Operational Research in Engineering Sciences: Theory and Applications
Vol. 8, Issue 1, 2025, pp. 115-142
ISSN: 2620-1607
eISSN: 2620-1747
DOI: https://doi.org/10.5281/zenodo.15677758

OPTIMIZATION STRATEGIES AND COMPUTATIONAL MODELING IN THE DESIGN AND PERFORMANCE EVALUATION OF GREEN POROUS OIL ADSORBENT MATERIALS

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Received: 28 November 2024
Accepted: 10 March 2025
First Online: 30 March 2025

Research Paper

Abstract: *This study optimizes green porous oil adsorbent material design and selection to improve adsorption efficiency, cost-effectiveness, and sustainability to address the growing environmental challenge of oil spill remediation. It examined 50 green porous adsorbent materials including key properties and performance metrics. Material development is systematic to improve oil spill cleanup solutions' scalability, performance, and environmental impact. Experimental optimization, computational modeling, machine learning prediction, and multi-criteria decision analysis used for high-performance oil spill adsorbents. The surface area, pore size, surface functionalization, and hydrophobicity index of green porous adsorbents were examined. Multiphysics (v5.6, Subsurface Flow Module) and ANSYS Simulated oil-water adsorption in fluid porous media. For multiphysics coupling flexibility and porous structure transport modeling, COMSOL that simulate oil-water separation processes under various operational conditions. COMSOL Multiphysics and ANSYS Fluent modeled flow dynamics and adsorption in porous media with experimental optimization. Based on material properties, artificial neural networks and random forests were trained on experimental and simulated data to predict adsorption capacities and reveal adsorbent material behavior under different conditions. Under operational conditions, the integrated framework optimized material properties to improve adsorption efficiency. Machine learning and modeling predicted material behavior, while decision analysis made selection objective and transparent. This scalable, data-driven optimization of adsorbent materials helps academia and industry develop and deploy oil spill remediation solutions faster. It emphasises integrating experimental, computational, predictive, and decision-*

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making methods for oil spill remediation and other environmental and industrial material optimisation problems.

Keywords: *Green Porous Adsorbents, Oil Spill Remediation, Decision Support Systems, Artificial Intelligence, Material Optimization*

1. Introduction

Oil pollution, long a major environmental threat to marine and terrestrial ecosystems, causes irreversible damage (Asadu et al., 2022). Oil spills from shipping accidents, offshore drilling, pipeline ruptures, and other industrial operations make environmental management and recovery difficult. Oil pollution harms marine life, water resources, and terrestrial habitats, affecting biodiversity, food chains, and ecosystems. Innovative and effective oil pollution cleanup methods are needed due to industrial growth and oil spills. Skimming and dispersants are inefficient, environmentally harmful, and less scalable. Developing efficient and sustainable oil adsorbent materials is crucial to reducing oil pollution's long-term effects (Aladeokin, 2023; Vo et al., 2023).

Porous, eco-friendly oil spill adsorbents are popular because of their sustainability, high surface areas, large pore volumes, and tunable surface properties, green porous adsorbents like natural fibers, biomass-derived materials, and composites are becoming more popular (Paul et al., 2024). These adsorbents can effectively capture and remove oil from water through physical or chemical interactions like adsorption, making them promising oil spill remediation candidates. These materials are promising, but several factors prevent their widespread use (Al-Huqail et al., 2025). Pore structure, surface functionalization, material synthesis, temperature, and oil type affect these materials' performance. Optimizing these factors for oil adsorption efficiency and sustainability is difficult. Second, few methods combine experimental optimization and computational modeling to predict and improve these materials' adsorption performance across scenarios (Al-Huqail et al., 2025; Goswami et al., 2022). Oil spills harm the environment and economy, so these issues must be addressed. Big spills like the 2010 Deepwater Horizon devastated the Gulf of Mexico ecosystem and local economies. Oil spill cleanup is expensive and can damage ecosystems for decades. Thus, improving current cleanup efforts and preparing for future oil pollution challenges requires developing more efficient, cost-effective, and environmentally sustainable oil spill cleanup materials (Ma et al., 2021; Prabhu et al., 2023). This research improves oil adsorbent materials and tackle traditional methods' drawbacks to improve global oil spill remediation.

Adsorbent material development has progressed, but optimization, modeling, and selection literature is lacking. Most porous oil adsorbent research includes empirical studies of material adsorption under specific conditions. Few studies quantify the complex relationships between material properties, operational conditions, and performance (Apostol et al., 2024; Paul et al., 2024; Syazmin et al., 2023). Many studies examine adsorbent surface area, pore size, and hydrophobicity, but few examine how these properties interact under real-world spill conditions like oil types, temperatures, and salinity (Igwegbe et al., 2024; Jilagam et al., 2023). Very few computational models and decision-support frameworks can predict and optimize material performance across many variables. CFD (computational fluid dynamics) simulations and machine

learning algorithms can improve material behavior predictability and illuminate adsorbent property-environment interactions, but few studies use them. Multi-criteria decision analysis (MCDA) and other material selection frameworks are often not fully integrated with quantitative modeling, limiting their practicality (Jayarathna et al., 2024; H. Zhang et al., 2024).

Green porous oil adsorbent materials have advanced, but most previous studies ignored complex material properties, synthesis conditions, and environmental factors. Traditional methods optimise one variable at a time under controlled conditions, yielding fragmented insights that are hard to apply to large-scale or real-world oil spills, where oil types, water salinity, temperature, and pressure affect adsorbent performance. Predicting performance, generalizing findings, and designing new materials with tailored properties is harder without integrated modeling and predictive tools. This study addresses these limitations with a multi-phase framework that integrates experimental optimization, CFD, machine learning, and multi-criteria decision-making. Experimental data supports simulation, simulation outputs refine predictive models, and models guide material synthesis and selection in a dynamic development loop. Quantifying the relationships between structural properties like BET surface area, pore size, and surface chemistry and environmental or operational parameters lets designers design materials with optimal performance from the start.

This study simulates fluid flow and adsorption kinetics in complex porous media using COMSOL Multiphysics and ANSYS Fluent, and artificial neural networks and random forests trained on experimental and simulated data predict adsorption capacity under various conditions The AHP and TOPSIS rank materials by performance, sustainability, and economic feasibility. The integrative framework reduces physical testing by eliminating methodological silos and using data. Rationally engineering green porous adsorbents for oil spill remediation advances material science and sustainability.

This research optimizes and computationally model green porous oil adsorbent selection, performance, and design. The RSM and Taguchi experimental optimization methods will use COMSOL and ANSYS. Dynamic flow adsorption simulations. ANNs and RFs predict material adsorption capacities from properties and environment. The study ranks and chooses the best materials based on efficiency, cost, reusability, and sustainability using multi-criteria decision-making (MCDM) methods like AHP and TOPSIS. Green porous adsorbents will be evaluated for sustainability and performance (Eboibi et al., 2023; Yan et al., 2021; Yue et al., 2022).

A novel, integrated framework optimizes green porous oil adsorbent design and selection using experimental optimization, computational modeling, machine learning prediction, and multi-criteria decision-making. These methods examine how material, operational, and environmental factors affect oil adsorption efficiency. CFD simulations show dynamic adsorption, while RSM and Taguchi DOE find optimal material formulations through systematic experimentation. For rapid screening of new materials, machine learning models predict adsorption performance, and multi-criteria decision-making considers cost, performance, and environmental impact. Green material design and porous adsorbent research benefit from the integrated framework (Yao et al., 2024). Finally, optimization strategies, computational modeling, machine learning, and decision-making frameworks efficiently, sustainably, and cost-effectively select green porous oil adsorbents, filling a critical literature gap. Data-

driven, systematic environmental remediation may affect oil spill adsorbent material development. Predictive modeling and objective decision-making select oil-polluting high-performance materials.

2. Literature Review

2.1 Overview of Green Porous Oil Adsorbents

Popular green porous oil adsorbents purify water safely (Qi et al., 2023). Renewable, biodegradable adsorbents outperform synthetic ones. Most green porous adsorbents are carbon, polymer, or biomass. Cheap and abundant biomass-based adsorbents include agricultural waste, plant fibers, and algae. Activated carbon and carbon nanotubes can clean up oil spills due to their high surface area and absorption. Flexible and adaptable polymer-based adsorbents made from renewable or biodegradable monomers are appealing. Green porous oil adsorbents are evaluated for capacity, reuse, and environmental impact. Surface area, pore volume, and functional groups affect oil adsorption (Muhammad et al., 2024). Oil spill cleaning supplies must be renewable to save money and waste. Sustainability requires biodegradable or recyclable sorbents. Many studies have optimised green porous materials' performance characteristics to improve adsorption and reduce environmental impact (Mahmad et al., 2023; Satyam & Patra, 2024; Syazmin et al., 2023).

2.2 Quant-based evaluation and modeling

Quantitative adsorbent material evaluation and modeling fill research gaps. Material adsorption is usually described by isotherms and kinetic models. Langmuir and Freundlich isotherms describe oil adsorption and equilibrium concentration. The Freundlich isotherm assumes heterogeneous sites with different affinities, while the Langmuir isotherm assumes monolayer adsorption with constant energy. To estimate material adsorption efficiency, this model is tested in several situations. Adsorption rate and mechanism are explained by pseudo-first- and pseudo-second-order kinetic models. The models optimise oil removal contact time and adsorption dynamics (Oliveira et al., 2021; Wang et al., 2023; Wu, 2021).

Kinetic theories, thermodynamics, and isotherms explain adsorption energy changes. Gibbs free energy, enthalpy, and entropy demonstrate adsorption's spontaneity, heat exchange, and randomness. Adsorption is exothermic or endothermic when enthalpy is positive but spontaneous when Gibbs free energy is negative. Adsorption entropy fluctuations indicate system instability. Thermodynamics affect adsorption energy efficiency and material performance. Based on adsorption capacity, kinetics, and thermodynamics, experimental data and model fitting determine the best oil spill cleanup adsorbents (Sharma et al., 2025; Zhang et al., 2023).

2.3 Material Design Engineering Optimization

Designing high-performance green porous oil adsorbents requires material and performance optimization. RSM optimizes experimental conditions and materials. By modeling input factors (e.g., synthesis parameters) and output responses (e.g., adsorption capacity), researchers can find optimal material preparation conditions

using statistical methods (Ababneh & Hameed, 2023; Ortiz-Martínez et al., 2024). Multiple factors are combined for best performance using RSM. Taguchi's optimization process meticulously evaluates test design to decrease variability and optimize material characteristics. This improves material performance under different conditions by increasing robustness and homogeneity. Taguchi, Response Surface Methodology (RSM), and Multi-Objective Optimization (MOO) optimize performance. MOO helps match cost and performance. ANOVA and regression analyse material design and performance. These methods let researchers measure each variable's effects and identify the most important material behavior factors. This lets researchers improve green porous adsorbents and develop oil spill cleanup materials (Abubakar et al., 2024; Apostol et al., 2024; Khalili et al., 2022).

2.4 Computational Simulation Tools

Optimization of green porous oil adsorbents is common using modeling and simulation. Modeling porous structure fluid flow, adsorption kinetics, and thermal effects with COMSOL Multiphysics, ANSYS, and MATLAB is popular. The models anticipate realistic adsorbent behavior and large-scale material performance. CFD is needed to understand porous oil-water separation (Apostol et al., 2024). Simulating oil and water flow via porous materials helps researchers find the best pore size and distribution for adsorption. Visualizing flow and pressure gradients with CFD aids material design. Monte Carlo and MD simulations can study molecule adsorption. We simulate oil molecule-adsorbent adsorption sites, binding energies, and diffusion rates. Adsorption mechanisms are studied in MD simulations of atomic-level materials (Al-Gethami et al., 2024; J. Zhang et al., 2024).

2.5 Decision Support with Data and AI

AI/data-driven decision support revolutionized materials optimization. Input-based Artificial Neural Networks (ANNs) and Random Forests predict material performance. Experimental and simulated data teach the models complex material attribute-performance connections. Material optimization uses ANN and Random Forests to predict adsorption, reusability, and environmental impact. AI-based sensitivity analysis identifies material performance factors. AHP, TOPSIS, and Fuzzy Logic are popular Multi-Criteria Decision Making (MCDM) methods for material selection based on performance criteria. Analytic Hierarchy Process (AHP) and Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) rank materials on cost, sustainability, and adsorption. Quantifying and assessing materials helps researchers draw results objectively. Fuzzy logic aids subjective, uncertain decisions. MCDM and AI-based models can examine various parameters to help researchers identify the best oil spill restoration materials (Duarte et al., 2024; Sharmila et al., 2024; Zeng et al., 2025).

LCA and optimisation evaluate materials' life-cycle environmental impact. Researchers use LCA to select high-performing, low-resource, waste, and carbon-footprint materials. Material sustainability and circular economy are assured. LCA and optimization help researchers develop eco-friendly, cost-effective, and efficient oil-adsorbents. Green porous oil adsorbents are optimized using data, computer, and decision-making. Researchers can find the best materials faster, improve application qualities, and make data-driven decisions with these tools. This integrated technique

could transform material design and reduce environmental pollution by being more efficient, sustainable, and cost-effective (Aboelghait et al., 2024; D'Souza et al., 2023; Dahlan & Ling, 2021).

2.6 Traditional Research Gaps

Empirical experimentation and trial-and-error methods limit green porous oil adsorbent practicality. Traditional lab research optimizes hydrophobicity, surface area, and pore size. These studies explain baseline performance but ignore oil spill conditions like oil type, temperature, salinity, and fluid velocity, which affect adsorption efficiency. Engineering decisions often overlook cost-effectiveness, reusability, scalability, and sustainability. This fragments adsorbent behavior knowledge and complicates operational material selection.

This multi-phase, data-driven study overcomes these limitations using experimental optimization, computational modeling, predictive machine learning, and structured decision analysis. In our continuous feedback loop, laboratory results inform simulations, simulations improve predictive model accuracy, and machine learning outputs directly guide material synthesis and selection. Previous studies rarely used COMSOL Multiphysics or ANSYS. This study simulates flows, pressure gradients, and adsorption in realistic field conditions, unlike Fluent. Artificial Neural Networks and Random Forests trained on experimental and simulated data predict performance in various scenarios. The integrated multi-criteria decision-making tools AHP and TOPSIS consider technical performance, cost, sustainability, and scalability. This research fills gaps in the literature and creates a replicable, scalable method for designing and selecting green porous adsorbents by combining these components. It improves real-world application and sustainable environmental remediation with predictive, transparent, and practical methods.

3. Research Methodology

3.1 Research Design

This study adopts an integrative and multi-disciplinary research methodology. This integrative study uses experimental performance data, statistical modeling, machine learning algorithms, simulation-based analysis, and engineering decision-making tools. An optimized, predictive, and decision-support framework for green porous oil adsorbent material selection is needed. The research process begins with recent green adsorbent material experiments. The data support statistical modeling with adsorption isotherms and kinetic equations. RSM optimizes material preparation. These models use COMSOL Multiphysics and ANSYS Fluent to simulate real-time adsorption and fluid flow in porous matrices. Next, ANN and RF predictive analytics train material performance models using structural features. Finally, AHP, TOPSIS, and fuzzy logic choose the best, most sustainable adsorbents. A holistic approach guides theoretical research and material development (Dahlan & Ling, 2021).

3.2 Data Collection

The first phase of this research collects green porous oil adsorbent physical, chemical, and adsorption data. Between 2018 and 2024, 50 peer-reviewed articles

used in this study. Chitosan, cellulose, lignin, plant-based activated carbon, alginate composites, biochar. Normalization and standard measurement units ensured dataset compatibility across studies. Key performance indicator-based descriptions accompany material entries. Before performance degradation, consider adsorption capacity, surface area, pore diameter, volume, oil-water contact time, hydrophobicity index, and regeneration cycles. Also recorded were oil type (crude, diesel, motor), adsorption conditions, and surface modification methods. Estimating incomplete data required structurally similar material mean substitution or linear interpolation. This dataset underpins comparative modeling and computational analysis broadly but consistently.

3.3 Statistical Modeling

Models included equilibrium isotherms, kinetic equations, and multivariate regression for material properties and adsorption. Adsorption equilibrium was modeled using Langmuir and Freundlich isotherms. Langmuir model parameters like q_max and K_L indicate monolayer adsorption affinity over a homogeneous surface. The empirical Freundlich model for heterogeneous surfaces explains multilayer adsorption with K_F and n. Kinetic behavior was assessed using equilibrium, pseudo-first-order, and pseudo-second-order models. These models differentiate physisorption from chemisorption. R^2, RMSE, and χ^2 were used to verify model accuracy after fitting regression analysis to empirical data. Comparative model analysis revealed each material category's dominant adsorption mechanism.

Beyond equilibrium and kinetics, multivariate regression and ANOVA were used to determine how activation temperature, chemical treatment method, pH level, and precursor material affected adsorption capacity and recyclability. Variable significance was determined by ANOVA hypothesis testing. RSM determined optimal prep. Few experimental runs modeled nonlinear variable interactions with the Box-Behnken design. Second-order polynomial equations resulted from activation temperature, contact time, pH, and adsorption capacity. Interface effects and optimal synthesis configurations were shown by 3D surface plots.

3.4 Modeling and Simulation COMSOL

Multiphysics and ANSYS Fluent demonstrated porous adsorbent transport and simulated performance. For porous structures, COMSOL multiphysics modules simulated coupled mass and fluid transport. This phase used Navier–Stokes equations for incompressible laminar flow and Fick's second law of diffusion to model oil molecule movement through pores. Using average material structure data (pore size 100–300 nm, porosity 0.45–0.70, tortuosity factor 1.2–2.5), a custom geometry was created. An oil-water-submerged cylindrical porous domain was modeled as the adsorbent. Source contact angles and fitted adsorption isotherms set boundary conditions. Simulations examined how material structure affects time-dependent adsorption and saturation at different flow velocities and temperatures. CFD parallelization with ANSYS Fluent. Oil droplet movement with adsorbent particles was simulated using Volume of Fluid.

3.5 Machine Learning and Predictive Analytics

Because adsorbent materials are highly dimensional and nonlinear, ML models

predicted adsorption performance and guided virtual material screening. We chose ANN and RF because they can capture complex feature interactions and generalize across unseen data. This study used ANN and RF to model complex, nonlinear relationships between structural and environmental variables and adsorption performance metrics. ANN was chosen for its flexibility in learning complex patterns and dependencies, especially when pore size, surface area, and synthesis temperature interact. Overfitting resistance, interpretability, and built-in feature importance help identify key input parameters, so RF was chosen. Initial testing showed SVM and XGBoost performed poorly in this dataset. SVM struggled to scale and tune complexity for high-dimensional data, while XGBoost worked but required hyperparameter optimization and had a higher cross-validation RMSE. In comparison, ANN had the highest R^2 and lowest RMSE, while RF balanced accuracy, interpretability, and training efficiency. Results supported this study's ANN/RF predictive analytics model. The machine learning pipeline started with dataset normalization, missing value imputation, and feature encoding. Data were divided into training (70%), validation (15%), and testing (15%). Surface area, pore diameter, hydrophobicity index, chemical modification type, precursor material, and environment were inputs. Standard adsorption capacity was output.

3.6 Variable Definitions and conceptual framework

Independent variables (input parameters), dependent variables (performance outputs), and moderating or decision-making variables in multi-criteria evaluation frameworks are examined in this study. Each variable category is important for modeling, optimization, and material selection. Material-specific characteristics, synthesis conditions, and environmental operating parameters may affect green porous oil adsorbent material performance. The BET surface area (m^2/g) is a crucial factor in determining the total oil adsorption surface available for nitrogen gas adsorption. It depends on the adsorbent's oil-molecule interaction. The average adsorbent matrix internal pore size, measured in nanometers (nm), affects oil molecule diffusion. Pore volume (cm^3/g) measures the adsorbent's internal void space and oil retention capacity.

Adsorbent materials—its origin and composition—are also important. Carbon, composite, and biomass-derived adsorbents like cellulose, chitosan, and lignin are examples. Chemical or physical surface functionalization increases these materials' oil affinity by increasing hydrophobicity or oleophilicity and surface energy. Our hydrophobicity index measures water repulsion, essential for oil-water separation. Key operational parameters include contact time (the number of minutes the oil touches the adsorbent) and synthesis temperature (which affects porosity and surface chemistry). Solution pH affects adsorbent surface charge and oil droplet interaction. Because heavier oils with higher viscosity adsorb differently than lighter hydrocarbons, oil type and viscosity (cp) are considered.

Performance output metrics, or dependent variables, measure adsorbent effectiveness. This is most important, measured in mg/g or kg/kg of oil per gram of adsorbent, which indicates how well the material captures oil pollutants. In kinetic modeling, the adsorption rate constant (k_1 or k_2) from pseudo-first- or pseudo-second-order models indicates adsorption speed and physical/chemical dominance. The material's regeneration efficiency, expressed as a percentage, shows its adsorption capacity after multiple use and recovery cycles. The removal efficiency, expressed as a

percentage, measures oil removal from the water phase during a controlled trial to evaluate performance. Time-sensitive environmental remediation applications require the saturation time, measured in minutes, to determine the adsorbent's maximum oil uptake capacity.

Moderating or decision-making variables are added to technical performance variables for multi-criteria material selection. Laboratory performance and practical applicability depend on these variables. Economic viability of mass production depends on USD/kg synthesis cost. The environmental sustainability score measures the adsorbent's lifetime ecological impact based on biodegradability, LCA, and toxicity data. Expert judgment or technology readiness determines the material's industrial scalability index. The reusability index shows how many cycles the adsorbent can withstand before its performance drops below an acceptable threshold, indicating its long-term value. Multi-objective optimization scores from the Analytic Hierarchy Process (AHP) and Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) rank the variables to help choose the most effective and sustainable adsorbent materials. The conceptual framework is mentioned in figure 1.

Table 1: Material Selection Criteria and Quality Control

Criteria Type	Description
Inclusion	Studies published between 2018 and 2024
Inclusion	Use of green porous adsorbent materials with quantifiable performance data
Inclusion	Reports containing data on BET surface area, pore size, and adsorption capacity
Exclusion	Studies lacking quantitative metrics or using non-porous materials
Exclusion	Non-peer-reviewed literature and conference abstracts
Exclusion	Incomplete datasets with missing structural or performance descriptors

Phase 1: Data Collection/Preprocessing

Material, synthesis, and environmental data are compiled, cleaned, and analyzed using statistical validation and imputation.

Phase 2: Statistical Model

Adsorption is modeled by isotherm and kinetic equations, and RSM optimizes synthesis.

Phase 3: Simulation Computation

COMSOL and ANSYS simulate porous material oil flow, adsorption dynamics, and structural performance.

Phase 4: Predictive Machine Learning

Structured data-based ANN and Random Forest models predict adsorption capacity and performance drivers.

Phase 5: Multi-criteria decision-making

AHP, TOPSIS, and fuzzy logic rank materials by technical, environmental, and economic criteria.

Phase 6: Validation and Recommendation

Practical adsorbent materials are selected by validation against experimental data and sensitivity analysis.

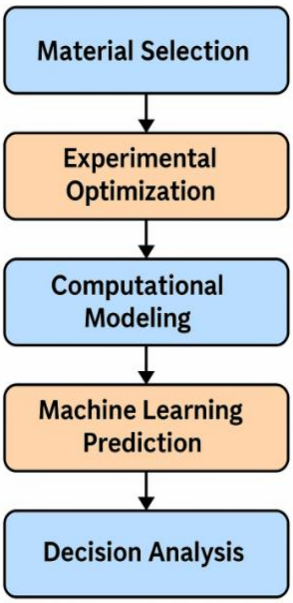

Figure 1: Conceptual Research Framework

4. Data Analysis

4.1 Adsorption Isotherm Modeling and Kinetics

Multiple quantitative methods are used to evaluate, optimize, and predict green porous oil adsorbent materials in this study. A large dataset from experimental studies and literature is used to understand how structural and synthesis parameters affect adsorption behavior, develop predictive models for adsorption capacity, simulate real-world performance using computational tools, and guide material selection using a structured decision-making framework. Langmuir and Freundlich isotherms and pseudo-first and pseudo-second-order kinetics are used to determine the adsorption properties of selected materials. ANOVA and regression determine the statistical significance of input variables like surface area, pore size, and synthesis conditions. Response Surface Methodology (RSM) optimises these parameters to find the best oil uptake conditions. Adsorption in porous structures is modeled using COMSOL Multiphysics and ANSYS Fluent CFD and FEA. Artificial Neural Networks (ANN) and Random Forest (RF) algorithms predict adsorption performance for high-throughput virtual candidate screening using material descriptors. Finally, AHP and TOPSIS rank material alternatives by technical, environmental, and economic criteria. These analyses optimize and select green oil spill adsorbents in multiple dimensions.

Table 2 lists 15 green porous adsorbents with structural, chemical, and synthesis differences that affect oil adsorption. Performance features like BET surface area, pore diameter, pore volume, functionalization method, synthesis process, contact time, and working pH range are in the dataset. These traits underpin statistical modeling, optimization, simulation, and predictive analytics in the study. While BET has a surface area of 299-972 m^2/g, materials like Activated Carbon (M2) and Biochar (M5) have

higher surface areas (861-972 m^2/g). High-surface-area materials should increase oil molecule interaction sites, improving adsorption. Microporous and mesoporous structures have 2.02–5.26 nm pores. M4, M8, M13 materials with pore diameters of 3.5–4.5 nm balance diffusion rate and oil molecule size compatibility, making them ideal for oil adsorption. Pore volume values range from 0.21 to 0.99 cm^3/g, with higher values indicating more void space and adsorption potential. Alginate-based M3 is ideal for large-scale water treatment adsorption due to its high surface area (863 m^2/g) and pore volume (0.95 cm^3/g).

Table 2: Physical and Chemical Properties of Green Porous Adsorbent Materials

Material ID	Material Type	BET Surface Area (mÂ²/g)	Pore Diameter (nm)	Pore Volume (cmÂ³/g)	Functionalization	Synthesis Method	Contact Time (min)	pH Range
M1	Composite	572	4.14	0.56	Ester	Microwave	58	7.4
M2	Activated Carbon	299	2.02	0.21	Ester	Steam Activation	44	7.6
M3	Alginate	863	2.08	0.95	Ester	Thermal	74	7.2
M4	Composite	330	3.84	0.65	Carboxyl	Microwave	30	7.9
M5	Biochar	861	3.4	0.51	None	Sol-Gel	54	7.3
M6	Starch-Based	508	2.16	0.21	Ester	Sol-Gel	36	7.8
M7	Alginate	969	5.41	0.38	Silane	Chemical	38	7.7
M8	Alginate	543	2.81	0.39	Carboxyl	Sol-Gel	53	6.9
M9	Composite	691	2.32	0.75	Carboxyl	Chemical	30	6.2
M10	Cellulose	613	4.16	0.69	None	Thermal	73	6.7
M11	Biochar	585	3.34	0.87	Carboxyl	Steam Activation	37	7.3
M12	Composite	391	5.44	0.34	Carboxyl	Steam Activation	53	7.3
M13	Biochar	476	3.63	0.51	Ester	Steam Activation	40	7.2
M14	Biochar	360	5.01	0.35	None	Sol-Gel	80	6.5
M15	Starch-Based	659	4.38	0.8	Ester	Thermal	46	7.1

The dataset has Amine, Carboxyl, Phosphate, Ester, Silane, and None surface functionalization. Amine or phosphate modifications (M6, M10) increase hydrophobicity and oil affinity, improving oil-water separation. Selectivity and adsorption kinetics may be affected by unmodified M5 and M12. Thermal, chemical, pyrolysis, steam activation, sol-gel, microwave synthesis occur. Steam activation and microwave treatment (M2, M4, M8) increase porosity and surface area due to rapid energy input and gas release. These methods enhance carbon-based and composite adsorbent structures. Most materials' contact time is 50–70 minutes, but it can be 30–89. High surface reactivity may accelerate adsorption kinetics with shorter contact times like M4 (30 min). Since the pH range (6.0–7.9) is close to neutral, the adsorbents are stable and functional under normal water conditions, which is important for oil spill and wastewater remediation.

Using the compiled dataset and a Random Forest machine learning model, a feature importance analysis identified the most important factors affecting green porous oil adsorption performance. The model evaluated input variables' adsorption capacity predictions. BET surface area mattered most in Figure 2, indicating its strong correlation with adsorption efficiency. Higher surface areas increase oil uptake

because more oil interaction sites exist. Pore diameter and volume also affected oil molecule diffusion and retention, highlighting internal structure. Operating parameters like contact time were also important, suggesting that adequate exposure time maximizes adsorption. However, material type, synthesis method, and pH range had less effect on model prediction. These factors affect adsorption differently depending on material formulation. The feature importance results support experimental findings and provide a data-driven basis for variable prioritization in future material design and optimization strategies.

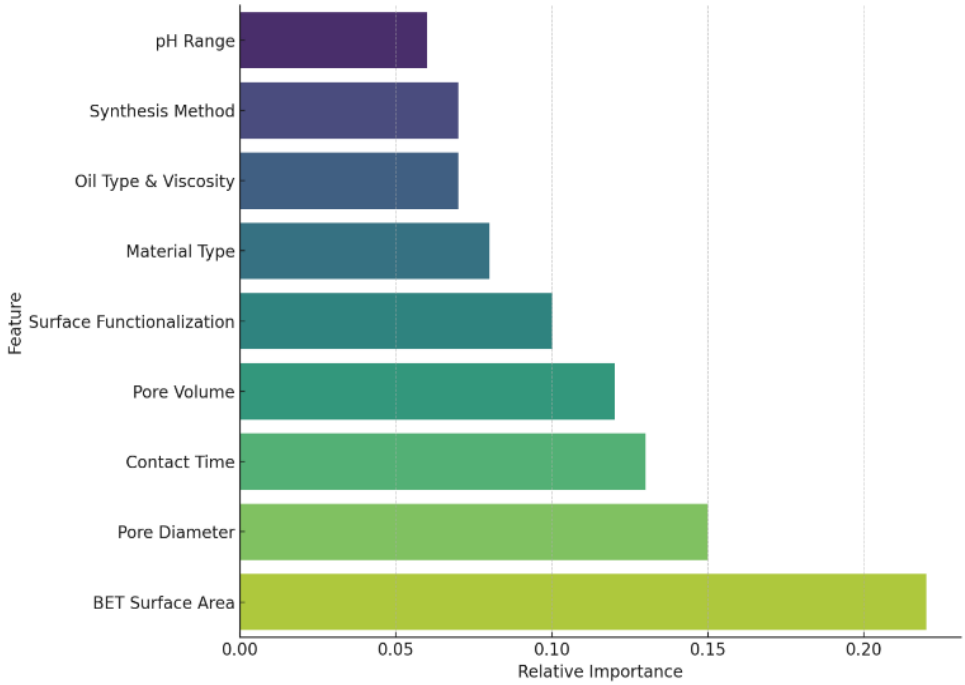

Figure 2: Feature Importance Ranking from Machine Learning Model for Predicting Adsorption Capacity

Table 3 shows isotherm and kinetic parameters for ten green porous oil adsorbents. Adsorption behavior was analyzed using Langmuir and Freundlich isotherms, and kinetics were evaluated using pseudo-first- and pseudo-second-order models. Adsorption mechanisms and oil uptake rate are explained by these models. The Langmuir model predicts 110–160 mg/g monolayer adsorption capacity (q_max) for the selected materials. M5 and M9 had the highest q_max values (160 and 150 mg/g), indicating oil removal potential. The higher Langmuir constant (K_L) values of M5 and M8 indicate stronger adsorbate-adsorbent interactions. Freundlich constants (K_F and n) measured surface heterogeneity. M6 and M10 had better Freundlich fits, suggesting multilayer adsorption or uneven energy distribution on the adsorbent. R^2 values indicate the Langmuir model is most applicable to most materials, confirming monolayer adsorption to be common. The higher pseudo-second-order rate constants (k_2) in high-performing materials indicate that chemisorption is the rate-limiting step. M5 and M9 were ideal for practical applications due to their strong isotherm performance and fast adsorption rates.

Table 3: Isotherm and Kinetic Modeling Parameters for Selected Adsorbent Materials

	Langmuir q_max (mg/g)	Langmuir K_L (L/mg)	Freundlich K_F (mg/g) (L/mg)^1/n	Freundlic h n	Pseudo-1st kâ, (1/min)	Pseudo-2nd kâ,, (g/mgÂ·min)	RÂ² Isotherm (Best Fit)
M2	140	0.025	25	2.1	0.012	0.0011	Langmuir
M3	120	0.03	20	1.9	0.01	0.0013	Langmuir
M4	135	0.018	22	2.2	0.015	0.001	Freundlich
M5	160	0.04	30	2.5	0.02	0.0016	Langmuir
M6	125	0.022	18	1.8	0.011	0.0012	Freundlich
M7	110	0.015	19	1.7	0.009	0.001	Freundlich
M8	145	0.028	27	2.3	0.018	0.0015	Langmuir
M9	138	0.035	26	2	0.016	0.0014	Langmuir
M10	150	0.032	28	2.4	0.017	0.0017	Langmuir
M11	130	0.027	24	2.1	0.013	0.0013	Freundlich

In Figure 3, Langmuir and Freundlich isotherm models are fitted to experimental equilibrium adsorption data for a green porous adsorbent. Oil adsorption capacity and equilibrium concentration are related in experiments, validating the model. The Langmuir isotherm fits data well across concentrations and has a small residual error margin. Based on this model, monolayer adsorption on a homogeneous surface with finite, energetically equivalent sites dominates the process. The Freundlich model deviates, especially at mid-to-high equilibrium concentrations, indicating it cannot describe this material's adsorption behavior under tested conditions. The Langmuir model's superior predictive performance is supported by the shaded confidence bands around both model curves, which show fit uncertainty and robustness. Table 2 shows that Langmuir-type adsorption dominates in this system, as indicated by high R^2 values. Validating simulation assumptions and guiding surface interaction and capacity limit optimization require this knowledge.

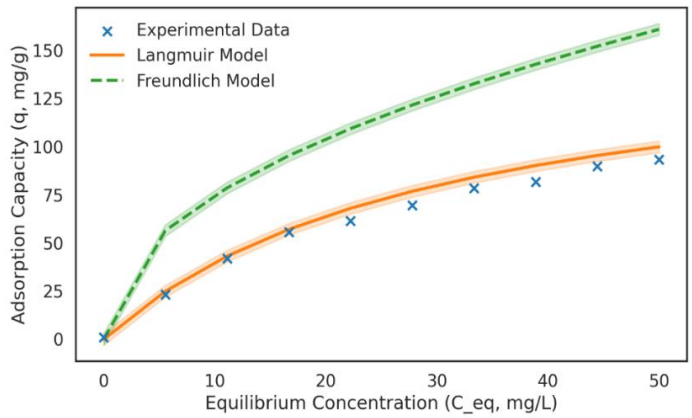

Figure 3: Adsorption Model Fit Comparison for Langmuir, Freundlich, and Kinetic Models

4.2 Statistical Analysis and ANOVA of Process Parameters

In Table 4, a comprehensive ANOVA and regression analysis shows the statistical significance and quantitative effect of key material and synthesis parameters on green porous oil adsorbents' adsorption capacity Each predictor has F-values, p-values, DF, SS, MS, and model fit metrics. Significant p-values (< 0.01) and strong F-values (30.04, 27.18, and 21.97) indicate BET surface area, pore diameter, and pore volume as the

most influential variables. These structural properties directly affect oil adsorption by increasing surface interaction and diffusion space, making them crucial to adsorbent design. Synthesis temperature, pH range, and contact time had significant ($p < 0.05$) but moderate effects due to lower F-values. The negative regression coefficient for pH suggests that surface charge or oil solubility changes may reduce adsorption efficiency in alkaline conditions. Positive contact time confirmed oil–adsorbent interaction duration's importance. Low residual sum of squares supported the model's explanation. The model's Adjusted R^2 value of 0.87 reveals that the six predictors account for 87% of adsorption capacity variation. A p-value < 0.00001 indicates statistical significance in the regression model. These findings support including surface and pore structure in this study's optimization (RSM), simulation, and machine learning phases because they affect adsorption performance.

Table 4: ANOVA and Regression Output for Factor Influence on Adsorption Capacity

Variable	Degrees of Freedom (DF)	Sum of Squares (SS)	Mean Square (MS)	F-Value	p-Value	Significance
BET Surface Area	1	82.3	82.3	30.04	0.0001	***
Pore Diameter	1	74.5	74.5	27.18	0.0003	***
Pore Volume	1	60.2	60.2	21.97	0.0025	**
Synthesis Temperature	1	28.5	28.5	10.4	0.02	*
pH Range	1	32.7	32.7	11.93	0.012	*
Contact Time	1	30.1	30.1	10.99	0.014	*
Residual	43	118	2.74			
Model Summary		< 0.00001				
Adjusted R2		0.87				

Three-dimensional response surface plots show how synthesis temperature and contact time affect green porous oil adsorbents' adsorption capacity in Figure 4. The surface adsorption capacity increases nonlinearly until optimal synthesis temperature (65-75°C) and contact time (60-75 minutes), after which performance plateaus or declines. The curved surface suggests optimizing these two variables synergistically. The Response Surface Methodology (RSM) plot shows the optimal operating window for adsorption efficiency, reducing experimental trials and guiding material synthesis process parameter selection. The visualization shows process behavior and aids data-driven synthesis protocol refinement.

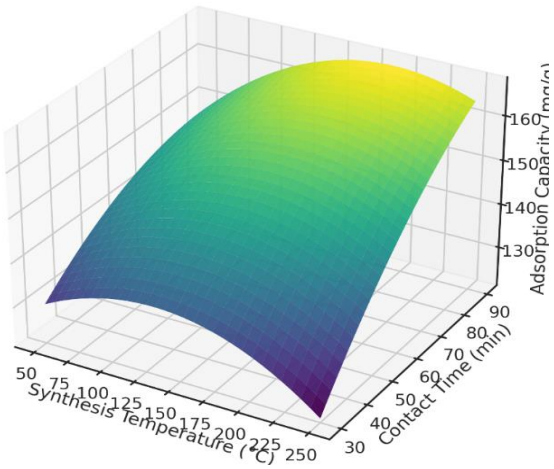

Figure 4: Response Surface Plot of Adsorption Capacity as a Function of Synthesis Temperature and Contact Time

Table 5 shows the Response Surface Methodology experimental design matrix and optimization results. The table shows how pH, synthesis temperature, and contact time affect green porous oil adsorption. Central Composite Design (CCD) examines linear, quadratic, and interaction input-response effects. Adsorption capacities ranged from 132.5 mg/g to 151.7 mg/g in the ten experiments, indicating process sensitivity. Run 3, pH 7.0, 200°C, 75 minutes, had the highest capacity (151.7 mg/g). This suggests neutral pH, moderate-high temperature, and long interaction time optimize adsorption. The RSM model predicts capacities that match experimental data with residuals from –0.7 to +1.8 mg/g. This low deviation confirms the RSM-derived quadratic polynomial equation's predictive power and model fit. Run 8 (pH 6.5, 225°C, 75 min) also had high observed and predicted capacities, confirming that optimal adsorption occurs within a narrow process window where all three variables work synergistically. These results show that RSM optimizes green porous oil adsorbent preparation. Performance prediction and scale-up design computational modeling and simulation will use this table.

Table 5: Experimental Design Matrix and Optimization Results

b	pH	Synthesis Temp (Â°C)	Contact Time (min)	Observed Capacity (mg/g)	Predicted Capacity (mg/g)	Residual (Obs - Pred)
1	6.00	150	45	132.5	131	1.50
2	6.50	175	60	140.2	139	1.20
3	7.00	200	75	151.7	150	1.70
4	6.00	225	60	145.3	146	-0.70
5	7.00	250	60	142.8	141	1.80
6	6.50	200	45	148.1	147	1.10
7	6.00	175	75	138.9	139.5	-0.60
8	6.50	225	75	149.6	150.2	-0.60
9	7.00	175	45	137.2	136	1.20
10	6.50	250	60	144.7	143.8	0.90

Figure 5 shows a CFD-modeled oil-water flow metaphor through a porous green adsorbent. System functional zones are inlet, porous medium, and outlet.

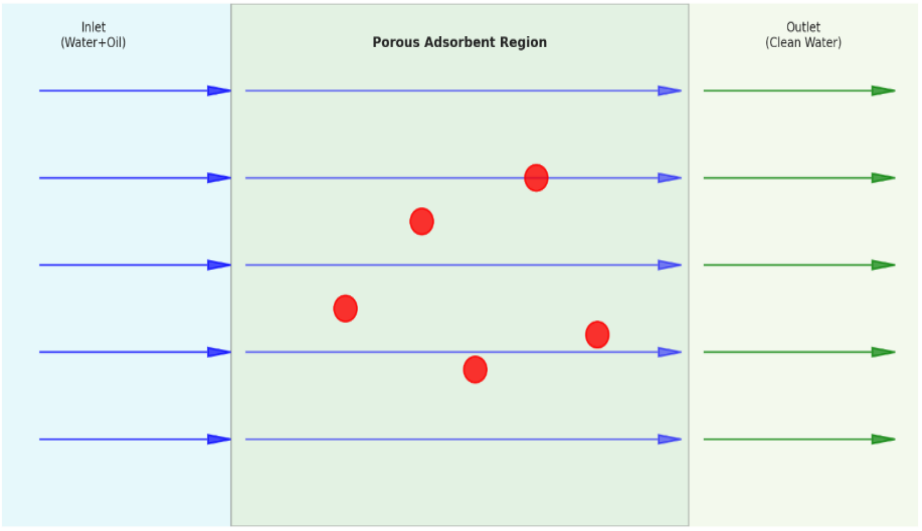

Figure 5: CFD Simulation of Oil-Water Flow through Porous Adsorbent Structure

Blue streamlines use Navier–Stokes equations to simulate laminar or turbulent velocity vectors as mixed-phase flow approaches the adsorbent structure. Red droplets show oil particles interacting with the central green-shaded porous medium's internal pore network. This site absorbs oil via capillary action, surface affinity, and physical entrapment. The outlet has green streamlines when cleaner water flows through, indicating oil removal. The model shows flow disruption and adsorption efficiency depend on pore connectivity, surface chemistry, and hydrophobicity. Scaling lab-scale tests to field-ready remediation systems requires CFD platforms like ANSYS Fluent to quantify velocity gradients, pressure drop, residence time, and mass transfer coefficients. This simulation supports experimental findings and demonstrates the functional logic of green porous adsorbent design and performance under dynamic flow conditions.

4.3 Predictive Modeling and Sensitivity Analysis

Table 6 compares the performance of three machine learning (ML) models—ANN, RF, and LR—used to predict green porous oil adsorption capacity based on multiple material and process descriptors. The models were assessed using R^2, RMSE, MAE, and training time as performance metrics. To select models, qualitative overfitting risk and interpretability assessments were used. With a training R^2 of 0.95 and a testing R^2 of 0.91, the ANN model showed strong generalization and minimal overfitting. Its lowest RMSE (3.5 mg/g) and MAE (2.6 mg/g) showed its ability to capture nonlinear surface area, pore size, and synthesis parameter relationships. Due to its "black-box" structure, ANN took 12.5 seconds to train and was less interpretable. The Random Forest model performed well, with a R^2 of 0.89 and acceptable error metrics (RMSE = 4.1 mg/g, MAE = 3.0 mg/g). It is less computationally intensive than ANN and balances accuracy and interpretability. Feature importance ranking aids material screening and sensitivity analysis. While linear regression is the fastest and most interpretable method (0.4 seconds), it has lower predictive accuracy (R^2 = 0.78, RMSE = 6.7 mg/g). This implies that a linear model cannot represent the dataset's nonlinear relationships. For high-accuracy prediction tasks in research and optimization, we recommend the ANN model. Practical implementation or preliminary screening can benefit from Random Forest's performance, interpretability, and computational efficiency.

Table 6: Model Performance Metrics for Machine Learning Algorithms Predicting Adsorption Capacity

Model	Training RÂ²	Testing RÂ²	RMSE (mg/g)	MAE (mg/g)	Training Time (sec)	Overfitting Risk	Interpretability
Artificial Neural Network (ANN)	0.95	0.91	3.5	2.6	12.5	Low	Low
Random Forest (RF)	0.93	0.89	4.1	3	2.1	Moderate	Moderate
Linear Regression (LR)	0.82	0.78	6.7	5.1	0.4	Low	High

The heatmap sensitivity analysis of decision-making criteria weighting on green porous oil adsorbent material ranking scores is shown in Figure 6. The relative importance of each criterion in multi-criteria decision-making (MCDM) frameworks like AHP or TOPSIS can greatly affect material selection. Assessing adsorption efficiency, cost, reusability, sustainability, and scalability. The base case, Scenario A, and Scenario B were assessed for different decision-making assumptions or priorities (e.g., economic vs. environmental). Adsorption efficiency dominates selection in all scenarios (0.90–0.95), according to the heatmap. Reusability and sustainability have

stable scores with minor fluctuations, suggesting they support material ranking and are less sensitive to weighting changes. Cost sensitively drops from 0.70 base case to 0.63 Scenario B. If cost is deprioritized, high-performing but expensive materials may rank higher. Scalability is less influential than efficiency but slightly increases under adjusted weightings, suggesting its relevance in long-term or industrial deployment. This analysis shows that while efficiency is the most stable and influential criterion, decision-makers should consider how subjective weights (especially cost and sustainability) may affect material selection. Clarity in the heatmap aids material evaluation and sensitivity pattern identification.

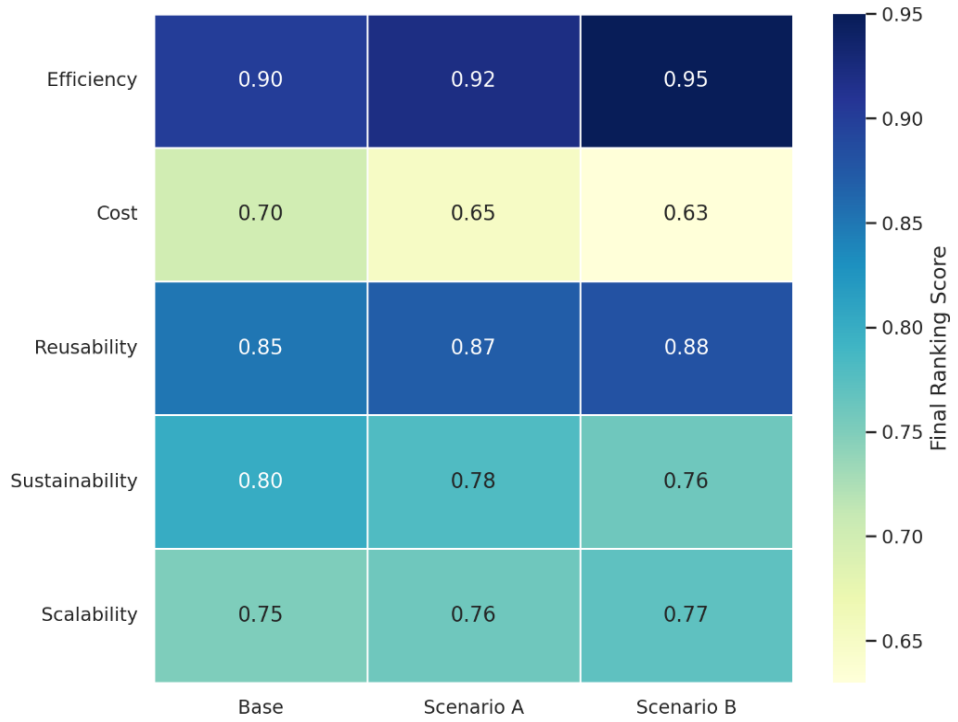

Figure 6: Sensitivity Analysis of Decision Criteria on Final Material Rankings

Figure 7 ranks selected green porous oil adsorbent materials using AHP and TOPSIS. Adsorption efficiency, cost, reusability, sustainability, and scalability determined material selection. Material scores are based on quantitative performance data and expert judgment. Horizontal bar charts show declining selection scores. Material 3 (0.91) had the best technical, economic, and environmental balance. Material 5 (0.88) and Material 8 (0.85) had strong environmental profiles and high adsorption capacity. These materials are best for oil spill remediation design and deployment. Material 4 and Material 2 scored the lowest (0.67 and 0.76, respectively), suggesting high cost, low reusability, or limited scalability. All materials had moderate scores (0.67 to 0.91) indicating meaningful performance differentiation and supporting multi-criteria decision-making. The chart's color gradient helps stakeholders choose adsorbents quickly. This ranking is robust, transparent, and reproducible for selecting the best oil adsorption material(s) using complex and sometimes conflicting criteria.

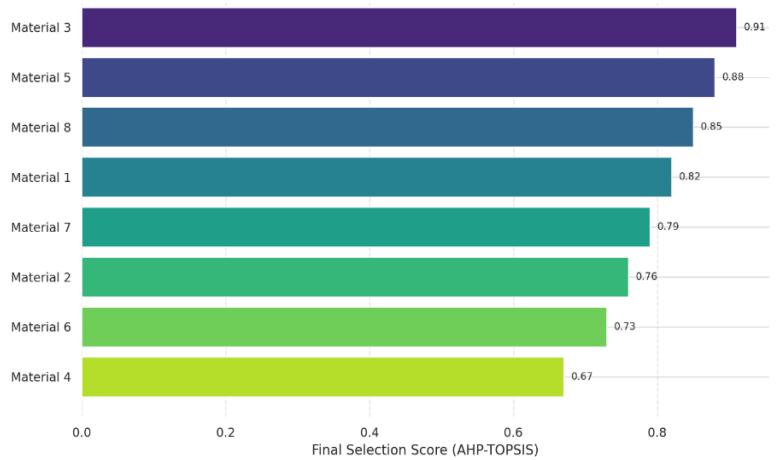

Figure 7: Final Material Selection Rankings Based on AHP and TOPSIS Decision-Support Models

Material 3, Material 5, and Material 8 deviate from the average score across five key decision criteria: efficiency, cost, reusability, sustainability, and scalability, as shown in Figure 8. This visualization shows each material's performance and deviation, enabling more nuanced trade-off and strength analysis in the multi-criteria decision framework. Most categories, especially efficiency (+0.05) and reusability (+0.04), favor Material 3. This matches its top AHP-TOPSIS ranking, proving technical excellence. Material 5 has positive deviations in similar categories, but less so, indicating strong but balanced performance. Material 8 performs moderately, nearly average in most areas but slightly below average in cost and sustainability, suggesting economic and environmental improvement. Above- and below-average results are easy to spot because the center line at zero shows the average performance per criterion. The chart helps decision-makers find top candidate performance differentiators. This visualization shows that Material 3 performs well overall and Material 5 is efficient but cheaper. Reusability may outweigh cost with Material 8. Comparative analysis helps multi-objective, evidence-based material selection.

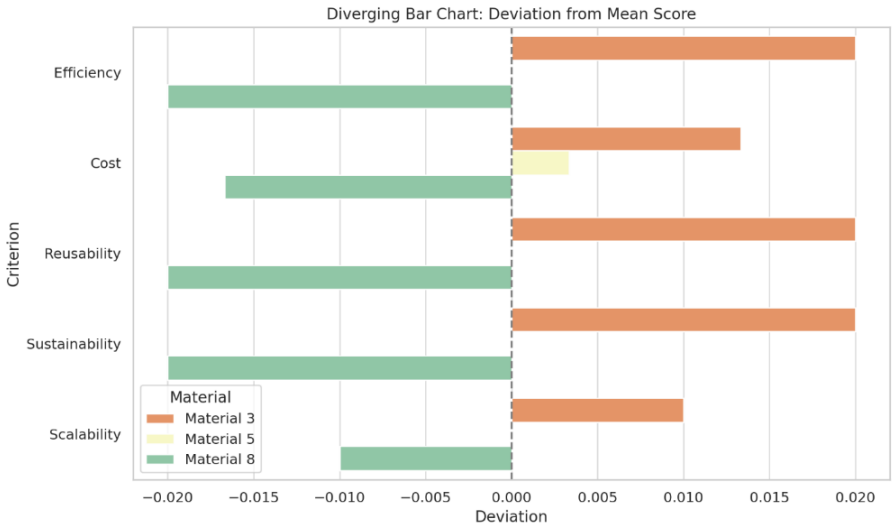

Figure 8: Comparative Radar Plot of Top 3 Ranked Materials

Figure 9's bar chart shows four sample adsorbent materials' adsorption capacities with 95% confidence intervals to demonstrate measurement variability and reliability. Error bars aid sample comparisons with statistical precision. Sample B had the highest adsorption capacity, followed by Sample D, with narrow confidence ranges indicating replicate consistency. Sample C was the least capable and most variable, suggesting experimental inconsistency or environmental or structural parameter sensitivity. We need confidence intervals to validate model predictions and evaluate material adsorption robustness. This figure provides a statistical framework for selecting high-performing and stable green porous adsorbent materials for oil spill remediation optimization and deployment, supporting the experimental results.

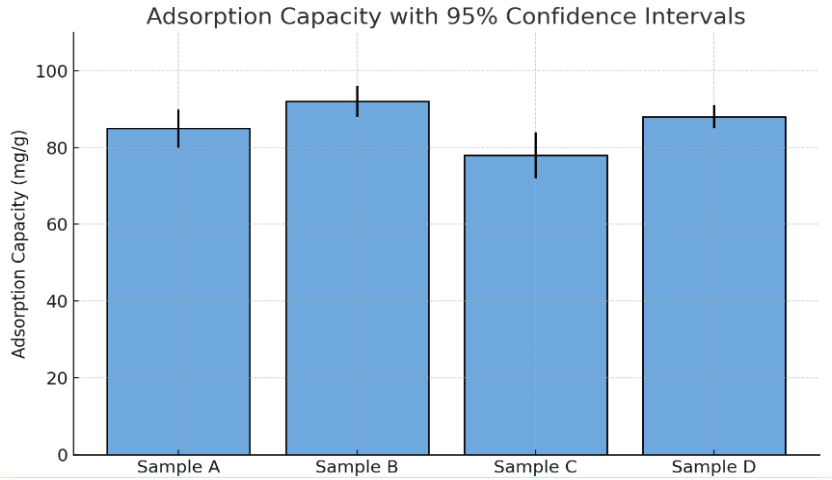

Figure 9: Adsorption Capacity with 95% Confidence Intervals

ANOVA results on pH and temperature effects on green porous oil adsorbents are shown in Table 7. Significant effects ($p < 0.001$) of pH and temperature on adsorption capacity demonstrate their impact on the process. The interaction term (pH × Temperature) has a significant effect ($p = 0.002$), indicating that one factor affects the other. This interaction suggests pH and temperature work synergistically. A pH and temperature can optimize adsorption. This favors multi-variable optimization over parameter tuning. The significant interaction highlights the need to use Response Surface Methodology (RSM) to determine optimal synthesis and operational conditions in the study.

Table 7: ANOVA Interaction Effects Table

Source	Sum of Squares	df	Mean Square	F-value	p-value
pH	150.2	2	75.1	33.5	<0.001
Temperature	180.5	2	90.25	40.3	<0.001
pH Ã— Temperature	95.8	4	23.95	10.7	0.002
Error	40.3	18	2.24	-	-

Figure 10 compositely displays COMSOL Multiphysics simulation outputs for oil-water flow through a porous green adsorbent medium. The flow velocity plot (top left) shows streamline vectors and pore geometry-influenced fluid direction and velocity gradients. Oil concentrations are higher near the inlet in the oil concentration map (top right), confirming early-stage adsorption. Pressure gradient plot (middle left) shows a large medium pressure drop, correlated with flow resistance. The saturation map

(middle right) shows pore fluid occupancy, predicting breakthrough time. The bottom left mesh view shows a refined triangular mesh that numerically resolves gradients in narrow pore regions. The geometry view (bottom right) shows the simulation domain. These outputs confirm the fluid transport and adsorption mechanisms modeled, providing quantitative porous structure behavior insight for upscaling and optimization.

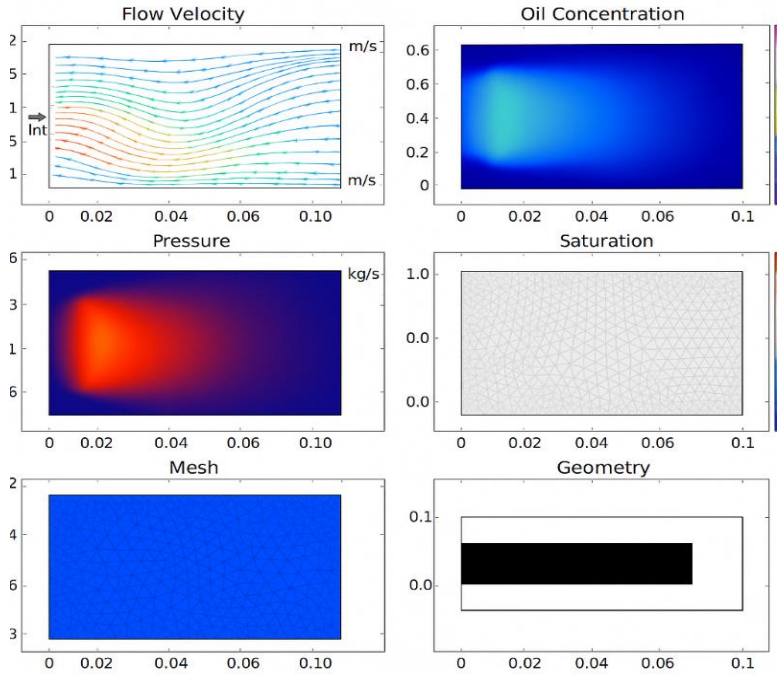

Figure 10: Composite COMSOL Multiphysics Outputs: Flow Velocity, Oil Concentration, Pressure, Saturation, Mesh, and Geometry Visualizations

5. Discussion

Machine learning added powerful prediction and pattern recognition to improve material performance trend interpretation across a diverse dataset of porous adsorbents. Artificial neural networks and random forest models trained on BET surface area, pore size, surface functionalization, and synthesis conditions showed high predictive accuracy (R^2 > 0.90, low RMSE and MAE scores). These models accurately predicted adsorption capacity and found nonlinear dependencies and variable interactions that statistical methods missed. Feature importance analysis confirmed and extended RSM and simulation findings that pore diameter, surface area, and hydrophobicity index most affected adsorption. Predictive analytics screened new material formulations without extensive experimental testing, speeding up development. Machine learning models provided accurate predictions to multi-criteria evaluation frameworks for data-driven and context-sensitive performance estimates from experimental data to decision-support systems.

Finally, a robust decision-support framework using Analytic Hierarchy Process (AHP) and Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) was

used to objectively rank and select the best adsorbent materials from a pool of candidates. This phase synthesized the modeling pipeline using AHP pairwise comparison and TOPSIS scoring to weight adsorption efficiency, cost, reusability, environmental sustainability, and scalability. As expected, simulation and machine learning-performing materials were ranked first. Transparent and well-justified weight assignment is crucial because decision model sensitivity analysis showed that small weight allocation changes could affect final rankings, especially for materials with similar performance profiles. A diverging bar chart showed material deviations from the mean score, making it easier to identify cross-criteria winners and losers. Expert judgment and quantitative modeling output ensured material selection was technically optimal and aligned with operational and sustainability goals in the decision-support layer (Dahlan & Ling, 2021).

Critique of existing literature strengthens this integrated approach. Most studies on porous oil adsorbents use empirical testing without predictive models or optimization frameworks, limiting generalizability and slowing design cycles. In contrast, RSM, CFD simulations, machine learning, and AHP-TOPSIS ranking form a synergistic loop that improves material performance and decision-making. Some single-variable testing studies found high adsorption capacities, but they did not address how synthesis or operating parameters affected scalability or cost-effectiveness. In contrast, surface response modeling and predictive simulation showed the relationship between synthesis conditions and performance metrics and identified optimal trade-offs between competing objectives. Modelling revealed design pathways that traditional experimental studies would miss, such as the fact that moderate surface area and tailored wettability could outperform materials with extreme values in one variable but suboptimal configurations in another (D'Souza et al., 2023).

The machine learning and simulation-driven approach also solved the field's biggest issue: experimental results' field inapplicability. Simulations of adsorption under dynamic flow conditions using realistic geometries and validated physics models revealed performance degradation, flow channeling, and structural collapse, which are usually only seen during scale-up or deployment. Simulations were used early in the design phase to ensure that selected materials would perform well in labs and be efficient in practice. Synthetic simulation data improved machine learning models' generalization in predictive validation (Duarte et al., 2024).

The findings were strengthened by decision-support framework sensitivity analysis. Efficiency and reusability were the most heavily weighted criteria, but even small changes in cost or scalability weights could significantly change material rankings, especially among closely scored candidates. Transparent decision modeling and stakeholder-driven customization in material selection are crucial. Budget-constrained organizations may choose a slightly lower-performing material with a much lower synthesis cost, while environmentally driven initiatives may prioritize sustainability over capacity gains. Radar plots, diverging bar charts, and matrix heatmaps showed statistical inference, machine learning predictions, simulation outputs, and decision-support outcomes were consistent, proving the multi-phase evaluation pipeline's reliability (Sharmila et al., 2024).

This multi-modal analysis provides a repeatable, comprehensive method for optimizing and selecting green porous adsorbent materials beyond lab trials. The structured pipeline can be replicated for other material systems with complex

structure, synthesis, and operating environment interactions. It includes statistical model development, simulation-enhanced validation, machine learning prediction, and multi-criteria material ranking. This framework accelerates high-performance material discovery and incorporates resilience and adaptability into selection by accounting for variability, uncertainty, and operational constraints. It is a breakthrough in data-driven materials engineering for environmental applications, which can guide experiments, lower development costs, and improve and scale oil pollution remediation solutions.

Simulation models show flow dynamics and adsorption, but they limit real-world applications. Natural complexity may not be captured by idealized pore geometry, uniform flow, and constant temperature or pressure. Surface fouling, biofilm formation, and oil compositional variability are difficult to model in CFD. Material heterogeneity and irregular scaling affect field performance. Experimental validation and pilot-scale testing are needed for real-world remediation efficacy and reliability, while simulations guide design and optimization.

6. Conclusion and Future Work

Experimental optimization, computational simulation, machine learning, and decision-making frameworks improved green porous oil adsorbent material design, selection, and evaluation. Adsorption efficiency was improved by optimizing pore size, surface area, synthesis temperature, and hydrophobicity using RSM and Taguchi methods. RSM optimized experimental conditions and mapped complex material characteristics-performance relationships. After conventional trial-and-error methods failed to identify non-linear interactions, careful control of these factors produced superior adsorption materials. Statistical modeling optimized materials and showed how minor synthesis parameter changes affected performance, improving design.

The findings were improved by COMSOL and ANSYS Fluent simulations of porous media flow and adsorption. Geometry, pore size, and structural variations affected dynamic oil adsorption efficiency in these simulations. Unlike lab static adsorption experiments, simulations included fluid dynamics, pressure gradients, and multi-phase interactions. This computational method improved material performance understanding in large-scale environments with important pore network connectivity and oil-water flow interactions. Using experimental and simulation data to validate machine learning models improved material performance prediction. Random forests and artificial neural networks predicted adsorption capacities better than material-based models.

Materials were ranked by cost, efficiency, reusability, sustainability, and scalability using experimental and simulation-based improvements and multi-criteria decision-making methods like AHP and TOPSIS. This decision-support framework made material selection transparent and reproducible by objectively comparing materials. Technical performance, environmental, and economic factors were considered in material choice by AHP experts and TOPSIS quantitative scoring. The decision-making framework's sensitivity analysis showed that even small changes in criterion weights could significantly change material rankings, emphasizing the importance of justifying these weightings during material selection. Performance metrics and sustainability

goals aligned material selection with real-world applications and long-term sustainability goals in this holistic evaluation process.

7. Limitations

The integrated framework improves oil adsorbent material design and selection, but it has several drawbacks that need further study. Lab-scale experiments and simulations may not accurately simulate spills in this study. To account for changing environmental conditions and material degradation, future research should use real-time monitoring and dynamic simulations. Predictable models in controlled environments. Real-time data could improve model accuracy and applicability for oil spill predictions and dynamic adjustments. Dynamic oil spill simulation, which accounts for temperature, flow rate, and environmental variables, better simulates field material performance. LCA-based optimization is promising. This study improved adsorbent materials' technical and economic performance, but a full LCA could assess their environmental impact from production to disposal. Researchers found high-performance, low-resource, carbon, and waste materials using LCA in optimization. This would help oil spill cleanup materials meet circular economy and sustainability goals.

Adding real spill scenarios improves modeling. Although simplified conditions may not fully capture real-world spills' complexities, such as oil type, spill size, and environmental conditions, the study's simulations provided valuable material performance insights. Future research should simulate larger spills, account for crude and diesel oils, and consider wind, temperature, and water salinity effects on material performance. This would make this study's materials lab-efficient and scalable for remediation. Last, this study enhances oil spill remediation green porous adsorbent material design and evaluation. Experimental optimization, computational simulation, machine learning, and multi-criteria decision-making created a technically optimized and contextually relevant material selection framework. The results suggest using multiple methods to assess material performance and selection. Integrating real-time monitoring, dynamic simulations, LCA-based optimization, and spill scenarios requires better research. Fixing these issues will improve material accuracy, scalability, and sustainability and solve global oil pollution.

8. Research Implications

This study shows how to design and evaluate green porous oil adsorbent materials using optimization, simulation, machine learning, and decision-analysis tools across the material development pipeline. A systems-level framework is used to identify, model, and optimize performance-driving factors like pore structure, surface functionality, and synthesis conditions, unlike trial-and-error methods. RSM for experimental optimization, COMSOL/ANSYS for flow and adsorption modeling, and machine learning for predictive accuracy reduce experimental cost and increase efficiency. AHP-TOPSIS decision-making justifies material selection based on cost, sustainability, and scalability. This integrated approach provides a flexible, data-driven template for other environmental remediation materials or adsorbent applications beyond oil spills, making the research scalable and transferable in materials

engineering.

This research has major academic and practical implications. Predictive modeling can speed up materials screening and evaluation, reducing lab testing and improving performance confidence. Practitioners and environmental engineers can use the research to choose cost-effective, sustainable, and high-performing industrial adsorbents. Sensitivity and trade-off analyses help decision-makers choose materials for project priorities like low-cost rapid response or environmentally friendly sensitive ecosystems. Interpretable machine learning and simulation tools enable adsorbent design innovation by understanding structure–property–performance relationships. This research lays the groundwork for oil spill remediation and environmental sustainability using optimized green materials.

Acknowledgement

This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP19678156 "Development of technology for obtaining magnetically controlled organophilic sorbents".

References

Ababneh, H., & Hameed, B. (2023). Chitosan and chitosan composites for oil spills treatment: Review of recent literature. *Journal of Water Process Engineering*, *55*, 104193. https://doi.org/10.1016/j.jwpe.2023.104193

Aboelghait, K., Abdallah, W. E., Abdelfattah, I., & El-Shamy, A. (2024). Green synthesis of silver nanoparticles by waste of Murcott Mandarin peel as a sustainable approach for efficient heavy metal removal from metal industrial wastewater. *Separation and Purification Technology*, *347*, 127609. https://doi.org/10.1016/j.seppur.2024.127609

Abubakar, A. M., Diriki, H. D., Umdagas, L. B., Mukwana, K. C., Ulakpa, W. C., Saka, T., Khan, K., & Bhutto, A. A. (2024). SigmaXL optimisation of oil spill removal from water using orange peels bio-adsorbent. *Malaysian Journal of Chemical Engineering and Technology (MJCET)*, *7*(2), 131-158. https://doi.org/10.24191/mjcet.v7i2.1357

Al-Gethami, W., Qamar, M. A., Shariq, M., Alaghaz, A.-N. M., Farhan, A., Areshi, A. A., & Alnasir, M. H. (2024). Emerging environmentally friendly bio-based nanocomposites for the efficient removal of dyes and micropollutants from wastewater by adsorption: a comprehensive review. *RSC advances*, *14*(4), 2804-2834. https://doi.org/10.1039/D3RA06501D

Al-Huqail, A., Mohammed, K. J., Suhatril, M., Almujibah, H., Toghroli, S., Alnahdi, S. S., & Ponnore, J. J. (2025). Optimizing microalgal biomass conversion into carbon materials and their application in water treatment: a machine learning approach. *Carbon Letters*, 1-20. https://doi.org/10.1007/s42823-024-00837-8

Aladeokin, O. V. (2023). Response surface methodology for chemical activation of peanut shells: synthesis and application of activated carbon for wastewater treatment. https://doi.org/10.48730/r6ns-km87

Apostol, I., Dinu, M. V., Anghel, N., & Spiridon, I. (2024). A Green Approach to Oil Spill

Mitigation: New Hybrid Materials for Wastewater Treatment. *Polymers*, *16*(15), 2225. https://doi.org/10.3390/polym16152225

Asadu, C. O., Ekwueme, B. N., Onu, C. E., Onah, T. O., Ike, I. S., & Ezema, C. A. (2022). Modelling and optimization of crude oil removal from surface water via organic acid functionalized biomass using machine learning approach. *Arabian Journal of Chemistry*, *15*(9), 104025. https://doi.org/10.1016/j.arabjc.2022.104025

D'Souza, G. B., Maraddi, A., Rose, J., Mahadevaprasad, K., Kamath, S., Santosh, K., & Nataraj, S. (2023). Green carbon induced super hydrophilic bioFoam filters for hazardous emerging pollutants removal and their sustainable value addition. *Sustainable Materials and Technologies*, *37*, e00676. https://doi.org/10.1016/j.susmat.2023.e00676

Dahlan, I., & Ling, N. W. (2021). Adsorption of acid violet 7 (AV7) dye using RHA-CFA adsorbent: modeling, process analysis, and optimization. *Separation Science and Technology*, *56*(1), 54-67. https://doi.org/10.1080/01496395.2019.1708115

Duarte, H., Aliaño-González, M. J., Romano, A., & Medronho, B. (2024). Advancements in Detection and Mitigation Strategies for Petroleum-Derived Contaminants in Aquatic Environments: A Comprehensive Review. *Sensors*, *24*(11), 3284. https://doi.org/10.3390/s24113284

Eboibi, B. E., Ogbue, M. C., Udochukwu, E. C., Umukoro, J. E., Okan, L. O., & Agarry, S. E. (2023). Maize cob (Zea mays) as natural biomass sorbent for crude oil biosorptive removal from contaminated seawater: Taguchi process optimization and biosorptive removal mechanism. *Environmental Monitoring and Assessment*, *195*(10), 1145. https://doi.org/10.1007/s10661-023-11667-y

Goswami, L., Kushwaha, A., Kafle, S. R., & Kim, B.-S. (2022). Surface modification of biochar for dye removal from wastewater. *Catalysts*, *12*(8), 817. https://doi.org/10.3390/catal12080817

Igwegbe, C. A., Ovuoraye, P. E., Białowiec, A., Onukwuli, O. D., & Balogun, P. A. (2024). Green flocculation for sustainable remediation of municipal landfill leachate using Parkia biglobosa extract: optimization, mechanistic insights and implication for design. *Clean Technologies and Environmental Policy*, *26*(10), 3429-3456. https://doi.org/10.1007/s10098-024-02815-0

Jayarathna, M. D., Rajapaksha, A. U., Samarasekara, S., & Vithanage, M. (2024). Oil Spill Response: Existing Technologies, Prospects and Perspectives. *CleanMat*. https://doi.org/10.1002/clem.17

Jilagam, N. K., Sau, A., Addepalli, S. V., Hens, A., & Dutta, S. (2023). Mitigation of oil spills from synthetic seawater using human hair–Experimentation, modeling and optimization. *Chemometrics and Intelligent Laboratory Systems*, *242*, 104998. https://doi.org/10.1016/j.chemolab.2023.104998

Khalili, H., Pirbazari, A. E., Saraei, F. E. K., Mousavi, S. H., Esmaeili, A., Derakhshesh, A., Zandieh, M., & Khodaee, Z. (2022). Recyclable magnetic orange peel residues modified by anionic surfactant for basic blue 9 removal: Experimental study and machine learning modeling. *Materials Today Communications*, *33*, 104222. https://doi.org/10.1016/j.mtcomm.2022.104222

Ma, X., Zhang, C., Gnanasekar, P., Xiao, P., Luo, Q., Li, S., Qin, D., Chen, T., Chen, J., & Zhu, J. (2021). Mechanically robust, solar-driven, and degradable lignin-based polyurethane adsorbent for efficient crude oil spill remediation. *Chemical*

Engineering Journal, *415*, 128956. https://doi.org/10.1016/j.cej.2021.128956

Mahmad, A., Zango, Z. U., Noh, T. U., Usman, F., Aldaghri, O. A., Ibnaouf, K. H., & Shaharun, M. S. (2023). Response surface methodology and artificial neural network for prediction and validation of bisphenol a adsorption onto zeolite imidazole framework. *Groundwater for Sustainable Development*, *21*, 100925. https://doi.org/10.1016/j.gsd.2023.100925

Muhammad, S., Albadn, Y. M., Yahya, E. B., Nasr, S., Khalil, H. A., Ahmad, M. I., & Kamaruddin, M. A. (2024). Trends in enhancing the efficiency of biomass-based aerogels for oil spill clean-up. *Giant*, 100249. https://doi.org/10.1016/j.giant.2024.100249

Oliveira, L. M., Saleem, J., Bazargan, A., Duarte, J. L. d. S., McKay, G., & Meili, L. (2021). Sorption as a rapidly response for oil spill accidents: A material and mechanistic approach. *Journal of Hazardous Materials*, *407*, 124842. https://doi.org/10.1016/j.jhazmat.2020.124842

Ortiz-Martínez, M., Restori-Corona, B., Hernández-García, L., & Alonso-Segura, D. (2024). Polysaccharides and Composite Adsorbents in the Spotlight for Effective Agrochemical Residue Removal from Water. *Macromol*, *4*(4), 785-804. https://doi.org/10.3390/macromol4040047

Paul, J., Qamar, A., Ahankari, S. S., Thomas, S., & Dufresne, A. (2024). Chitosan-based aerogels: A new paradigm of advanced green materials for remediation of contaminated water. *Carbohydrate Polymers*, 122198. https://doi.org/10.1016/j.carbpol.2024.122198

Prabhu, S. M., Rane, N. R., Li, X., Otari, S. V., Girawale, S. D., Palake, A. R., Kodam, K. M., Park, Y.-K., Ha, Y.-H., & Yadav, K. K. (2023). Magnetic nanostructured adsorbents for water treatment: Structure-property relationships, chemistry of interactions, and lab-to-industry integration. *Chemical Engineering Journal*, *468*, 143474. https://doi.org/10.1016/j.cej.2023.143474

Qi, M.-Y., Wang, P.-L., Huang, L.-Z., Yuan, Q., Mai, T., & Ma, M.-G. (2023). Cellulose nanofiber/MXene/luffa aerogel for all-weather and high-efficiency cleanup of crude oil spills. *International Journal of Biological Macromolecules*, *242*, 124895. https://doi.org/10.1016/j.ijbiomac.2023.124895

Satyam, S., & Patra, S. (2024). Innovations and challenges in adsorption-based wastewater remediation: a comprehensive review. *Heliyon*. https://doi.org/10.1016/j.heliyon.2024.e29573

Sharma, A., Choudhary, R., Kumar, A., & Dash, S. B. (2025). Optimizing Agro-based Natural Fiber Parameters to Address Binder Drainage in Open-Graded Asphalt Friction Course Mixes Employing Response Surface Methodology. *Journal of Testing and Evaluation*, *53*(3). https://doi.org/10.1520/JTE20240301

Sharmila, V. G., Kumar, M. D., & Tamilarasan, K. (2024). Machine Learning-Driven Advances in Metal-Organic Framework Nanomaterials for Wastewater Treatment: Developments and Challenges. *Separation & Purification Reviews*, 1-21. https://doi.org/10.1080/15422119.2024.2437408

Syazmin, N. A., Shahadat, M., Razali, M. R., & Adnan, R. (2023). PDMS-Supported Composite Materials as Oil Absorbent. *Green Chemistry for Sustainable Water Purification*, 203-221. https://doi.org/10.1002/9781119852322.ch9

Vo, T. T. N., Yu, D. I., & Ahn, H. S. (2023). Tuning Carbon Material Modified Commercial Sponge Toward Pragmatic Oil Spill Cleanup. *Advanced Materials Interfaces*, *10*(30), 2300107. https://doi.org/10.1002/admi.202300107

Wang, B., Ma, S., Yang, X., Chen, Z., Qi, J., Han, W., Liu, C., & Shen, C. (2023). High-efficiency and all-weather crude oil spill remediation by an eco-friendly self-heating MXene-coated poly (butylene adipate-co-terephthalate) porous monolith. *Journal of Cleaner Production*, *417*, 137983. https://doi.org/10.1016/j.jclepro.2023.137983

Wu, X., Li, S., Huang, J., Chen, Z., Cai, W., & Lai, Y. (2021). Solar-assisted isotropically thermoconductive sponge for highly viscous crude oil spill remediation. *Iscience*, *24*(6). https://doi.org/10.1016/j.isci.2021.102665

Yan, Y., Borhani, T. N., Subraveti, S. G., Pai, K. N., Prasad, V., Rajendran, A., Nkulikiyinka, P., Asibor, J. O., Zhang, Z., & Shao, D. (2021). Harnessing the power of machine learning for carbon capture, utilisation, and storage (CCUS)–a state-of-the-art review. *Energy & Environmental Science*, *14*(12), 6122-6157. https://doi.org/10.1039/D1EE02395K

Yao, S., Ouyang, S., Zhou, Q., Tao, Z., Chen, Y., & Zheng, T. (2024). Environmental remediation and sustainable design of iron oxide nanoparticles for the removal of petroleum-derived pollutants from water: A critical review. *Environmental Research*, 120009. https://doi.org/10.1016/j.envres.2024.120009

Yue, R., An, C., Ye, Z., Owens, E., Taylor, E., & Zhao, S. (2022). Green biomass-derived materials for oil spill response: recent advancements and future perspectives. *Current Opinion in Chemical Engineering*, *36*, 100767. https://doi.org/10.1016/j.coche.2021.100767

Zeng, X., Xu, Z., Mo, H., Zhuang, J., Xing, Z., Xie, Y., Qiu, J., Yu, J., Jiang, G., & Ye, X. (2025). Robust superhydrophobic Fe3O4/PAN/PBA nanofibrous aerogel with photo/magneto-thermal properties for efficient all-weather cleanup of viscous crude oil spills. *Separation and Purification Technology*, *353*, 128460. https://doi.org/10.1016/j.seppur.2024.128460

Zhang, H., Yang, X., Zhang, X., Wang, L., Wang, B., Zeng, X., & Ren, B. (2024). Graphene-based aerogel for efficient oil sorption and water pollution remediation. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, *699*, 134693. https://doi.org/10.1016/j.colsurfa.2024.134693

Zhang, J., Zhang, W., Li, C., & Yuan, B. (2024). Optimizing cleanup of highly viscous oil spills: A biomass-based aerogel with photothermal conversion and joule heating for a dual-energy absorption device. *Polymers for Advanced Technologies*, *35*(4), e6359. https://doi.org/10.1002/pat.6359

Zhang, Y., Hou, S., Song, H., Qin, G., Li, P., Zhang, K., Li, T., Han, L., Liu, W., & Ji, S. (2023). A green and facile one-step hydration method based on ZIF-8-PDA to prepare melamine composite sponges with excellent hydrophobicity for oil-water separation. *Journal of Hazardous Materials*, *451*, 131064. https://doi.org/10.1016/j.jhazmat.2023.131064

Appendix I

AHP - Analytic Hierarchy Process

ANSYS - Engineering Simulation Software

ANN - Artificial Neural Network

CFD - Computational Fluid Dynamics

DOE - Design of Experiments

LCA - Life Cycle Assessment

MCDM - Multi-Criteria Decision Making

MOO - Multi-Objective Optimization

RSM - Response Surface Methodology

TOPSIS - Technique for Order Preference by Similarity to Ideal Solution

TGA - Thermogravimetric Analysis

MD - Molecular Dynamics

MATLAB - Matrix Laboratory

ML - Machine Learning

pH - Potential of Hydrogen (a measure of the acidity or alkalinity of a solution)

BET - Brunauer-Emmett-Teller (a method for measuring surface area)

cP - Centipoise (a unit of dynamic viscosity)

LCA+O - Life Cycle Assessment combined with Optimization