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REGULAR ARTICLE

Enhancing Nanocomposite Filtration Membranes: Refined SVM Approach for Precise Estimation of Permeate Flux and Foulant Rejection

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The nanocomposite filtration membranes have emerged as potential water purification and separation technologies. However, reliable estimation of foulant rejection and permeate flux remains difficult due to the complicated interaction of many components. Traditional modeling techniques fail to capture the complex dynamics at work. In this paper, we provide a Refined Support Vector Machine (RSVM) strategy to solve this issue and increase the performance of nanocomposite filtration membranes. To normalize the features, the data are pre-processed using min-max normalization. Data features like foulant rejection rates, permeate flux values, membrane features, and experimental setup are displayed. Furthermore, the proposed RSVM to determine the best input factors for the effectiveness of each nanocomposite membrane. Due to the strong resilience of RSVM and the great generalization ability of the ML model, the obtained results demonstrated that the RSVM model's prediction efficiency (R_2 = 0.995) outperformed the mathematical model in terms of prediction performance. To conduct training, validation and testing for this work, we employed statistical data including 764 samples of the input variables (five) and output variables (two). The RSVM approach provides a dependable and effective way to forecast membrane fouling and water filtration by predicting foulant rejection and permeate flux.

Keywords: Thin-film nanocomposite (TFN), Machine learning, Permeate flux, Foulant rejection, Refined Support Vector Machine (RSVM).

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1. INTRODUCTION

The thin film nanocomposite filtration membrane has been conducted during the past two decades for both industrial and domestic uses, with a focus on nanocomposite-filtered membranes. Both organic materials (polymers) and inorganic materials (ceramics) can be used to make membranes; polymeric materials have been studied due to their chemical stability, mechanical strength and flexibility. The term "permeate flux" defines the rate at which a fluid that has been filtered or treated permeates the membrane surface per unit area throughout a particular period. The capacity of the membrane to prevent or reject the passage of unwanted chemicals (foulants) between the permeate side and the feed solution is referred as foulant rejection. To extend the membrane's life and increase its function, nanocomposites are used in membrane technology [1]. Polymeric membrane performance, mainly ultra filtration (UF) membranes, the application of nano-filtration such as TiO_2, SiO_2, GO, Ag, SWCNTs, and Cuinpolymer matrices has generated significant. Commercialization of membranes modified with nanocomposite was impeded by concerns for the long-term effects of exposure to nano-filtration leached from the polymer and a reluctance to change their current manufacturing lines [2], which include the combination of polymer, solvent and nano-filtration filler, without an accurate cost-benefit analysis. A design platform to speed up the development of innovative nanocomposite membranes is desired by membrane groups. When machine learning (ML) is used instead of conventional experimental and computational methods, the production time of UF nanocomposite membranes can be decreased [3-4].

2. RELATED WORK

The article [5] suggested that commercial and in-

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house polyether sulfone (PES) membranes, and thin TiO_2 nanoparticle mesoporous coatings in a range of pore sizes were produced utilizing a hydrothermal low temperature (HLT) method. After dip-coating titanic sol-gel particles onto membrane substrates, the other organic templates were separated using heat and Ultraviolet (UV) light treatments. To improve the coating's surface qualities and microstructure, dip-coating parameters were varied, such as the number of coating cycles, dipping and withdrawal velocities drying and holding times. The research [6] proposed these membranes to vast regions are visible, Graphene-based membranes have great potential for creative separation platforms because of their accurate molecular filtration of dissolved molecules and gas as well as their rapid water transfer. The ideal filtration membrane structure consists of a thin, dense, and defect-free serving as a practical filter; porous and more permeable support is mechanical strength.

The study [7] suggested the wastewater from the production of cheese puts pressure on the environment. The use of the convolutional neural network (CNN)modelling in dynamic whey flux data studies has wider use, as it can be used to improve whey recovery efficiency by sensor tuning that in effect enables online flux monitoring. The author [8] proposed that membrane technologies have become increasingly prevalent in wastewater and water treatment operations. AI allows simpler system operation, including better planning, tracking, and real-time comprehensive understanding of resource loss, thus maximizing revenue capture and water quality satisfaction. The research [9] presented the difference between the output values of the model and the real values suggested by the study. To create materials with intrinsic composite features, membrane technology and polymeric materials have continued to concentrate on membrane modification. The article [10] proposed the ML approach can handle complex nonlinear interactions; it has been widely used in many fields, such as water chemistry. The possible use of ML in desalination research holds great potential in developing sustainable and effective desalination technologies. The author [11] suggested membrane technologies are becoming more useful and adaptable for sustainable development. An optimal framework for integrating ML techniques with particular application goals in membrane design and discovery is provided along with best practices. The study [12] developed membranes using nanotechnology that are gaining widely recognized as an eco-friendly technology for significant separation processes, capable of resolving the trade-off dispute seen in conventional methods for the separation of membranes. The main topics of this area include desalination, food, energy and biomedical fields, as well as air and water purification, as well as the latest developments in advanced nanocomposite membranes and their potential applications. The article [13] suggested that Green nanotechnology is the generation of safe technology to reduce potential risks for the health of humans and the environment both the manufacturing and consumption of nanotechnology products [14-16].

3. METHODOLOGY

In this section, the proposed RSVM attempts to predict two essential parameters in membrane filtering processes: permeate flux (the rate of fluid flux through the membrane) and foulant rejection (the membrane's capacity to reject or remove undesired substances).

3.1 Dataset

The materials, architectures, and production methods for incorporating various nanomaterial types into TFN membranes are designed to raise the efficiency of the membranes exceeding the level achievable with conventional manufacturing. The statistical data 764 samples were used in this study. Table 1 show the statistics data for five input and two output variables.

Table 1 – Input and output variable of statistical data

Variables	Means± SD	Range	Description
Input Variables			
Thin layer Thickness	224 ±200.4	31.75–2250	–
Temperature post-treatment(◦C)	70.68±16.23	26–121	–
Location of theNPs	1.40	0–6	"Organic solution," "PVA solution," "Aqueous solution," "Grafted on the TFC membrane," "Membrane support," "PSF support," and "Polymer support casting solution." was changed to 0, 1,2,…,6respectively.
Duration of post-treatment (minutes)	17.19±41.45	1–241	–
Operation pressure (PSI)	161.3±91.88	14.51–30.01	–
Output Variables			
Foulant rejection (%)	54.60–99.70	92.95 ± 8.45	–
Permeate flux	0.38–137.79	35.24 ± 23.60	–

Note: Pounds per square inch (PSI), polyvinyl alcohol (PVA), Price per Square Foot (PSF)

Input Variables:

1. Thin layer thickness: This refers to the thickness of the thin layer in the filtration process, which has an impact on foulant accumulation and permeates flow.
2. Location of nanoparticles (NPs): The arrangement or spatial distribution of nanoparticles in the filter, which can have an impact on fouling and filtered efficiency.
3. Temperature post-treatment: The temperature at

which membrane properties and fouling behavior are affected by post-treatment performed after filtration.

4. Duration of post-treatment: The length of post-treatment, which impacts the membrane is cleaned or rejuvenated.
5. Operation pressure: The pressure at which the filtration system operates, affecting the driving force for permeation and fouling dynamics.

Output Variables:

1. Permeate flux: The rate which the filtrate passes through the membrane per unit area and time is known as the filtration flux or permeation rate.
2. Foulant rejection: The percent of retained foulants compared to the total amount in the feed shows the membrane rejects contaminants or foulants.

3.2 Data Pre-processing Using Min-Max Normalization

We use Min-Max Normalization for normalize the input variables to improve accuracy and speed up the learning phase. Normalization of the RSVM's input data is becoming more popular in the classification process of RSVMs. Translation of data into the range (or any other range) or transferring information onto the unit sphere is called normalization in ML. Standardization and normalization can be beneficial for some ML algorithms, particularly when Euclidean distance is used.

$$W_{norm} = \frac{M_{max} - M_{min}}{W_{max} - W_{min}} \times (W - M_{min}) + M_{min} \quad (1)$$

When vector X is used as the input or output, the normalized form of W_{norm} is the same. M_{min} and M_{max} are the input values, whereas W_{max} and W_{min} are the min values and max values of the output vectors, − 1 and +1, respectively

3.3 Refined Support Vector Machine (RSVM)

The supervised ML algorithm that can be applied to regression and classification problems is a refined support vector machine (RSVM). RSVM can be used for a variety of tasks in the context of nanocomposite filtration membranes, including the calculation of membrane presentation, the classification of various membrane types, and the optimization of membrane properties. In general, ML uses kernel function implementation and high dimensional space simplification to perform data classification and reduce structural risk.

The RSVM technique aims to offer precise and reliable estimations of permeate flux and foulant rejection. This accuracy is critical for maximizing membrane filtering operations, increasing system efficiency, and maintaining constant product quality. The RSVM was highly accurate in predicting the pore and fracture pressures if the coefficient of determining reporting responsibility (R^2) was more than 0.995. It is a crucial component in membrane structure. With a few real-time surface drilling measurements, it is feasible to calculate the fracture pressure and estimate the pore pressure without the necessity for pressure trends.

Using a dataset that includes observations of the input variables (thin layer thickness, NP location, temperature post-treatment, duration of post-treatment, operation pressure) and corresponding values of the output variables (permeate flux, foulant rejection), the RSVM approach involves creating an ML model. To create accurate predictions or estimations for unseen data, the model is trained to identify the underlying patterns and connections between the inputs and outputs.

$$min_{\omega,a,f} I\ (\omega, f) = \frac{1}{2}\omega^2 + \gamma\ \sum_{j=1}^{n} W_s \quad (2)$$

Such that

$$Zj(\omega' Wi + a) + \varepsilon i \geq 1;\ \varepsilon i \geq 0;\ i\ =\ 1, 2, \dots, n \quad (3)$$

$$min_{\omega,a,f} I\ (\omega, f) = \frac{1}{2}\|\omega^2\| + \frac{1}{2}\gamma\ \sum_{l=1}^{n} f_l^2 \quad (4)$$

Here I, W_j, and Z_j are representative of the binary target, slack variable and the risk bound, respectively. Along with the bias, slack variable, weight matrix, error and regularization parameter are represented by the symbols $\mu, \tau, a, \varepsilon i, \varphi$, W_j and Z_j in that order. This method of determining the Lagrangian function was used to solve the problem:

$$K_{LSSVM} == \frac{1}{2}\|\omega^2\| + \frac{1}{2}\gamma\ \sum_{l=1}^{n} f_l^2 - \sum_{l=1}^{M} \alpha_l\ \{(\omega.\theta\ (\omega_l)) + a + f_l - z_l\} \quad (5)$$

The Lagrangian multipliers are represented by α_k in Eq. (3) Eq. (4) provides the derivatives of Eq. (3) for $a, f, \omega,$ and αk are used to determine the parameters.

$$\frac{\partial K_{LSSVM}}{\partial \omega} = \frac{\partial K_{LSSVM}}{\partial a} = \frac{\partial K_{LSSVM}}{\partial f_l} = \frac{\partial K_{LSSVM}}{\partial \alpha_l} = 0 \quad (6)$$

$$\omega = \sum_{l=1}^{M} \alpha_l\, \emptyset(w_l) \quad (7)$$

$$\sum_{l=1}^{M} \alpha_l = 0 \quad (8)$$

$$\alpha l = \gamma f_l l = 1, \dots, M \quad (9)$$

$$(\omega. \emptyset(wl)) + a + fl - zl = 0\ l = 1, \dots M \quad (10)$$

$$\begin{bmatrix} 0 & J_M^S \\ J_M \Omega + \gamma^{-1/M} \end{bmatrix} \begin{bmatrix} a \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ Q \end{bmatrix} \quad (11)$$

Using the equations mentioned above, the definition of a linear system as follows:

$$\Omega_{se} = \emptyset\ (w_s)\emptyset(w_e) = L(w_s, w_e) \quad (12)$$

In several domains, such as water treatment, wastewater management, membrane filtered process, the application of RSVM for measuring penetrates flux and foulant rejection is important. By reducing energy consumption and maintenance needs, precise estimation of these parameters can enhance the performance of systems for filtration, increase process efficiency and reduce operating expenses. In conclusion, an RSVM technique was developed to predict foulant rejection and permeate flow in a filtered or separation system based on two output variables and five input variables.

4. RESULT AND DISCUSSION

4.1 Statistical Analysis

The data indicates that the polyamide layer (PA) is the primary polymer utilized in the production of TFN. An attribute of nanocomposite membranes, which consist of two or more polymers which is produced one or more support layers that are porous is a thin polymer barrier layer. TFN fabrication has the use of major polymers. One important feature of membrane construction that will affect TFN economics is the ability to coat the porous sub-layer with a thick, ultrathin layer of material specialized to nanoparticles using a variety of ways. The existing focus on membrane research must be on developing with creating efficient nanocomposite membranes that have high solute rejection, improved water flux, improved physicochemical integrity, and small surface fouling.

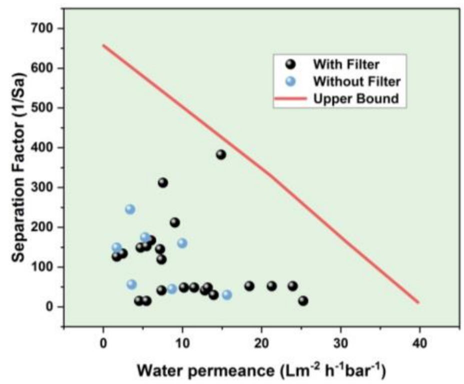
The PIP solution and trimethyl chloride solution react at a slow rate. An acid acceptor with a higher concentration value and acyl halide is required for the polyamide-increased activity layer. However, the integrated acid acceptor in MPD-based membranes is the high tertiary amine focused. The trend shows that the two common reactive monomers are increasing. Table 2 shows the evaluation of TFN membrane performance.

Table 2 – TFN membrane performance

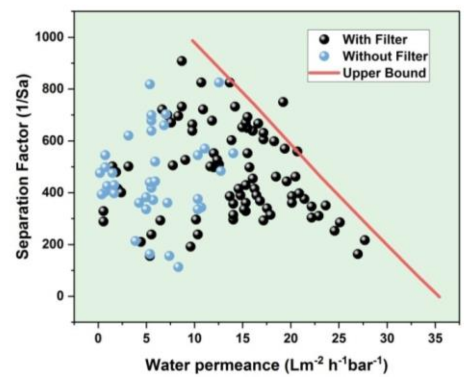
Name	No of membranes
Water	62
Na_2SO_4	55
$MgCl_2$	30
$MgSO_4$	46
NaCl	111

4.1.1. Evaluation of TFN Membrane Performance

In spite of being widely used in separation methods, polymeric membranes, the TFN membrane's performance has been restricted by the compatibility of their permeability and selectivity. Robeson's upper bound can be used to show this trade-off in gas separation applications. They investigate whether this upper bound idea can also apply to water separation in this study, in addition to restricted gas separation membranes. Desalination and water purification are two uses for TFN membranes, a type of membrane technology. To confirm laboratory-scale results and evaluate real-world performance, pilot- or field-scale testing is frequently required. In general, more permeable membranes reflect an increase in Na_2SO_4 and a decrease in $MgCl_2$ and $MgSO_4$ separation factor. Fig. 1 (a) and (b) shows a scatter plot of the water permeance of PA nanocomposite membranes in TFN with and without nanoparticles against the separation factors of $MgCl_2$ (1/Sa), and Na_2SO_4 (1/Sa).



(a)



(b)

Fig. 1 – Water penetration scatter graph a) $MgCl_2$, b) Na_2SO_4

4.2 Correlations of Input Variables

Evaluating the connection between each set of variables is essential for machine learning models since high correlation coefficients between RSVM models' input parameters could result in excessive fitting. Table 3 shows the RSVM models permeate flux input variables correlation coefficients. Because of the extremely low correlation coefficient values (less than 0.6), the suggested RSVM models' inputs haves no bond.

Table 3 – Input variables for correlation coefficients in the RSVM model for permeate flux

	Operation pressure	Thickness of thin layer	NPs location	Temperature post-treatment	Duration of post-treatment
Operation pressure	1.00				
Thin layer thickness	0.33	1.00			
Location of the NPs	– 0.39	– 0.03	1.00		
Temperature post-treatment	0.50	0.06	–0.12	1.00	
Duration of post-treatment	0.02	0.17	0.06	– 0.10	1.00

The trimethyl chloride (TMC in n-hexane) organic phase concentration, rejection, NP position, operation pressure, particle concentration, temperature, duration, contact angle, and thin layer thickness, were chosen as the eight variables of the RSVM models to estimate foulant rejection and permeate flux.

5. CONCLUSION

This study utilizes ML for nanocomposite filtration membranes, to calculate foulant rejection and permeates flux. Through an extensive study of various input variables including thin layer thickness, post-treatment duration, operation pressure, NP location and post-treatment temperature the study effectively utilized Refined Support Vector Machine (RSVM) models to accurately estimate foulant rejection and permeate flux. After that, the RSVM models' initial weights were modified to increase R_2 and reduce MSE. The results demonstrated the efficiency of the RSVM model as a high-accuracy, general-purpose method for predicting permeate flow and foulant rejection using training, validation, test and unseen data. Without performing expensive and time-consuming real experiments, the suggested approach can be utilized to determine permeate flow and foulant rejection as well as takes into consideration the effects on nanocomposite filtration membranes of each experimental condition.

REFERENCES

1. M. Fetanat, M. Keshtiara, Z.X. Low, R. Keyikoglu, A. Khataee, Y. Orooji, V. Chen, G. Leslie, A. Razmjou, *Ind. Eng. Chem. Res.* **60** No 14, 52365250 (2021).
2. C. Wang, L. Wang, A. Soo, N.B. Pathak, H.K. Shon, *Separation Purification Technology* **304**, 122328 (2023).
3. M. Asghari, A. Dashti, M. Rezakazemi, E. Jokar, H. Halakoei, *Rev. Chem. Eng.* **36** No 2, 265 (2020).
4. L. Wang, Z. Li, J. Fan, G. Lu, D. Liu, Z. Han, *J. Environ. Chem. Eng.* **11** No 5, 111154 (2023).
5. Y. Liu, X. Wang, X. Gao, J. Zheng, J. Wang, A. Volodin, Y.F. Xie, X. Huang, B. Van der Bruggen, J. Zhu, *J. Membr. Sci.* **596**, 117717 (2020).
6. M.B.M.Y Ang, J.M. Pereira, C.A. Trilles, R.R. Aquino, S.-H. Huang, K.-R. Lee, J.- Y. Lai, *Sep. Purif. Technol.* **210**, 521 (2019).
7. L.T. Yogarathinam, K. Velswamy, A. Gangasalam, A.F. Ismail, P.S. Goh, A. Narayanan, M.S. Abdullah, *J. Environ. Manag.* **301**, 113872 (2022).
8. N.D. Viet, D. Jang, Y. Yoon, A. Jang, *Crit. Rev. Environ. Sci. Technol.* **52** No 20, 3689 (2022).
9. M.J. Talukder, A.S. Alshami, A. Tayyebi, N. Ismail, X. Yu, *Separation & Purification Rev.* 53 No 2, 216 (2023).
10. N. Baig, J. Usman, S.I. Abba, M. Benaafi, I.H. Aljundi, *J. Cleaner Prod.* **418**, 138193 (2023).
11. H. Yin, M. Xu, Z. Luo, X. Bi, J. Li, S. Zhang, X. Wang, *Green Energy Environ.* **9** No 1, 54 (2024).
12. O. Gupta, S. Roy, *Nanocompos. Membrane. Water Gas Separat.* 29 (2020).
13. K.C. Khulbe, T. Matsuura, *Nanotechnology in Membrane Processes* (Springer Nature Switzerland AG: 2021).
14. T.H. Lee, J.Y. Oh, S.P. Hong, J.M. Lee, S.M. Roh, S.H. Kim, H.B. Park, *J. Membr. Sci.* **570–571**, 23 (2019).
15. N.A. Ahmad, P.S. Goh, K.C. Wong, A.K. Zulhairun, A.F. Ismail, *Desalination* **476**, 114167 (2020).
16. N. Li, L. Yu, Z. Xiao, C. Jiang, B. Gao, Z. Wang, *Desalination* **473**, 114162 (2020).

Покращення нанокомпозитних фільтраційних мембран: удосконалений підхід SVM для точної оцінки потоку пермеату та відторгнення забруднень

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Нанокомпозитні фільтраційні мембрани з’явилися як потенційні технології очищення та розділення води. Однак надійна оцінка відторгнення забруднюючих речовин і потоку пермеату залишається важкою через складну взаємодію багатьох компонентів. Традиційні методи моделювання не можуть повністю проконтролювати складну динаміку в роботі. У цій статті запропонована стратегія удосконаленої опорної векторної машини (RSVM) для вирішення цієї проблеми та підвищення продуктивності нанокомпозитних фільтраційних мембран. Для нормалізації функцій дані попередньо обробляються за допомогою мінімально-максимальної нормалізації. Відображаються характеристики даних: рівень відторгнення забруднюючих речовин, значення потоку пермеату, характеристики мембрани та експериментальна установка. Крім того, запропонований RSVM для визначення найкращих вхідних факторів для ефективності кожної нанокомпозитної мембрани. Завдяки високій стійкості RSVM і великій здатності моделі ML до узагальнення, отримані результати продемонстрували, що ефективність прогнозування моделі RSVM (R_2 = 0,995) перевершує математичну модель з точки зору ефективності прогнозування. Для проведення навчання, перевірки та тестування для цієї роботи були використані статистичні дані, включаючи 764 зразки вхідних змінних (п’ять) і вихідних змінних (дві). Підхід RSVM забезпечує надійний і ефективний спосіб прогнозування забруднення нанокомпозитної мембрани та фільтрації води шляхом прогнозування відторгнення забруднюючих речовин і флюсу пермеату.

Ключові слова: Тонкоплівковий нанокомпозит (TFN), Машинне навчання, Пермеатний потік, Відмова від забруднень, Вдосконалена опорна векторна машина (RSVM).