

Review

Toward Intelligent and Sustainable Membrane Engineering: Integrating Computational Fluid Dynamics, Machine Learning, and Material Assessment

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Abstract

Membrane technologies play a role in water treatment, energy conversion, and industrial separation processes; however, their performance is limited by fouling, polarization phenomena, transport inefficiencies, and energy consumption. This study presents a review of the integration of computational fluid dynamics and machine learning in membrane technologies, complemented by an environmental and engineering assessment of representative membrane materials. A systematic literature screening based on PRISMA guidelines was conducted using the Scopus (Elsevier B.V., Amsterdam, The Netherlands) and Web of Science (Clarivate, Philadelphia, PA, USA) databases, yielding 1421 records, of which 54 studies met the predefined relevance criteria. The analysis revealed a transition from conventional physics-based approaches toward hybrid simulation–machine learning frameworks, with artificial neural networks, surrogate models, and optimization emerging as the dominant methodologies. Energy consumption was identified as the most frequently investigated variable, particularly in desalination, fuel cell, electrodialysis, and hydrogen production systems. A complementary material-level assessment showed that conventional polymeric membranes, especially polyamide-based systems, remain dominant due to their performance and economic feasibility, whereas advanced materials such as graphene, carbon nanotubes, and perovskites offer promising functional properties but face challenges. The findings highlight the potential of integrated simulation–machine learning–material assessment frameworks to accelerate the development of intelligent and sustainable membrane technologies for future applications.

Keywords: computational fluid dynamics; machine learning; membrane technologies; sustainable material selection

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1. Introduction

Membrane technologies (MTs) are widely recognized as enabling technologies for water purification, wastewater treatment, energy conversion, hydrogen production, and industrial separation processes. Due to their high separation efficiency, modularity, and reduced chemical requirements compared with conventional methods, membrane processes are considered enabling technologies for achieving several Sustainable Development Goals (SDGs), particularly those related to clean water, affordable energy, responsible consumption, and climate action [1–3]. Despite these advantages, membrane systems

still face operational limitations, including fouling, concentration and thermal polarization, pressure losses, and nonuniform flow distribution. Some membrane processes remain limited by relatively high energy requirements, particularly pressure-driven desalination and electrochemical separation technologies. Consequently, membrane performance is ultimately reflected in key indicators such as permeate flux, selectivity, operational stability, and membrane lifetime. In addition, the interaction among hydrodynamics, heat transfer, mass transport, electrochemical reactions, and material properties makes membrane systems inherently multiphysics in nature, increasing the complexity of their analysis and design.

Computational fluid dynamics (CFD) has become one of the principal tools used to investigate transport behavior in membrane systems [4,5]. CFD simulations enable detailed characterization of velocity fields, pressure distributions, shear stress, concentration gradients, and thermal effects within membrane channels and porous structures. Previous studies have applied CFD to optimize spacer geometries, assess flow maldistribution, analyze fouling mechanisms, and improve electrochemical membrane reactor performance [4,6,7]. More recently, multiphysics CFD models have been adopted to simultaneously represent coupled hydraulic, thermal, electrochemical, and mass transport phenomena [5,8–10]. These capabilities have expanded the role of CFD from a diagnostic tool toward a framework for performance optimization. Nevertheless, although CFD provides detailed physical insight, high-fidelity simulations often require significant computational resources, particularly when large design spaces, multiple operating conditions, or iterative optimization procedures must be evaluated.

Consequently, machine learning (ML) techniques have gained increasing attention in this field. Artificial neural networks (ANNs), surrogate models (SMs), and ML for optimization frameworks have been widely implemented for performance prediction, operational control, and accelerated process evaluation. These approaches enable prediction of membrane system performance while reducing the need for repeated numerical simulations [11–13].

The integration of CFD and ML has enabled the development of hybrid frameworks in which ML models are trained using CFD-generated datasets to construct surrogate representations of membrane processes. These approaches have demonstrated potential for performance prediction, design optimization, fouling mitigation, energy reduction, and enhanced hydrogen production [7,14–16]. More recently, Physics-Informed Machine Learning (PIML) has emerged as a complementary paradigm that incorporates governing equations and physical constraints directly into the learning process, improving model generalization and physical consistency while reducing dependence on large training datasets [17].

In addition to process modeling, recent advances in membrane engineering have emphasized sustainable material selection. Membrane materials influence permeability, selectivity, mechanical stability, chemical resistance, durability, and environmental impact. Conventional polymeric membranes remain dominant in water treatment (WT) applications, whereas emerging materials are attracting growing interest in energy systems and selective separation processes [18–21]. However, limited attention has been devoted to integrating environmental assessment with CFD and ML-based membrane optimization strategies.

Despite the relevance of this topic, studies integrating CFD, ML, sustainability indicators, and environmental evaluation of membrane materials remain scarce, as the available literature remains fragmented across these fields. To address this gap, this study presents a systematic review of the integration of CFD and ML in MTs for water and energy applications, emphasizing intelligent and sustainable membrane engineering through SMs, PIML, and integrated CFD and ML methods. Representative membrane materials

were also evaluated using ANSYS Granta Selector (ANSYS Inc., Canonsburg, PA, USA) based on embodied energy, carbon footprint, mechanical performance, and economic indicators. This integrated approach provides a framework for the future development of intelligent and sustainable MTs.

The remainder of this paper is structured as follows: Section 2 details the methodological approach adopted in this study. Section 3 reports the key results derived from the literature. Finally, Section 4 offers concluding remarks.

2. Materials and Methods

The methodology consisted of eligibility criteria, literature search strategy, study selection and screening, the data collection process and data items, scoring-based relevance classification, material level assessment, synthesis strategy, and bias and limitations assessment, which are described in the following sections.

2.1. Eligibility Criteria

The eligibility criteria were defined to ensure the selection of studies relevant to membrane systems and emerging modeling approaches. The inclusion criteria were (i) peer-reviewed journal articles; (ii) studies focused on MTs; (iii) studies employing CFD, ML, or SM approaches; and (iv) studies reporting performance indicators and, when available, environmental or sustainability variables such as energy consumption (EC), efficiency, fouling, or mass transfer.

The exclusion criteria included (i) conference proceedings, editorials, and non-peer-reviewed publications; (ii) studies not focused on membrane systems; (iii) studies without explicit modeling approaches; and (iv) articles without accessible full text. Studies were grouped for synthesis based on modeling approach, application domain, and scale of analysis.

2.2. Literature Search Strategy

The literature search was conducted using the Scopus (Elsevier B.V., Amsterdam, The Netherlands) (SCOPUS) and Web of Science Core Collection (Clarivate, Philadelphia, PA, USA) databases (WOS). The search was last conducted in April 2026. The search strategy was designed to capture studies at the intersection of membrane systems, CFD modeling, ML, and environmental performance variables. The search query was constructed using Boolean operators and truncation symbols as follows: (membrane OR desalination OR electrodialysis) AND (CFD OR “computational fluid dynamics”) AND (“surrogate model ” OR “machine learning” OR ANN OR kriging) AND (“energy consumption” OR “environmental impact” OR LCA OR optimization). This query was consistently applied across both databases to ensure reproducibility and comparability of the retrieved records. The search strategy was iteratively refined to minimize ambiguity in model classification, particularly by avoiding generic terms that could overlap between CFD and ML approaches. In cases of uncertainty during the study selection process, discrepancies were resolved through consensus among the authors. A summary of the search strategy and retrieved records is presented in Table 1.

Table 1. Summary of literature search strategy and retrieved records.

Database	Search Query Components	Records Retrieved
SCOPUS	Membrane + CFD + ML/Surrogate + Environmental indicators	627
WOS	Membrane + CFD + ML/Surrogate + Environmental indicators	794
	TOTAL	1421

2.3. Study Selection and Screening

The selection followed a multi-stage screening process based on PRISMA guidelines [22]. A total of 1421 records were initially identified from the selected databases. After removing duplicate records ($n = 110$), 1311 records were screened based on titles and abstracts, resulting in the exclusion of 965 records. Subsequently, 346 reports were sought for retrieval, of which 2 were not accessible. A total of 344 reports were assessed for eligibility through full-text evaluation. At this stage, 290 studies were excluded for not meeting the predefined relevance criteria ($\text{score} < 4$), as defined by the scoring-based relevance classification. The remaining 54 studies met the inclusion threshold and were considered eligible for analysis. The screening and selection processes were conducted using predefined criteria and a structured, reproducible approach. The complete study selection process is illustrated in the PRISMA flow diagram (Figure 1). The complete database of the 1,311 records screened during the study-selection process is provided as: Supplementary-Material-File-S1.

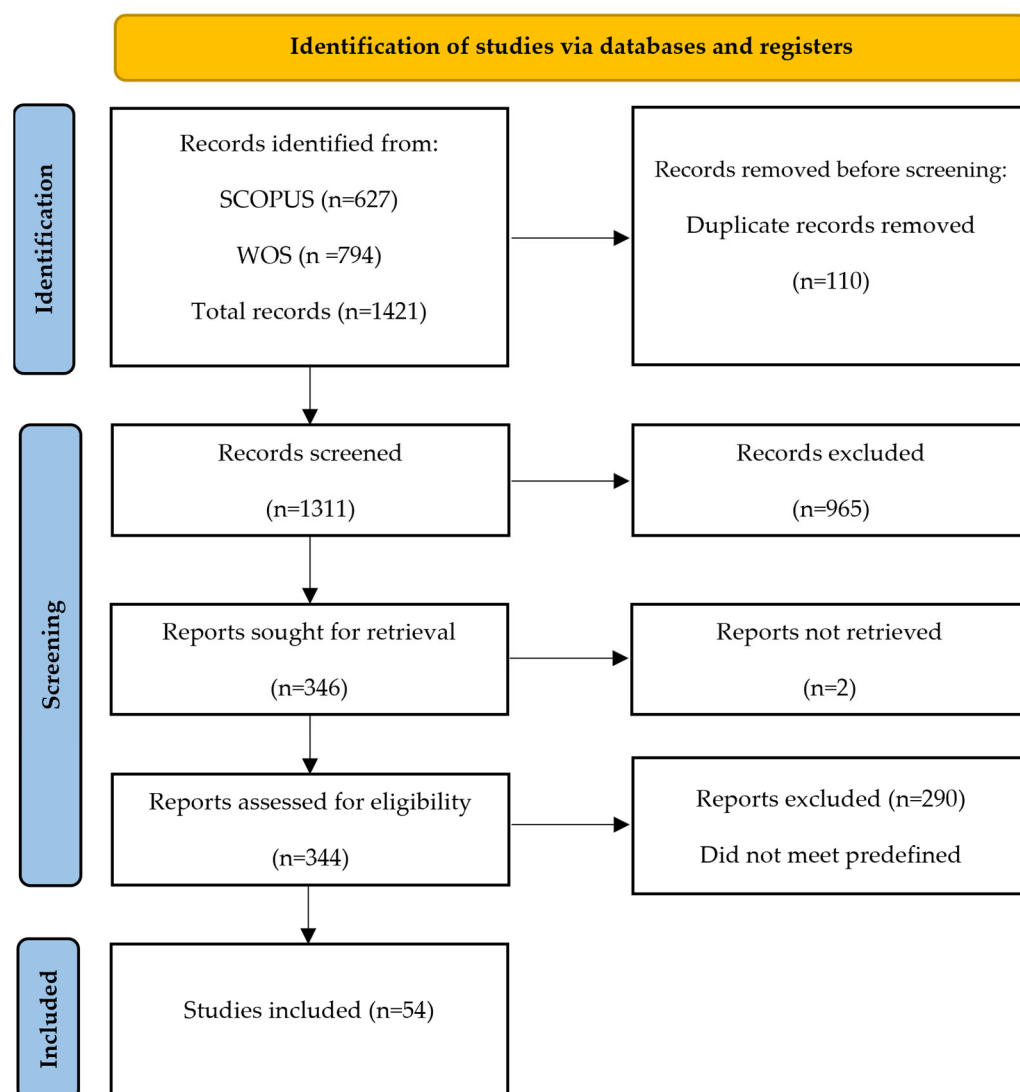


Figure 1. PRISMA flow diagram of the study selection process.

2.4. Data Collection Process and Data Items

Data were extracted from the title, abstract, and full text of each study using a structured database. The collected information included the type of model, application area,

main variables, environmental indicators, and analysis scale. This information was used to organize and compare selected studies.

2.5. Scoring-Based Relevance Classification

A scoring system was developed to evaluate the relevance of each study. Five criteria were considered: (i) focus on membrane systems; (ii) use of CFD; (iii) use of ML or SMs; (iv) inclusion of key variables such as energy, pressure, mass transfer, or fouling; and (v) inclusion of environmental or sustainability indicators. Each criterion received a score of 0 or 1, resulting in a maximum score of 5.

2.6. Material-Level Assessment Using ANSYS Granta Selector

To complement the analysis of CFD and ML methodologies, the environmental and engineering characteristics of the membrane materials most frequently reported in the reviewed literature were evaluated using ANSYS Granta Selector (ANSYS Inc., Canonsburg, PA, USA). Since material selection directly influences transport behavior, fouling resistance, durability, and the energy efficiency of membrane processes, this assessment provides a complementary perspective for the design of intelligent and sustainable membrane systems. The evaluated materials were selected based on their recurrence in studies related to desalination, water treatment processes (including reverse osmosis, ultrafiltration, nanofiltration, and pervaporation), electrodialysis, and membrane-based energy applications. The following metrics were considered: (i) embodied energy (MJ/kg); (ii) carbon footprint (kg CO₂/kg); (iii) water consumption (L/kg) during material manufacturing; (iv) price (USD/kg); (v) density (kg/m³); (vi) Young's modulus (GPa); and (vii) tensile strength (MPa).

2.7. Synthesis Strategy

The selected studies were analyzed using a combination of quantitative and qualitative approaches. Quantitative analysis was used to determine the distribution of modeling approaches, performance variables, and system scales across the dataset. Qualitative synthesis was used to identify methodological trends, integration patterns, and research gaps. The results were organized using tabular and graphical representations, including distributions of modeling approaches (CFD, ML, and hybrid methods), key process variables (energy, fouling, flux, and pressure), and frequency-based material classifications.

2.8. Bias and Limitations

A formal risk-of-bias assessment was not conducted, as the primary objective of this study was to identify methodological trends rather than evaluate intervention outcomes. However, potential sources of bias related to database selection, keyword definition, and publication availability were considered.

To mitigate these limitations, the search strategy was iteratively refined, and a structured scoring system was implemented to ensure objective and reproducible study selection. This approach enhances the transparency and robustness of the review process.

3. Results

3.1. Overview of Selected Studies

Figure 2 summarizes the selected studies according to relevance level (score ≥ 4), modeling approach, and application domain related to water and energy systems. The selected studies encompass a wide range of membrane-related applications, including desalination, electrodialysis, fuel cells, hydrogen production, and membrane separation processes, highlighting the growing use of integrated computational approaches across water

and energy technologies. Percentages are calculated with respect to the total number of studies ($n = 54$), and categories are not mutually exclusive.

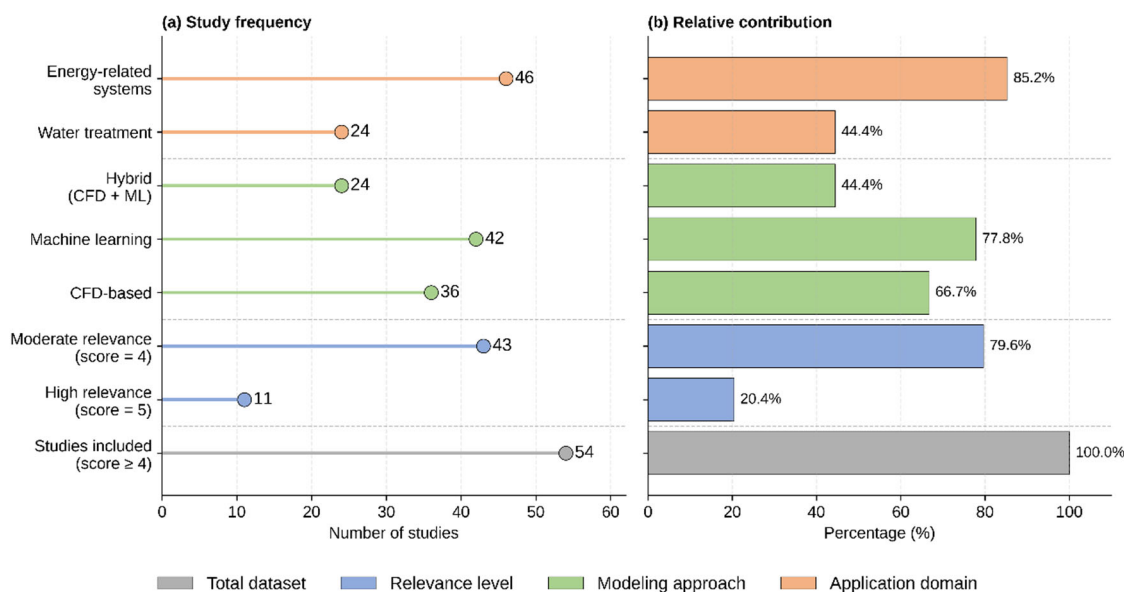


Figure 2. Distribution of the reviewed studies according to relevance level, modeling approach, and application domain.

The distribution of studies reveals that only a limited number achieve full methodological integration, combining membrane systems, emerging modeling approaches, and environmental performance indicators. Although more than 60% of the reviewed studies rely on computational tools, the results indicate a growing interest in ML approaches. This trend reflects a transition from models based only on physical principles toward hybrid methods and methods based on data analysis, motivated by the need to improve computational efficiency and system optimization. The increasing presence of hybrid models further supports this evolution, suggesting that ML methods are not replacing traditional approaches but rather complementing them within integrated modeling frameworks.

Additionally, energy applications appeared more frequently than WT applications within the reviewed studies. However, these categories were not mutually exclusive, since several investigations simultaneously addressed WT and energy membrane systems.

3.2. Distribution of Modeling Approaches

Table 2 summarizes the CFD approaches, physical scales, and AI strategies reported in the reviewed studies and indicates whether each of the 54 publications employed CFD, ML, or an integrated CFD–ML framework. Moreover, it reveals that ML strategies for optimization and performance prediction dominated the 54 reviewed studies, with ANN-based models representing the most frequently adopted approach, either as standalone algorithms or integrated with SM, physics-aware frameworks, and optimization techniques. Their use reflects the ability of conventional ANNs to provide a balance between predictive accuracy, computational efficiency, and simple implementation. This trend parallels the increasing complexity of multiphysics membrane simulations [23–25] and the growing integration of CFD with ML methodologies [16,26,27]. Most hybrid frameworks coupled multiple transport phenomena, including mass transfer [28], heat transfer [27], fluid dynamics [24,29], species transport [30], and electrochemical interactions [8,14,17,23], indicating a progressive transition from purely hydrodynamic analyses toward comprehensive multiphysics representations of membrane systems.

Table 2. Classification of the reviewed studies according to CFD approach and ML techniques.

Studies	CFD	ML	CFD Approach	Physical Scale	AI/ML Strategy
[31,32]		✓		Multiscale	Optimization ML
[11,25,26,33–38]		✓		Multiscale	ANN-based modeling; Optimization ML;
[39–43]	✓	✓	Multiphysics	Multiscale	ANN-based modeling; Optimization ML
[7,15,28,44–47]	✓	✓	Multiphysics	Multiscale	ANN-based modeling; SM; Optimization ML
[48,49]		✓		Membrane/System	ANN-based modeling; SM; Optimization ML
[50]		✓		Pore	PSM; Optimization ML
[51]	✓	✓	Multiphysics	Module	ANN-based modeling; SM; PSMs; HPM; Optimization ML
[5,8–10,52–58]	✓		Multiphysics	Multiscale	ANN-based modeling; Optimization ML
[59]		✓		Pore	ANN-based modeling.
[60,61]	✓	✓	Hydrodynamic	Membrane/System	ANN-based modeling; SM; Optimization ML
[62]		✓		Membrane/Module	SM; Optimization ML
[63]		✓		System	ANN-based modeling; Optimization ML
[16,30]	✓	✓	Multiphysics	Pore/Membrane	ANN-based modeling; PSM; PINN; OL; Optimization ML
[17]		✓		Pore	ANN-based modeling; PSM; Optimization ML
[23,24]	✓	✓	Multiphysics	Multiscale	Optimization ML
[64]	✓	✓	Multiphysics	Multiscale	PINN; OL
[14]	✓	✓	Multiphysics	Membrane	PSM; ANN-based modeling
[27]	✓	✓	Multiphysics	Module	ANN-based modeling; SM; PINN
[65]	✓	✓	Multiphysics	Multiscale	ANN-based modeling; SM; HPM, PINN; Optimization ML
[66]	✓		Hydrodynamic	Pore	ANN-based modeling.
[29]	✓	✓	Multiphysics	Pore/Module	DDML

The reviewed studies reveal two methodological families. The first is related to conventional data-driven machine learning models (DDMLs), including ANN, tree-based, kernel-based, Support Vector Machine (SVM), Bagging SVM (B-SVM), Multi-Task Learning (MTL). The second family encompasses PIML approaches. In this review, the term PIML is used to include methodologies that incorporate physical knowledge through different mechanisms to improve predictive robustness, extrapolation capability, and computational efficiency.

Several studies employed ANN [11,60], Kriging [48], Random Forest [41], and Extreme Gradient Boosting algorithms [41,63] to approximate CFD results and accelerate optimization workflows. These methods enable the representation of complex relationships while accelerating optimization processes without repeatedly executing full physical simulations. The increasing incorporation of tree-based, kernel-based, and ensemble learning methods suggests that recent methodological advances have focused on improving prediction robustness, computational efficiency, and model generalization, while complementing rather than replacing conventional ANN-based SMs.

The analysis further indicates that optimization-oriented ML represents one of the dominant methodological directions. The category “Optimization ML” appeared across most identified groups, demonstrating that current research is not restricted to predictive tasks alone, but increasingly prioritizes the identification of optimal operating conditions, geometric configurations, and transport strategies to improve membrane system performance.

Four methodological strategies were identified according to how physical knowledge is incorporated into model development. Physics-data-driven surrogate models (PSMs) employ high-fidelity CFD or molecular dynamics (MD) simulations to generate training datasets for conventional ML algorithms, enabling rapid prediction while preserving the physical fidelity of the underlying simulations [7,14,16,25,26,44,45,50,51,60]. Hybrid physics-guided models (HPMs) use physical or theoretical knowledge to structure the model, preprocess the data, constrain variable limits, or analytically couple with the

neural network, without embedding differential equations into the loss function [15,38,43]. Physics-Informed Neural Networks (PINNs) directly incorporate governing equations, conservation laws, and boundary conditions into the training process, reducing dependence on large, labeled datasets while improving physical consistency and extrapolation capability [17,64,65]. Finally, operator-learning approaches (OL), such as Fourier Neural Operator (FNO) or DeepONet, learn mappings between functional spaces from physics-generated datasets, providing efficient approximations of complex multiphysics fields without explicitly embedding governing equations during optimization [24,30,64].

Although all four strategies integrate physical knowledge, they address different challenges and offer advantages. PSMs accelerate high-fidelity numerical simulations but remain dependent on the quality and representativeness of CFD or MD-generated datasets. Hybrid physics-guided models improve interpretability by preserving mechanistic formulations while enhancing predictive flexibility. PINNs are particularly attractive for problems with limited labeled data because physical constraints reduce dependence on purely data-driven learning and improve extrapolation beyond the training domain. In contrast, operator learning methods approximate solution operators for high-dimensional multiphysics systems, making them well suited for rapid field prediction and digital twin applications.

Despite their growing potential, the adoption of physics-informed approaches remains limited. Recent methodological advances have instead focused on integrating explainable AI, hybrid optimization strategies, and digital twins with conventional SMs rather than fully transitioning toward physics-informed learning. Moreover, the predictive performance of most current frameworks remains dependent on the quality of training datasets, while experimental validation, uncertainty quantification, and model transferability across different operating conditions continue to represent methodological challenges. Consequently, these approaches should be regarded as complementary rather than competing methodologies, each offering distinct advantages depending on the physical scale, data availability, and computational objectives of the membrane process.

Beyond offline prediction and design optimization, the computational efficiency of CFD–ML frameworks are enabling intelligent real-time applications. Recent studies have demonstrated their integration into model predictive control [11], energy management systems [65], and IoT-enabled automated control frameworks [38], thereby enabling continuous adjustment of operating conditions under transient process dynamics. In addition, recurrent architectures such as Long Short-Term Memory neural networks have been employed to anticipate process dynamics and support adaptive membrane operation [64]. These developments represent a transition from static optimization toward adaptive and autonomous membrane systems.

In membrane processes, the dominant issues include membrane fouling and concentration polarization [33,39], thermal polarization, and high specific EC [9,65]. In electrochemical systems and proton exchange membrane fuel cells, the primary limitations involve nonuniform reactant distribution, inadequate liquid water management, and pressure drop losses. These challenges have driven the integration of CFD and ML to improve geometric design, flow distribution, and operating conditions while reducing the computational effort associated with iterative optimization.

Despite the rapid adoption of hybrid CFD–ML frameworks, high-fidelity CFD simulations remain indispensable for resolving complex multiphysics transport phenomena and generating the datasets required to develop reliable SMs. The reviewed studies further show that the contribution of each methodology depends on the physical scale of the problem. At the pore scale, CFD provides detailed transport information, whereas ML accelerates material design and property prediction. At the membrane and module scales, hybrid frameworks primarily reduce the computational cost of iterative design and

optimization while preserving the underlying transport physics. In contrast, system-scale applications emphasize process optimization, control, and digital twin implementation. Overall, the effectiveness of CFD–ML integration lies in balancing physical fidelity and computational efficiency according to the objectives of each application.

Beyond the classification presented in Table 2, only the original research articles ($n = 41$) were further assessed in terms of dataset generation, model development, validation strategies, performance evaluation, and reproducibility.

Table 3 compares representative implementations of DDML, PIML, and OL approaches by evaluating their training data requirements, predictive accuracy, and computational speedup relative to CFD or MD simulations. The accuracy indexes are coefficient of determination (R^2), mean square error (MSE), root mean square error (RMSE), and mean absolute error (MAE). Because an objective of this review is to analyze the integration of CFD and ML for membrane engineering, both the training data requirements and the reported computational speedups are referenced to CFD/MD simulations. These physics-based numerical models constitute the source of high-fidelity training data in the reviewed literature and provide the computational baseline against which the efficiency of ML surrogates and physics-informed approaches is commonly assessed.

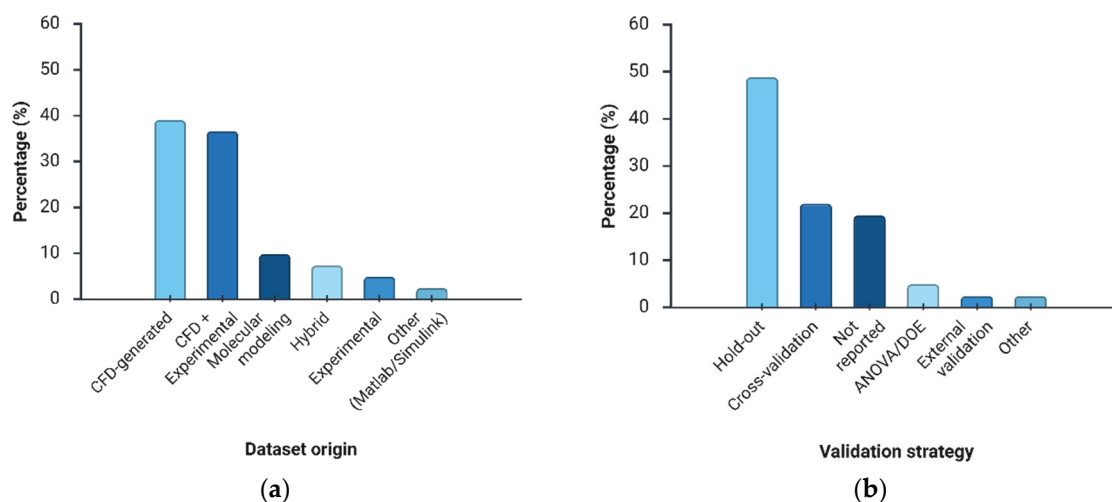
Table 3. Comparison of representative approaches.

Modeling Approach	Specific Algorithm	Training Data Requirement	Predictive Accuracy	Computational Speedup (vs. CFD/MD)	Studies
DDML	ANN	600 synthetic samples	MSE = 0.001479 – 0.003267 $R^2 = 0.952735 - 0.983839$	Mechanistic models based solely on CFD are too computationally intensive for real-time applications or assessments.	[15]
	ANN	3125 CFD data points	$R^2 = 0.9997$, RMSE = 0.0444, MAE = 0.0152	Reduces prediction from hours to fractions.	[60]
	SVM	350 CFD samples	$R^2 = 0.9953$, RMSE = 0.0371, MAE = 0.0202	Immediate inference once trained, bypassing CFD bottlenecks.	[14]
	B-SVM	60 CFD simulations	$R^2 = 0.9669$, MAPE = 12.817%	Replaces CFD in Genetic Algorithm for saving computational resources.	[44]
	MTL	1473 plant simulation data points	$R^2 = 0.9948$, RMSE = 1.59, MAE = 0.86	Solves simultaneous regressions without full flow simulation.	[35]
PIML	PINN	400 MD simulations	$R^2 = 0.980$ (400 points)/ $R^2 = 0.939$ (200 points)	Predicts nanoscale electrokinetics directly, avoiding full MD.	[17]
	PINN	10–20% of the data required by standard ANNs	<5% relative error/ $R^2 > 0.95$	Reduces full spatial simulation runtimes.	[65]
	PINN+TL	By leveraging transfer learning, the model generalizes to new geometries and flow conditions without requiring complete re-training.	Achieves 98% to 99% predictive accuracy.	Achieves an order-of-magnitude efficiency gain (approx. 10x) compared to traditional numerical computation.	[64]
OL	FNO	960 CFD models	$0.967 < RMSE \leq 0.995$, $0.961 < R^2 \leq 0.995$ 0.989.	Several times faster than CFD (e.g., 105 times)	[67]
	DeepONet	800 spatially heterogeneous CFD samples	RMSE = 0.05% to 1.31%	Provides real-time continuous physical field predictions.	[30]

DDML methods, particularly ANN-based surrogate models, generally achieve the highest predictive accuracy when trained with sufficiently large CFD-generated datasets [7,44]. However, their performance remains highly dependent on the availability, quality, and physical fidelity of these datasets and is largely restricted to interpolation within the training domain. In contrast, PINNs incorporate the governing equations directly into the optimization process, reducing their reliance on labeled CFD data while improving physical consistency and extrapolation capability [65]. Similarly, OL approaches rapidly approximate complete multiphysics solution fields, making them particularly suitable for digital twins, real-time prediction, and multiscale simulations [30]. Consequently, selecting an appropriate CFD–ML methodology requires balancing predictive accuracy, computational cost, data availability, and physical fidelity according to the specific objectives of the membrane engineering application. These trade-offs also explain the methodological trends observed in the reviewed literature, where the characteristics and origin of the training datasets largely determine the selection and performance of the implemented ML framework.

The resulting methodological trends are summarized in Figures 3 and 4. Figure 3a–d collectively indicate that current CFD–ML frameworks are predominantly supported by simulation-generated datasets. Although this distribution is partly influenced by the eligibility criteria adopted in this review, CFD-generated datasets and CFD models complemented with experimental validation account for nearly 76% of the selected research articles, highlighting the central role of CFD in SM development. Within the reviewed studies, CFD serves not only as a numerical simulation tool but also as the principal source of training data, making the predictive capability of ML models dependent on both the learning algorithm and the physical fidelity of the simulations used to generate the datasets.

This methodological dependence is reinforced by the widespread use of hold-out validation, whereas more rigorous approaches such as cross-validation and external validation remain comparatively uncommon. When combined with the limited availability of datasets and the inconsistent reporting of dataset characteristics, these practices restrict independent validation and objective benchmarking across studies, making it difficult to determine whether improvements in predictive performance arise from algorithmic advances or differences in the underlying training data. Collectively, these findings suggest that the current challenge in CFD–ML membrane research is no longer limited to developing more sophisticated ML algorithms, but also to improving the quality, transparency, and validation of the datasets supporting them. Future progress will therefore depend on strengthening methodological rigor through standardized dataset reporting, broader data availability, robust validation protocols, and closer integration of CFD, experimental measurements, and ML.



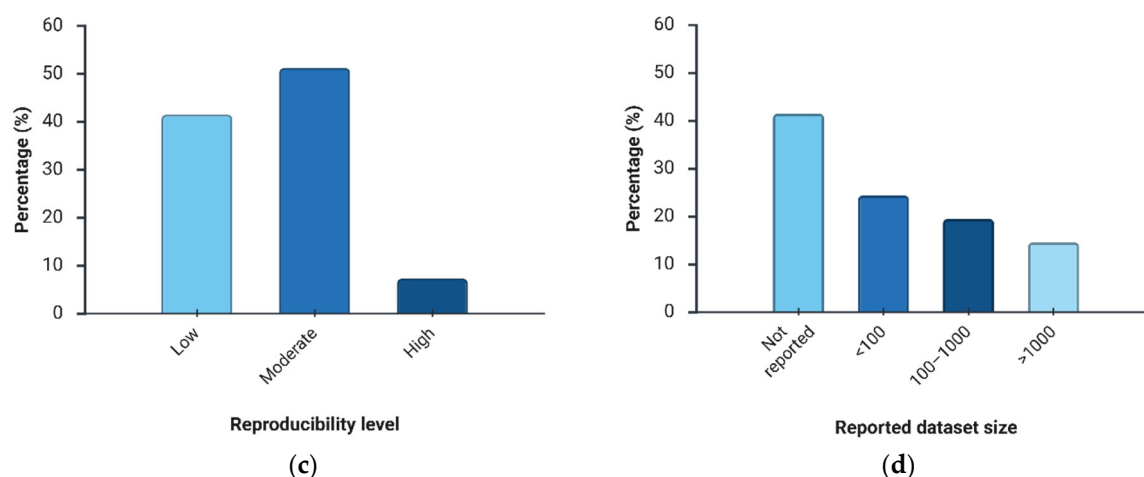


Figure 3. Quantitative distribution of the main methodological characteristics identified in the 41 CFD–ML research articles included in this review: (a) dataset origin, (b) validation strategy, (c) reproducibility level, and (d) reported dataset size. Review articles were excluded from this analysis because they do not develop original computational models.

Figure 4 complements the methodological assessment presented in Figure 3 by examining how current CFD–ML frameworks are implemented and evaluated in practice. The predominance of experimental validation (Figure 4a) reflects increasing efforts to improve the credibility and practical applicability of simulation-driven models. However, purely numerical validation remains common, indicating that comprehensive computational–experimental integration has not yet become standard practice.

This methodological limitation is also reflected in model performance evaluation (Figure 4b). R^2 , MSE, RMSE, and MAE, are the most widely adopted performance indicators because they provide objective measures of predictive accuracy. Nevertheless, the absence of standardized benchmarking protocols continues to hinder meaningful comparisons among models developed using different datasets, validation strategies, and computational frameworks.

The computational infrastructure adopted by the reviewed studies (Figure 4c) further supports these findings. Most investigations rely on well-established commercial platforms, particularly ANSYS Fluent (ANSYS Inc., Canonsburg, PA, USA) and COMSOL Multiphysics (COMSOL AB, Stockholm, Sweden), whereas open-source and alternative computational environments remain comparatively underrepresented. Although commercial software provides mature and robust simulation capabilities, its predominance may limit methodological diversity, reproducibility across software ecosystems, and the broader accessibility of CFD–ML research.

Taken together with the methodological trends identified in Figure 3, these findings indicate that future advances in CFD–ML membrane research will depend less on the development of new computational tools than on improving methodological standardization through reproducible workflows, rigorous validation, standardized benchmarking protocols, and consistent model evaluation.

The analyzed studies show a progressive transition toward the integration of CFD and ML methods for the prediction and optimization of membrane processes. In this context, EC was the most investigated variable, appearing in 46 studies, particularly in desalination systems, fuel cells, and hydrogen production units. In these applications, CFD simulations were widely used to describe fluid flow, heat transfer, mass transport, and electrochemical reactions [54,68,69]. Several studies focused on geometric optimization of membrane channels, spacers, and flow configurations in order to improve transport

efficiency and reduce pressure losses. In parallel, ML was employed to rapidly predict operational performance and optimize operating conditions [25,38,42,62,70]. These approaches enabled accelerated evaluation of membrane system behavior during optimization.

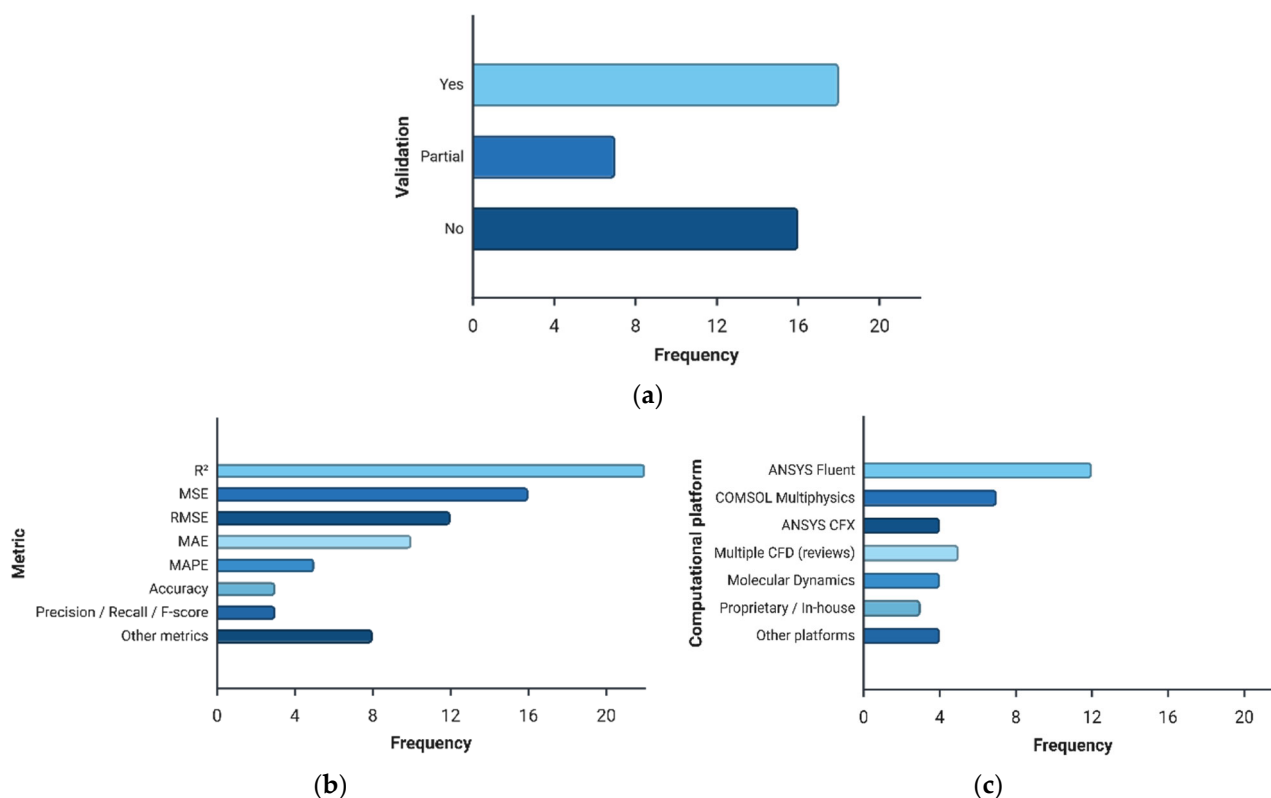


Figure 4. Computational implementation and model evaluation practices reported in the reviewed CFD–ML studies. **(a)** Experimental validation of the developed models. **(b)** Performance metrics used for model evaluation. **(c)** Computational platforms employed for CFD model development. Frequencies represent the number of studies reporting each category; a single study may contribute to more than one category where applicable.

3.3. Analysis of Performance Variables

Figure 5 presents the main variables used to evaluate MTs, their environmental relevance, modeling approaches, and associated scales.

WT applications accounted for 24 studies, mainly focused on desalination, waste treatment, membrane distillation, and contaminant removal. Across the analyzed studies, flux and pressure were among the most frequently investigated variables, particularly in reverse osmosis, nanofiltration, ultrafiltration, fuel cells, electrodialysis, and hydrogen production systems. CFD analyses were applied to evaluate velocity distribution, wall shear stress, concentration polarization, and pressure drop inside membrane channels [4,71,72], while ML methods were used to predict permeate flux, hydrodynamics, and contaminant removal efficiency [17,63].

In studies addressing membrane fouling phenomena, CFD simulations were mainly used to analyze particle deposition, shear stress distribution, and concentration boundary layers near membrane surfaces, whereas ML models were employed to predict fouling evolution and permeate flux decline using operational and imaging data. Some studies additionally incorporated control strategies based on ML to optimize aeration and back-washing conditions, contributing to lower energy demand and longer membrane service life [33,39,73].

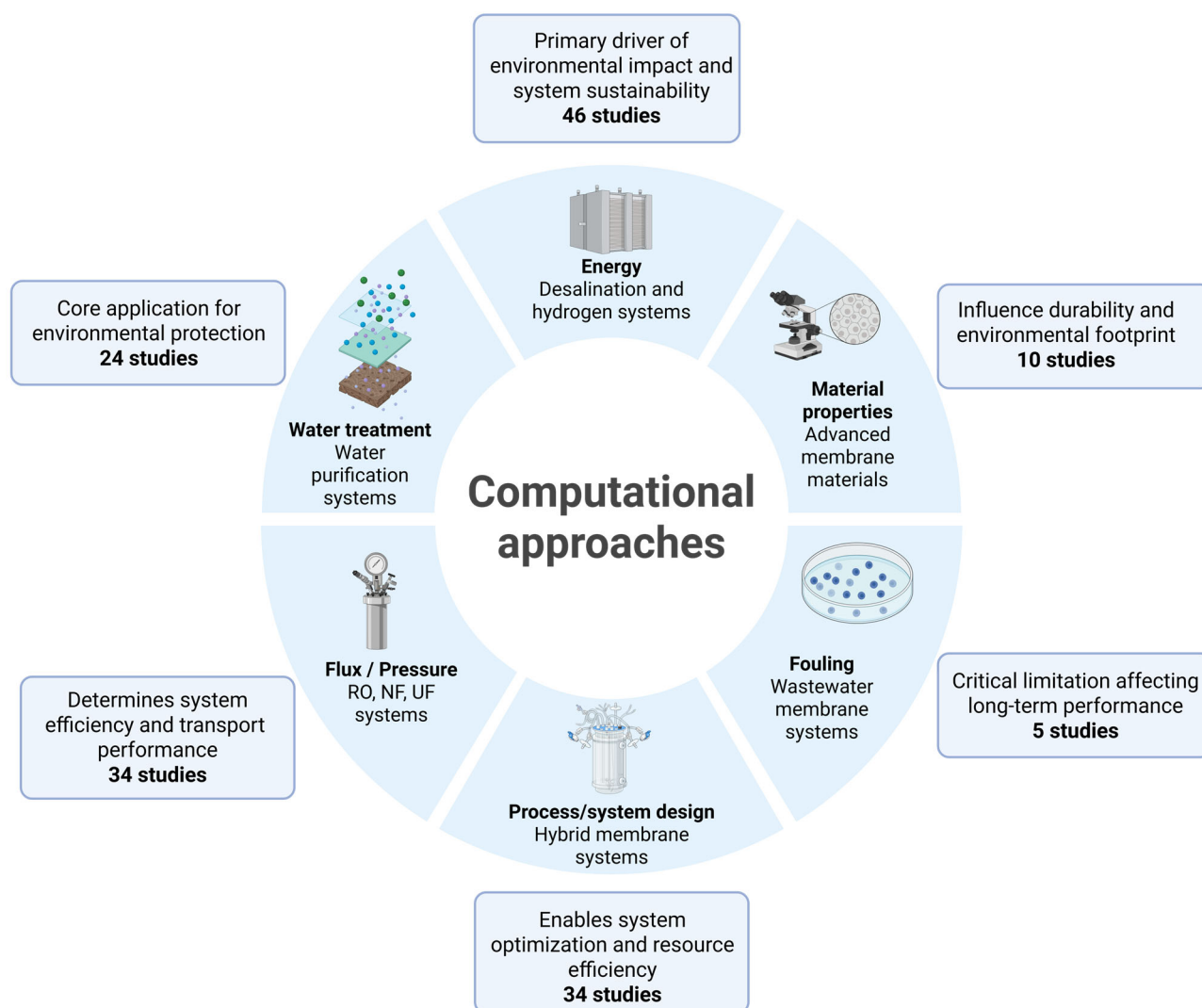


Figure 5. Computational approaches, key variables, and application domains in membrane systems.

3.4. Environmental and Engineering Assessment of Membrane Materials

As discussed in Section 2.6, membrane materials directly affect several variables commonly optimized through CFD and ML approaches, including flux, fouling, transport efficiency, and EC [46]. Therefore, a complementary material-level assessment was performed to evaluate the environmental and engineering characteristics of the membrane materials most frequently reported in the reviewed studies. Figure 6 summarizes the occurrence frequency of the principal membrane materials according to their dominant application domains, including WT, ES, and advanced membrane separation processes.

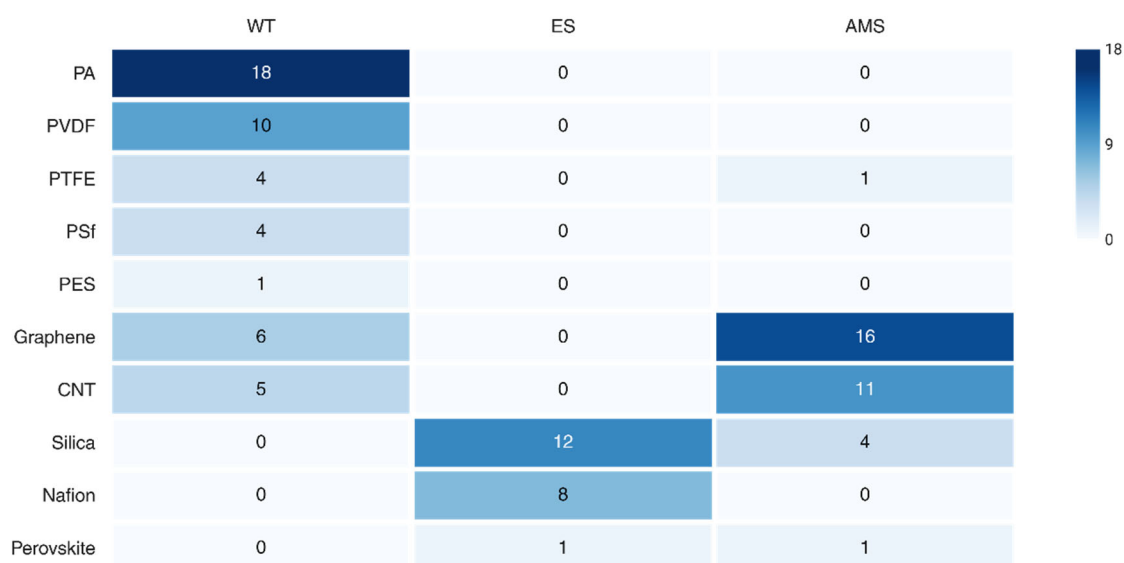


Figure 6. Frequency distribution of membrane materials across application domains.

The heatmap shows that recent computational studies are mainly focused on commercial polyamide (PA) and polyvinylidene fluoride (PVDF) membranes, particularly for WT applications. PA membranes exhibit the highest occurrence frequency due to their extensive use in reverse osmosis and nanofiltration systems, attributed to their high salt rejection and tunable chemical structure, which enhances water permeability. Similarly, polysulfone (PSf) and polyethersulfone (PES) are employed as porous support materials because of their elevated mechanical strength and resistance to high operating pressures [31]. Polyvinylidene fluoride (PVDF) and polytetrafluoroethylene (PTFE) are also investigated owing to their hydrophobic nature, which is essential for membrane distillation processes and for minimizing flooding phenomena in gas diffusion layers used in fuel cells [9,74,75].

In contrast, membranes based on graphene and carbon nanotubes (CNTs) are more frequently used in advanced separation applications due to their high chemical stability, large specific surface area, and enhanced separation performance. Graphene-based materials also exhibit high thermal and electrical conductivity, which contributes to fouling mitigation, electrochemical contaminant removal, and improved transport efficiency. In particular, multilayer graphene membranes and graphene oxide have attracted significant attention because their tunable surface chemistry and nanoscale architecture enable enhanced ionic selectivity and permeability during seawater desalination processes [17,76]. Similarly, Nafion membranes are widely used in fuel cells and electrochemical ES because of their high proton conductivity, chemical stability, and favorable ionic transport properties [77].

The reviewed literature also highlights the growing implementation of ceramic, inorganic, and catalytic membrane materials, including perovskites (e.g., BSCF and LSCF), silica membranes, palladium-based membranes, metallic catalysts (e.g., Pt and Ni), and covalent organic frameworks (e.g., COF, SNW-1). Perovskite materials are particularly attractive because their mixed ionic–electronic conductivity enables selective oxygen transport at elevated temperatures while maintaining high thermochemical stability [24]. Silica membranes have been investigated for selective hydrogen separation and continuous hydrogen production in membrane reactors, whereas Pt- and Ni-based materials are widely evaluated due to their electrocatalytic activity in ammonia decomposition and fuel cell applications [54]. Likewise, nanostructured porous materials and COF-based

additives have emerged as promising alternatives for improving porosity, interconnectivity, and hydrophilicity in thin-film composite membranes [78,79].

Given the increasing structural complexity and functional diversity of membrane materials, the evaluation of their environmental and engineering performance has become essential for assessing industrial feasibility and long-term sustainability. Despite the growing implementation of advanced membrane materials, comparative environmental and engineering assessments remain limited within the reviewed literature. Therefore, a quantitative comparative analysis was conducted using Ansys Granta Selector (ANSYS Inc., Canonsburg, PA, USA) with representative engineering materials selected to approximate the membrane systems most frequently reported in the literature.

The analysis employed a material database containing engineering grade materials with physicochemical and functional properties comparable to those commonly used in membrane fabrication and separation processes. Specifically, PA membranes were represented by PA66 unfilled molding grade, PVDF membranes by general purpose PVDF, PTFE membranes by virgin PTFE, PSf membranes by polysulfone (PSU), PES membranes by polyethersulfone (PESU), Nafion membranes by PFSA ionomer (sodium), graphene membranes by graphite, carbon nanotube membranes by multi-walled carbon nanotube composites (PC CNT composite), silica membranes by fused silica, and perovskite membranes by barium titanate. Graphite was selected because no graphene material was available in the database. Therefore, it was used only as a qualitative surrogate and should not be interpreted as representing the environmental profile of graphene, which depends strongly on the synthesis route and functionalization. When multiple variants were available, materials representative of membrane applications were selected.

The assessment included environmental indicators associated with material production, including carbon footprint, embodied energy, and water consumption, together with intrinsic material properties such as density, mechanical strength, and chemical stability. The results are presented in Tables 4 and 5.

Table 4. Environmental indicators of representative membrane materials.

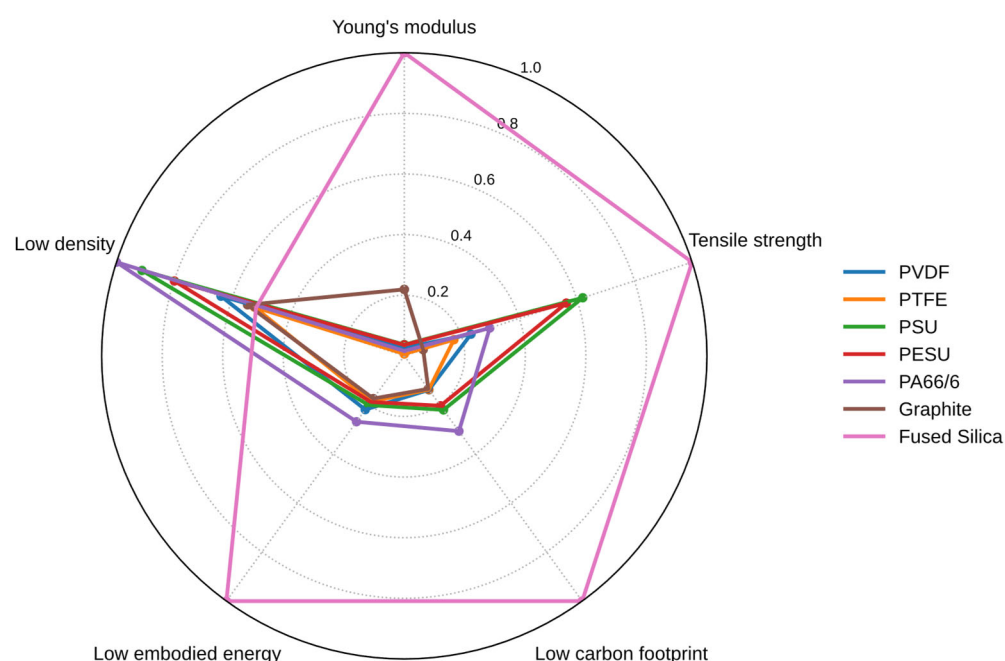
Material	Carbon Footprint (kg CO ₂ eq/kg)	Embodied Energy (MJ/kg)	Water Consumption (L/kg)
PVDF	15.3–16.9	165–183	434–480
PTFE	15.4–17.0	195–215	372–411
PSU	9.64–10.6	181–199	495–547
PESU	10.4–11.5	193–213	NA
PA66/6	6.91–7.61	135–149	147–163
Ionomer (sodium)	5.19–5.73	106–117	267–295
Graphite	15.7–17.4	208–230	291–322
PC CNT Composite	8.33–9.18	154–170	2.96–3.27
Fused Silica	2.12–2.34	36.2–40.1	NA
Barium Titanate	NA	NA	NA

NA: Not available in ANSYS Granta (ANSYS Inc., Canonsburg, PA, USA) database.

The comparative analysis of membrane materials reveals substantial differences in environmental impact, mechanical performance, and economic feasibility, highlighting the compromises currently associated with the design and optimization of membrane systems. The results obtained using ANSYS Granta Selector (ANSYS Inc., Canonsburg, PA, USA), together with the radar chart presented in Figure 7, demonstrate that no single material simultaneously maximizes all desirable engineering and sustainability properties. Consequently, membrane material selection remains strongly dependent on operational requirements and the target application domain.

Table 5. Engineering and economic properties of representative membrane materials.

Material	Price (USD/kg)	Density (kg/m ³)	Young's Modulus (GPa)	Tensile Strength (MPa)
PVDF	11.1–16.2	1770–1780	1.30–2.53	24.1–50
PTFE	10.7–17.2	2140–2200	0.40–0.55	20.7–34.5
PSU	12.7–12.8	1230–1250	2.62–2.76	94.4–104
PESU	20–26	1370–1460	2.41–2.83	85–95.2
PA66/6	2.58–3.84	1120–1140	0.95–1.40	35–60
Ionomer (sodium)	5.06–5.25	934–950	0.10–0.38	21–43
Graphite	11.2–17.0	1900–2250	7–25	10–11
PC CNT Composite	10.5–11.6	1170–1240	2.07–2.76	58.6–65.5
Fused Silica	6.21–10.4	2170–2220	71.2–74.8	152–168
Barium Titanate	13.3–16.0	5500–6020	67	59–100


Figure 7. Comparative environmental and engineering performance of representative membrane materials.

From an environmental perspective, silica exhibited the most favorable profile among all evaluated materials, presenting the lowest carbon footprint (2.12–2.34 kg CO₂ eq/kg) and embodied energy (36.2–40.1 MJ/kg), together with the highest tensile strength (152–168 MPa) and Young's modulus values exceeding 71 GPa. The reported properties confirm the suitability of silica membranes for applications requiring high thermal stability, chemical resistance, and operation under elevated pressure and temperature conditions. Similarly, barium titanate exhibited high mechanical rigidity due to its ceramic structure, although environmental indicators were not directly available in the ANSYS Granta (ANSYS Inc., Canonsburg, PA, USA) database.

Despite their excellent structural properties, ceramic materials generally possess high density, low flexibility, and elevated manufacturing complexity, factors that may limit industrial implementation at large scale. Among the polymeric materials, PA and sodium ionomers, used here as ionomeric approximations for Nafion type membranes, exhibited the most balanced environmental performance. PA66/6 presented a relatively low carbon footprint, low embodied energy, reduced water consumption, and the lowest cost among all evaluated polymeric membranes, which may explain its widespread industrial

implementation, although challenges related to recyclability still remain. Similarly, sodium ionomers displayed lower environmental impacts compared with fluorinated polymers, supporting their increasing use in ion exchange membrane systems and electrochemical applications such as electrodialysis and proton exchange membranes. In contrast, PVDF and PTFE showed high environmental impacts due to the energy intensive production of fluorinated polymers, although they remain widely used because of their excellent chemical resistance, thermal stability, and hydrophobic properties.

The analysis also highlights the growing relevance of carbon-based nanostructured materials in advanced membrane engineering. The representative graphite material and PC CNT composites exhibited multifunctional characteristics associated with improved transport characteristics and enhanced mechanical performance. In particular, the representative graphite material exhibited the highest Young's modulus among the evaluated carbon materials (7–25 GPa), indicating high rigidity and structural stability. However, the graphite approximation used to represent graphene-based materials also showed elevated embodied energy and carbon footprint values, reflecting the environmental characteristics of the graphite surrogate adopted for comparison. Therefore, these results should be interpreted only as a qualitative reference for carbon materials and not as the environmental profile of graphene membranes. By comparison, PC CNT composites displayed a more balanced profile, combining moderate embodied energy with relatively high tensile strength and extremely low water consumption. This combination of properties supports the growing interest in CNT membranes for applications requiring enhanced permeability, mechanical stability, and selective transport properties. The limited availability of environmental indicators highlights the current lack of environmental information for several emerging functional materials, particularly ceramic materials and electrochemical membrane systems.

Economic considerations also revealed important differences among the materials analyzed. Conventional engineering polymers such as PA66/6 exhibited the lowest cost range (2.58–3.84 USD/kg), reinforcing their suitability for large-scale industrial applications. In contrast, materials such as PESU exhibited considerably higher costs due to the greater manufacturing complexity and processing requirements associated with advanced MTs. Nevertheless, these costs may be justified in applications requiring superior thermal stability or enhanced separation efficiency.

Overall, the results indicate that conventional polymeric materials, particularly PA membranes, continue to dominate recent membrane research due to their balanced operational performance, economic viability, and manufacturing feasibility, which supports their widespread use in CFD and ML based optimization studies.

4. Conclusions

The reviewed literature demonstrates a clear transition in membrane engineering from conventional physics-based analyses toward integrated computational frameworks combining CFD, ML, and surrogate modeling (SM). Among the 54 analyzed studies, optimization-oriented ML methodologies, particularly ANN-based and hybrid CFD–ML approaches, emerged as the predominant strategies because of their predictive capability, computational efficiency, and suitability for complex membrane systems. Energy consumption (EC), coupled transport phenomena, fouling, and concentration polarization remain the principal drivers of membrane process optimization across desalination, electrodialysis, fuel cells, hydrogen production, and advanced separation technologies. Within this framework, CFD continues to provide high-fidelity descriptions of multiphysics transport, whereas ML increasingly enables rapid prediction, optimization, and surrogate-assisted design.

Regarding membrane fabrication materials, conventional polymeric membranes, particularly PA-based systems, continue to dominate industrial and computational applications because of their balanced performance, manufacturing feasibility, and economic viability. In contrast, emerging materials such as graphene, CNT composites, perovskites, covalent organic frameworks (COFs), and ceramic membranes exhibit promising functional and mechanical properties but remain largely confined to laboratory-scale research because of manufacturing complexity, scalability limitations, production costs, and the scarcity of environmental datasets. The eco-engineering assessment further revealed important trade-offs between sustainability indicators and engineering performance, highlighting the need to integrate CFD, ML, material selection, and sustainability metrics into unified computational frameworks capable of accelerating material screening, design optimization, and industrial implementation of next-generation membrane technologies.

Beyond predictive modeling, intelligent membrane systems (IMS) are progressively evolving toward adaptive and autonomous operation through the integration of surrogate models, digital twins, adaptive control, and reinforcement learning. From a broader sustainability perspective, combining CFD, ML, and sustainable material selection enables simultaneous optimization of membrane materials, module configurations, and operating conditions, promoting process intensification while reducing energy consumption and improving resource utilization. These integrated computational frameworks further support circular economy strategies through resource recovery, waste valorization, carbon capture, and integrated membrane processes that maximize material and energy efficiency across the process lifecycle.

Future advances in IMS will depend on improving data quality, model transparency, multiscale integration, and automated design capabilities rather than solely increasing predictive accuracy. A major challenge remains the limited availability of standardized experimental datasets, which restrict model reproducibility, increase the risk of overfitting in data-driven black-box models, and hinder objective benchmarking across computational approaches. Addressing these limitations will require open-access databases, standardized benchmarking protocols, and rigorous experimental validation to support the development of reliable and transferable ML models. Within this framework, broader implementation of explainable AI and PIML is expected to improve model interpretability, physical consistency, and confidence in industrial decision-making. Likewise, hierarchical CFD–ML frameworks capable of linking pore-, membrane-, module-, and system-scale phenomena represent a key step toward reliable digital twins with broader industrial applicability. Ultimately, advancing from predictive modeling to inverse and automated design will accelerate the discovery of high-performance membrane materials and process configurations, strengthening the transition toward intelligent and sustainable membrane engineering.

Supplementary Materials: The supporting information can be downloaded at <https://www.mdpi.com/article/doi/s1> as: Supplementary-Material-File-S1. The file contains the complete database of the 1,311 records screened during this review. It provides the authors, article titles, publication years, source titles, DOIs, web links, abstracts, and keywords that support the literature screening, study selection, and analyses presented in this review.

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Abbreviations

The following abbreviations are used in this manuscript:

ANN	Artificial neural network
B-SVM	Bagging support vector machine
CFD	Computational fluid dynamics
CNT	Carbon nanotubes
DDML	Data-driven machine learning model
EC	Energy consumption
FNO	Fourier Neural Operator
HPM	Hybrid physics-guided model
IMS	Intelligent membrane system
MAE	Mean absolute error
MAPE	Mean absolute percentage error
MD	Molecular dynamics
ML	Machine learning
MSE	Mean square error
MT	Membrane technology
MTL	Multi-Task Learning
OL	Operator learning
PIML	Physics-Informed Machine Learning
PINN	Physics-Informed Neural Network
PSM	Physics-data-driven surrogate model
R ²	Coefficient of determination
RMSE	Root mean square error
SVM	Support Vector Machine
SDG	Sustainable Development Goal
SM	Surrogate model
TL	Transfer Learning
WT	Water treatment

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