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Approach for Predicting Filtration Efficiency in Nanocomposite Membranes Using 2D Materials

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Potential water purification and separation technologies include nanocomposite filtration membranes. The complex relationships between numerous components make it difficult to estimate the rejection rate and filtration flux accurately. To address this issue and improve filtration performance in nanocomposite membranes, this research presents a novel Adaptive Golden Jackal Infused Random Forest (AGJ-RF) technique to predict the filtration efficiency in nanocomposite membranes. Polyvinylidene fluoride (PVDF) is the traditional membrane used for water treatment along with the two-dimensional (2D) materials, such as MXenes and graphene oxide (GO). The characterization technique known as permeability testing is employed for maintaining the effective filtration quality. A statistical technique known as analysis of variance (ANOVA) is employed to determine the variance. This analysis utilizes the SPSS software for the performance. The proposed method's efficiency in water filtration is conducted through Python platform. It evaluates the filtration flex and rejection rate by comparing the GO, Mxenes, and traditional membranes. The proposed AGJ-RF technique was performed in various matrices like RMSE (2.1), MAE (1.5) and R^2 (0.88). The experimental finding shows that the proposed technique performed more significantly in the field of predicting filtration efficiency in nanocomposite membranes using 2D material.

Keywords: Nanocomposite membrane, Two-dimensional (2D) materials, Water filtration, Graphene oxide (GO), Filtration quality.

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1. INTRODUCTION

The reverse osmosis process contributes over half of the global desalination capacity. The reverse osmosis, a membrane-based technique, makes it possible to separate pure water from brackish and saltwater with less power [1]. Membrane techniques like reverse and forward osmosis, nanofiltration, and ultrafiltration are some of the most effective techniques for eliminating both established and emerging contaminants from streams [2]. Untreated wastewater discharge has a strong relationship with environmental pollution, which impacts the quality of groundwater and surface water. Modern membrane technologies are the primary technique for the reuse of wastewater, as biological techniques are limited in their capacity to remove different types of pollutants from sewage [3]. A feasible approach to achieving the demanding drinking water regulations with the issue of disinfection by-products (DBPs) is the use of nanofiltration in water surface treatment [4]. An amine including m-phenylenediamine (MPD), piperazine (PIP), and phenylenediamine (PPD) that dissolves in an aqueous solution and a polyfunctional acid chloride like trimethyl chloride (TMC) dissolves in an organic solvent are the two monomers used to create nanocomposite membrane of the interfacial polymerization process [5]. Distillation and other traditional water purification techniques are efficient in extracting minerals, bacteria, and substances that stiffen water; they are ineffective at eliminating chlorine or organic pollutants and require an excessive amount of energy [6]. The significant benefits of membrane technology on alternative techniques for filtration have contributed to its potential validity throughout a wide range of research fields and businesses, including food processing, gas separation, water treatment, pharmaceutical production, etc [7]. The reverse osmosis membranes are typically made to create a thin

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layer of polyamide active filtration of permeable substrate [8]. Permeation, congestion, and stickiness of particles, organic compounds and substances impair pores in the membrane and hold the membrane position, connected through complicated chemical and experimental procedures, resulting in a fouling layer. The membrane fouling is a complicated phenomenon [9].

This research aims to develop a novel predictive technique known as AGJ-RF for effectively predicting the filtration efficiency in nanocomposite membranes with 2D materials. It utilizes PVDF as a traditional membrane and 2D materials, such as GO and MXenes. These nanocomposites membranes is compared with various parameters like rejection rate and filtration flux in the research.

2. RELEVANT RESEARCH

The assessment of the flux of permeate and foulant resistance in nanocomposite filtering membranes was performed in the study [10] employing the machine learning (ML) technique. With the support of the suggested approach, it could be feasible to establish permeate flow and foulant rejection and take into consideration how each of the conditions affects the nanocomposite filtration membrane without performing costly and time-consuming experiments. The bismuth telluride and graphene oxide (GO) coatings were used in the research [11] to create composite membranes made of polymers for membrane crystallization. It compared the polyvinylidene fluoride membrane (PVDF)-pristine membranes with PVDF-based membranes that had several layers of graphite or bismuth telluride. By employing a non-solvent phase separation technique, hydroxyapatite/boron nitride (HAp/BN) was created in polyethersulfone membranes were explored in the article [12]. Polyethersulfone (PES) ultrafiltration membranes enhanced the hydrophilicity, liquid flow, and anti-fouled properties, HAp/BN intercalation with the PES matrix effectively provided the alternate option. The paper [13] presented the 2D nano-materials that could be modified and the applications in water management. The basics of 2D nanomaterials were provided, with information on their types, synthesis approaches, and important features related to water management. It investigated the possibility of 2D nanomaterials for application in water quality monitoring devices, such as field-effect transistors, electrochemical sensors, colorimetric sensors, and fluorescent sensors. The developments in 2D smart membranes (2DSMs) were gathered in the examination [14].

3. RESEARCH METHODOLOGY

In this phase, the material synthesis and characteristic techniques are explored in detail. The statistical analysis ANOVA was employed in the research and performed for the prediction of filtration efficiency. The proposed AGJ-RF method was extensively explained in this phase.

3.1 Material Synthesis

The nanocomposite membranes were synthesized using a combination of solvent casting and phase inversion techniques. In this research, the polymer matrix known as PVDF is the traditional membrane that was employed for water purification and it was dissolved by utilizing the solvent called N-dimethylformamide (DMF) to generate the homogeneous solution. Filtration membrane made of polyvinylidene fluoride for filtration without moisture resistance. PVDF micropore membranes have an effective elimination rate for nanoparticles from the solution. The 2D materials, such as MXenes and GO, can be utilized to evaluate the effectiveness of the filter by comparing the traditional membrane (PVDF). They were employed in the polymer solution at various concentrations, such as GO with 0.5 % and MXenes with 1.0 %. The Hummer's method was utilized to GO. The chemical process known as Hummer's technique generates GO by reacting potassium permanganate, sodium nitrate, and sulphuric acid. It is a typical technique for producing enormous quantities of GO in technical and laboratories. The MXenes were obtained from MAX phases through selective printing and were created and distributed in the polymer solution through ultrasonic treatment in the final membrane. MAX phases are the class of triple carbides and nitrides possessing a hexagonal structure with a transitional material and the group component.

3.2 Characterization Techniques

To evaluate the properties of nanocomposite membranes, permeability testing was utilized. Filtration permeability testing evaluates a filter's capacity to allow chemical flow and its outcomes can be utilized to increase the efficiency and efficacy of filters along with developing and specifying filtration for specific usage. Maintaining substance homogeneity in manufacturing areas requires permeability control. Maintaining consistent good quality can be improved by this test. Measurement of the filtration flux and rate of rejection for several contaminants, including salts and dyes, was performed to determine the membranes' filtration efficiency.

3.3 Statistical Assessment

Filtration can be used to determine the shape, dimension, concentration, and composition of nanoparticles by statistical analysis. The evaluation of the solid pollutants that have been eliminated in the filter process and the portion of the filter membrane need to be taken out, and the contents need to be placed in the filter patches. This research employed the statistical analysis technique called ANOVA for the prediction of filtration efficiency. It employs the SPSS v20 software to perform the function. The ANOVA test compares research findings from several unrelated samples or groups to determine differences.

3.4 Predicting Filtration Efficiency in Nanocomposite Membranes using 2D Materials by Employing Adaptive Golden Jackal Infused Random Forest (AGJ-RF)

In this research, the machine learning method was developed AGJ-RF, which combines adaptive golden jackal (AGJ) optimization and random forest (RF) for predicting the filtration efficiency in the nanocomposite membrane. It is particularly developed to capture and analyze the complex relationships between nanocomposites and filtering effectiveness by integrating 2D materials into the membranes. By providing updated standards for filtering efficiency evaluations in nanocomposite materials with significant application potential, it enhances prediction reliability.

3.4.1 Random Forest (RF)

The RF is applied to regression instances in which predicting filtration efficiency in nanocomposite is the objective. To explain it another way, the RF generates a large number of decision trees during its filtering phase and uses the average outcome value of each tree as the effective outcome. Evaluating the important factors in the filtering, it is a reliable technique. Combining several classification regression trees with lower performance into the forest using specific filtration regulations along with selecting across all of the decision trees in the framework to predict filtering outcomes is the fundamental principle of the RF model. The RF method e can be defined by Equation (1) and can be produced of decision trees.

$$\{g(A,\theta_l), l = 1,2, \dots N\} \tag{1}$$

Where θ_l and A, define the random vector and the input. At the N^{th} decision tree, the distribution of θ_l occurs independently. Through B categories are present in the input vector A. Equation (2) computes the edge function of filtration considering the input vector A and output vector B.

$$L(A,B) = x_l J[g(A,\theta_l) = B] - {}^{Maxx_l}_{i \neq B} J[g(A,\theta_l) = i] \tag{2}$$

Where x_l represents the effective filtration function and the training set types are indicated as i. The reliability of categorization is highly correlated with a higher edge filtration function. Equation (3) is used to formulate the RF model's generalization error.

$$F^* = Q_{A,B}(L(A,B) < 0) \tag{3}$$

Converging the variance of the RF model (F^*), which is represented by Equation (4), to zero is probable when the number of trees increases for each θ_l.

$$Q_{A,B}\big(Q_\theta(g(A,\theta) = B)\big) - {}^{MaxQ_\theta}_{i \neq B}\big(g\big((A,\theta) = i\big) < 0\big) \to 0 \tag{4}$$

Equation (5) uses the represented to determine the upper bound in the RF model generalization error.

$$F^* \leq \frac{\bar{\rho}(1-t^2)}{t^2} \tag{5}$$

Where t is the tree's average strength and ρ represents the average correlation coefficient. It indicates that the upper bound in the generalization error can be effectively controlled by decreasing the tree connectivity and enhancing the filtration efficiency.

3.4.2 Adaptive Golden Jackal (AGJ) Optimization

The optimization is employed to improve the reliability of the predicting performance of filtration. The AGJ optimization technique mimics the natural hunting behavior of golden jackals. Three steps are included in a golden jackal's hunting motions: hunting, killing, and impacting the prey until it appears as an effective filtration process, followed by leaping in the path of the filtration. During the initialization phase, Equation (6) generates a collection of filtration position matrices that are randomly distributed.

$$\begin{bmatrix} A_{1,1} & \cdots & A_{1,i} & \cdots & A_{1,n} \\ A_{2,1} & \cdots & A_{2,i} & \cdots & A_{2,n} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{N-1,1} & \cdots & A_{N-1,i} & \cdots & A_{M-1,n} \\ A_{N,1} & \cdots & A_{N,i} & \cdots & A_{1,n} \end{bmatrix} \tag{6}$$

In the filtration instance, N represents the number of prey populations and n for dimensions. Based on the mathematical framework of the filtration predicting search for ($|E| > 1$) is determined in Equations (7 and 8).

$$A_1(t) = A_N(t) - E \cdot |A_N(t) - Rl \cdot prey(t)| \tag{7}$$

$$A_2(t) = A_{FN}(t) - E \cdot |A_{FN}(t) - Rl \cdot prey(t)| \tag{8}$$

The prey's position vector is denoted by $prey(t)$, the female golden jackal's position is given by $A_{FN}(t)$, and its current iteration is indicated by t. The regions where golden jackals, both male and female, have been regularly observed are indicated by $A_1(t)$ and $A_2(t)$. The eliminated filters are represented by Equations (9 and 10) to calculate E.

$$E = E_1 \cdot E_0 \tag{9}$$

$$E_1 = c_1 \cdot (1 - (t/T)) \tag{10}$$

Where T represents the maximum number of repetitions in predicting the filtration process, c_1 is a constant set of 0.5 and E_1 indicates that the predicting strength is decreasing the filters. E_0, a random value in the range [– 1,1], represents the filtration's initial prediction. Equations (7) and (8) show that Rl represents a vector of random numbers derived from the Levy flight functions. The symbol represents the distance between a target $|A_n(t) - Rl \cdot prey(t)|$ and the filtration predictions are represented in Equations (11 and 12).

$$Rl = 0.05 \cdot Levyflight(a) \tag{11}$$

$$Levyflight(a) = 0.01 \times (\mu \times \sigma)/(|v^{1/\beta}|) \quad \sigma = \left\{\frac{\Gamma(1+\beta)\times\sin(\pi\beta/2)}{\Gamma\left(\frac{1+\beta}{2}\right)\times\beta\times(2^{\beta-1})}\right\}^{1/\beta} \tag{12}$$

Where, v is a random value in the filtration interval (0,1) and the constant β is 1.5. $A(t+1)$ is a representation of the updated filtration predicting position (Equation (13)).

$$A(t+1) = \frac{A_1(t)+A_2(t)}{2} \tag{13}$$

Prediction expends less energy to avoid the filter when it is processed. The following Equations (14 and 15) represent the mathematical representation of prediction surrounding and filtration prediction: ($|E| \le 1$).

$$A_1(t) = X_N(t) - E \cdot |Rl \cdot A_N(t) - Prey(t)| \tag{14}$$

$$A_2(t) = X_{FN}(r) - E \cdot |Rl \cdot A_{EN}(t) - Prey(t)| \tag{15}$$

To predict the filtration effectiveness in nanocomposite membranes with 2D materials, it proposed the AGJ-RF techniques. It improves the water purification technology and provides the efficient application of nanocomposite membranes in a variety of circumstances.

4. RESULTS AND DISCUSSIONS

This section clearly demonstrates the outcome of the statistical method and predictive method, as well as giving their system configurations.

4.1 Experimental Setup

The performance of the proposed AGJ-RF techniques requires certain system specifications (hardware and software). Table 1 explores the experimental setup.

Table 1 – Experimental Setup

Components	Details
Operating System (OS)	Windows 10
Programming Language	Python 3.10.0
RAM	32GB
Processor	Intel core i7

4.2 Filtration Performance Evaluation

The change in solvent concentration or contaminant particle concentration in the filtration process can be used to measure the filtration performance analysis. Measurement of the filtration flows and rates of rejection for several pollutants, including dyes and salts was performed to determine the membranes' filtration efficiency. In the 2D materials, such as GO and MXenes along with traditional membrane (PVDF) were employed in the filtration performance evaluation for dye contaminants. Table 2 and Figure 1 (a and b) depict the outcomes of dye. The results of salts are determined in Table 3 and Figure 2 (a and b) in various types of nanocomposite membranes.

Table 2 – Outcomes of Dye with Various Nanocomposite Membranes

Types of Nanocomposite Membrane	Filtration Flux (L/m²/h)	Rejection Rate (%)
0.5 % of GO	50	95
1.0 % of MXenes	60	98
Traditional Membrane	35	85

The outcomes of dyes determine that 0.5 % of GO has 50L/m²/h of flux and a 95 % rejection rate. 1.0 % of MXenes, provides rejection rate (98 %) and flux (60 L/m²/h). The traditional membrane explores 35 L/m²/h of filtration flux and an 85 % rejection rate.

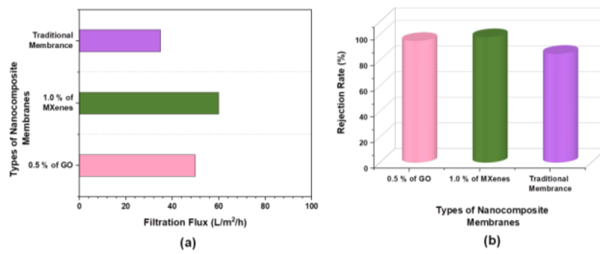

Fig. 1 – (a) Filtration Flux in Dyes and (b) Rejection Rate in Dyes

Table 3 – Results of Salt with Various Nanocomposite Membranes

Types of Nanocomposite Membrane	Filtration Flux (L/m²/h)	Rejection Rate (%)
0.5 % of GO	45	90
1.0 % of MXenes	65	98
Traditional Membrane	30	80

The findings of the salt contaminant of GO with 0.5 % (rejection rate (90 %) and filtration flux (45L/m²/h)), traditional membrane (filtration flux (30L/m²/h) and rejection rate (80 %)) and 1.0 % of MXenes (95 % of rejection rate and 55L/m²/h of filtration flux) are examined.

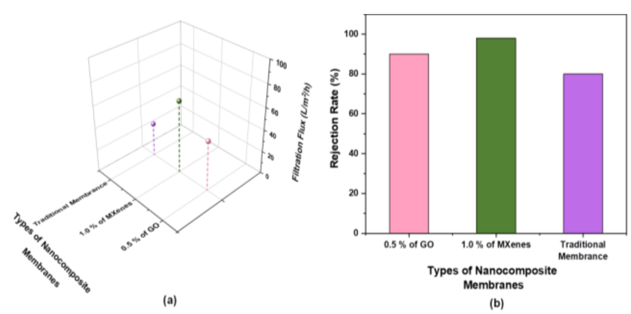

Fig. 2 – (a) Filtration Flux in Salt and (b) Rejection Rate in Salt

1.1 Evaluation of Statistical Assessment

The statistical technique called ANOVA was evaluated between the group and within the group for the performance of filtration prediction. The results of ANOVA were explored in Table 4. The distinct groups' (between and within the group) means are compared to determine the statistically significant variations using the ANOVA.

Table 4 – Evaluation Outcomes of ANOVA

Variation	SS	DF	MS	F-value
Between Group	1200	2	600	15.0
Within Group	800	27	29.63	–
Total	2000	29	–	–

The foundation of ANOVA is the regulation of total variance, which divides the variance found in a specific parameter into components attributed to several sources of variations. SS represents the sum of squares. The mean square is presented as MS, and the degrees of freedom are represented as DF.

5. CONCLUSION

Establishing filtration flux and accurately estimating rejection rate was complex for the interactions between multiple components. A unique AGJ-RF technique was presented in the research for predicting the filtration efficiency in nanocomposite membranes, effectively solving the issue and improving the filtration performance in the membranes. The efficacy of a filter can be assessed by water samples taken in front of and behind 2D materials like GO and MXenes. The particle concentration was measured to calculate the filtration efficiency. The material synthesis employed for the traditional membrane for water treatment is PVDF. Permeability testing as a characterization approach was used to maintain the effective filtration quality. The variance was determined by applying a statistical method identified as ANOVA. For the performance analysis, SPSS software was implemented. The effectiveness of the proposed water filtration technology is tested using Python. It evaluated the different nanocomposite membranes for filtering flex and rejection rates. A variety of matrices, such as RMSE (2.1), MAE (1.5), and R2 (0.88), were used to test the proposed AGJ-RF approach. Based on the testing results, the proposed approach outperformed the 2D material in terms of forecasting filtration efficiency for nanocomposite membranes.

5.1 Limitations and Future Scope

The efficacy of the proposed method could vary depending on the 2D materials and foulants utilized in the research, which limits its generalizability in the range of water conditions. The proposed method could be applied to different membrane materials in the future and other 2D materials, including MoS_2 could be included. To enhance the model's effectiveness, it could be optimized for instant filtration applications and scalability in industrial environments.

REFERENCES

1. C.S.H. Yeo, Q. Xie, X. Wang, S. Zhang, *J. Membrane Sci.* **606**, 118135 (2020).
2. I. Alam, L.M. Guiney, M.C. Hersam, I. Chowdhury, *J. Membrane Sci.* **599**, 117812 (2020).
3. S. Yadav, I. Ibrar, A. Altaee, A.K. Samal, R. Ghobadi, J. Zhou, *Sci. Total Environ.* **745**, 141088 (2020).
4. S. Abdikheibari, L.F. Dumée, V. Jegatheesan, Z. Mustafa, P. Le-Clech, W. Lei, K. Baskaran, *J. Water Process Eng.* **34**, 101160 (2020).
5. J. Yang, Z. Li, Z. Wang, S. Yuan, Y. Li, W. Zhao, X. Zhang, *Adv. Mater. Technol.* **6** No 10, 2000862 (2021).
6. X. Liu, L. Zhang, X. Cui, Q. Zhang, W. Hu, J. Du, H. Zeng, Q. Xu, *Adv. Sci.* **8** No 23, 2102493 (2021).
7. A. Elahi, S. Chaudhuri, *ChemEngineering* **7** No 6, 108 (2023).
8. Y. Liu, X.P. Wang, Z.A. Zong, R. Lin, X.Y. Zhang, F.S. Chen, L.L. Zhang, X.M. Meng, J. Hou, *J. Membrane Sci.* **653**, 120520 (2022).
9. W. Zheng, Y. Chen, X. Xu, X. Peng, Y. Niu, P. Xu, T. Li, *J. Water Process Eng.* **59**, 104876 (2024).
10. M. Fetanat, M. Keshtiara, R. Keyikoglu, A. Khataee, R. Daiyan, A. Razmjou, *Separ. Purification Technol.* **270**, 118383 (2021).
11. M. Frappa, F. Macedonio, A. Gugliuzza, W. Jin, E. Drioli, *Membranes* **11** No 5, 302 (2021).
12. P. Kallem, G. Bharath, K. Rambabu, C. Srinivasakannan, F. Banat, *Chemosphere* **268**, 129306 (2021).
13. J. Fatima, A.N. Shah, M.B. Tahir, T. Mehmood, A.A. Shah, M. Tanveer, R. Nazir, B.L. Jan, S. Alansi, *Front. Environ. Sci.* **10**, 766743 (2022).
14. D. Han, X. Dong, G. Yu, T. Gao, K.G. Zhou, *Adv. Membran.* **2**, 100045 (2022).

Підхід до прогнозування ефективності фільтрації в нанокомпозитних мембранах з використанням 2D-матеріалів

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Потенційні технології очищення та розділення води включають використання нанокомпозитні фільтраційних мембран. Складні взаємозв'язки між численними компонентами ускладнюють точну оцінку коефіцієнта відторгнення та фільтраційного потоку. Щоб вирішити цю проблему та покращити ефективність фільтрації в нанокомпозитних мембранах, це дослідження представляє новий метод адаптивного випадкового лісу, наповненого Golden Jackal (AGJ-RF), для прогнозування ефективності фільтрації в нанокомпозитних мембранах. Полівініліденфторид (PVDF) є традиційною мембраною, що використовується для очищення води разом з двовимірними (2D) матеріалами, такими як MXenes та оксид графену (GO). Для підтримки ефективної якості фільтрації використовується метод характеристики, відомий як тестування на проникність. Для визначення дисперсії використовується статистичний метод, відомий як дисперсійний аналіз (ANOVA). Цей аналіз використовує програмне забезпечення SPSS для оцінки продуктивності. Ефективність запропонованого методу фільтрації води проводиться за допомогою платформи Python, за допомогою якої можна оцінити гнучкість фільтрації та коефіцієнт відторгнення шляхом порівняння GO, Mxenes та традиційних мембран. Запропонований метод AGJ-RF був виконаний у різних матрицях: RMSE (2.1), MAE (1.5) та R2 (0.88). Експериментальні результати показують, що запропонована методика має більшу ефективність у прогнозуванні якості фільтрації в нанокомпозитних мембранах з використанням 2D-матеріалів.

Ключові слова: Нанокомпозитна мембрана, Двовимірні (2D) матеріали, Фільтрація води, Оксид графену (GO), Якість фільтрації.