

Mathematical Modelling Of Diesel Fuel Hydrodesulfurization kinetics For Reduction Of Environmental health impacts

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المخلص

يعد الديزل أحد أكثر أنواع الوقود استخدامًا على مستوى العالم، وخاصة في صناعة النقل. تعد عملية إزالة الكبريت بالهيدروجين عملية تكرير بترولية بالغة الأهمية تهدف إلى إنتاج وقود نقل أنظف. وقد نمت أهمية عملية إزالة الكبريت بالهيدروجين في السنوات الأخيرة بسبب اللوائح الأكثر صرامة على انبعاثات المركبات وجودة الوقود، فضلاً عن الحاجة المتزايدة لمعالجة الزيوت الخام ذات الجودة المنخفضة التي تحتوي على تركيزات أعلى من الكبريت. للمركبات الكبريتية الموجودة في الوقود تأثيرات بيئية وصحية شديدة؛ أثناء الاحتراق، تشكل أكاسيد الكبريت (SOx)، والتي تساهم في هطول الأمطار الحمضية وتدهور كفاءة المحولات الحفازة المستخدمة لتقليل انبعاثات أول أكسيد الكربون وأكاسيد النيتروجين. تعمل عملية إزالة الكبريت بالهيدروجين عن طريق تحويل مركبات الكبريت العضوية إلى كبريتيد الهيدروجين (H₂S) والهيدروكربونات، عادةً في مفاعلات ثابتة ومنقطرة باستخدام محفزات (Co-Mo/γ-Al₂O₃) في درجات حرارة مرتفعة (300-425 درجة مئوية) وضغوط (1-20 ميجا باسكال). تبحث هذه الدراسة في حركية تفاعلات HDS باستخدام مركبات الكبريت النموذجية - الثيوفين، والبنزوثيوفين، والداي بنزوثيوفين - المستندة إلى الديزل الخام الليبي. تم استخلاص المعلمات الحركية، والتي تختلف حسب ظروف التفاعل وخصائص المحفز، باستخدام بيانات المصنع الفعلية من مصفاة تعالج 60.000 برميل من النفط الخام يوميًا. تم إجراء نمذجة التفاعل باستخدام Polymath و Excel لمحاكاة عملية HDS التحفيزية. الكلمات المفتاحية: النمذجة الرياضية، عملية المعالجة الهيدروجينية، حماية الصحة البيئية، جزء الديزل، البنزوثيوفين، الداى بنزوثيوفين، حركية التفاعل.

ABSTRACT

Diesel is one of the most widely used fuels globally, particularly in the transportation industry. Hydrodesulfurization (HDS) is a critical petroleum refining process aimed at producing cleaner transportation fuels. The significance of HDS has grown in recent years due to stricter regulations on vehicular emissions and fuel quality, as well as the increasing need to process lower-quality crude oils containing higher sulfur concentrations. Sulfur compounds in fuels have severe environmental and health impacts; during combustion, they form sulfur oxides (SO_x), which contribute to acid rain and degrade the efficiency of catalytic converters used to reduce CO and NO_x emissions. HDS operates by converting organosulfur compounds into hydrogen sulfide (H₂S) and hydrocarbons, typically in fixed- and trickle-bed reactors using (Co-Mo/ γ -Al₂O₃) catalysts at elevated temperatures (300–425°C) and pressures (1–20 MPa). This study investigates the kinetics of HDS reactions using model sulfur compounds—thiophene, benzothiophene, and dibenzothiophene—based on Libyan crude diesel. The kinetic parameters, which vary depending on reaction conditions and catalyst properties, were derived using actual plant data from a refinery processing 60,000 barrels of crude oil per day. Reaction modeling was conducted using Polymath and Excel to simulate the catalytic HDS process.

Keywords: Mathematical modeling, hydrotreating process, environmental health protection, diesel fraction, benzothiophene, dibenzothiophene, reaction kinetics.

INTRODUCTION

Diesel fuel is a primary energy source in the global transportation industry. However, its combustion generates sulfur oxides (SO_x) through the oxidation of organic sulfur compounds. SO_x emissions significantly contribute to environmental degradation by forming acid rain, which damages infrastructure, depletes forest ecosystems, and disrupts ecological balance[1,2]. Furthermore, exposure to SO_x has been associated with severe health issues, including asthma, pulmonary diseases, cardiovascular disorders, and increased risk of heart attacks. Consequently, many countries have established stringent regulations for diesel refining to reduce SO_x emissions. For instance, South Africa has mandated that by 2020, petroleum distillates must contain less than 5 ppm sulfur to comply with the Euro 5 emission standards[4,5]. This regulatory shift necessitates advanced

desulfurization methods to achieve such low sulfur levels. Various techniques, including hydrodesulfurization (HDS), adsorption (AD), biodesulfurization (BDS), oxidation, and solvent extraction, are under investigation to address this critical issue. The removal of sulfur from petroleum products is crucial for both environmental and industrial reasons [6]. Sulfur compounds in fuel not only cause corrosion in internal combustion engines and refinery equipment but also deactivate catalytic converters, reducing their efficiency. Catalytic hydrotreating (HDT) is a pivotal process in the refining industry for removing sulfur, nitrogen, oxygen, and metals while improving the quality of petroleum products. HDT is employed for various refinery streams, including straight-run distillates, vacuum gas oil, and light cycle oil[7]. The process involves the use of sulfided catalysts, such as cobalt-molybdenum (CoMo) or nickel-molybdenum (NiMo) supported on γ -alumina, under specific operating conditions, including elevated temperatures and hydrogen partial pressures. Hydrodesulfurization (HDS), a subset of the HDT process, is particularly critical for sulfur removal. While the HDS process efficiently removes simple sulfur compounds like sulfides, disulfides, and mercaptans, it struggles with more complex compounds such as benzothiophenes and dibenzothiophenes (DBTs). Specifically, sterically hindered molecules like 4-methyldibenzothiophene and 4,6-dimethyldibenzothiophene exhibit high resistance to desulfurization, thereby limiting the efficiency of conventional HDS processes. Current HDS technologies rely on exothermic reactions conducted in adiabatic fixed-bed or trickle-bed reactors, depending on the feedstock composition. While these methods have been in use since the 1930s, their optimization remains a focus of ongoing research to address economic and environmental challenges effectively. Stringent global regulations for ultra-low sulfur diesel (ULSD) emphasize the importance of advancing HDS technology[4]. In the United States, for example, the Environmental Protection Agency (EPA) has mandated a sulfur limit of 15 ppm for highway diesel, replacing the previous standard of 500 ppm. Similarly, California has adopted even stricter policies with accelerated implementation schedules and broader controls, including off-road and stationary sources. South Africa's alignment with Euro 5 standards underscores the global commitment to reducing SO_x emissions. Thus, enhancing desulfurization technologies is essential to comply with these regulations and

mitigate the environmental and health impacts of sulfur emissions[11]. Table (1) Sulfur standards for gasoline and diesel fuel [1].

Table (1) Sulfur standards for gasoline and diesel fuel [1].

Country	Regulation	Date	Sulfur Limit (ppm)
US	Tier 2-gasoline Heavy-duty-diesel	2006	80
		1993	500
		2005	50
		2006	15
EU	Heavy-duty-diesel	1997	350
		2003	350
		2005	50
		2008	10
Japan	National regulations	2004	50
Libya	Heavy Naphtha	2007	275
	Kerosene	2007	55
	Diesel	2007	800

The sulfur content of crude oil varies significantly depending on its origin. Highly paraffinic crudes from regions such as North Africa (Libya and Algeria), Nigeria, and Indonesia typically contain as little as 0.2 wt% sulfur and have a very low metal content (e.g., approximately 3 ppm). Deposits formed within catalyst pores or on the outer surfaces of catalyst pellets due to sulfur content can lead to plugging and eventual catalyst deactivation. Consequently, increasingly stringent sulfur content regulations have been implemented to mitigate emissions of sulfur oxides, which contribute to acid rain, ozone depletion, and smog. Additionally, automobile manufacturers are advocating for low-sulfur diesel, as advanced sulfur-sensitive technologies can reduce nitrogen oxide (NO_x) emissions by up to 75% and particulate matter by as much as 80%, provided sulfur content is minimized (EPA, 1999; Manufacturers of Emission Controls Association, 1999)[3,4]. Beyond air pollution prevention, operational and production requirements also necessitate that jet fuel feedstocks undergo hydrotreatment to achieve minimal sulfur content[9,10]. Deep desulfurization, broadly defined as the reduction of sulfur content in middle distillates to below **500 wppm**, poses a

challenge. Conventional hydrodesulfurization (HDS) technology efficiently reduces sulfur levels to **2500 wppm** and, with some difficulty, to **500 wppm**, but it has limited capacity to achieve the levels required for deep desulfurization [5,6]. Sulfur compounds are particularly present in the diesel fraction with a boiling point range of **250–350°C**, where sulfur content varies between **0.1 and 1.4 wt%** [7,8].

Main Objectives of the Research:

1. Selection and Validation of Rate Expressions:

- Identify the most suitable rate expression for catalytic hydrotreating from literature data.
- Utilize the selected rate expression to predict the behavior of industrial reactors.
- Compare the predictions with actual Libyan crude oil data, focusing on diesel fuel properties.

2. Kinetic Study of Sulfur Removal:

- Investigate the kinetic behavior of model sulfur compounds to simulate catalytic hydrotreating.
- Determine the required catalyst weight to achieve sulfur removal that complies with specification limits.

3. Assessment of Sulfur's Environmental and Health Impacts:

- Enhance understanding of the adverse effects of sulfur on human health and the environment, emphasizing the importance of its removal.

Modeling and Mechanism of Hydrodesulfurization (HDS)

The modeling and mechanisms of hydrodesulfurization (HDS) have been extensively studied using both model organosulfur compounds and industrial fuels. However, discrepancies in the data reported across studies arise due to variations in reaction conditions, reactor types, catalysts, and feedstock compositions. Despite these differences, several general conclusions regarding the reaction mechanisms and catalyst performance can be drawn from the literature.

Organosulfur compounds are ubiquitous across almost all fractions of crude oil distillation, with heavier fractions containing higher sulfur content and more complex sulfur compounds. Consequently, it is essential to consider a diverse range of sulfur-containing compounds in the context of hydrotreating processes. The key organosulfur compounds of interest include mercaptans, sulfides, disulfides, thiophenes, benzothiophene (BT), and their alkylated derivatives. Furthermore, for achieving ultra-deep desulfurization, polynuclear organic sulfur compounds warrant attention.

The HDS process, which involves the removal of sulfur from organic compounds, is exothermic and irreversible under industrial operating conditions. For thiophenic compounds, two primary reaction pathways are observed. In the first pathway, sulfur atoms are directly cleaved from the molecule via hydrogenolysis. In the second pathway, the aromatic ring undergoes hydrogenation, followed by sulfur removal. Both pathways occur simultaneously on different catalytic active sites. The dominant pathway depends on the nature of the sulfur compound, reaction conditions, and the catalyst used. For instance, under similar reaction conditions, dibenzothiophene (DBT) predominantly follows the hydrogenolysis pathway. In contrast, alkylated DBTs, particularly those substituted at the 4 and 6 positions, exhibit significant activity through both the hydrogenolysis and hydrogenation pathways[6].

Health and Safety Considerations

Sulfur and sulfur compounds of petroleum fractions are undesirable impurities so must be reduced for a variety of reason:

Environment

Sulfur and its compounds in fuels are converted, when burnt in air, to Sulfur dioxide (SO₂), which, if emitted in combustion gases to atmosphere, causes "Acid rain", an acidic solution formed by SO₂ dissolving in falling rain. Acid rain is currently a subject of great controversy because of widespread environmental damage for Which it has been blamed, including eroding buildings and structures, injuring crops And forests and threatening or depleting life in freshwater lakes[10].

Human Health Risks and Environmental Effects

The general population may be exposed to diesel fuel and other middle distillates through various means, including at fueling stations, during accidental spills, while handling these fuels, or when using kerosene for domestic cooking or heating. Occupational exposure is more frequent among workers handling and discharging fuel at terminals, storage facilities, and fueling stations; during the manufacturing, repair, maintenance, and testing of diesel engines and related equipment; when using diesel fuel as a solvent or cleaning agent; and during routine sampling and handling of diesel fuel in laboratories. Due to the low volatility of diesel fuel, vapor concentrations are typically minimal at room temperature. However, in confined spaces or at elevated temperatures, significant vapor accumulation may occur. Under standard handling conditions, vapor exposure is generally limited. Dermatitis caused by skin contact is the most frequently reported health issue, as diesel fuel is a known skin irritant. However, it typically does not cause eye irritation. Acute kidney toxicity has been documented following dermal exposure, though the long-term effects of prolonged, low-level dermal absorption remain uncertain. Ingestion of diesel fuel may lead to regurgitation and aspiration, potentially causing chemical pneumonia, similar to other hydrocarbons with comparable viscosity. Notably, practices such as washing hands with diesel fuel are highly discouraged based on evidence of acute human toxicity. Groundwater contamination by diesel fuel, which could lead to entry into drinking water, poses potential health risks. However, such contamination would likely be detectable through taste or odor, making accidental ingestion unlikely. A case-control study investigating workers exposed to diesel fuel suggested a potential association with increased risks of lung cancer (excluding adenocarcinoma) and prostate cancer. Nevertheless, due to the limited number of studies, small sample sizes, and wide confidence intervals, no definitive conclusion regarding the carcinogenic potential of diesel fuel in humans can be drawn. Diesel fuel spills have immediate and severe environmental impacts, resulting in significant mortality among affected biota[26,27,28,29].

Health and Safety

A significant hazard associated with atmospheric sulfur dioxide (SO₂) pollution, often referred to as petrochemical smog, arises under specific local and

meteorological conditions that enable the accumulation of SO₂ in the air. This can result in severe respiratory health issues when inhaled by humans. Hydrogen sulfide (H₂S) and other volatile sulfur compounds are acutely toxic, even at concentrations as low as 50 parts per million. Additionally, H₂S and related sulfur compounds are acidic and react readily with metals, leading to two critical technical challenges. First, they cause corrosion of equipment and pipelines. Second, they react with catalysts—typically metals or metal oxides—rendering them "poisoned," meaning the catalysts lose their catalytic activity. Catalysts, which are substances that facilitate or accelerate chemical reactions without being consumed, are extensively used in refining and petrochemical processes. The widespread adoption of catalytic converters in gasoline-powered vehicles over the last two decades has significantly reduced emissions of harmful nitrogen oxides. However, the presence of sulfur compounds in gasoline can impair the efficiency of these devices by poisoning the catalysts[12].

Diesel Hydrodesulfurization

Kerosene, diesel fuel, and aviation turbine fuel (jet fuel) belong to the class of petroleum products known as middle distillates. As the term suggests, these fuels have boiling points higher than gasoline but lower than gas oil, typically within the range of 175–375°C, with carbon numbers from approximately C8 to C24. While these products share similar properties, they differ in specifications tailored to their respective applications. Diesel fuels were originally derived as straight-run products from crude oil distillation. However, modern diesel formulations often include varying proportions of selected cracked distillates to enhance production volumes. Diesel fuel generally boils within the range of 125–328°C. Its appearance, including color, serves as a practical indicator to detect contamination by residual high-boiling constituents, water, or fine particulate matter. Therefore, visual inspections are crucial to ensure the delivery of clean fuel [20]. Diesel fuels are broadly categorized into two types: high-quality fuel for high-speed engines in cars and trucks, and heavier, lower-quality diesel for slower engines, such as those in marine vessels and stationary power plants [21]. Increasing environmental concerns have prompted stricter fuel specifications, necessitating improvements in combustion quality and emission control. Processes like hydrodesulfurization are implemented to enhance the chemical

stability, color, odor, and cetane number of these fuels. Moreover, sulfur content must be drastically reduced to meet stringent future regulations, which require sulfur levels below 50 ppm [25]. In middle distillates like diesel and kerosene, sulfur predominantly exists in the form of condensed heterocyclic compounds, such as benzothiophenes, dibenzothiophene, benzonaphthothiophenes, and derivatives of dibenzothiophene [22].

Hydrodesulfurization reactions and reactivities

The reactivity of sulfur compounds in hydrodesulfurization (HDS) processes follows a distinct order, ranked from most to least reactive: thiophene > alkylated thiophene > benzothiophene (BT) > alkylated BT > dibenzothiophene (DBT) and alkylated DBT without substituents at the 4- and 6-positions > alkylated DBT with a single substituent at either the 4- or 6-position > alkylated DBT with substituents at both the 4- and 6-positions. Achieving deep desulfurization of fuels requires the conversion of increasingly less reactive sulfur compounds, which poses significant challenges for process optimization and catalyst development [6].

Reaction Kinetics and Modeling

To determine the weight required for the hydrodesulfurization unit under specific temperature and pressure conditions, computer programs were employed to provide rapid and accurate calculations. The hydrodesulfurization of thiophene and dibenzothiophene (DBT) compounds was modeled using either the Langmuir-Hinshelwood-Hougen-Watson (LHHW) theory or a simple power-law equation, as illustrated in Table 2. These models are based on the premise that each reacting component is initially chemisorbed onto the catalyst surface, followed by surface rearrangement and subsequent desorption of the reaction products. The kinetics and mechanisms of desulfurization for diesel and kerosene were investigated using model compounds such as benzothiophene (BT) and DBT. The proposed rate equations for BT and DBT desulfurization, as shown in Table 2, were analyzed. The kinetic rate constants and equilibrium constants for these models were calculated through computer simulation tools such as Polymath, Excel, and Origin.

Table (2)kinetics models for benzothiophene and dibenzothiophene HDS

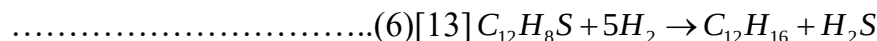
no	Model of benzothiophene and dibenzothiophene
I.	$r_{DBT}^* = \frac{kK_{DBT}K_{H_2}C_{DBT}C_{H_2}}{(1 + K_{DBT}C_{DBT} + K_{H_2S}C_{H_2S})^2 + (1 + K_{H_2}C_{H_2})} \dots\dots\dots(1)[23]$
II.	$r_{DBT}^{**} = \frac{kK_{DBT}K_{H_2}C_{DBT}C_{H_2}}{(1 + K_{DBT}C_{DBT} + K_{H_2S}C_{H_2S})} \dots\dots\dots(2)[14]$
III.	$r_{DBT} = \frac{kK_{DBT}K_{H_2}C_{DBT}P_{H_2}}{(1 + K_{DBT}C_{DBT} + K_{H_2}P_{H_2} + K_{H_2S}P_{H_2S})} \dots\dots\dots(3)[14]$
IV.	$r_{DBT} = \frac{kK_{DBT}K_{H_2}C_{DBT}C_{H_2}}{(1 + K_{DBT}C_{DBT} + K_{H_2S}C_{H_2S}) + (1 + K_{H_2}C_{H_2})} \dots\dots\dots(4)[24]$
V.	$r_{DBT} = \frac{kK_{DBT}P_{DBT}}{(1 + K_{DBT}P_{DBT} + K_{H_2S}C_{H_2S})} \dots\dots\dots(5)[18]$

* For DBT hydrogenolysis and ** For DBT hydrogenation

The equation (3) is used for any sulfur compound.

The reaction rates for benzothiophene (BT) and dibenzothiophene (DBT) are primarily governed by hydrogenolysis and hydrogenation mechanisms, both of which yield similar products as described by the following reaction:

The reaction for dibenzothiophene is given as:



The rate of desulfurization for DBT is typically slower compared to other sulfur-containing compounds. As a result, the desulfurization of DBT is often considered the rate-limiting step and is commonly used to represent the kinetics of kerosene and diesel fuel desulfurization. Table 3 summarizes the typical ranges of process variables employed in hydrotreating operations [9]. Table (3) shows typical ranges of process variables in hydrotreating operations [9].

Table (3) shows typical ranges of process variables in hydrotreating operations [9].

process variables	Typical range
Temperature	300–425°C
Pressure	1–20MPa
Hydrogen, per unit of feed:	-

Recycle	360 sm ³ /m ³
Consumption	36–142 sm ³ /m ³
Space velocity (LHSV)	1.5–8.0

Estimation of weight of diesel HDS catalyst

The determination of the hydrotreating catalyst weight is based on the reaction rate equations of organosulfur compounds. An isothermal plug flow reactor (tubular reactor) model was employed as the foundational design equation for the hydrodesulfurization (HDS) reactor.

Diesel is fed to HDS = yield (%) × amount of crude.....(7)

Diesel weight = $\rho_D \times V_D$(8)

$$\left(\frac{W}{F_{A^0}} \right) = \int_0^{x_A} \frac{d\chi_A}{r_p} \dots\dots\dots(9)[15]$$

The global rate r_p which includes itraparticle diffusion is given as:

$$r_p = \eta r_A \dots\dots\dots (10)[15]$$

This section details the steps undertaken to calculate the effectiveness factor, as outlined below:

$$\eta = \frac{1}{\phi_c} \left(\frac{1}{\tanh(3\phi_c)} - \frac{1}{(3\phi_c)} \right) \dots\dots\dots(11)[15]$$

Thiele-modulus for cylindrical porous catalyst

$$\phi_c = \frac{r_s}{3} \sqrt{\frac{(n+1) \times k \times \rho_p \times C_{AS}^{n-1}}{2D_e}} \dots\dots\dots(12)[16]$$

The catalyst used in this study consists of cobalt and molybdenum oxides supported on alumina, with its specifications provided in literature. The bulk diffusivity of sulfur compounds in the binary liquid mixture is:

$$D_{AB} = 7.4 \times 10^{-12} \frac{(\psi_B M_B)^{1/2} T}{\mu_B \hat{V}_A^{0.6}} \dots\dots\dots(13)[17]$$

$$\hat{V}_A = 0.285(V_c)^{1.048} \dots\dots\dots(14)[18]$$

Knudsen diffusivity

$$D_{K,A} = 0.97 \times a \times \left(\frac{T}{M_A} \right)^{0.5} \dots\dots\dots(15)[19]$$

Combined diffusivity

$$D = \frac{1}{\left(\frac{1}{D_{AB}} \right) + \left(\frac{1}{D_K} \right)} \dots\dots\dots(16)[15]$$

Tortuosity factor

$$\delta = \frac{1}{\varepsilon_B} \dots\dots\dots(17)[15]$$

Effective diffusivity

$$D_e = \frac{\varepsilon_B \times D}{\delta} \dots\dots\dots(18)[15]$$

The critical properties and acentric factor of diesel were calculated using the Riazi-Daubert equations.

Table (4) amount reactor outlet materials in function of conversion

Component	Wight (kg mol/hr)
Sulfur left (dibenzothiophene)	6.1436 (1-x)
Cyclohexylebenzene formed	6.1436 x
Hydrogen sulfide formed	6.1436x
Hydrogen gas left	1671.288-(5×6.1436x)
Diesel in	305.275

Gases	129.181
Total	2111.89-24.574x

Table(5) mole fraction of reactor outlet materials in function of conversion

Component	Mole fraction(y_i)
Sulfur left(dibenzothiophene)	$\frac{6.1436(1-x)}{2111.89-24.574x}$
Cyclohexylebenzene formed	$\frac{6.1436(x)}{2111.89-24.574x}$
Hydrogen sulfide formed	$\frac{6.1436(x)}{2111.89-24.574x}$
Hydrogen gas left	$\frac{1671.288-(5 \times 6.1436x)}{2111.89-24.574x}$
Diesel in	$\frac{305.275}{2111.89-24.574x}$
Gases	$\frac{129.181}{2111.89-24.574x}$
Total	1.00

The theoretical amount of catalyst was calculated using Equation (9) in conjunction with the reaction rate equations presented in Table 3. These equations were applied in Equations (1–5). The results, summarized in Tables 6 to 10, show the calculated catalyst weight required for diesel hydrotreating based on the kinetics models outlined in Table 3.

Table(6) results of weight of catalyst of diesel HDS at various temperatures and pressure by model (I), (W in kg)

T,°C	300		341.66		383.33		425	
P,Mpa	η	W	η	W	η	W	η	W
1	0.966	14300	0.848	9390	0.884	8570	0.898	7880
7.33	0.808	43000	0.509	50900	0.571	49500	0.601	48800
13.66	0.708	80400	0.400	110000	0.456	108000	0.485	107000
20	0.638	124000	0.342	183000	0.392	179000	0.418	178000

Table(7) results of weight of catalyst of diesel HDS at various temperatures and pressure by model (II), (W in kg)

T, ^o C	300		341.66		383.33		425	
P,Mpa	η	W	η	W	η	W	η	W
1	0.932	356000	0.937	366000	0.941	376000	0.945	378000
7.33	0.686	9330	0.701	9280	0.715	9210	0.727	9160
13.66	0.569	3240	0.585	3200	0.600	3160	0.614	3120
20	0.497	1730	0.513	1700	0.527	1680	0.541	1650

Table(8) results of weight of catalyst of diesel HDS at various temperatures and pressure by model (III), (W in kg)

T, ^o C	300		341.66		383.33		425	
P,Mpa	η	W	η	W	η	W	η	W
1	0.961	97800	0.965	98700	0.968	99300	0.971	100000
7.33	0.789	16300	0.805	16100	0.818	16100	0.831	15900
13.66	0.685	10000	0.704	9910	0.721	97700	0.737	9620
20	0.614	7660	0.634	7520	0.653	73600	0.670	7220

Table(9) results of weight of catalyst of diesel HDS at various temperatures and pressure by model (IV), (W in kg)

T, ^o C	300		341.66		383.33		425	
P,Mpa	η	W	η	W	η	W	η	W
1	0.881	39400	0.889	41400	0.896	43700	0.903	45600
7.33	0.566	22400	0.582	22200	0.598	22000	0.612	21800
13.66	0.452	24800	0.467	24200	0.481	23700	0.494	23200
20	0.388	27500	0.402	26600	0.415	26000	0.427	25300

Table(10) results of weight of catalyst of diesel HDS at various temperatures and pressure by model (V), (W in kg)

T, ^o C	300		341.66		383.33		425	
P,Mpa	η	W	η	W	η	W	η	W
1	0.936	16100	0.942	16300	0.947	16400	0.952	16500
7.33	0.700	21500	0.719	21300	0.736	21100	0.752	20900
13.66	0.584	25800	0.604	25400	0.624	24900	0.641	24600
20	0.512	29400	0.532	28800	0.551	28200	0.569	27700

CONCLUSIONS

Model II (Equation 2 in Table 2) for diesel hydrodesulfurization provided the most accurate predictions of hydrodesulfurization reactor performance. Consequently, Models I, II, IV, and V can be recommended for simulating hydrodesulfurization reactors. The optimal operating conditions were identified as a temperature range of 300–425°C, a pressure range of 1–20 MPa, and a hydrogen-to-feed ratio of 400 scm/cm³ of feed. As a result, models (I, II), (IV, V), and (II) have been identified as the most suitable for further evaluation of plant performance in diesel hydrodesulfurization processes. To achieve the production of ultra-low-sulfur fuels, significant advancements are required in three key areas: catalyst performance, process optimization, and reactor design. Moreover, the strategic incorporation and enhancement of transformative refining units will not only enable refineries to produce cleaner fuels but also contribute to increased economic profitability and the sustainable development of the refining industry.

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