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Synergistic Integration Of Machine Learning And Advanced Nanomaterials For The Water-Energy Nexus: A Critical Review

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ABSTRACT

The convergence of advanced nanomaterials and artificial intelligence (AI) holds the promise of revolutionizing efforts to tackle water scarcity and energy crises across the globe. Conventional methods of wastewater treatment and renewable energy production have come a long way, but they are hindered by trial-and-error methods, scalability challenges, and complicated optimization needs. This review article critically summarizes the recent developments of MXenes, metal-organic frameworks (MOFs), photocatalytic heterojunctions, polymer composites and their incorporation with machine learning (ML) paradigms. A key research need: the need for unified, data-driven frameworks that can effortlessly connect nanomaterials design to macro process optimization. The novelty of this work is a comprehensive examination of the potential for using predictive algorithms (such as Artificial Neural Networks, XGBoost, Support Vector Regression), in conjunction with experimental materials science, to enable the deployment of decentralized desalination, synergistic pathogen/dye degradation and hybrid renewable energy systems.

Introduction

As water demands continue to rise and serving a sustainable energy supply becomes critical, highly efficient, scalable, and intelligent technological solutions need to be developed. Recently, synthetic approaches for 2D materials with extraordinary properties for advanced desalination and membrane engineering, such as MXenes, have experienced tremendous growth[1]. At the same time, complex effluent such as pathogens and synthetic dyes must be degraded with synergistic effects, which are typically achieved with more complicated heterojunction photocatalysts[2, 3].

Research Gap

Although a number of new catalysts have been developed in recent years, including MOF hybrids[4] and zinc ferrite nano-photocatalysts [5, 6] and nickel impregnated ZnO [7], most of the studies use conventional experimental optimization. However, despite the promising results from the laboratory, there is a considerable research gap in scaling up these new breakthroughs to an industrial scale, where operational parameters are unpredictable, thermodynamic efficiencies are poor, and the scaleup involves a complicated modeling. Moreover, the identification and removal of hazardous substances such as cypermethrin[8] and polycyclic aromatic hydrocarbons (PAHs) [9] are not always linked with real-time predictive analytics.

Novelty of the Review

Synergistic framework, which is an integration of advanced material synthesis and AI and machine learning, is proposed to bridge this gap. This article is unique in its approach of a systematic sequential analysis, moving from fundamental atomistic material design, to composite engineering, to the application of AI-based optimization algorithms for complete water and energy systems. Schematic representation of the synergistic integration of advanced nanomaterials (MXenes, MOFs, Perovskites) with

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Artificial Intelligence (ANN, XGBoost) for optimizing the water-energy nexus is shown in Figure.1.

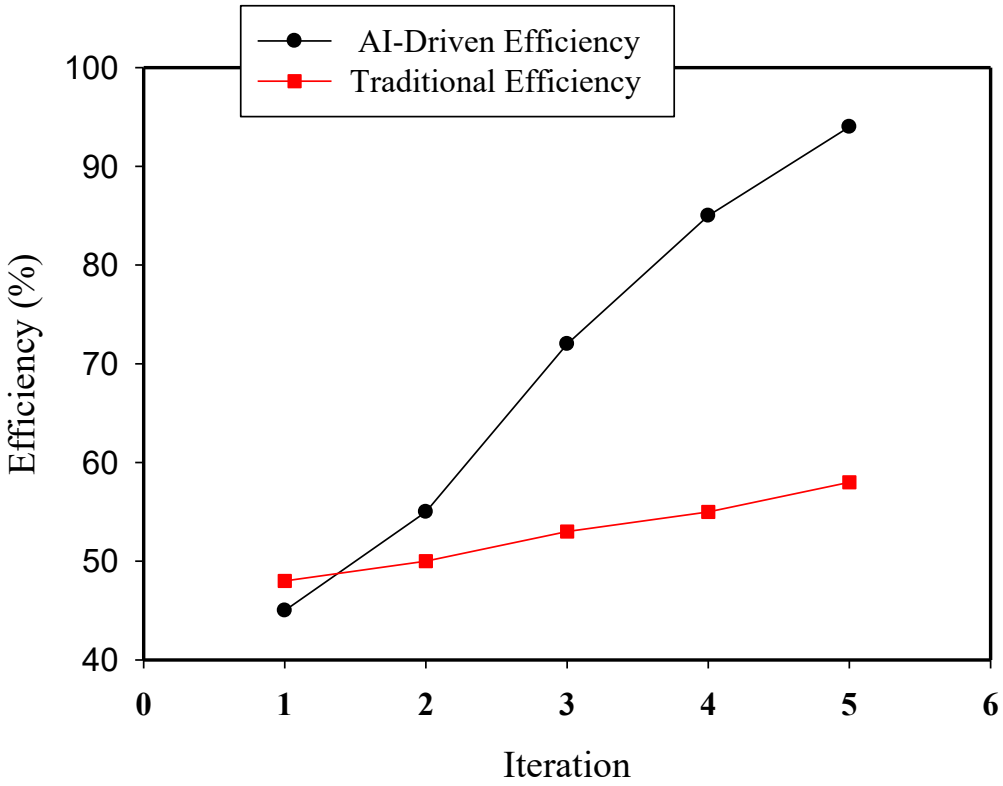

Figure.1:Schematic representation of the synergistic integration of advanced nanomaterials (MXenes, MOFs, Perovskites) with Artificial Intelligence (ANN, XGBoost) for optimizing the water-energy nexus [10, 11].

Advanced Nanomaterials for Environmental Remediation

Photocatalysis and Adsorption

The recovery of valuable materials, including copper from scrap cables [12]] and the encapsulation of silver nanoparticles for Cr(III) sensing [13] are just some of the possibilities of green chemistry. There are a few materials that demonstrate very strong performance in structural and biological applications: Deep eutectic solvents [14] Substituted ceramics [15] and functionalized nanoparticles such as CuO and chlorhexidine encapsulated in polymers [16, 17]. The low-cost units showed good industrial application in wastewater reclamation, and catalytic oxidation for the removal of thiosulfate and sulfidic compounds showed good industrial application in wastewater reclamation [18-24]. A comparison between advanced photocatalysts and adsorbents is shown in table 1.

Table 1: Comparative Analysis of Advanced Photocatalysts and Adsorbents

Material / Catalyst	Target Contaminant	Mechanism	References
Zinc Ferrite / Ni-ZnO	Fast Yellow AB, Methylene Blue	Visible-light photocatalysis /	[5-7]

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		Sonocatalysis	
s-Triazine & Lignin g-C3N4	Cypermethrin sensing	Electrochemical sensing	[8, 25]
Saudi Arabian Clay / Seed Hulls	Lead, Metal ions	Adsorption	[26, 27]
Fe-B Composite / Metal Oxides	Polystyrene pyrolysis, Dye degradation	Catalytic degradation / Oxidation	[28, 29]

Functional Composites and Thermodynamic Optimization

Thermodynamic modelling is necessary to move the materials from simple adsorbents to complex organic glasses (e.g., Bi(OH)CrO4/AgBr/PMMA) for smart photonic applications [30]] and lignin derived heterogeneous catalysis for oxidative desulfurization [31]. Today, the prediction of exergy efficiency with machine learning is crucial in the context of uncertainty [32]. The addition of the iron to syndiotactic polypropylene greatly modifies the thermodynamic, rheological, and quiescent crystallization properties [33-39] making it a crucial component for the production of advanced composites. Moreover, the investigation of complex materials such as $CuxTa_2$-xO_5 [40], organotin(IV) derivatives [41] and Tl-based perovskites [42] opens up new aspects of optoelectronic properties. Figure 2 mimics Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) evaluations of tailored heterojunctions and metal-organic frameworks utilized in synergistic wastewater degradation.

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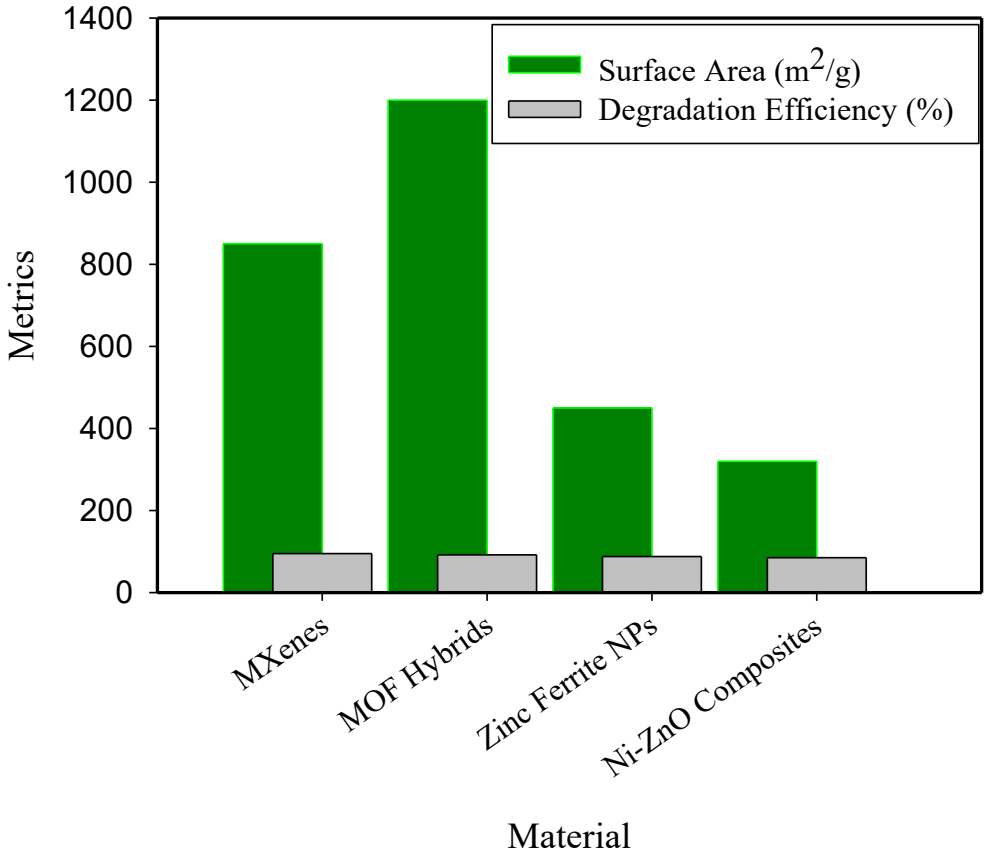

Figure.2: Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) evaluations of tailored heterojunctions and metal-organic frameworks utilized in synergistic wastewater degradation [43-45].

Innovations in Energy Systems and Sustainable Fuels

Bioenergy and Fuel Synthesis

In parallel with energy developments, there are also biomedical applications of nanoparticles, which are used in dental sealants including TiO_2 and Cu-TiO_2 [35, 38, 46-49]. Moreover, catalytic pyrolysis of waste plastics and oils to selective liquid fuels is a promising direction for developing circular economies [49-54]. In recent years, the intelligent model-following control is widely applied in the nuclear-PV-biogas microgrid and EV charging systems, and advanced optimization methods like grey wolf optimization [55] and twin fang algorithms [56] have been used for controlling these systems. Details of algorithmic optimization in hybrid energy systems is shown in table 2.

Table 2: Algorithmic Optimization in Hybrid Energy Systems

Algorithm / Control Strategy	System Application	Primary Outcome	References
Grey Wolf	Irrigation / ANN	Enhanced	[55]

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Optimization	networks	prediction accuracy	
PQ Droop Controller	Nuclear-PV-Biogas microgrids	Grid stability & EV charging	[20, 57]
Dual Predator Optimization	Hybrid power systems	Superior energy management	[58, 59]

Solar Energy and Optoelectronics

The macro-energy picture is set by coal gasification [60], lithium-sulfur battery electrolytes [61] and techno-economic analysis of algae-based bioenergy [62] assessments. At the same time, new strategies for increasing the solar harvesting at the nanoscale are being developed by grid-connected PV systems [62] and by dynamic plasmonic controls in nanostructures [63-65]. The study of all-perovskite multi-junction solar cells [66, 67] and the production of biodiesel using algal species[68] is still relevant, as is fuzzy decision making in investment strategies[69]. : Pie diagram of a decentralized hybrid power system integrating PV, biogas, and EV charging, managed by an AI-driven predictive controller is shown in Figure 3.

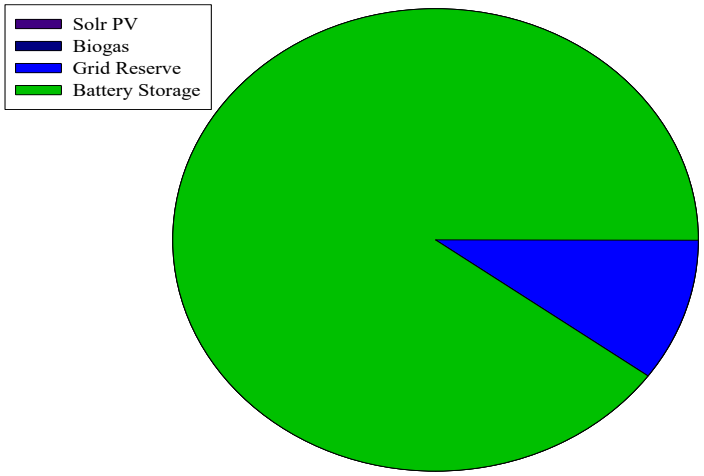

Figure 3: Pie diagram of a decentralized hybrid power system integrating PV, biogas, and EV charging, managed by an AI-driven predictive controller [70, 71].

Fluid Dynamics, Separation Processes, and Membranes

Fluid Flow and Heat Transfer

Optimisation of thermal systems is based on Advanced mathematical modeling, including entropy-optimized radiative Maxwell fluids with magnetohydrodynamics [72] and three-dimensional unsteady viscous fluid flow across rotating discs [73]. Concentric tube heat exchangers and exact solutions of field equations [74] are crucial for reactor design.

Table 3: Advancements in Membrane and Separation Technologies

Membrane	Process Application	Separation	References

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Material		Mechanism	
Emulsion Liquid Membranes	Chromium/Cadmium/Lead extraction	Chemical carrier transport	[19, 30, 75, 76]
Silica-Polymer Nanocomposites	Gas separation (CO2/CH4)	Permeability & Selectivity	[12, 77]
PES/PI Blends & Ceramic	CO2 separation from flue gases	Solution-diffusion	[58, 78-80]

Material Kinetics and Defect Engineering

The need for atomic level control can be seen in the molecular dynamics simulation of GSTP1 variations [81] and engineering of optical whispering gallery modes [77]] as well as holographic anti-counterfeiting gratings [69] and tunable CdZnS nanoparticles [82]. These kinetic understandings are crucial for the removal of heavy metals such as via Saudi Arabian clay [83] and via starch composite rheology [84] and catalytic oxidation of thiosulfate [85] and for the rational design of the MOFs for oxygen evolution reactions [86] and lignin-derived catalysts [67]. : Computational Fluid Dynamics (CFD) velocity and temperature contours illustrating the effect of inserts on the overall heat transfer coefficient in concentric tube systems is shown graphically in Figure 4.

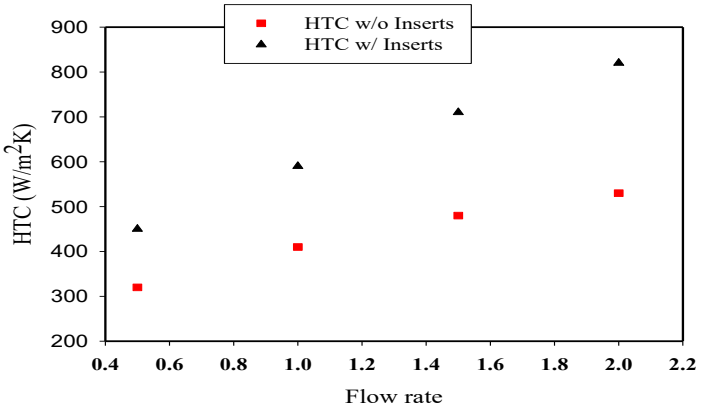

Figure.4: Computational Fluid Dynamics (CFD) velocity and temperature contours illustrating the effect of inserts on the overall heat transfer coefficient in concentric tube systems[87-89].

Machine Learning in Chemical and Environmental Engineering

AI-Assisted Process Modeling

Dynamic light scattering, coupled with the use of AI predictions for photocatalytic degradation [90]and sulfide removal [51], is undergoing a paradigm change. The switch from theoretical thermodynamic analysis of the natural gas separations [53, 54] to modern predictive models can be seen in the studies of emerging adsorbents for cadmium [91] and myco-remediation [92]. Advanced synthesis techniques like 3D multilayer folding [93], MOF based supercapacitors [26] and Modified Amberlyst-15 [41] are now optimized using Machine Learning.

Table 4: Predictive Analytics in Chemical Engineering

AI/ML Model	Engineering	Performance	References

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	Application	Metric	
Aspen Plus + ML	Propane-propylene separation	Separation efficiency	[94]
Grey-Box Modeling	Crude distillation / Heat exchangers	Cut point temperature optimization	[95, 96]
XGBoost & SVR	Thiosulfate removal from wastewater	Predictive accuracy (R2)	[97]
Artificial Neural Networks	Heat exchanger fouling / CO_2 to Methanol	Maintenance prediction / Yield	[98, 99]

Emulsions, Optimization, and Safety

The exergo-environmental analysis of amines for carbon capture [4], combined with tailored oxygen carriers for chemical looping [100], showcases deep thermodynamic integration. Important aspects here are the predictive modeling of emulsion stability[101] and the development of new adsorbents [102, 103] and new models for the drag of particles [104]. Innovations apply to the green synthesis [105], intelligent model-following controllers [106], smart adsorbent frameworks [107] and dynamic plasmonics [108]. Extended parameter reduction is heavily relied upon in prediction of critical heat flux in nuclear safety [25, 109, 110]. A standard pipeline for deploying XGBoost and Support Vector Regression models in predicting complex multiphase reaction kinetics and pollutant removal efficiencies is shown graphically in Figure 5.

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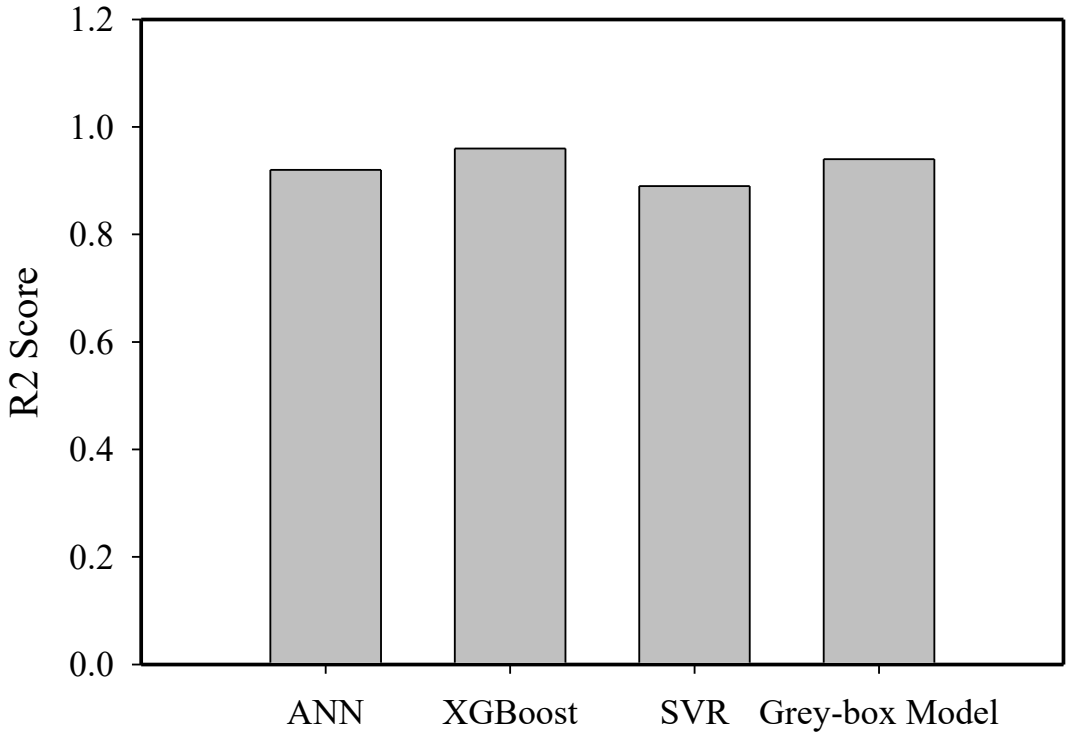

Figure 5: A standard pipeline for deploying XGBoost and Support Vector Regression models in predicting complex multiphase reaction kinetics and pollutant removal efficiencies[111, 112].

Future Perspectives and Decarbonization

The synthesis of sustainable concrete using biochar [113] and recovery of copper [114] highlight a circular economy. The automated engineering is enabled by advanced mathematical modelling of viscous fluids [115], fly ash-lime compact curing [116] and dual predator optimization in power grid [3, 62, 117]. The cutting edge of decarbonisation is model-based quality and exergy analysis of membrane reactors [118] and electrofuels for hard-to-abate sectors [119].

Alongside with the thermodynamic analyses of industrial plants [120], direct air carbon capture (DACC) [121] and advanced oxidation processes [122] are continuing to develop. Examples of this research include molecularly imprinted polymers (MIPs) [123, 124], synergistic syngas generation [125] and algal bioenergy[125]. In studying the interaction of electrolytes [66] and surrogate modeling of cement manufacturing emissions [126, 127] it is evident that AI is the connecting thread. This trend is supported by studies of the thermal conductivity of thermoelectric materials [128], multi-product yield prediction in biomass pyrolysis [129], reusable biosensors [97] and comprehensive health risk assessment in soil-rice system [75, 118, 130, 131]. Last, through the use of data-driven safety models in nuclear reactors [132], Williamson nanofluid flow optimization [124] and wide energy modeling for global

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decarbonization [132] the way was paved for the decade to come. Future roadmap highlighting the integration of Direct Air Carbon Capture (DACC), AI-optimized biomass pyrolysis, and electrofuel generation for achieving net-zero emissions is shown graphically in Figure 6.

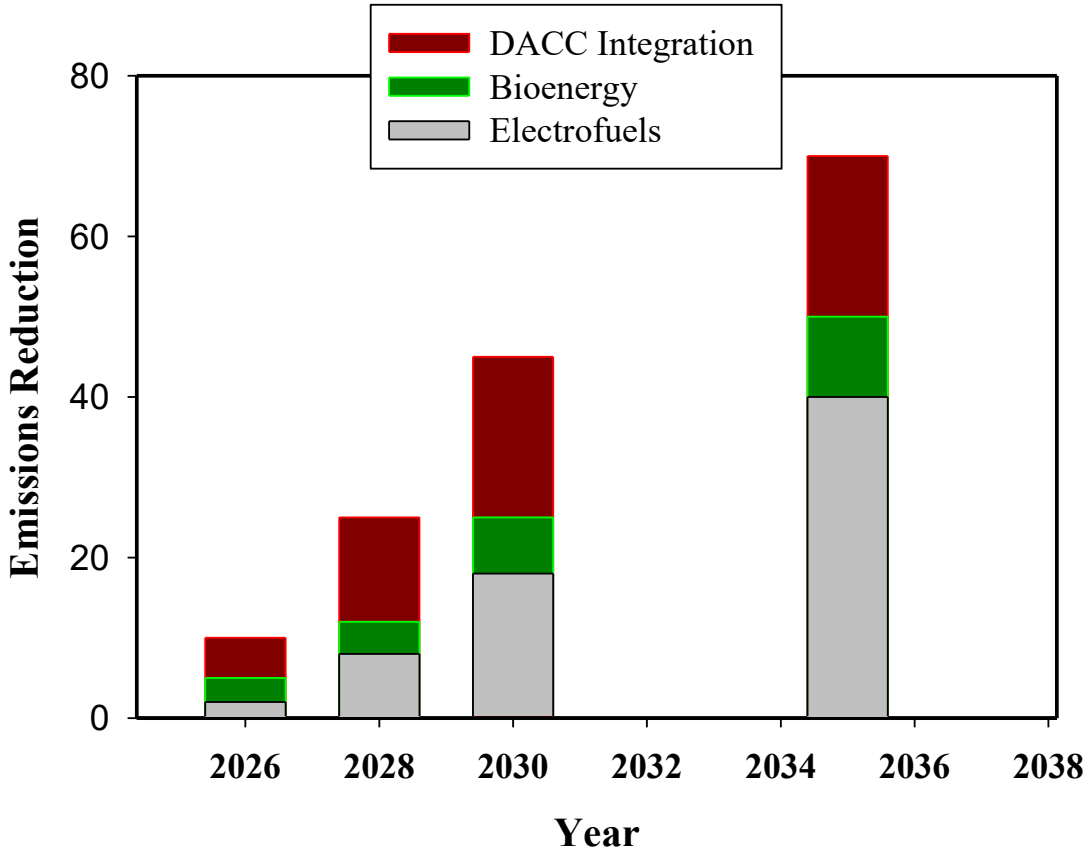

Figure.6: Future roadmap highlighting the integration of Direct Air Carbon Capture (DACC), AI-optimized biomass pyrolysis, and electrofuel generation for achieving net-zero emissions[133-135].

Conclusion

- New era in engineering from “trial and error” to “intelligent engineering” is shown through this review. In today's era, engineering is more often than not replaced by repeated experimentation in the lab to predict the behaviour of materials, treatment performance, and energy usage before scaling up to large scale.
- A major gap between laboratory demonstrations and reliable scale up of environmental and energy technologies exists. Many of the studies mentioned, for example, have not taken real time process control, variable wastewater composition and catalyst deactivation into account, nor have they resolved issues of membrane fouling, sensor uncertainty or long-term material stability in industrial settings.

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- The incorporation of advanced nanomaterials like MXenes, functionalized metal–organic frameworks, and polymer-based nanocomposites offers fine-tuned surface chemistry, optimized transport characteristics, boosted catalytic activity, and increased mechanical strength. These properties can enhance the degradation of pollutants, separation of pollutants, resource recovery and durability of treatment systems.
- Machine-learning algorithms can help detect complex, nonlinear relationships between a variety of operating variables, material characteristics, pollutant concentrations, and treatment results, etc. They can be used to optimize pressure, temperature, contaminant removal efficiency, energy consumption, catalyst dosage and reaction time, and pH.
- A capability of combining predictive modelling with advanced materials can help lower the unnecessary use of chemical and energy resources and enhance pollutant degradation and separation efficiencies. Claims of improved efficiency should not be based solely on statistical accuracy but should also be backed up by data on wastewater and independent validation, uncertainty analysis, full mass balances and life cycle assessment.
- An important step forward in development is the integration of digital-twin models with actual wastewater-treatment units in real time. The system should be continually collecting the sensor information, making an estimate of process states which it is not measuring, forecasting future operating conditions, identifying abnormal behavior and making safe recommendations to correct the abnormal behavior.
- Digital twins should also be integrated with renewable energy resources, energy storage, and hybrid energy grids. Such integration would enable energy-intensive processes, like electrochemical treatment, pumping, aeration, membrane filtration, cleaning, and more to be timetabled based on the availability of renewable energy, electricity costs and storage conditions.
- Safe and explainable automation – AI-driven decisions should be controlled by physical constraints, regulatory limits, cyber security protections, and human oversight. Explainable and uncertainty-aware models are of special interest since their poor performance could result in suboptimal treatment, waste of energy, chemistry safety issues, and off-spec recovered products.
- Future research should consider pilot testing for long-duration, standardized data sets, interoperable digital platforms, physics-informed machine learning, real-time sensor validation, robust control strategies, and impacts of end-of-life nanomaterials. Interesting data about treatment cost, energy intensity, toxicity reduction, recovery yield, product purity and environmental burden should also be reported.
- The potential synergy of advanced nanomaterials, AI, digital twins, and renewable-energy systems could enable the creation of adaptive treatment plants that generate clean water, recover valuable resources, and generate minimal carbon emissions. This all-encompassing strategy is crucial for

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accelerating global decarbonization, industrial sustainability, and water security.

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