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A Study Using Simulation to Remove Petroleum Hydrocarbons through Bioremediation and Resource Recovery

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Abstract. Petroleum hydrocarbons are one of the most widespread and persistent organic pollutants, caused by the worldwide dependence on oil as an energy source. The presence of petroleum hydrocarbons in soil and wastewater around oil refineries and oil handling facilities is a serious threat to the environment and human health, as these substances are highly toxic and persistent. This paper proposes a bioremediation approach for petroleum hydrocarbons, with toluene used as a representative aromatic contaminant for simulation purposes, while simultaneously producing methane as valuable byproduct. The system uses kinetic modeling and real-time optimization in MATLAB based on simplified lumped Monod-type and first-order kinetic assumptions, while Aspen HYSYS is used for process simulation, material and energy balance calculations. The simulation results, obtained under steady-state anaerobic conditions at mesophilic temperature, show substantial removal of petroleum hydrocarbons and efficient methane-rich gas production, thus emphasizing the potential of system for sustainable resource management. The proposed method is consistent with SDG-United Nations for clean water, responsible production, and climate action. The study is fully simulation-based relies on literature-derived and assumed parameters, the quantitative results should be interpreted as indicative trends rather than exact predictions, and experimental validation is required to reduce uncertainty.

1 Introduction

1.1 Problem Statement

The dependence on oil as the primary source of energy has consistently resulted in the land and water being polluted with petroleum hydrocarbons. Different types of hydrocarbon compounds like alkanes, aromatics, asphaltenes, and resins are the main contributors to such pollution [1]. These pollutants are not only extremely toxic but also very slow to degrade, hence they pose great threats to both the environment and human health as shown in

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Figure 1. Commonly used techniques for soil decontamination, such as removal of the soil, incineration and chemical oxidation, are to a certain degree effective but still prohibitively expensive and most often result in the generation of secondary environmental problems.

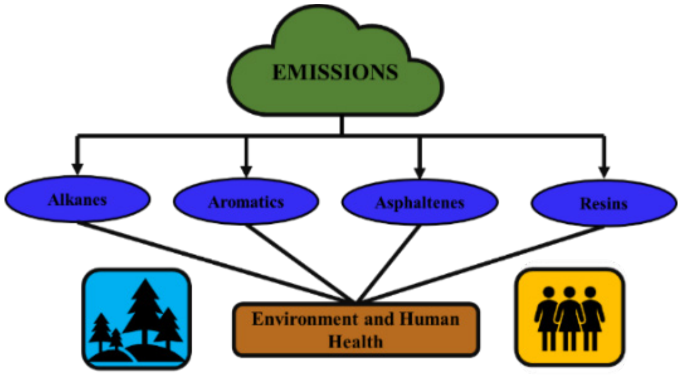

Fig. 1. Emission from petroleum hydrocarbons.

Thus, green and cost-effective remediation techniques are desperately needed that would not only eliminate the contaminants but also let the precious resource recover. The turning point is bioremediation with resource recovery through computational modeling and process simulation using MATLAB and Aspen HYSYS. The collaboration between bioremediation and resource recovery not only can reduce the time of pollutant's degradation but also facilitate the optimal methane and nutrient recovery while adhering to the circular economy and global sustainability goals [2].

1.2 Research Gap

Countless investigations have focused on bioremediation as a method for petroleum hydrocarbon degradation [1]. A large number of these works have concentrated on the removal of pollutant, whilst the integration of resource recovery mechanisms has been neglected. The opportunity to eliminate the contamination of the environment and at the same time obtain useful materials, for instance, methane, treated water, and compostable residues, is still not much explored. Additionally, computational modeling and simulation tools such as MATLAB and Aspen HYSYS have been used in isolation in environmental studies, but their combination for the purpose of dynamic process optimization in bioremediation systems is still rare. Furthermore, the lack of existence of well-developed and predictive models that correlate laboratory-scale biodegradation kinetics with industrial-scale process simulation is another area of concern.

Moreover, the sustainability assessment and circular economy implications of the bioremediation and resource recovery system have rarely been quantitatively assessed in the literature. This lack of assessment further emphasizes the need to adopt an integrated approach to bioprocess development, modeling, and sustainability assessment to develop an efficient and reproducible bioremediation and resource recovery system for petroleum-contaminated environments.

1.3 Justification of the Study

Bioremediation is an environmentally friendly practice that supports the sustainability of the environment through the degradation of pollutants in the environment. However, the application of bioremediation is limited due to the lack of resource recovery. Furthermore, the integration of co-biotechnology with methane and nutrient recovery transforms the conventional bioremediation process from waste treatment to a value-added process, which is in accordance with the circular economy concept.

The application of simulation tools like MATLAB and Aspen HYSYS in bioprocess development is highly beneficial in simulating the bioprocess, optimizing the process parameters, and scaling up the process from laboratory to industrial scale through computational integration. Moreover, the recovery of valuable by-products from the petroleum-impacted wastewater is not only helpful in the remediation of the environment from pollutants but also aligns with the global sustainability goals and objectives [3]. Even though the present study is focused on the simulation of the bioprocess, the integration of bioremediation and resource recovery is in accordance with the sustainability goals and objectives like SDG 6: Clean Water and Sanitation and SDG 7: Affordable and Clean Energy.

1.4 Solution

This article aims to showcase the computer-based method that integrates the process of bio-remediation and resource production to clean up oil-contaminated environments in an environmentally friendly manner. It is not simply a theoretical process but is based on data and computer modeling using data and parameters and the use of computer-based data to validate the results.

The process aims to break down the petroleum hydrocarbon biodegradation process into two steps: not only to clean the environment but also to produce useful by-products such as methane gas, clean water, and compost materials. The process works by introducing a mixed microbial consortium, which is already known to thrive in both aerobic and anaerobic environments. In the anaerobic section, methanogenic archaea play an important role in the production of methane gas. The process also produces a treatment residue that is converted to compost and clean water [4].

To check the viability of this process, the main computer programs used to simulate the process were MATLAB and Aspen HYSYS.

- MATLAB was used to carry out the simulations. The parameters and the values of the parameters such as the maximum specific growth rate (μ_{ma}), saturation constant (K_s), and yield ($Y_x/_s$) obtained from the literature were used to carry out the simulations.
- Aspen HYSYS was used to carry out the process simulations and to check the efficiency and scaling potential. The output from the bioreactor in MATLAB was fed into HYSYS which was used to model the phases of methane recovery, composting, and water treatment- using virtual reactor and separator blocks for each of the phases respectively.
- This combined modeling system illustrates that the process of petroleum bioremediation can be optimized and evaluated through the hands-on experimental approach. The incorporation of biological principles, process engineering, and computational analysis results into a conceptual and predictive model that gives the solution both pollution mitigation and resource recovery.

Hence, the combined study provides a data-driven foundation for next experimental validation and industrial-scale application, which is altogether in line with circular economy principles and UN Sustainable Development Goals (SDGs 6, 7). The composition of the simulated results, which stem from literature-validated assumptions, indicates that the integration of such a system can very likely lead to over 85-90% removal of hydrocarbon along with significant methane enrichment in the recovered gas stream and recoverable by-products.

2 Methods

This research paper presents a detailed computational methodology for the investigation of petroleum hydrocarbons removal via microbial bioremediation in combination with recycling of resources and process simulation. The research was carried out in two main stages:

- Stage 1 – Kinetic Modeling (MATLAB): Generation and refinement of kinetic models for the purposes of imitating the degradation behaviour, calculating the reaction parameters, and carrying out sensitivity analysis for various environmental and nutrient conditions.
- Stage 2 – Resource Recovery Simulation (Aspen HYSYS): Simulating and appraising the processes of methane recovery, compost production, and water reuse by means of steady-state material and energy balance calculations.

Although anaerobic petroleum biodegradation proceeds through multiple microbial stages, a lumped kinetic representation was adopted in this work. This approach captures the overall substrate degradation trend and is suitable for simulation-based process analysis, while detailed microbial interactions were beyond the scope of the present study. Note that MATLAB and Aspen HYSYS were not directly connected via dynamic coupling or real-time data sharing. Instead, they were used as independent but complementary tools within a sequential modeling framework. MATLAB-based kinetic modeling was performed to study representative biodegradation behaviour and estimate conversion trends under anaerobic conditions. These results were then used to inform the selection of reaction assumptions and operating parameters in the Aspen HYSYS process simulation, which focused on steady-state material and energy balance analysis and resource recovery evaluation.

2.1 Simulation and Modelling

2.1.1 MATLAB Modelling

MATLAB software was used for the simulation of biodegradation kinetics and for process parameter optimization as well. The data obtained from published literature sources were applied to the first-order and Monod models to evaluate the kinetic constants (μ_{max}, K_s, $Y_x/_s$). A dynamic differential equation model predicting the decay of hydrocarbons and the growth of biomass was created.

The microbial consortium used in this study was chosen on the basis of functional compatibility with petroleum hydrocarbon biodegradation and anaerobic methane production, as described in existing literature. Instead of focusing on the isolation of particular strains, the model postulates a mixed microbial consortium consisting of hydrocarbon-degrading bacteria (including facultative and obligate anaerobes) and methanogenic archaea. The criteria used for selection were (i) the capacity to degrade a wide range of petroleum hydrocarbons and intermediate degradation products, (ii) resistance to toxic hydrocarbon fractions and fluctuating environmental conditions (pH, temperature, and nutrient availability), and (iii) established syntrophic relationships between fermentative bacteria and methanogenic archaea that facilitate the efficient utilization of complex organic substrates for methane production in anaerobic environments. The kinetic parameters characterising these microbial populations were sourced from established literature to facilitate the simulation model in accurately replicating the concurrent processes of contaminant biodegradation and methane production.

2.1.2 MATLAB Model Assumptions and Scope

This study employs a MATLAB model, which gives a simplified kinetic picture of the degradation of petroleum under anaerobic conditions [4]. Due to the complex nature of the microbial communities, the model applies a global rate expression, which gives a simplified picture of the degradation of petroleum under anaerobic conditions. The model was not designed to give a detailed mechanistic or predictive picture of the degradation of petroleum. Consequently, MATLAB results are interpreted qualitatively and used for comparative analysis. Kinetic parameters were selected within ranges reported in the cited literature for anaerobic petroleum hydrocarbon degradation and methanogenic systems. Model-defined feeding parameters were used to simulate fed-batch operational behavior rather than site-specific conditions.

Table 1. Kinetic parameters used in the MATLAB-based anaerobic bioremediation model and their literature sources.

Parameter	Description	Value Used	Unit	Literature Source
μ_{max}	Maximum specific microbial growth rate	0.20	h^{-1}	Imam et al., 2021; Agarry et al., 2020
K_s	Half-saturation constant for hydrocarbons	100	mg L^{-1}	Agarry et al., 2020; Sun et al., 2021
K_n	Nitrogen half-saturation constant	10	mg L^{-1}	Sun et al., 2021
K_p	Phosphorus half-saturation constant	5	mg L^{-1}	Sun et al., 2021
$Y_x/_s$	Biomass yield coefficient	0.10	g g^{-1}	Jamal & Pugazhendi, 2018; Imam et al., 2020
Y_{CH_4}	Methane yield coefficient	0.30	g g^{-1}	Jamal & Pugazhendi, 2018; Borah & Yadav, 2017
k_d	Microbial decay rate constant	0.005	h^{-1}	Raper et al., 2018
F_s	Hydrocarbon feed rate (fed-batch phase)	2	mg L^{-1} h^{-1}	Assumed (scenario-based simulation)
$t_{feed,start}$	Start time of substrate feeding	60	h	Model-defined
$t_{feed,end}$	End time of substrate feeding	120	h	Model-defined

2.1.3 Justification for Kinetic Model Selection

The Monod model and the first order kinetic model were chosen as both continue to be widely used and supported in the bioremediation literature to be effective in predicting microbial growth and petroleum hydrocarbon biodegradation due to most studies being in the two parameters. The Monod model is a good example to use to analyse and predict microbial growth state in substrate limiting conditions (Kennes et al., 1998) as it is found in anaerobic hydrocarbon biodegradation systems where the level of nutrients and hydrocarbons concentration are main factors which affect microbial growth. On the other hand, the first order kinetic model was a good fit for oil biodegradation processes where the concentration of hydrocarbons is low or when there is no need to know the details of the process. Therefore, the use of Monod model together with the first order kinetic model provides a balanced approach for simulation studies in bioremediation and bio-catalyzed recovery processes.

2.1.4 Aspen HYSYS Simulation

The bioremediated sludge and gas streams produced were brought into Aspen HYSYS for the purpose of simulating and analysing the resource recovery phase. The whole system comprised the subsystems for anaerobic digestion, solid residue management, and water recovery. Aspen HYSYS was used for steady-state process simulation to perform mass and energy balance analysis and evaluate product recovery, rather than to represent detailed biological kinetics. Several generalizations were implemented in the Aspen HYSYS model, including lumped reaction stoichiometry, steady-state operation, and ideal phase separation. These conventions are suitable for process-level viability analysis.

2.1.5 Model Components in HYSYS:

- Mixers: Used before the reactor units to combine inlet components.
- Reactors: Biological conversion reactor and gas formation.
- Separators: Two-phase separators for gas and water phase separation.

2.1.6 Reaction Stoichiometry and Modeling Assumptions

The degradation of petroleum hydrocarbons under anaerobic conditions takes place through a series of complex biochemical reactions, which involve the participation of diverse microbial consortia. In the model, a single, overall lumped reaction stoichiometry represents the net anaerobic degradation of petroleum hydrocarbons to stable end products. The stoichiometric coefficients of the reaction are obtained from the elemental mass balance of the components of petroleum, as well as the pathways of the degradation of petroleum, as reported in the literature [5,6].

Material balance was carried out to determine the efficiency of the processes, the yield of methane, the yield of energy (MJ kg^{-1} sludge), which was subsequently used to determine the various parameters, such as:

- Energy recovery efficiency, which was obtained from the methane yield.
- Water reuse efficiency and quality parameters.
- Nutrient content in the sludge
- Carbon credits.

The variables used in the model, both in MATLAB and Aspen HYSYS, have a single unit system, which is the International System of Units, i.e., the variables used in the model have the following units:

- Concentration, (kg/m^3).
- Time, (hours).
- Reaction rate constants, (h^{-1}).
- Temperature, (kelvin).
- Pressure, (bar).

Although this approach is not as accurate as a detailed mechanistic model for petroleum degradation under anaerobic conditions, it is adequate for process simulation as required for Aspen HYSYS. The kinetic parameters employed in this study were obtained from literature for a better representation of petroleum degradation under anaerobic conditions. Although this approach is not as accurate as a detailed mechanistic model for petroleum degradation under anaerobic conditions, it is adequate for process simulation as required for Aspen HYSYS.

3 Results and Discussion

3.1 Simulation Results for Anaerobic Bioremediation with Methane Recovery

Figure 2 indicates the time course of the anaerobic bioremediation model using MATLAB, which predicts the time course of the hydrocarbon substrate, the biomass, and the methane produced as a byproduct of the reaction. The level of the hydrocarbon substrate drops dramatically from 1000 mg/L to less than 50 mg/L at the very outset of the simulation, indicating the effectiveness of the microbes in degrading the easily degradable fractions of the hydrocarbon [7]. After the dramatic drop, the level of the hydrocarbon substrate remains almost flat at a very low level, gradually increasing to indicate that the easily degradable fractions of the hydrocarbon have been completely consumed.

The level of the biomass initially increases as the microbes use the hydrocarbon as a food source to carry out the degradation of the hydrocarbon. The level of the biomass peaks and gradually starts to decline towards the very end of the simulation [8]. The level of methane, on the other hand, gradually increases throughout the simulation, indicating the constant production of methane as a byproduct of the anaerobic degradation of the hydrocarbon [9]. The production of methane, apart from contributing to the degradation of the hydrocarbon, can be used as a source of energy, which can improve the economic viability of the remediation of the hydrocarbon using the anaerobic degradation method as compared to the traditional degradation methods. In short, the findings indicate that hydrocarbons were thoroughly removed along with the growth of biomass and the continuous production of methane, thus verifying the kinetic model's ability to reflect changes in key variables typically observed in anaerobic bioremediation combined with resource recovery.

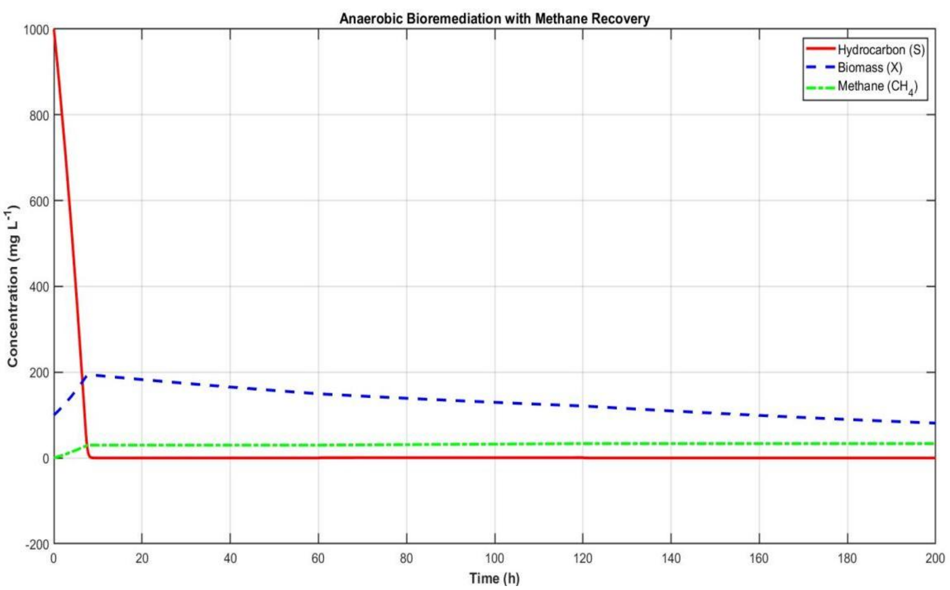

Fig. 2. Temporal variation of hydrocarbon (S), biomass (X), and methane (CH_4) concentrations during the anaerobic bioremediation process with methane recovery.

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3.2 Aspen HYSYS-Based Simulation of Bioremediation and Resource Recovery

Aspen HYSYS has been utilized to perform process simulation for recovering downstream resources from the bioremediated product streams. Parameters taken from the literature were used to model methane purification, gas- liquid separation, and water recovery.

3.2.1 Methane Recovery

The methane stream that was simulated showed that the mass flow rate was about 10.06 kg h^{-1}. The low levels of impurities like CO_2 and water vapor prove that phase separation and gas purification were very efficient. These figures are comparable to those published for simulation based anaerobic digestion and biogas recovery, thus the modeling approach is representative of the real system.

3.2.2 Separator Performance

Gas-liquid separator (V-100) separated well the outlet of the reactor into gas and liquid streams. The liquid fraction was mainly water (99.7 %) which means that the water can be reused provided that only a small amount of post-treatment is carried out. The methane concentration in the gas phase was very high with the hydrocarbon losses being negligible, hence the separation efficiency was very high.

3.2.3 Process Efficiency and Sustainability

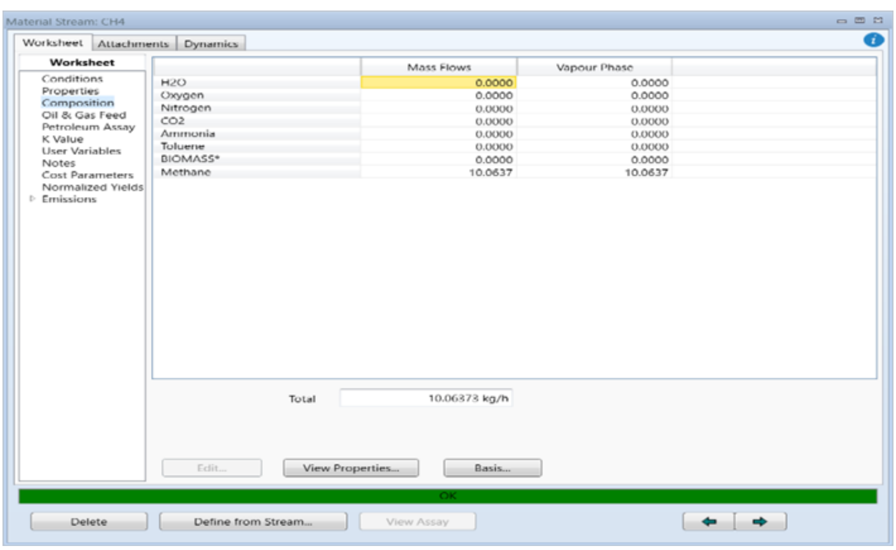

Fig. 3. Material stream data for methane output from the anaerobic bioremediation process as simulated in Aspen HYSYS, showing component mass flow rates and vapor-phase composition.

It was estimated that the recovery of potential energy from methane would be roughly 500 MJ h^{-1} based on the simulated methane flow rate and its lower heating value that the integrated process is energy-positive. Simulation results further reveal that the CO_2 concentration in the vent gas is quite low relative to methane, which indicates a high carbon conversion efficiency in the bioreactor (Figures 3 and 4). The water treated in the process came out to be highly pure, and the biomass produced had solid residues left behind, which could be used as fertilizer once the stabilization is complete [10]. Overall, these results indicate that the integration of bioremediation and resource recovery is not only technically feasible but also environmentally sustainable, which aligns well with the circular economy and similar simulation-based studies in the area.

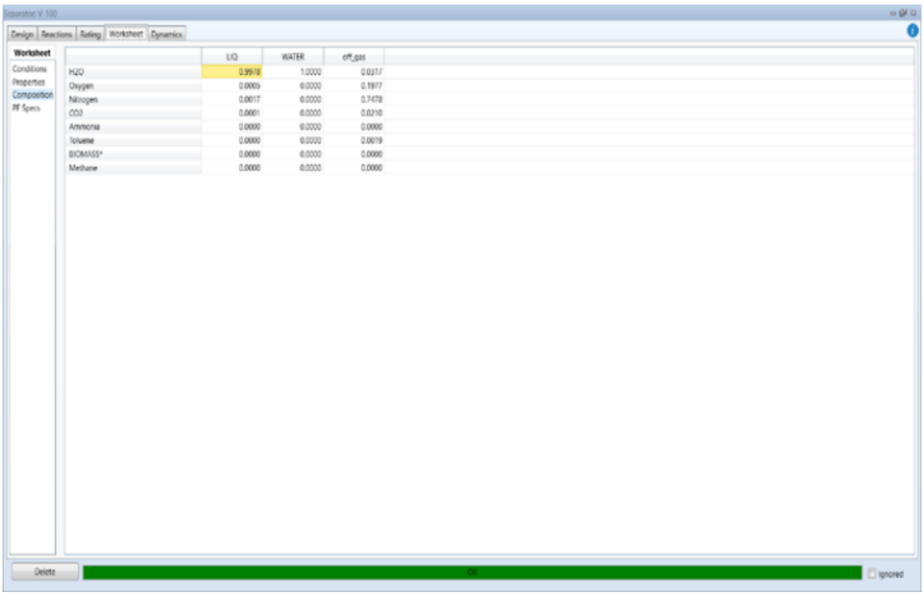

Fig. 4. Composition data of the bioreactor inlet stream from Aspen HYSYS simulation, showing liquid and vapor phase distribution of major components during the bioremediation process.

All reactions implemented in the simulation were atomically balanced, and mass conservation was enforced by the Aspen HYSYS solver. The overall material balance was verified across the bioreactor and separation units. Gas-phase products such as methane and carbon dioxide were separated in downstream flash units, which may give the appearance of mass loss when only liquid-phase streams are considered. No net mass violation occurs when all phases are accounted.

3.3 Discussion

One of the characteristics that distinguish the anaerobic biodegradation processes in the model is the extremely rapid initial decrease in hydrocarbon concentration. Similar trends were observed in the investigations on anaerobic petroleum hydrocarbon degradation, particularly during the exponential phase of microorganism development, due to the microorganism consortia's preferential consumption of the readily degradable hydrocarbon fractions. The production of methane, which grew gradually with the lag following the initial timing, is consistent with the anaerobic metabolic pathways that have been theoretically described. Syntrophic bacteria have been observed to form a chain to degrade hydrocarbons into intermediate compounds such as volatile fatty acids and alcohol, which are further converted into methane by methanogenic archaea [11]. However, methane production is slower than the consumption of the substrate due to the two-step degradation process.

Using Aspen HYSYS software to simulate the process along with the kinetic model, the study was able to quantify the resource recovery potential. These results suggest that the process is technically feasible with significant energy recovery, efficient gas-liquid separation, and high purity methane production. This is further supported by the predictive ability of the model due to simulated hydrocarbon removal efficiencies in excess of 90% and methane production yields in accordance with similar comprehensive simulation studies in the area.

3.4 Limitations and Need for Experimental Validation

The combined package of the MATLAB and Aspen HYSYS program presents an exciting new perspective on the viability and efficiency of anaerobic bioremediation and resource recovery processes. However, due to the simulated nature of the study, the results have some limitations in and of themselves. For instance, all the parameters used in the study were assumed and simulated from the literature and not from actual on-site studies and sampling of the target compounds in the environment. Therefore, the results of the study should be considered as having the potential to occur rather than actual quantitative results.

Furthermore, the study on bioremediation and resource recovery has shown that methane production is an advantage in the production of bioenergy. However, the study does not consider the actual problems in methane production at the larger scale in the model simulation. For instance, methane production in the actual case may be limited in several ways, including the mass transfer limitations and the actual process controls in the reactors. These limitations may have contributed to the results not being exactly as the model simulation had predicted.

The model simulation used the MATLAB program, which is not accurate in the actual case due to the simplification of the actual process in the model simulation. For instance, the actual process of the degradation of petroleum in the environment is not simple and involves several steps in the metabolism of the microorganisms involved in the bioremediation process. Therefore, the actual results may not have been exactly as the model simulation had predicted due to the simplification of the model simulation. Furthermore, the actual process in the environment is difficult to model in the computer program due to the actual complexities involved in the bioremediation process in the environment. Confirmation of this through experiments at different scales will considerably raise the assurance of the integrated methodology's use not only in the field of remediation but also in the industrial implementation.

4 Conclusion

The current investigation indicates that an integrated system of bioremediation and resource recovery has a great potential for the eco-friendly treatment of petroleum-contaminated sites, and it was based on simulation. The modeling of kinetics was carried out in MATLAB while the process simulation was done in Aspen HYSYS; as a result, the study excellently predicted the biodegradation of peat and fungi production through a combination of anaerobic conditions. The Kinetics at MATLAB confirmed that the suggested anaerobic biodegradation pathway was effective as there was no more than 10% left of the total hydrocarbons at the end of the simulation period. Besides that, there was a significant microbial growth and a slow formation of CH_4.

The study also indicated through the process of Aspen HYSYS that the resource recovery was indeed possible as there was methane constituting the dominant fraction of the recovered biogas, treated water which was very less polluted or even reusable, and the composited soil which was nutrient-rich could be produced from the process. The collaboration of biotic, abiotic, and computational models draws a very important and energetic path to the positive and circular remediation systems. Even though the research relies on assumed and literature-derived data, the outcomes provide a firm conceptual and predictive base for experimental validation and industrial-scale application. To provide a more thorough examination of environmental impacts, future research may include quantitative sustainability indicators including life cycle assessment (LCA), carbon footprint, and energy return on investment. From a sustainability perspective, the integrated bioremediation and resource recovery approach demonstrates potential relevance to selected Sustainable Development Goals, particularly those related to water treatment and energy recovery. These links are only examples, and they are meant to show how the proposed framework can be used in more situations, not to claim that it directly leads to SDG achievement.

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