{API} = \frac{141.50}{sp.gr_{15.6}} - 131.50$	(19)	[31]

Table 2. Optimizing parameter estimation

Given	Obtain	So as to minimize	Subjected to
· Catalyst Type. · Experimental parameters for oxidative desulfurization · DBBR formation.	Pre-exponential factor (ko), reaction order (n), and activation energy (EA) for (ZnO/ γ -Al_2O_3)	The sum of squared error (SSE).	Constraints of operation

The following equation can also be used in calculating the conversion of DBT:

$$X_{DBT} = 1 - \frac{C_{DBT}}{C_{DBT.t}} \tag{21}$$

5. Formulation of the Optimization Problem for Kinetic Parameter Estimation

Table 2 is explained the parameters used in estimating the ODS problem:

Following is the mathematical form of the optimization problem:

Min: **SSE**

n^j, EA^j, k_i^j, (j = catalyst number 1, 2, …)

S.t.f (z, x(z), $\dot{x}$(z), u(z), v) = 0

$C_L \le C \le C_U$

$n_L^j \le n^j \le n_U^j$

$EA_L^j \le EA^j \le EA_U^j$

$k_{oL}^j \le k_i^j \le k_{oU}^j$

Where:

S.t.f(z, x(z),$\dot{x}$(z), u(z),v) = 0 : ODS model.
z : independent variable.
u(z) : the decision variable.
x(z) : the set of all variables.
$\dot{x}$(z) : the derivative of the variables based on time.
v : the design variable.
L,U : lower and upper bounds.

6. Findings and Discussion

6-1. Characterizing the prepared catalyst

6-1-1. Prepared nanocatalyst surface area

The Brunauer-Emmett-Teller (BET) test was utilized to evaluate the nanocatalyst surface area, pore volume, and pore size. Table 3 displays the results of the BET test conducted on the produced nano-catalyst (12% ZnO/γ-Al_2O_3). The pore volume and specific surface area were shown to decrease following zinc oxide loading. ZnO occupancy in specific catalyst regions accounts for this phenomenon [32]. Also, the surface area and pore volume of catalyst were decreased after the impregnation step due to the blockage of the pores of alumina with the deposited metals. These promising outcomes demonstrate the catalyst possesses a high specific surface area, which boosts the number of functional active sites and enhances the adsorption of reactants. N2 adsorption and desorption isotherm for γ-Al_2O_3 and 12% ZnO/γ-Al_2O_3 catalyst are explained in Figs. B.3 and B.4.

Table 3. BET study of nano-catalyst

Sample	Specific surface area (m^2/gm)	Pore size (nm)	Pore volume (cm^3/gm)
γ-Al_2O_3	500	48	1.5
12% ZnO/γ-Al_2O_3	353. 5	20	0.037

6-1-2. Scanning electron microscopy (SEM)

Scanning electron microscopy is used to investigate the composition of the engineered catalyst's surface (SEM). Images of the nano-catalyst surface (12% ZnO/γ-Al_2O_3) are shown in Fig. B.5. The SEM examination does not reveal the precise distribution of ZnO particles on alumina support, but the presence of bright spots on the γ -Al_2O_3 surface may refer to the presence of heavier components. In addition, the small particles of nanomaterials are more easily dispersed in a medium of γ-Al_2O_3's large surface area [1].

6-2. Oxidative desulfurization results

6-2-1. The influence of temperature on reaction

The level of effectiveness achieved by the oxidative desulfurization process is strongly influenced by the temperature at which the reaction is carried out. The results of a study into the effects of raising the reaction temperature at 25, 40, 55, and 70 ℃ on the ODS reaction rate are shown in Fig. 1. A higher reaction temperature has been proven to hasten the decomposition of DBT compounds. This effect is caused by an increase in the collision probability between DBT compounds and the oxidizing agent. Further, using high temperatures permits the effortless elimination of the most strongly adsorbed sulfones from the catalyst surface active sites [33]. In a reaction with an initial concentration of 600 ppm DBT and an 80-minute time constant, a rise in temperature from 25℃ to 70℃ boosts DBT removal from 82.5% to 95.5%.

6-2-2. Influence of response time

The impact of reaction times on DBT chemical elimination is seen in Fig. 2. Experiments revealed that a longer reaction period resulted in more complete elimination of DBT because more sulfur compounds and the oxidant had time to contact each other on the active sites exhibited on the surface of nanocatalyst [34,35]. Increasing the oxidation time from 20 to 80 minutes at 70 ℃. with DBT level initially of 600 parts per million improved the percentage of DBT compounds removed from 80.6% to 95.5%.

6-2-3. Effect of initiating sulfur content

Fig. 3 depicts the findings from an investigation into the effects of

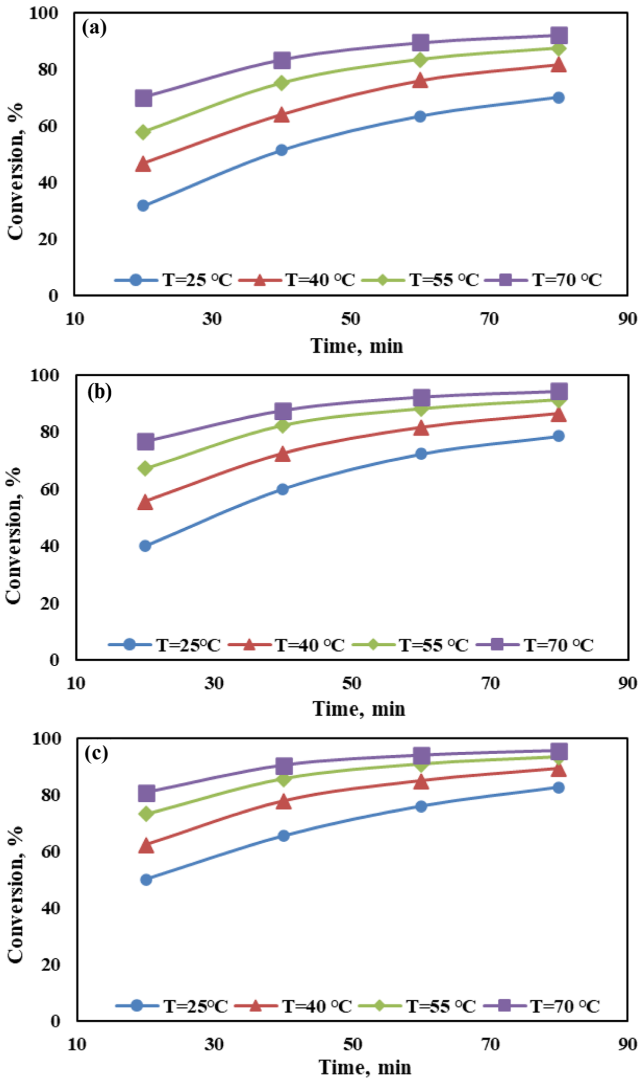

Fig. 1. At varied reaction times for starting DBT content, reaction temperature affects ODS reaction activity (a) Concentration Levels: (a) 300 ppm (b) 450 ppm (c) 600 ppm.

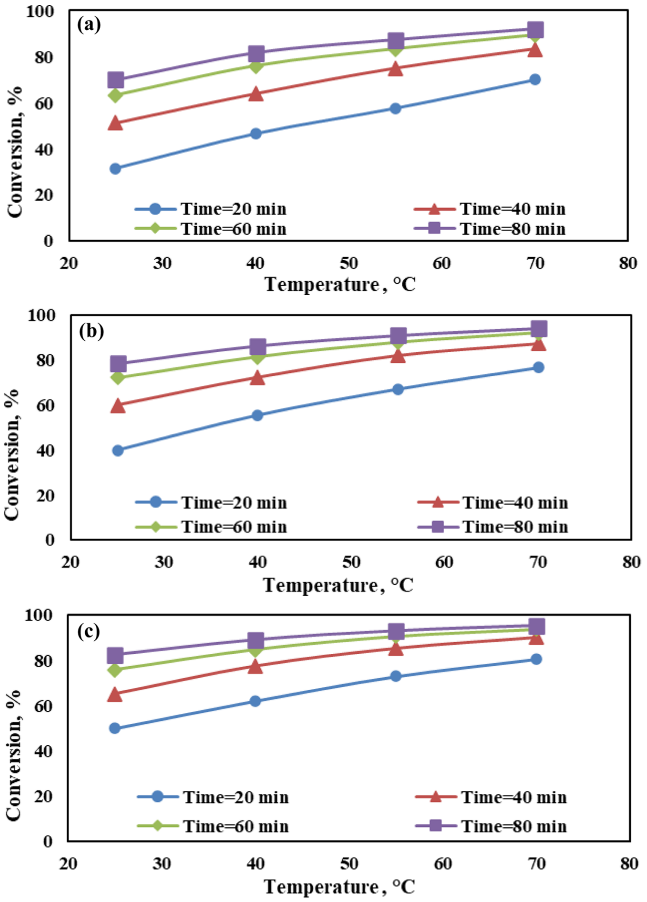

Fig. 2. The impact of initial DBT content on ODS reaction activity across a range of reaction temperatures (a) Concentration Levels: (a) 300 ppm, (b) 450 ppm, (c) 600 ppm.

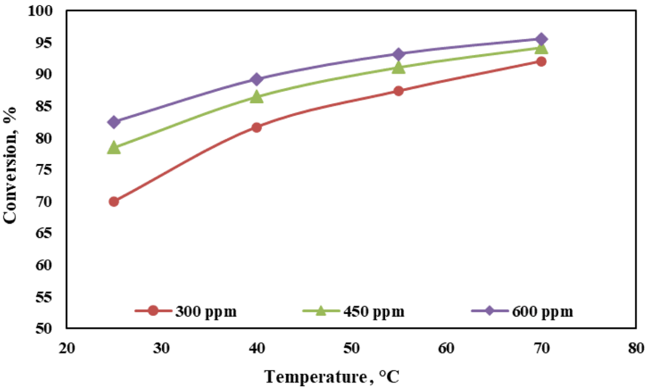

Fig. 3. ODS reaction activity and starting DBT content (reaction time = 80 min).

300, 450, and 600 ppm starting sulfur compounds on DBT conversion. It was shown that initial sulfur concentration had a significant impact on DBT conversion and that lowering it resulted in a lower overall conversion rate. Initiating an ODS reaction is more likely when more sulfur compounds are present. As a result, the number of reactions occurring between the reactants on the active sites of the produced catalyst increases when there is a high concentration of DBT in the oil feedstock[32] . In a study conducted at 80 minutes and 70 degrees Celsius, the DBT elimination degree rose from 92% to 95.5% as the starting DBT concentration enhanced from 300 ppm to 600 ppm.

6-2-4. The effect of γ-Al_2O_3 with a large surface area

To study how catalyst support affects ODS process activity, ZnO was loaded on high-surface-area gamma alumina (γ -Al_2O_3). By comparing these findings to those of comparable prior studies [19, 20], the results proved that catalyst support plays a crucial role in increasing sulfur compound removal throughout the ODS process. Because of its high surface area, γ-Al_2O_3 helps to ensure that active metal (ZnO) is evenly distributed across the surface of the catalyst [1]. As a result of its increased surface area, Al_2O_3 generate a bigger area for contacting area of reactants, producing a more complete eliminating for DBT. Due to γ-Al_2O_3's wide surface area, DBT molecules diffuse rapidly to the catalyst’s active sites [36].

Table 4. ODS modelling constant parameter values

Parameter	Unit	Value
Initial content of DBT compounds (Ct1,2,3)	ppm	300, 450, 600
Batch time1,2,3,4	min	20, 40, 60, 80
Reaction temperature (T1,2,3,4),	℃	25, 40, 55, 70
Density of kerosene at 15 ℃	gm/cm^3	0.523
T_{meABP}	°R	756
Acceleration gravity (g)	m/sec^2	9.810
R	J/mole. °K	8.314
Vg	cm^3/gm	0.037
Sg	cm^2/gm	3534350
Vp	cm^3	2.567×10^{-17}
Sp	cm^2	2.208×10^{-11}
$\rho_{B.}$	gm/cm^3	0.513
M.Wt of kerosene (M_{wL})	gm/mole	170
M.Wt of DBT (M_{wi})	gm/mole	184
r_g,	nm	0.209

Table 5. ODS reaction models with the most precise specifications

Parameter	Value	Unit
n	1.7560	-
EA	24.7470	KJ/mol.
k_o	7799.4320	$wt^{-0.756}.min^{-1}$
SSE	5.3570×10^{-6}	-

Table 6. Optimal parameters for ODS technology

Factors, unit	Value
$C_{DBT.i}$, ppm	899.0
T, ℃	87.0
Time, min	140.0
Conversion, %	99.1

6-3. ODS reaction's proposed mechanism

Fig. B.6 depicts the proposed mechanism for the ODS process, which is dependent on the H_2O_2 and prepared catalyst. It is based on these processes that the desulfurization reaction is carried out. At first, the DBT molecules undergo an adsorption process, wherein they are taken up into the pore channel of the catalyst (12% $ZnO/\gamma\text{-}Al_2O_3$). The second stage involves oxidizing the DBT molecules to the corresponding sulfoxides (DBTO) using the oxygen generated from the oxidizing agent (H_2O_2). By oxidizing the sulfoxides (DBTO), more polar sulfones ($DBTO_2$) are produced.

6-4. Determination of kinetic parameters

Table 4 lists the constants used in the modelling procedure. The application of the modelling led to the discovery of the most correct value of the kinetic parameters, which is displayed in Table 5 below.

6-5. Results from simulation and experiment

The results of the experimental runs and the predicted data for different oxidation temperature, oxidation time and initial DBT content are illustrated Figs B.7-B.10. As illustrated in these figures the difference between the results that experimental work and predicted values obtained via the process model gives low error (<5%) for all results. These figures show an excellent agreement between the data obtained experimentally and by modeling (each point represents the data generated experimentally (X axis) and by modeling (Y axis)) under the same ODS conditions. The correlation between the experimental and predicted data explains to be straight line with a slope close approximately to 1.0, which proves a significant agreement between it.

7. Optimized Operating Conditions based on DBT Concentration Minimization

7-1. Formulation of a maximal removability optimization problem

To maximize DBT chemical conversion, the obtained kinetic parameters are used to determine optimal working conditions. Consequently, the following creates the optimization problem:

Obtain: settings ideal for DBT removal using the ODS technique.

So as to minimize: Kerosene DBT content.

Subjected to: Operational Restriction(s)

The optimization problem can be mathematically expressed as follows:

Min: C_{DBT}

$T,\ t_i,\ C_{DBT}$

S.t. $f(z, x(z), \dot{x}(z), u(z), v) = 0$

$time_L \le time \le time_U$

$C_{DBT.tL} \le C_{DBT.t} \le C_{DBT.tU}$

$T_L \le T \le T_U$

$X_{DBT.tL} \le X_{DBT.t} \le X_{DBT.tU}$

The optimization solution is conducted using the gPROMS application.

7-2. Maximum DBT conversion process conditions

The optimal circumstances for the operation are presented in Table 6, which shows how using an optimization technique can offer these conditions.

The optimal operating parameters for producing high-quality kerosene fuel while still meeting environmental regulations, according to Table 6, are a reaction time of 140 minutes, a reaction temperature of 87 degrees Celsius, and an initial concentration of 899 parts per million DBT. More than 99% of the DBT had to be removed to achieve this goal. At the optimal conditions (temperature of 87 ℃ and time of 140 minute), an experimental run was conducted to check the reliability of the prediction. The DBT removal efficiency was 98.4% at the best experimental conditions and this obtained result is remarkably close to the predicted removal efficiency.

8. Conclusion

It was found that oxidative desulfurization of DBT in kerosene cut at 25-70 ℃, 20~80 min, and 300~600 ppm using high surface of 12% ZnO/-Al_2O_3 and hydrogen peroxide yielded the greatest removal of DBT components. Baffles were installed in digital baffled batch reactors to reduce fluid whirling and improve mixing. According to the conclusions of this study, the ODS system is very effective at removing DBT pollutants from kerosene fuel. This conclusion was reached after the ODS system was put through its paces. With an initial DBT concentration of 600 ppm, a reaction temperature of 70 degrees Celsius, and an 80-minute reaction period, the ODS system was able to remove 95.5% of the DBT. Furthermore, the rate of DBT conversion increased dramatically with the use of mathematical modelling techniques. Removing more than 99% of DBT from fuel with ODS took 140 minutes, a process temperature of 87 degrees Celsius, and an initial DBT concentration of 899 parts per million.

Nomenclature

k_{App}	: Apparent Rate Constant
$Sp.gr_{15.6}$	: Specific gravity of kerosene at 15.6°C
M_{wL}	: Liquid molecular weight of kerosene
M_{wi}	: Molecular weight of DBT
R	: Gas constant
$-r_{DBT}$	: Reaction rate of DBT
r_g	: Pore radius (nm)
r_p	: Particle radius
V_g	: Pore volume
T_{meABP}	: Mean average boiling point
ρ_B	: Bulk density
$\rho_{L15.6}$	: Density of kerosene at 15.6 ℃(gm/cm^3)

Supporting Information

Additional information as noted in the text. This information is available via the Internet at https://doi.org/10.9713/kcer.2023.61.2.226.

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