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Original article

Mathematical Modeling and Analysis of Diesel Hydrodesulfurization Kinetics for Sustainable Environmental Health Solutions

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Abstract
Diesel remains a globally essential fuel, especially in transportation, yet its sulfur content poses significant environmental and health risks by forming sulfur oxides (SOx) during combustion. This study presents a mathematical modeling and kinetic analysis of diesel hydrodesulfurization (HDS) as a sustainable solution to produce cleaner fuels. Using catalysts such as Co-Mo/γ-Al_2O_3 in fixed-bed and trickle-bed reactors operating between 300–425°C and 1–20 MPa, the research simulates sulfur removal reactions involving thiophene, benzothiophene (BT), and dibenzothiophene (DBT) present in Libyan crude diesel. Models developed in Polymath and Excel compare kinetic expressions, notably the Langmuir-Hinshelwood-Hougen-Watson (LHHW) and power-law models, with findings indicating that the model corresponding to Equation 2 (Model II) best predicts reactor performance. The study also contrasts HDS with alternative desulfurization methods—such as biodesulfurization, adsorptive, oxidative, and extractive approaches—highlighting HDS's superior efficiency and refinery compatibility despite challenges in deep desulfurization. Furthermore, the analysis identifies an optimal operating condition at approximately 383°C and 7.33 MPa, balancing catalytic efficiency with durability. Evaluations of catalyst effectiveness and diffusion limitations via the Thiele modulus reinforce the need for optimized catalyst design. Overall, the research underscores the potential of targeted process optimization to enhance sulfur removal, contributing to cleaner diesel fuels and improved environmental health.

Keywords. Hydrodesulfurization, Mathematical Modeling, Diesel, Sulfur Compounds, Environmental Health.

Introduction

Diesel fuel remains a pivotal energy source in the global transportation sector due to its high energy density and widespread availability [1]. However, its use comes with significant challenges, particularly the emission of sulfur oxides (SOx), which are major environmental pollutants. Formed through the oxidation of sulfur compounds in petroleum, SOx contribute to issues such as acid rain, which accelerates infrastructure degradation, disrupts ecosystems, and poses threats to biodiversity [2]. Moreover, SOx exposure is linked to severe public health risks, including respiratory ailments, cardiovascular diseases, and elevated mortality rates [3]. To address these challenges, many countries have implemented stringent regulations on sulfur content in diesel fuel. For example, South Africa adopted Euro 5 standards in 2020, mandating sulfur levels about 10 ppm. Similarly, nations such as the United States, Europe, and Japan have introduced measures promoting ultra-low sulfur diesel (ULSD). These regulatory frameworks have significantly advanced the global transition toward cleaner fuels, emphasizing the need for innovative desulfurization technologies to meet environmental compliance and sustainability goals [4].

Desulfurization is crucial for meeting stringent regulatory standards and addressing operational challenges in refining processes and end-use applications. The presence of sulfur in fuels risks corrosion of internal combustion engines, deactivation of catalytic converters, and diminished refinery efficiency. Catalytic hydrotreating (HDT) is widely employed for sulfur removal and eliminating nitrogen, oxygen, and metals while enhancing petroleum product quality [5]. Within HDT, hydrodesulfurization (HDS) is particularly effective for sulfur removal, relying on sulfided catalysts such as cobalt-molybdenum (CoMo) or nickel-molybdenum (NiMo) on γ-alumina. Although HDS efficiently reduces simple sulfur compounds like sulfides and mercaptans, it faces limitations with sterically hindered compounds such as 4,6-dimethyldibenzothiophene, impeding deep desulfurization. Traditional HDS technologies, often implemented in trickle-bed or adiabatic fixed-bed reactors, struggle to achieve ULSD standards below 15 ppm, especially when processing high-sulfur and high-metal-content crude oils, which accelerate catalyst deactivation and reduce operational efficiency. These challenges highlight the pressing need for advanced desulfurization technologies to effectively address economic, operational, and environmental constraints [6].

Fuel sulfur content regulations vary significantly across the globe, driven by differences in refining capabilities and regulatory frameworks. In developed regions, such as the United States, stringent sulfur <15 ppm has been implemented [7]. In contrast, regions like Libya and Nigeria face significant challenges due to limited refining capacities, resulting in diesel sulfur content often exceeding 500 ppm. Consequently, these disparities emphasize the need for advancing desulfurization technologies to meet environmental

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standards and reduce sulfur-related emissions. For example, in the United States, the Environmental Protection Agency (EPA) reduced the highway diesel sulfur limit to 15 ppm in 2006, replacing the previous standard of 500 ppm. Similarly, California has adopted even stricter regulations, including accelerated schedules and broader controls. Furthermore, South Africa's alignment with Euro 5 standards further highlights the global commitment to reducing sulfur oxide (SOx) emissions. However, regions with limited refining capabilities, such as Libya, face difficulties meeting these stringent targets.

The sulfur content of crude oil varies depending on its origin. For example, paraffinic crudes from regions like North Africa, Nigeria, and Indonesia typically contain as little as 0.2 wt% sulphur. However, sulfur accumulation within catalysts can lead to deactivation, highlighting the need for efficient desulfurization processes [8]. Moreover, reducing sulfur levels significantly benefits air quality, as it can reduce nitrogen oxide (NOx) emissions by up to 75% and particulate matter by 80%, thereby improving both environmental health and fuel quality. Despite these benefits, deep desulfurization remains a major challenge. While conventional HDS technologies can reduce sulfur levels to 2500 wppm, achieving the ultra-low sulfur requirements, particularly for diesel fractions with sulfur content ranging from 0.1 to 6 wt%, requires further advancements in desulfurization technology [9].

This disparity highlights the urgent need for global policy alignment and investment in capacity-building initiatives to achieve sustainable fuel standards. Beyond reducing sulfur emissions, low-sulfur fuels enable the use of advanced sulfur-sensitive emission control technologies, which mitigate the formation of nitrogen oxides (NOx) and particulate matter. Consequently, these fuels significantly reduce air pollution and improve public health outcomes. Recognizing these benefits, there is an increasing emphasis on deep desulfurization processes to address environmental and health concerns associated with high sulfur fuels. However, achieving ultra-low fuel sulfur levels presents technical and economic challenges, particularly with conventional HDS technologies. To meet stringent regulatory standards, continued research is essential for developing innovative desulfurization solutions that enhance efficiency, reduce costs, and promote sustainability [32].

This study systematically examines the mathematical modeling of diesel fuel HDS kinetics, aiming to reduce environmental and public health impacts while addressing the limitations of existing HDS methods. To begin with, the study explores advanced strategies for optimizing desulfurization processes and provides actionable insights to facilitate compliance with current and future global fuel standards. In doing so, it supports broader environmental and public health goals. Specifically, a key focus of this research is selecting and validating suitable rate expressions for catalytic hydrotreating. To achieve this, the study identifies the most appropriate rate expression from existing literature data and uses it to predict the behavior of industrial reactors. Subsequently, these predictions are compared with actual data obtained from Libyan crude oil, emphasizing diesel fuel properties. Moreover, the research delves into the kinetic study of sulfur removal by investigating the kinetic behavior of model sulfur compounds under catalytic hydrotreating conditions. As a result, the analysis determines the required catalyst weight to achieve sulfur removal within specification limits, offering practical guidelines for optimizing industrial processes. In addition, this paper assesses the environmental and health impacts of sulfur in diesel fuels, highlighting its adverse effects on human health and the ecosystem. This discussion further highlights the critical importance of sulfur removal in achieving cleaner fuel standards and minimizing the ecological footprint of diesel consumption. Finally, by addressing these interconnected aspects, this study advances hydrodesulfurization technology [33].

Comparative Analysis of Desulfurization Methods

Desulfurization is a crucial process in the refining industry, aimed at reducing sulfur content in fuels to meet environmental standards. Various desulfurization methods, such as Hydrodesulfurization (HDS), Biodesulfurization (BDS), Adsorptive Desulfurization (ADS), Oxidative Desulfurization (ODS), and Extractive Desulfurization (EDS), each offer unique advantages and challenges [10]. In comparison, HDS remains the most widely used and established method due to its efficiency and scalability, alternative methods like BDS, ADS, ODS, and EDS present promising solutions, though they face hurdles in terms of cost, scalability, and reaction rates. Table 1 presents a comparative analysis of these desulfurization techniques, highlighting their respective advantages and challenges. The table provides a clear overview of each method's effectiveness, operational requirements, and limitations, offering valuable insights into their potential applications and areas for further development.

Hydrodesulfurization in Diesel Fuel Production

Kerosene, diesel fuel, and aviation turbine fuel (jet fuel) are collectively classified as middle distillates, a group of petroleum products defined by intermediate boiling points (150-380°C) and carbon chain lengths (C_8 to C_{24}). Positioned between the lighter gasoline and heavier gas oil fractions, these fuels share general physical and chemical properties but are specified and used differently depending on their applications. For example, diesel fuel was traditionally produced as a straight-run distillate from crude oil with a typical

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boiling range of 180-380 °C [11]. However, modern refining techniques employ a blend of cracked distillates to optimize yield.

Table 1. Comparative Analysis of Desulfurization Methods [34]

Method	Advantages	Disadvantages
Hydrodesulfurization (HDS)	Well-established and widely implemented technology. Efficiently removes thiols, sulfides, and thiophenes. Proven scalability and integration into existing refineries. Suitable for light fractions with hydrogen gas. Compatible with pre-treatment for refractory sulfur compounds.	Requires moderate to high pressure/temperature. Catalyst deactivation over time.
Biodesulfurization (BDS)	Operates under mild conditions. Eco-friendly with low emissions. Produces valuable by-products. Effective for complex sulfur compounds.	Extremely slow reaction rates. Costly and challenging microbial cultivation. Limited scalability and storage issues. Highly sensitive to microbial viability and conditions.
Adsorptive Desulfurization (ADS)	Effective at low temperatures. No hydrogen gas required. Targets stubborn sulfur compounds. Prevents hydrogen sulfide emissions.	High sorbent consumption and regeneration challenges. Limited selectivity and adsorption capacity. Requires frequent replacement of adsorbents
Oxidative Desulfurization (ODS)	Cost-effective for light fractions. High reaction rates. Avoids hydrogen gas use. Complements HDS processes. Converts complex sulfur compounds effectively.	Expensive oxidizing agents. Limited data on effectiveness for heavy fractions. Catalyst requirements for deep desulfurization increase costs. Potential for unwanted by-products formation.
Extractive Desulfurization (EDS)	Operates under low-pressure/temperature conditions. Easily integrates into refineries. Reusable solvents reduce waste. Extracted sulfur can be repurposed.	Limited sulfur solubility in solvents without modification. Efficiency improves with oxidation, adding complexity. Potential for hydrocarbon loss during extraction.

Diesel fuel is broadly categorized into two primary types high-quality diesel for high-speed engines (used in vehicles like cars and trucks) and lower-quality diesel for slow-speed engines (such as those in marine vessels and stationary power generators). Over the years, growing environmental concerns and stringent emissions regulations have significantly influenced the refining and formulation processes for diesel. These regulations have driven advancements in fuel quality, particularly in reducing sulfur content to meet ultra-low sulfur diesel (ULSD) standards. Key fuel attributes such as chemical stability, odor, color, and cetane number have been enhanced through modern refining technologies, including Hydrodesulfurization (HDS). Some regulatory frameworks now require low sulfur levels in order to reduce harmful sulfur oxide (SO_x) emissions and their associated environmental impacts [12]. In particular, in middle distillate such as diesel and kerosene—sulfur predominantly exists in the form of stable, condensed heterocyclic compounds, including benzothiophenes, dibenzothiophenes, benzonaphthothiophenes, and substituted derivatives of dibenzothiophene [13]. These compounds exhibit considerable resistance to traditional desulfurization processes, presenting a significant challenge to compliance with ultra-low sulfur fuel standards. As a result, intensive research and development are being undertaken to enhance the efficiency of desulfurization technologies and meet increasingly demanding regulatory requirements.

Figure 1 shows a simplified flow diagram of a petroleum refinery illustrating various processing units, including the Diesel Hydrodesulfurization (HDS) unit. The Diesel Oil Hydrotreater, depicted at the bottom of the diagram, represents the Diesel HDS unit. This unit facilitates the removal of sulfur compounds from diesel oil through a catalytic reaction with hydrogen, producing ultra-low sulfur diesel (ULSD) that complies with modern environmental and regulatory standards. The adoption of advanced refinery units like Diesel

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HDS ensures cleaner-burning fuels that align with contemporary sustainability goals and emissions guidelines [35].

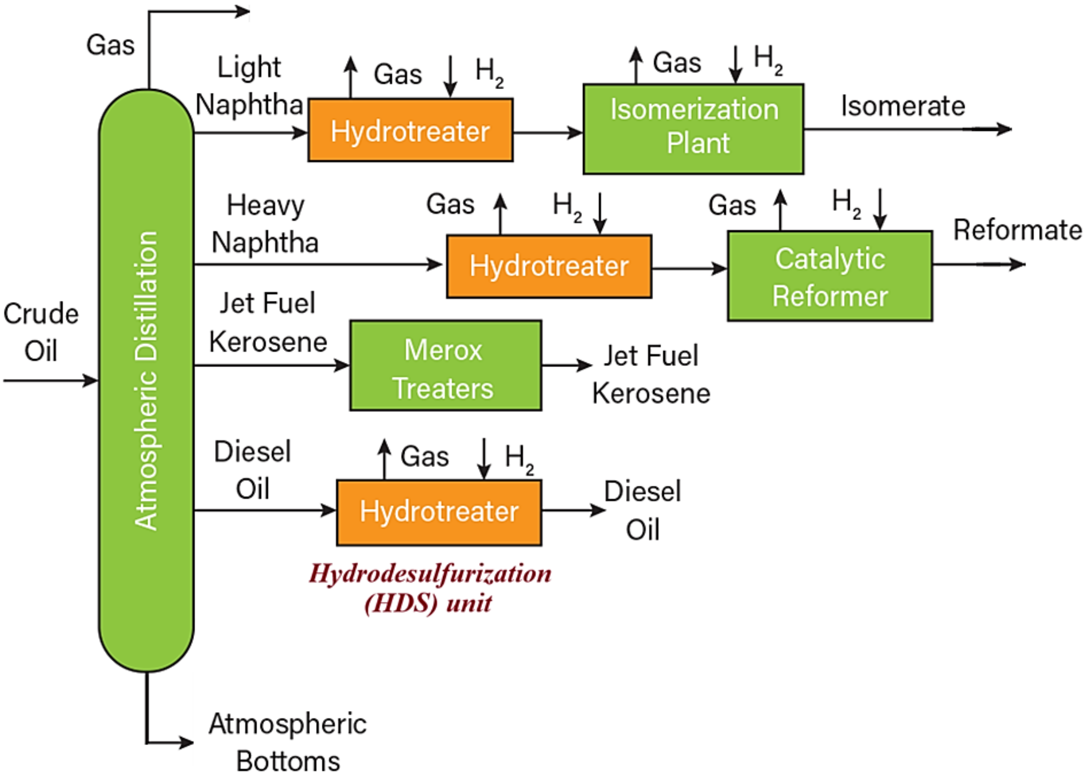

Figure 1. Simplified refinery flow diagram highlighting the HDS unit

Mechanistic Models and Mechanisms of HDS

Modeling HDS for Efficient Sulfur Removal

Modelling HDS processes is vital in understanding reaction kinetics, optimising process parameters, and designing efficient catalytic systems for sulfur removal from fuels. Two common approaches for modelling HDS are shown in Figure 2 [16]. The Langmuir-Hinshelwood-Hougen-Watson (LHHW) model assumes that reaction steps, such as adsorption, surface reaction, and desorption, occur on the catalyst surface under equilibrium or quasi-equilibrium conditions. This model provides a detailed mechanistic understanding of the HDS process by accounting for the competitive adsorption of reactants and intermediates on active sites, making it particularly suitable for describing complex behaviours in multicomponent systems. On the other hand, the simpler power-law model expresses the reaction rate as a function of reactant concentrations and experimentally derived rate constants, offering a more practical approach for large-scale process simulations with reduced computational complexity.

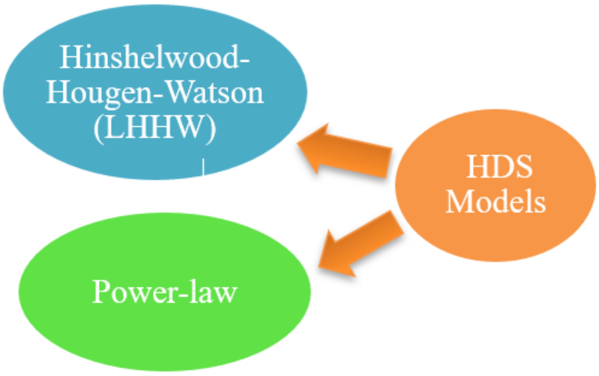

Figure 2. Common approaches for modelling HDS

The modelling of HDS also incorporates the use of sulfur-containing model compounds, such as thiophene, benzothiophene (BT), and dibenzothiophene (DBT), to represent the diverse range of sulfur species present in real fuel streams. These models enable the study of reaction kinetics for different sulfur compounds,

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including determining rate constants, equilibrium constants, and activation energies. Computational tools such as Polymath, MATLAB, Excel, and Origin are commonly employed to perform kinetic parameter estimation and validate the predictive accuracies of these models. By integrating experimental data with kinetic and reactor models, HDS process simulations have become essential for optimising reactor design, catalyst performance, and operational conditions. Ultimately, reliable modelling of HDS ensures efficient desulfurisation while minimizing operational costs and energy consumption, helping to meet the stringent environmental requirements for ultra-low sulfur fuels [17].

HDS Process Mechanisms

The mechanisms of HDS have been widely investigated using model organosulfur compounds and industrial fuels. However, discrepancies across reported studies often cause the HDS process to arise due to variations in critical factors, as presented in Figure 3 (A) While these differences influence specific outcomes, the literature broadens consensus on key reaction mechanisms and catalyst behaviours. Organosulfur compounds are present in nearly all crude oil fractions, with heavier fractions characterised by higher sulfur content and more chemically complex sulfur species [14]. It is crucial to account for the diversity of sulfur-containing compounds encountered in crude oil to optimise hydrotreating processes. The primary organosulfur compounds targeted in HDS reactions include mercaptans, sulfides, disulfides, thiophenes, benzothiophene (BT), and alkylated derivatives. For achieving ultra-deep desulfurisation, a requirement for ultra-low sulfur fuels, polynuclear aromatic sulfur compounds, such as alkylated DBTs, require particular consideration due to their recalcitrant nature.

The HDS process is exothermic and occurs irreversibly under typical industrial conditions. For thiophenic compounds, two dominant reaction pathways have been identified in the literature, as shown in Figure 3 (B). In the hydrogenolysis pathway, a direct cleavage of the sulfur atom occurs without altering the aromatic structure. The aromatic ring is first hydrogenated in the hydrogenation pathway, after which the sulfur atom is removed. These pathways proceed at distinct catalytic active sites, and the predominant mechanism is determined by the specific sulfur compound, reaction parameters, and catalyst properties. For example, DBT predominantly undergoes hydrogenolysis under industrially relevant reaction conditions [10]. However, alkylated DBTs, especially those substituted at the 4 and 6 positions, exhibit significant activity through both hydrogenolysis and hydrogenation pathways, highlighting the influence of molecular structure on reactivity. These insights reinforce the need for rational catalyst design and careful optimisation of reaction conditions to effectively target the diverse range of organosulfur species encountered in real feedstocks [15].

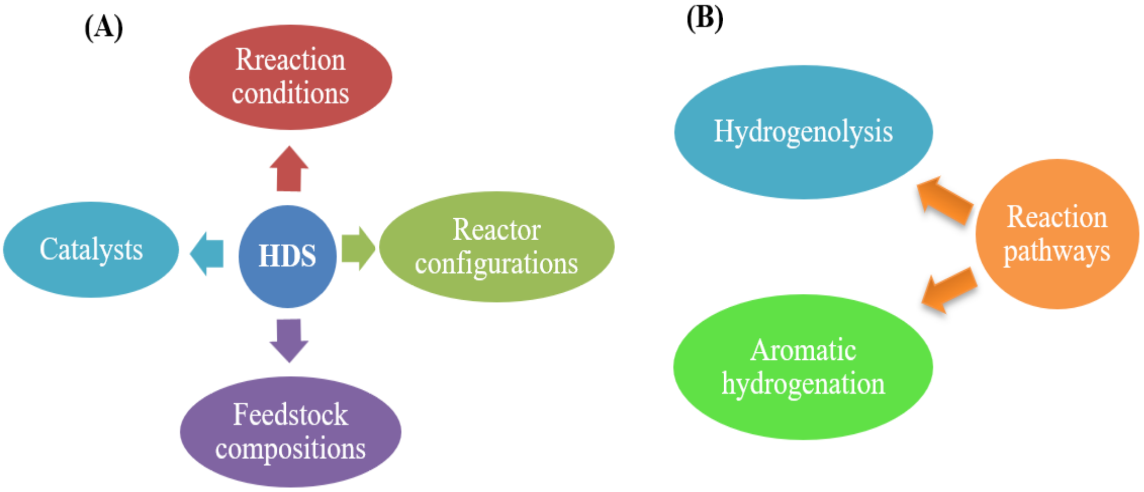

Figure 3. Factors influencing the HDS process: (A) Key variables affecting the HDS process and (B) Reaction pathways involved.

Reactions and Reactivities in HDS

The reactivity of sulfur compounds in hydrodesulfurisation (HDS) processes varies significantly, enabling their hierarchical classification from most to least reactive. The typical reactivity order is: thiophene > alkylated thiophene > benzothiophene (BT) > alkylated BT > dibenzothiophene (DBT) and its alkylated derivatives 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 [19]. This hierarchy is primarily governed by steric hindrance and chemical stability, with simpler compounds like thiophene being more readily removed due to their higher reactivity. In contrast, complex sulfur species, particularly heavily alkylated DBT derivatives, exhibit lower reactivity, making them more resistant to desulfurisation. These less reactive sulfur compounds present significant challenges as HDS processes evolve to achieve ultra-deep

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desulfurisation [10]. Advanced catalyst designs are required to enhance activity and selectivity, especially for breaking the strong bonds in sterically hindered sulfur species. Optimised reaction conditions, including temperature, pressure, and hydrogen availability, are equally critical for improving conversion efficiencies [20]. Addressing these challenges is pivotal for producing ultra-low sulfur fuels that comply with stringent environmental and regulatory standards.

Reaction Kinetics and Modeling

The desulfurisation of diesel and kerosene was systematically studied by examining the kinetics and mechanisms using representative sulfur-containing model compounds, such as benzothiophene (BT) and DBT. Rate equations describing the desulfurisation of these compounds, as detailed in Table 2, were thoroughly analysed to gain a deeper understanding of the reaction pathways and behaviours. By employing advanced computational tools, including Polymath, Excel, and Origin, key kinetic parameters, such as rate constants and equilibrium constants, were accurately determined. These simulations provided valuable insights into the intricate kinetics of hydrodesulfurisation and enabled a robust evaluation of process efficiency. The results are a foundation for optimising hydrodesulfurisation operations, enhancing sulfur removal performance, and advancing the design of more efficient catalytic systems.

Table 2. Kinetics models for benzothiophene and dibenzothiophene HDS

No.	Model of benzothiophene and dibenzothiophene
I.	$r^{*}_{DBT}=\dfrac{kK_{DBT}K_{H_2}C_{DBT}C_{H_2}}{\left(1+K_{DBT}C_{DBT}+K_{H_2S}C_{H_2S}\right)^2+\left(1+K_{H_2}C_{H_2}\right)}$……………………………………(1)[23] [21]
II.	$r^{**}_{DBT}=\dfrac{kK_{DBT}K_{H_2}C_{DBT}C_{H_2}}{\left(1+K_{DBT}C_{DBT}+K_{H_2S}C_{H_2S}\right)}$……………………………………………………………(2)[14] [36]
III.	$r_{DBT}=\dfrac{kK_{DBT}K_{H_2}C_{DBT}P_{H_2}}{\left(1+K_{DBT}C_{DBT}+K_{H_2}P_{H_2}+K_{H_2S}P_{H_2S}\right)}$………………………………………………(3)[14] [22]
IV.	
V.	$r_{DBT}=\dfrac{kK_{DBT}P_{DBT}}{\left(1+K_{DBT}P_{DBT}+K_{H_2S}C_{H_2S}\right)}$…………………………………………………………………(5)[18] [23]

** For DBT hydrogenolysis and ** For DBT hydrogenation. The equitation (3) is used for any sulfur compound.*

Two key mechanisms hydrogenolysis and hydrogenation predominantly control the reaction rates of benzothiophene (BT) and dibenzothiophene (DBT). Both mechanisms produce similar products, highlighting the analogous pathways these sulfur-containing compounds undergo during their transformation.
The specific reaction pathway for dibenzothiophene (DBT) can be represented as follows:

$$C_{12}H_8S+5H_2\rightarrow C_{12}H_{16}+H_2S\ \ldots\ldots\ldots\ldots\ldots\ldots\ \ (6)\ \ [24]$$

The desulfurisation rate of dibenzothiophene (DBT) is generally slower than other sulfur-containing compounds. Consequently, the desulfurisation of DBT is often considered the rate-limiting step in the process and is commonly used as a model to represent the desulfurization kinetics in kerosene and diesel fuel treatments. Table 3 summarizes the typical ranges of process variables employed in hydrotreating operations [37].

Table 3. Typical ranges of process variables in hydrotreating operations [37].

Process variables	Typical range
Temperature	300 - 425°C
Pressure	1 - 20 MPa
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 the Diesel HDS Catalyst Weight

The weight of the hydrotreating catalyst is determined using the reaction rate equations for organosulfur compounds. The foundational basis for the design of the HDS reactor is an isothermal plug flow reactor

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(PFR) model. This model provides a comprehensive framework for understanding the reaction dynamics and optimising reactor performance during desulfurisation.
Diesel is fed to HDS = yield (%) × amount of crude……….(7)

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

$$\left(\frac{W}{F_{A^0}}\right) = \int_0^{\chi_A} \frac{d\chi_A}{r_P} \text{……………………(9) [25]}$$

The global rate r_P, which includes intraparticle diffusion, is given as:

$$r_P = \eta r_A \text{…………………………………………………(10) [25]}$$

Estimation of the Catalyst Effectiveness Facto

The catalyst effectiveness factor (η) is a critical parameter in modeling Diesel HDS, reflecting the balance between chemical reaction rates and internal diffusion limitations within porous catalyst particles. Accurate estimation of (η) ensures reliable predictions of catalyst performance by incorporating intrinsic reaction kinetics and effective diffusivity, which are influenced by operating conditions such as temperature, pressure, and catalyst structure. This estimation is essential for optimizing HDS processes and achieving stringent sulfur content specifications in diesel fuels.

$$\eta = \frac{1}{\phi_c}\left(\frac{1}{\tanh(3\phi_c)} - \frac{1}{(3\phi_c)}\right) \text{…………………………… (11) [25]}$$

Estimation of the Thiele Modulus for a Cylindrical Porous Catalyst

The Thiele modulus is a dimensionless parameter that characterizes the relationship between reaction rates and diffusion limitations in porous catalytic systems. This study focuses on estimating the Thiele modulus for a cylindrical porous catalyst, providing insights into the interplay between diffusion and reaction kinetics, essential for optimizing catalytic performance in chemical processes.

$$\phi_c = \frac{r_s}{3}\sqrt{\frac{(n+1)\times k \times \rho_p \times C_{AS}^{\,n-1}}{2D_e}} \text{………………………(12)} \qquad [26]$$

The catalyst used in this study comprises cobalt and molybdenum oxides supported on alumina, with detailed specifications available in the literature. The bulk diffusivity of sulfur compounds in the binary liquid mixture is as follows:

$$D_{AB} = 7.4\times10^{-12}\,\frac{(\psi_B M_B)^{1/2}\,T}{\mu_B \hat{V}_A^{0.6}} \text{…………………………………(13) [38]}$$

$$\hat{V}_A = 0.285(V_c)^{1.048} \text{………………………………(14) [65]}$$

Estimation of the diffusivity

Accurate modeling of Diesel Hydrodesulfurization (HDS) requires a comprehensive understanding of mass transport within the catalyst pores. Key parameters such as Knudsen diffusivity, combined diffusivity, tortuosity factor, and effective diffusivity play a vital role in describing diffusion under varying conditions. Knudsen diffusivity governs transport when pore dimensions are small relative to the molecular mean free path, while combined diffusivity considers both molecular and Knudsen mechanisms. The tortuosity factor captures the impact of complex pore geometries, and effective diffusivity integrates these aspects to reflect actual transport behavior. Estimating these parameters is crucial for optimizing catalytic performance and improving sulfur removal efficiency in Diesel HDS processes.

Knudsen diffusivity

$$D_{K,A} = 0.97\times a\times\left(\frac{T}{M_A}\right)^{0.5} \text{…………………(15) [40]}$$

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Combined diffusivity

$$D = \frac{1}{\left(\frac{1}{D_{AB}}\right) + \left(\frac{1}{D_K}\right)} \quad \text{...(16) [25]}$$

Tortuosity factor

$$\delta = \frac{1}{\varepsilon_B} \quad \text{..(17) [25]}$$

Effective diffusivity

$$D_e = \frac{\varepsilon_B \times D}{\delta} \quad \text{..(18)[25]}$$

The critical properties of diesel, along with its acentric factor, were determined using the Riazi-Daubert equations for accurate characterization.

Table 4 presents the material balance at the reactor outlet as a function of conversion (x) in the hydrodesulfurization process. It details the quantities of key components, including unconverted sulfur (dibenzothiophene), reaction products like cyclohexylbenzene and hydrogen sulfide, residual hydrogen gas, and the total product stream. This analysis provides insights into how conversion impacts the distribution of reactor outputs, essential for optimizing process performance.

Table 4. Amount of reactor outlet materials as a function of conversion

Component	Weight (Kgmol/hr)
Sulfur left (dibenzothiophene)	6.1436 (1 - x)
Cyclohexylebenzene formed	6.1436 x
Hydrogen sulfide formed	6.1436 x
Hydrogen gas left	1671.288 - (5×6.1436 x)
Diesel in	305.275
Gases	129.181
Total	2111.89 - 24.574 x

Table 5 provides the mole fractions of reactor outlet materials as a function of conversion (x) during the hydrodesulfurization process. It highlights the relative composition of unconverted sulfur (dibenzothiophene), reaction products such as cyclohexylbenzene and hydrogen sulfide, remaining hydrogen gas, diesel, and gaseous components. The total mole fraction is normalized to 1.00, offering a clear representation of the changes in material distribution with varying conversion levels.

Table 5. Mole fraction of reactor outlet materials as a function of conversion

Component	Mole fraction(ii)
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

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Results and Discussion

The theoretical amount of catalyst was calculated using Equation (9) in combination 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 kinetic models outlined in Table 3.

Table 6 presents the effect of temperature (T) and pressure (P) on sulfur removal (W) and process efficiency (η). At higher temperatures, such as 425°C, sulfur removal and efficiency are generally higher due to enhanced catalytic activity, with sulfur removal reaching a maximum of 178,000 kg at 20 MPa. As the temperature decreases, both sulfur removal and efficiency decline at higher pressures, indicating a reduced catalytic rate. However, at lower pressures, such as 1 MPa, efficiency is relatively high even at reduced temperatures, suggesting that lower pressures minimize energy losses but limit sulfur removal. Conversely, increasing the pressure enhances sulfur removal due to higher hydrogen availability, but efficiency decreases, likely due to heat and mass transfer limitations. The highest efficiency is observed at 300°C and 1 MPa (η = 0.966), while the optimal balance between sulfur removal and efficiency occurs at 425°C and 7.33 MPa. These results highlight the trade-off between maximizing sulfur removal and maintaining process efficiency, underscoring the need to optimize operating conditions in HDS.

Table 6. Results of catalyst weight for diesel HDS at various temperatures and pressures by Model I.

T (°C)	**300**		**341.66**		**383.33**		**425**	
P (Mpa)	H	W(Kg)	η	W(Kg)	η	W(Kg)	η	W(Kg)
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

The results of Table 7 provide insights into the performance of the process under varying T and P, as measured by the catalyst W required and the η. At low pressure (1 MPa), the catalyst weight is extremely high across all temperatures, ranging from 378,000 kg at 425°C to 356,000 kg at 300°C. This indicates that lower pressures demand a significantly larger amount of catalyst to achieve effective desulfurization. Despite this, η is consistently high, decreasing only slightly from 0.945 at 425°C to 0.932 at 300°C. These results suggest that low pressure supports high process efficiency but at the cost of excessive catalyst consumption. As the pressure increases to moderate levels (7.33 MPa), the required catalyst weight decreases dramatically, with values such as 9,160 kg at 425°C and 9,330 kg at 300°C. However, efficiency declines more noticeably, from 0.727 at 425°C to 0.686 at 300°C. This demonstrates a trade-off where moderate pressure significantly reduces catalyst consumption and results in lower efficiency. In addition, at high pressures (13.66), the catalyst weight is minimized, with values as low as 1,650 kg at 425°C and 1,730 kg at 300°C for 20 MPa. However, the efficiency decreases significantly at these pressures, dropping from 0.541 at 425°C to 0.497 at 300°C for 20 MPa.

These results suggest that increasing pressure substantially reduces catalyst weight requirements but also leads to diminished process efficiency, likely due to mass transfer limitations and increased hydrogen partial pressure, which may alter reaction kinetics. It is clear that the effect of temperature is more pronounced at lower pressures, where higher temperatures improve both catalyst weight and efficiency. At higher pressures, the influence of temperature becomes less significant, with only small variations in W and η. The results highlight a clear trade-off between minimizing catalyst consumption and maintaining high efficiency. Low pressures are more efficient but demand excessive catalyst weight, while high pressures reduce catalyst requirements at the expense of efficiency. Optimal operating conditions for diesel HDS would require a careful balance between temperature and pressure to achieve the desired performance metrics.

Table 7. Results of catalyst weight for diesel HDS at various temperatures and pressures using Model II

T (°C)	**300**		**341.66**		**383.33**		**425**	
P (Mpa)	H	W(Kg)	η	W(Kg)	η	W(Kg)	η	W(Kg)
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 provides the catalyst W and η for diesel HDS at varying T and P based on Model III. The catalyst weight is quite high at a low pressure of 1 MPa, ranging from 100,000 kg at 425°C to 97,800 kg at 300°C.

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Despite this high catalyst requirement, the process maintains a high efficiency, with η slightly decreasing from 0.971 at 425°C to 0.961 at 300°C. This suggests that higher temperatures improve efficiency marginally at lower pressures while requiring more catalysts for effective desulfurization. When the pressure is increased to 7.33 MPa, the catalyst weight significantly decreases, ranging from 15,900 kg at 425°C to 16,300 kg at 300°C. However, there is a noticeable drop in efficiency, with η declining from 0.831 at 425°C to 0.789 at 300°C. This indicates that moderate pressure reduces catalyst demand but at the expense of a decrease in efficiency. As pressure increases further to 13.66 MPa, the catalyst weight continues to drop, with values as low as 7,220 kg at 425°C and 7,660 kg at 300°C for 20 MPa. However, the efficiency also decreases more markedly, from 0.737 at 425°C to 0.614 at 300°C at 20 MPa. This demonstrates a clear trade-off, while increasing pressure greatly reduces catalyst requirements, it also results in a significant reduction in desulfurization efficiency. This may be due to limitations in reaction kinetics and mass transfer at higher hydrogen partial pressures.

Table 8. Weight of the catalyst for diesel HDS at various temperatures and pressures, as predicted by Model III

T (^{o}C)	300		341.66		383.33		425	
P (Mpa)	H	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 shows the weight of the catalyst W and η for diesel HDS at varying T and P, predicted by Model IV. As the results indicate, the catalyst weight decreases significantly with the increase in pressure across all temperatures. At low pressure (1 MPa), the catalyst weight is relatively high, starting at 45,600 kg at 425°C and gradually decreasing as the temperature lowers, reaching 39,400 kg at 300°C. The efficiency also remains high at low pressure, with values between 0.903 and 0.881. This suggests that low pressure favors high efficiency but requires more catalyst to achieve effective desulfurization. As the pressure increases to 7.33 MPa, the catalyst weight drops significantly, from 21,800 kg at 425°C to 22,400 kg at 300°C. However, the efficiency also decreases, with values ranging from 0.612 at 425°C to 0.566 at 300°C. This trade-off demonstrates that while moderate pressures reduce catalyst consumption, they also lead to a decrease in efficiency. At even higher pressures, such as 13.66 MPa, the catalyst weight continues to decline. At 13.66 MPa, the catalyst weight ranges from 23,200 kg at 425°C to 24,800 kg at 300°C. At the highest pressure of 20 MPa, the catalyst weight increases further, from 25,300 kg at 425°C to 27,500 kg at 300°C. The efficiency, however, drops significantly at these pressures, with values ranging from 0.494 at 425°C to 0.388 at 300°C. This pattern shows that although higher pressures reduce catalyst requirements, the trade-off comes in the form of reduced efficiency, which is likely due to increased hydrogen partial pressures and the resulting changes in reaction kinetics.

Table 9. Weight of the catalyst for diesel HDS at various temperatures and pressures, as predicted by Model IV

T (^{o}C)	300		341.66		383.33		425	
P (Mpa)	H	W(Kg)	η	W(Kg)	η	W(Kg)	η	W(Kg)
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 illustrates the weight of the catalyst W and η at various T and P, predicted by Model V. At low pressure (1 MPa), the catalyst weight is relatively low, ranging from 16,500 kg at 425°C to 16,100 kg at 300°C, while the efficiency remains high, between 0.952 and 0.936. This indicates that at lower pressures, the process can achieve high efficiency with relatively low catalyst requirements. As the pressure increases to 7.33 MPa, the catalyst weight rises, with values ranging from 20,900 kg at 425°C to 21,500 kg at 300°C. Although the catalyst demand increases with pressure, the efficiency decreases slightly, from 0.752 at 425°C to 0.700 at 300°C. This suggests that while moderate pressures reduce the catalyst weight compared to lower pressures, there is a clear reduction in efficiency as pressure increases. Further increasing the pressure to 13.66 MPa and 20 MPa results in even higher catalyst weight. At 13.66 MPa, the catalyst weight ranges from 24,600 kg at 425°C to 25,800 kg at 300°C, with efficiency values decreasing from 0.641 at 425°C to 0.584 at 300°C. At the highest pressure of 20 MPa, the catalyst weight continues to increase, from

27,700 kg at 425°C to 29,400 kg at 300°C, while the efficiency declines further, from 0.569 at 425°C to 0.512 at 300°C.

Table 10. Weight of the catalyst for diesel HDS at various temperatures and pressures, as predicted by Model (V)

T (°C)	**300**		**341.66**		**383.33**		**425**	
P (Mpa)	H	W(Kg)	η	W(Kg)	η	W(Kg)	η	W(Kg)
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

Assessment of Diesel HDS as a Sustainable Solution for Environmental Health

Evaluating Diesel HDS for Sustainable Environmental Health Solutions

Diesel HDS represents a transformative approach in transitioning toward cleaner fuels and sustainable environmental health solutions. This catalytic process effectively eliminates sulfur compounds from diesel fuel, including mercaptans, disulfides, and thiophenes, thus enabling the production of ultralow-sulfur diesel (ULSD) with sulfur content as low as 10 - 15 ppm, in compliance with stringent environmental regulations. Reducing sulfur dioxide (SO_2) emissions from diesel combustion directly addresses critical public health concerns, as SO_2 is a known contributor to respiratory disorders, aggravated asthma symptoms, and cardiovascular diseases. Furthermore, the mitigation of sulfur emissions also hinders the atmospheric formation of fine particulate matter, which poses severe long-term health risks such as lung cancer, chronic bronchitis, and premature deaths [27]. From an environmental perspective, HDS minimizes the ecological damage caused by sulfur-related pollutants. The sharp reduction in SO_2 emissions prevents acid rain, degrades soil quality, alters water chemistry in aquatic systems, and disrupts ecosystems reliant on sensitive pH balances. Moreover, by enabling lower-sulfur fuels, HDS facilitates the effective operation of advanced emission control technologies like diesel particulate filters (DPFs) and selective catalytic reduction (SCR) systems, further reducing nitrogen oxide (NOx) and particulate matter emissions. These advancements improve air quality, less environmental degradation, and significantly reduce climate-warming phenomena linked to black carbon and ground-level ozone production. Thus, diesel HDS is pivotal in reducing the immediate and long-term risks posed by diesel emissions and plays a critical role in global efforts to shift toward sustainable energy practices and fulfill environmental health objectives [28].

Impact of Diesel on Human Health and the Environment

The widespread use of diesel fuel in transportation and industrial sectors has profound implications for human health and environmental systems due to the toxic pollutants generated during combustion. Diesel exhaust is a complex mixture of harmful compounds, including NOx, PM2.5, SO_2, CO, and hydrocarbons [29]. Among these, NOx and PM2.5 are particularly hazardous. NOx contributes to ground-level ozone and smog formation, exacerbating respiratory issues such as asthma, bronchitis, reduced lung function, and even long-term damage to the respiratory system. Additionally, PM2.5, a fine particulate pollutant, is capable of penetrating deep into the lungs and entering the bloodstream, leading to serious cardiovascular problems, lung cancer, and premature death. Diesel exhaust has been classified as a Group 1 carcinogen by the International Agency for Research on Cancer (IARC), highlighting its significant cancer-causing potential. Environmentally, diesel emissions pose several severe threats. NOx emissions play a substantial role in the chemical reactions that produce acid rain, which deteriorates soil quality, damages forests, and disrupts aquatic ecosystems by creating conditions unsuitable for marine life. Furthermore, diesel combustion is a significant source of black carbon and greenhouse gases, major contributors to climate change. Black carbon, a component of PM2.5, directly absorbs sunlight and accelerates glacier and polar ice melt, intensifying global warming and altering natural precipitation cycles. SO_2 emissions further harm the environment by increasing atmospheric acidity, leading to widespread biodiversity loss in terrestrial and aquatic ecosystems.These environmental effects are most pronounced in urban and industrial regions, where high diesel usage contributes to poor air quality and ecological degradation. Addressing these impacts requires adopting cleaner technologies such as ultralow-sulfur diesel (ULSD), stricter emissions regulations, and a transition to alternative energy sources to mitigate the long-term risks to human health and the planet [30].

Environmental and Health Benefits of Hydrodesulfurization

The HDS is essential in reducing sulfur emissions, delivering significant environmental and health benefits by enabling the production of ultralow-sulfur diesel (ULSD). The process eliminates sulfur-containing compounds from diesel fuel, drastically curbing SO_2 emissions during combustion. From a health

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perspective, this reduction in SO_2 levels addresses major respiratory and cardiovascular concerns. High concentrations of SO_2 in the air are linked to aggravated asthma, bronchitis, lung infections, and long-term chronic diseases, particularly in vulnerable populations such as children and the elderly [68]. Moreover, the removal of sulfur compounds minimizes the formation of PM2.5, which is associated with serious health hazards, including reduced lung function, cardiovascular diseases, and increased rates of premature mortality [31]. Cleaner emissions achieved through HDS decrease overall exposure to these harmful pollutants, improving air quality and reducing the burden on public health systems [18]. The environmental benefits of HDS are equally profound. By lowering SO_2 emissions, the process significantly reduces the occurrence of acid rain, which is responsible for soil acidification, aquatic ecosystem degradation, and biodiversity loss. The ecological damage caused by sulfur emissions is further mitigated as HDS supports advanced emission control technologies such as DPFs and SCR systems, which target other major pollutants like NOx and particulate matter. Additionally, decreasing sulfur content in diesel also reduces the formation of black carbon, a potent climate-forcing agent, thereby contributing to the global effort to combat climate change. HDS facilitates substantial strides toward meeting environmental regulations and sustainability goals, ensuring a cleaner, healthier, and more stable ecosystem while protecting human well-being. Hydrodesulfurization remains a cornerstone in achieving sustainable environmental health solutions because it can address both local air quality and broader ecological concerns [41].

Conclusion

In conclusion, this research paper emphasizes the critical need for advanced desulfurization technologies to meet increasingly stringent global environmental and regulatory standards, particularly through optimizing the hydrodesulfurization (HDS) process. It highlights the limitations of traditional HDS methods and underscores the importance of developing innovative techniques to achieve ultra-low sulfur diesel (ULSD) levels. By analyzing the reactivity and kinetics of sulfur compounds, along with the influence of catalyst design and operating conditions, the study underscores the necessity for accurate modeling and efficient catalytic systems to reduce sulfur emissions effectively. The study also stresses the significant health and environmental benefits of lowering sulfur emissions, demonstrating how improved HDS processes contribute to cleaner fuels and sustainable environmental health solutions. Among the models assessed, Model II (Equation 2 in Table 2) provided the most accurate predictions of hydrodesulfurization reactor performance. Consequently, Models I, II, IV, and V are recommended for simulating HDS 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 cm^3/cm^3. Models (I, II), (IV, V), and (II) were identified as the most suitable for further evaluation of plant performance in diesel hydrodesulfurization processes. Significant advancements are required in three key areas: catalyst performance, process optimization, and reactor design to produce ultra-low-sulfur fuels. Additionally, the strategic integration and enhancement of transformative refining units will enable refineries to produce cleaner fuels, increase economic profitability, and support the sustainable development of the refining industry. Finally, the paper highlights the risks associated with diesel fuel exposure, which can cause skin irritation and dermatitis. It advises avoiding skin contact and discourages the use of diesel for cleaning purposes. Furthermore, accidental releases of petroleum products into the environment should be prevented, and any spills must be promptly addressed to minimize environmental damage.

Conflict of interest. Nil

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الملخص

يظل الديزل وقودًا أساسيًا عالميًا، وخاصة في النقل، إلا أن محتواه من الكبريت يشكل مخاطر بيئية وصحية كبيرة من خلال تكوين أكاسيد الكبريت أثناء الاحتراق. تقدم هذه الدراسة نمذجة رياضية وتحليلًا حركيًا لإزالة الكبريت من الديزل كحل مستدام لإنتاج وقود أنظف. باستخدام محفزات مثل $Co\text{-}Mo/\gamma\text{-}Al_2O_3$ في مفاعلات ثابتة ومتقطعة تعمل بين 300-425 درجة مئوية و1-20 ميجا باسكال، يحاكي البحث تفاعلات إزالة الكبريت التي تنطوي على الثيوفين والبنزوثيوفين والداي بنزوتوفين الموجودة في الديزل الخام الليبي. تقارن النماذج التي تم تطويرها في Polymath وExcel بين التعبيرات الحركية، ولا سيما نماذج LHHW (Langmuir-Hinshelwood-Hougen-Watson) وقوانين الطاقة، مع نتائج تشير إلى أن النموذج المقابل للمعادلة 2 (النموذج الثاني) يتنبأ بشكل أفضل بأداء المفاعل. كما تقارن الدراسة بين طريقة إزالة الكبريت من الديزل وطرق إزالة الكبريت البديلة - مثل إزالة الكبريت الحيوي، والامتصاص، والأكسدة، والأساليب الاستخراجية - مما يسلط الضوء على كفاءة إزالة الكبريت من الديزل المتفوقة وتوافقها مع المصفاة على الرغم من التحديات في إزالة الكبريت العميقة. وعلاوة على ذلك، يحدد التحليل حالة تشغيل مثالية عند حوالي 383 درجة مئوية و7.33 ميجا باسكال، مما يوازن بين الكفاءة الحفزية والمتانة. تعزز تقييمات فعالية المحفز وقيود الانتشار عبر معامل ثيل الحاجة إلى تصميم محفز محسن. بشكل عام، يؤكد البحث على إمكانات تحسين العملية المستهدفة لتعزيز إزالة الكبريت، والمساهمة في الحصول على وقود ديزل أنظف وتحسين الصحة البيئية.لمحاكاة عملية إزالة الكبريت من الديزل الحفزية.

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