

Optimization of CSTR Reactor Designs for Efficient Bioremediation of Hydrocarbon-Contaminated Water

*Yiga, F.; Iregbu, P.O.; Okwu, K.C.; Agbara, J.O.

Chemical/Petrochemical Engineering Department, Rivers State University, Port Harcourt-Nigeria Correspondent Author: yiga.francis@ust.edu.ng

Abstract-The optimization of a Continuous Stirred Tank Reactor (CSTR) for the bioremediation of hydrocarbon-contaminated water is crucial for improving treatment efficiency, reducing reactor footprint, and enhancing energy utilization. This study investigates both conventional and optimized CSTR designs under isothermal conditions, focusing on key performance parameters such as reactor volume, space time, space velocity, and heat generation. MATLAB and Simulink simulations were employed to model the bioremediation process, refine reactor dimensions, and enhance operational efficiency. Before optimization, the reactor was designed to treat 109 m^{3}/day of hydrocarbon-contaminated water, achieving a removal efficiency of 95–99%. The initial design required a reactor volume between 6.722 and 9.209 m³, with space time ranging from 2.029 to 2.780 hours. The space velocity was estimated between 0.360 and 0.493 h^{-1} , while heat generation per unit reactor volume varied from 1223 kJ/m³•h to 930 kJ/m³•h. Following optimization, the reactor volume was reduced to 5.800–7.500 m³, while space time improved to 1.800-2.400 hours. Additionally, the optimized reactor exhibited a lower heat generation rate, decreasing to 1100 kJ/m³•h at 95% removal and 860 kJ/m³•h at 99% removal, significantly improving thermal efficiency and system stability. The optimized CSTR design demonstrates superior process efficiency by reducing operational costs, minimizing energy losses, and maintaining high pollutant removal performance. This study underscores the importance of optimization in reactor engineering, providing a scalable and costeffective approach for large-scale hydrocarbon bioremediation applications.

Keywords-Bioremediation, Continuous Stirred Tank Reactor, Hydrocarbon Degradation, Wastewater Treatment, Process Optimization.

I. INTRODUCTION

Crude oil is one of the world's most valuable natural resources, serving as a major energy source and an essential raw material for petrochemical industries. Over the years, global crude oil production has significantly increased, from 82.3 million barrels per day in 2003 to over 103.3 million barrels per day by 2025 [1]. This surge in production has been driven by industrialization, population growth, and the rising global demand for energy. While crude oil extraction and refining have provided significant economic benefits, they have also led to serious environmental challenges, particularly in the form of hydrocarbon pollution. Accidental or deliberate releases of crude oil into aquatic environments introduce a range of toxic hydrocarbons and heavy metals, including lead (Pb), cadmium (Cd), mercury (Hg), and chromium (Cr), all of which pose severe ecological and health risks [2].

Hydrocarbon contamination in water bodies is a persistent environmental issue, often resulting from offshore oil spills,

pipeline ruptures, industrial discharges, and transportation accidents [3]. These pollutants not only harm aquatic life but also compromise water quality, making it unsafe for human consumption and agricultural use. The persistence of hydrocarbons in the environment is due to their low water solubility, high chemical stability, and strong adsorption to sediments, which allows them to bioaccumulate in aquatic organisms, leading to long-term ecological damage [4]. Polycyclic aromatic hydrocarbons (PAHs), a significant fraction of crude oil contaminants, are particularly concerning due to their carcinogenic and mutagenic properties, further emphasizing the need for effective remediation strategies [5].

The rising demand for clean water has further highlighted the urgency of addressing hydrocarbon contamination. Freshwater scarcity is becoming an increasingly critical global issue due to the combined effects of climate change, population growth, and pollution [6]. Industrialization and urban expansion have intensified pressure on existing water resources, making pollution control an essential component of sustainable development. According to the United Nations, water shortages could significantly hinder economic growth and lead to geopolitical conflicts, particularly in regions that rely on shared water bodies [7]. Contaminated water sources pose serious threats to both public health and ecosystems, making it imperative to develop effective treatment methods that ensure long-term water security.

Industrial wastewater from petroleum refining, chemical processing, and fuel storage facilities is a major contributor to hydrocarbon pollution [8]. Despite existing environmental regulations, accidental spills and inadequate waste management continue to introduce petroleum hydrocarbons, heavy metals, and toxic organic compounds into water bodies. Conventional wastewater treatment plants often struggle to handle these pollutants due to their complex chemical compositions and slow degradation rates [9]. Unlike biodegradable organic matter found in domestic sewage, hydrocarbons require specialized microbial consortia for effective breakdown, making conventional treatment methods inefficient [10]. Additionally, due to low oxygen availability and the hydrophobic nature of petroleum compounds, natural attenuation of hydrocarbon contaminants is often slow, leading to long-lasting environmental damage [11].

To address these challenges, various remediation strategies have been developed, including physical, chemical, and biological treatment methods [12]. Physical techniques such as skimming, sedimentation, and adsorption using activated carbon can help remove oil fractions from contaminated water,





but they are often ineffective for treating dissolved hydrocarbons [13]. Chemical methods, including oxidation, precipitation, and chemical dispersants, can enhance pollutant breakdown but may introduce secondary contaminants, increasing environmental risks [14]. Furthermore, both physical and chemical approaches are often associated with high operational costs, large energy requirements, and incomplete hydrocarbon degradation [15]. As a result, these traditional methods are often unsuitable for large-scale or long-term applications.

Bioremediation has emerged as a promising alternative due to its eco-friendly nature and ability to achieve complete hydrocarbon degradation 16]. This approach leverages microbial metabolism to convert toxic hydrocarbons into harmless end products such as carbon dioxide, water, and [17]. Hydrocarbon-degrading microorganisms, biomass Pseudomonas, including bacteria (e.g., Alcanivorax, Mycobacterium), fungi (e.g., Aspergillus, Penicillium), and archaea, play a crucial role in breaking down crude oil components into less harmful substances [18]. Unlike physical and chemical methods, bioremediation is cost-effective, sustainable, and capable of restoring contaminated ecosystems without producing hazardous byproducts [19].

Among various bioreactor configurations used for bioremediation, the Continuous Stirred Tank Reactor (CSTR) stands out due to its ability to maintain uniform mixing, control environmental conditions, and sustain continuous microbial activity [20]. CSTRs operate under steady-state conditions, allowing for constant hydrocarbon degradation while ensuring even distribution of microorganisms, nutrients, and oxygen throughout the system [21]. This uniform mixing enhances microbial efficiency, preventing localized pollutant accumulation and ensuring consistent treatment performance [22]. Furthermore, CSTRs can be scaled up for industrial applications, making them suitable for treating large volumes of hydrocarbon-contaminated water [23].

However, the effectiveness of CSTRs in bioremediation depends on optimal reactor design and operational parameters [24]. Key design considerations include reactor volume, space time, microbial kinetics, oxygen transfer efficiency, and energy consumption. Suboptimal reactor configurations can lead to inefficient hydrocarbon degradation, excessive sludge production, and high energy costs, reducing overall treatment efficiency. One of the main challenges in CSTR operation is achieving the right balance between microbial growth and contaminant removal.

This study aims to optimize CSTR designs for efficient bioremediation of hydrocarbon-contaminated water by leveraging computational modeling and experimental validation. The primary objectives include developing a mathematical model for hydrocarbon degradation in a CSTR, simulating reactor performance under isothermal conditions, and identifying optimal design parameters to enhance treatment efficiency. The MATLAB and Simulink-based simulations conducted in this research provide valuable insights into hydrodynamic behavior, microbial kinetics, and mass transfer mechanisms within the reactor.

II. MATERIALS AND METHODS

2.1 Materials

Crude oil-contaminated water sample, Continuous Stirred Tank Reactor (CSTR) setup, Microbial consortia for bioremediation, MATLAB and Simulink software, pH meter, Dissolved oxygen meter, Gas chromatography-mass spectrometry (GC-MS), Total Organic Carbon (TOC) analyzer Spectrophotometer, Temperature controller, Agitator/stirring mechanism, Nutrient medium for microbial growth, Synthetic wastewater formulation, Analytical reagents (e.g., NaOH, HCl, buffer solutions), Bioreactor monitoring sensors (pH, temperature, and dissolved oxygen probes)

2.2 Methods

2.2.1 Experimental Setup

The CSTR was seeded with the microbial consortium and operated under controlled environmental conditions. The influent hydrocarbon concentration was varied to evaluate the reactor's performance. The reactor was continuously fed with contaminated water at a controlled flow rate, and samples were collected periodically for analysis.

2.2.2Hydrocarbon Degradation Analysis

GC-MS was used to quantify the concentration of hydrocarbon fractions before and after treatment. The degradation efficiency (%) was calculated using the formula: $\varphi = \frac{c_i - c_0}{(1)}$

$$=\frac{1}{C_i}$$
 (1)

where C_i and Co represent the initial and final hydrocarbon concentrations, respectively.

2.2.3 Heavy Metal Analysis

AAS was used to measure residual concentrations of Pb, Cd, Hg, and Cr in the treated water. The results were compared against regulatory limits set by the Environmental Protection Agency (EPA).

2.2.4 Reactor Design

Michaelis-Menten model was adopted, as it is one of the models that have been used for bioremediation studies But the growth rate decay is expressed as:

$$-r_s = \frac{\mu_{\text{max}}S}{K_s + S} \tag{2}$$

where: $-r_s =$ Hydrocarbon degradation rate (kmol/m³.h);

 μ_{max} = Maximum specific rate constant (kmol/m³.h); K_s = Constant relating to Michaelis-Menten equation (kmol/m³); S = Substrate (hydrocarbon) concentration (kmol/m³)

$$S = S_o (1 - X_s) \tag{3}$$

Substitution of equations (3) into (2) yields:

$$-r_{s} = \frac{\mu_{\max}S_{o}(1-X_{s})}{K_{s}+S_{o}(1-X_{s})}$$
(4)

2.2.4.1 Development of Reactor Performance Equations

The reactor performance equation was developed in this section using the principle of mass Conservation, and it is expressed as shown in equation (5)

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$$\begin{pmatrix} \text{Rate of accumulation} \\ \text{of material} \\ \text{with in CSTR} \end{pmatrix} = \begin{pmatrix} \text{Rate of input} \\ \text{of material} \\ \text{into CSTR} \end{pmatrix} - \\ \begin{pmatrix} \text{Rate of output} \\ \text{of material} \\ \text{from CSTR} \end{pmatrix} \pm \begin{pmatrix} \text{deplection/generation of material} \\ \text{by chemical reaction in CSTR} \end{pmatrix}$$

2.2.4.2 Material Balance on Continuous Stirred Tank Reactor (CSTR)

The schematic diagram of CSTR is shown in Figure 1. In CSTR, there is inflow and outflow of materials. The performance equation of CSTR was developed using equation (5) as follows.



Fig. 1. Continuous Stirred Tank Reactor

From equation (4) we have:

$$F_o = F + (-r_s)V_{CSTR} + \frac{dN_s}{dt} \quad (6)$$

Simplifying and taking into consideration that for a CSTR, $\frac{dN_s}{dN_s} = 0$ we have:

$$dt$$
2.2.4.3 Volume of CSTR
$$V_{CSTR} = \frac{F_o X_s [K_s + S_o (1 - X_s)]}{\mu_{max} S_o (1 - X_s)}$$
(7)
2.2.4.4 Height of CSTR
$$H_{CSTR} = \frac{F_o X_s [K_s + S_o (1 - X_s)]}{\pi D^2 \mu_{max} S_o (1 - X_s)}$$
(8)
2.2.4.5 Space Time of CSTR
$$S_s = \frac{F_o X_s [K_s + S_o (1 - X_s)]}{F_o X_s [K_s + S_o (1 - X_s)]}$$
(9)

 $v_o \mu_{\text{max}} S_o (1 - X_s)$ 2.2.4.6 Space Velocity of CSTR

$$S_{v} = \frac{v_{o}\mu_{\max}S_{o}(1-X_{s})}{F_{o}X_{s}[K_{s}+S_{o}(1-X_{s})]} \quad (10)$$

2.2.4.7 Heat Generated per unit Volume of CSTR

$$q_{CSTR} = \frac{(-\Delta H_r) v_o \pi R^2 \mu_{\text{max}} S_o (1 - X_s)}{K_s + S_o (1 - X_s)} \quad (11)$$

2.2.5 Optimization Strategy

Reactor optimization was conducted using a two-stage approach:

- 1. Pre-Optimization Data Collection: Baseline reactor performance was assessed in terms of hydrocarbon removal efficiency, residence time, microbial activity, and sludge formation.
- 2. Optimization via MATLAB and Simulink Modeling: Key reactor parameters such as hydraulic retention time, microbial kinetics, aeration rate, and mixing speed were adjusted to maximize hydrocarbon degradation while minimizing energy consumption.

2.2.6 Statistical Analysis

Data were analyzed using ANOVA to determine the significance of optimization parameters on reactor performance. A confidence level of 95% (p < 0.05) was used to assess statistical significance.

III. RESULTS AND DISCUSSION

The optimization results in the table 1 highlight the significant improvements in the design and operation of the Continuous Stirred Tank Reactor (CSTR) for hydrocarbon bioremediation. Before optimization, the reactor volume ranged from 6.722 m³ to 9.209 m³ as the conversion increased from 95% to 99%. However, after optimization, the volume was reduced to a range of 5.800 m³ to 7.500 m³. This reduction indicates a more efficient design, which minimizes material costs while maintaining high conversion efficiency. Space time, which measures the residence time of the contaminated water in the reactor, also decreased after optimization. Initially, space time ranged from 2.029 hours to 2.780 hours, but after optimization, it decreased to between 1.800 hours and 2.400 hours. This reduction suggests improved reaction kinetics and enhanced microbial activity, leading to faster hydrocarbon degradation. Space velocity, the inverse of space time, increased after optimization, indicating a higher throughput. Before optimization, it ranged from 0.360 h⁻¹ to 0.493 h⁻¹, whereas after optimization, it improved to 0.417 h⁻¹ to 0.555 h⁻¹. This improvement ensures greater treatment capacity within a given reactor volume. Finally, heat generation per unit reactor volume decreased post-optimization, reducing from 1223 kJ/m³·h to 930 kJ/m³·h before optimization and from 1100 kJ/m³·h to 860 kJ/m³·h after optimization, lowering operational energy costs.

Table I: The optimization results

Table 1. The optimization results								
Conversion	Volume(m ³)		Space Time (h)		Space Velocity(h-1)		Heat Generation(kJ/m ³ •h)	
	Before	After	Before	After	Before	After	Before	After
0.95	6.722	5.800	2.029	1.800	0.493	0.555	1223	1100
0.96	7.345	6.200	2.230	1.950	0.448	0.513	1150	1040
0.97	8.002	6.700	2.450	2.100	0.408	0.476	1080	980
0.98	8.745	7.100	2.610	2.250	0.383	0.444	990	920
0.99	9.209	7.500	2.780	2.400	0.360	0.417	930	860

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Fig. 2: Volume of CSTR vs. Conversion before and after Optimization

Fig. 2 shows the relationship between the volume of the CSTR and conversion before and after optimization. As conversion increases, the volume required for the reactor also increases. However, after optimization, the volume requirement is reduced, making the system more efficient. This optimization ensures that less space is required to achieve high conversion, leading to reduced material costs and better process scalability. The reduction in reactor volume indicates an improvement in reaction kinetics and operational efficiency, which is crucial for industrial-scale applications where space and capital investment play significant roles in process feasibility.



Fig. 3: Space Time vs. Conversion before and after Optimization

Fig. 3 represents space time versus conversion before and after optimization. Space time, which is the time required for reactants to be processed in the reactor, initially increases with conversion. However, after optimization, the space time decreases, meaning that the same level of conversion is achieved in a shorter duration. This reduction implies an improvement in reactor performance and throughput, making the bioremediation process more cost-effective. A lower space time means that more contaminated water can be treated within a given period, improving the overall efficiency of hydrocarbon removal in wastewater treatment facilities.



Fig. 4: Space Velocity vs. Conversion before and after Optimization

Fig. 4 illustrates the relationship between space velocity and conversion before and after optimization. Space velocity, the inverse of space time, measures how quickly the feed passes through the reactor. The optimized process shows higher space velocity, meaning that the reactor can handle more influent while still achieving high conversion. This improvement is crucial for large-scale operations where high processing rates are required to meet treatment demands. By increasing space velocity, the system ensures better utilization of reactor capacity while maintaining effective contaminant breakdown, which enhances the feasibility of continuous operation.



Fig. 5: Heat Generated per CSTR Volume vs. Conversion before and after Optimization

Fig. 5 depicts heat generated per CSTR volume versus conversion before and after optimization. Before optimization, the heat generated decreases with conversion, but the values are higher compared to the optimized system. The optimized process results in lower heat generation, reducing the thermal load on the system and minimizing energy consumption. This decrease is beneficial for industrial operations where excessive heat generation can lead to equipment degradation and increased cooling costs. By optimizing the reactor design, the

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system operates more efficiently, reducing both operational expenses and environmental impact while maintaining high hydrocarbon degradation rates.

IV. CONCLUSION

This study successfully optimized the design of a Continuous Stirred Tank Reactor (CSTR) for the efficient bioremediation of hydrocarbon-contaminated water. The results demonstrate that optimization significantly enhances reactor performance, leading to reduced reactor volume, decreased space time, increased space velocity, and lower heat generation per unit reactor volume. These improvements contribute to better efficiency, cost-effectiveness, and sustainability of the bioremediation process.

Before optimization, the CSTR required a larger reactor volume, ranging from 6.722 m³ to 9.209 m³ for 95% to 99% hydrocarbon conversion. However, after optimization, the volume was significantly reduced to 5.800 m³ to 7.500 m³. This decrease in reactor size implies lower material costs and a more compact design, making large-scale implementation more feasible. Additionally, the reduction in space time from 2.029–2.780 hours to 1.800–2.400 hours after optimization indicates an improvement in reaction kinetics. The optimized reactor allows for faster hydrocarbon degradation, increasing the efficiency of contaminant removal while ensuring sustained microbial activity.

The observed increase in space velocity after optimization, from 0.360–0.493 h^{-1} to 0.417–0.555 h^{-1} , further supports the enhancement in reactor throughput. This means that more contaminated water can be processed within the same reactor volume, improving overall treatment capacity. Another crucial finding is the reduction in heat generation per unit reactor volume, from 1223-930 kJ/m3·h before optimization to 1100-860 kJ/m3·h after optimization. This reduction in heat load contributes to lower operational energy costs, making the optimized CSTR more economical and sustainable in long-term applications. The study highlights the importance of reactor design optimization in achieving efficient and cost-effective bioremediation of hydrocarbon-contaminated water. By optimizing key parameters, such as reactor volume, space time, space velocity, and heat generation, the performance of CSTRs can be significantly improved. This research provides a framework for designing scalable wastewater treatment systems that minimize environmental impact while ensuring high hydrocarbon removal efficiency. Future studies can focus on integrating advanced process control strategies to further enhance reactor stability and performance under varying operational conditions.

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