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Review article

Micropollutant rejection by nanofiltration membranes: A mini review dedicated to the critical factors and modelling prediction

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A R T I C L E I N F O

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A B S T R A C T

Nanofiltration (NF) membranes, extensively used in advanced wastewater treatment, have broad application prospects for the removal of emerging trace organic micropollutants (MPs). The treatment performance is affected by several factors, such as the properties of NF membranes, characteristics of target MPs, and operating conditions of the NF system concerning MP rejection. However, quantitative studies on different contributors in this context are limited. To fill the knowledge gap, this study aims to assess critical impact factors controlling MP rejection and develop a feasible model for MP removal prediction. The mini-review firstly summarized membrane pore size, membrane zeta potential, and the normalized molecular size ($\lambda = r_s/r_p$), showeing better individual relationships with MP rejection by NF membranes. The Lindeman-Merenda-Gold model was used to quantitatively assess the relative importance of all summarized impact factors. The results showed that membrane pore size and operating pressure were the high impact factors with the highest relative contribution rates to MP rejection of 32.11% and 25.57%, respectively. Moderate impact factors included membrane zeta potential, solution pH, and molecular radius with relative contribution rates of 10.15%, 8.17%, and 7.83%, respectively. The remaining low impact factors, including MP charge, molecular weight, logKow, pKa and crossflow rate, comprised all the remaining contribution rates of 16.19% through the model calculation. Furthermore, based on the results and data availabilities from references, the machine learning-based random forest regression model was trained with a relatively low root mean squared error and mean absolute error of 12.22% and 6.92%, respectively. The developed model was then successfully applied to predict MPs' rejections by NF membranes. These findings provide valuable insights that can be applied in the future to optimize NF membrane designs, operation, and prediction in terms of removing micropollutants.

1. Introduction

With the continuous development of detection technology, various emerging trace organic micropollutants (MPs),such as pharmaceuticals and personal care products (PPCPs) or pharmaceutically active compounds (PhACs), disinfection by-products (DBPs), endocrine disrupting chemicals (EDCs), carcinogenic polycyclic aromatic hydrocarbons (PAHs), have been frequently detected in the aquatic environment (Bolong et al., 2009; Liu et al., 2020; Lv et al., 2017). Even though the concentrations of MPs in waters are low, usually in the order of ng L^{-1} to μg L^{-1}, they are very difficult to be naturally biodegraded, therefore posing potential risks to aquatic organisms (Lin et al., 2016; Pan et al., 2021). If the contaminated water is consumed by aquatic organisms, they may affect the functioning of nervous system, induce the production of drug-resistant strains, and cause biological reproduction disorders or abnormal development (Overturf et al., 2015).

Wastewater treatment plants (WWTPs) have been recognized as the primary sources of MPs in the water environment, as the traditional

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secondary biological treatment process is largely ineffective in removing MPs from wastewater (Roberts et al., 2016). To date, membrane technologies, such as microfiltration (MF), ultrafiltration (UF), reverse osmosis (RO), and nanofiltration (NF), have been widely used in advanced wastewater treatment with one of the specific targets being MPs (Goh et al., 2022; Luo et al., 2018). Among them, the NF membrane approach has broad application prospects for wastewater treatment, owing to the advantages of selective permeability, low monovalent ion rejection rates, and effective MP rejection (Ahmad et al., 2022; Garcia-Ivars et al., 2017; Li et al., 2022).

Previous studies have demonstrated that several factors can affect the MP rejection efficiencies of NF membranes. Those factors include membrane properties (e.g., pore size, hydrophilicity or hydrophobicity, zeta potential, surface groups, etc.), MPs properties (e.g., molecular radius, molecular weight, molecular structure, ionization state, etc.), NF system operation conditions (e.g., operation pressure, crossflow rate, and recovery rate), and properties of NF influent (e.g., influent temperature, inorganic ion concentration, organic matter concentration, and solution pH) (Azais et al., 2016; Garcia-Ivars et al., 2017; Yangali-Quintanilla et al., 2010). Several experiments have been conducted to assess the properties of NF membranes, characteristics of target MPs, and system operation conditions (Taheran et al., 2016). However, systematic quantitative assessment of these individual factors on MP rejection by NF membranes and the potential interactions are essential to facilitate the design and operation of effective NF membranes for MP removal.

Even though several classical mathematical models have been used to predict targeted MP rejection by NF membranes (Bowen and Mukhtar, 1996, Lab Ba N et al., 2017), relatively reliable models for the assessment of important available parameters related to MP rejection under different conditions are lacking. Therefore, machine learning-based models, such as support vector machine (SVM), multilayer perceptron (MLP), and extreme gradient boosting (XGBoost) models, have been developed in membrane process researches (Lyu et al., 2018; Wang et al., 2023; Zhu et al., 2023), which are powerful tools to deal with complex nonlinear problems and provide a higher accurate interpretation of membrane separation process. Due to fewer training variables, high prediction accuracy, and effective capacity to model complex nonlinear dimensional relationships, random forest regression (RFR) model has been deemed as an easy-to-use and powerful approach (Chang et al., 2023; Giri et al., 2023). Previous studies have successfully applied the RFR model to understand the organic solvent movement in membrane separation processes (Hu et al., 2021; Zhu et al., 2023). However, the feasibility and effectiveness of RFR model in predicting MPs rejections through NF membranes need further exploration.

Therefore, this study aims to investigate the contribution and interactions of individual impact factors on MP rejection by NF membranes, and further develop an effective machine-learning based prediction model. Firstly, a literature review was conducted to collect available data on MP rejection during NF membrane treatment. The individual relationships between the membrane properties (e.g., pore size and zeta potential), MP properties (e.g., molecular weight and molecular radius), and operation conditions (e.g., operation pressure, crossflow rate, and solution pH) were investigated. The Lindeman-Merenda-Gold (LMG) model was used to quantitatively assess the relative contributions of the related impact factors to MP rejection. The RFR theory was used to model the rejection of targeted organic MPs by NF membranes using primary parameters detected by the LMG model.

2. Materials and methods

2.1. Data selection

The Web of Science and Science Direct databases were used to extract literature using the search keywords "nanofiltration" and "micropollutant/trace organic pollutant/emerging contaminant/antibiotic/PPCPs/EDCs/PhACs". As the temperature at which a filtration experiment is carried out could lead to obvious differences in MP rejection (Xu et al., 2020), the summarized data were obtained at a temperature range 20–25 °C in this study. A total of 21 journal articles, covering six types of NF membranes and 30 species of MPs, were obtained (Table 1). The physicochemical properties of the MPs are listed in Table S1. In total, 290 rows of data were analyzed to investigate the impacts of individual factors on MP rejection and then quantitatively evaluate their contributions.

2.2. Data analysis

Relative contribution rate. The Lindeman-Merenda-Gold (LMG) model was used to quantitatively assess the relative importance of each impact factor, including membrane pore size, membrane zeta potential, operation pressure, crossflow rate, solution pH, molecular weight, pKa, LogKow, MP charge, and molecular radius to MP rejection. Based on multiple regression analysis, the LMG model offers the possibility to quantify the contribution of each individual impact factor to the variance of the model. Considering the correlation and sequential effect between dependent variables, it decomposes the variance of dependent variables by averaging all possible marginal contributions to the variables to calculate the relative contribution of each dependent variable (Gong et al., 2020; Liu et al., 2019; Meng et al., 2018). The "relaimpo" package (Groemping, 2006) in R studio (https://cran.r-project.org) was used to support the analysis following Eq. (1). (Carvalhais et al., 2014).

$$\mathrm{LMG}(x_j)=\frac{1}{p}\sum_{k=0}^{p-1}\sum_{\substack{S\subseteq\{x_1,\dots,x_p\}/\{x_j\}\\ n(S)=k}}\frac{seqR^2(\{x_j\}|S)}{C_{p-1}^{k}} \tag{1}$$

where x is the regression variable, S is the set of variables that were entered into the model, and R is the fit goodness of model.

Rejection prediction. The RFR is composed of a set of regression subtrees$\{h(x, \theta_t), t = 1,2, \dots, T\}$and selects the means of regression results of each decision tree$\{h(x, \theta_t)\}$as the regression prediction value (Eq. (2)).

$$\overline{h}(x)=\frac{1}{T}\sum_{t=1}^{T}\{h(x,\theta_t)\} \tag{2}$$

where θ_t represents the independent and identically distributed random variable, x represents the independent variable, T represents the number of regression decision trees, $h(x, \theta_t)$ represents the output based on x, $h(x)$ represents the predicted result of model.

In the summarized dataset, the explanatory variables included membrane pore size, operation pressure, membrane zeta potential, solution pH, and molecular radius, while the response variable was the rejection rate of MP. The dataset contained 201 sample groups. After normalization, the sample groups of the dataset was disordered and divided into training samples and testing samples according to the ratio of 7:3 (Chang et al., 2023). The training samples were used to optimize the random forest regression and develop the prediction model, while the testing samples were used to evaluate the model's accuracy. After the calculation results were denormalized, the root mean squared error (*RMSE*), mean absolute error (*MAE*) and goodness of fit (r^2) were used for model evaluation. RFR used Python 3.10 operations in the Pycharm development environment.

3. Results and discussion

3.1. Effect of membrane properties on MP rejection

Previous studies have demonstrated that the mechanisms of MP rejection by NF membranes primarily include adsorption, electrostatic

Table 1
Properties of NF membranes investigated in this study.

Membrane	Active layer material	Manufacturer	Water permeability (L/m^2 h bar)	$MgSO_4$ rejection (%)	Membrane molecular weight cut-off (Da)	Membrane zeta potential at pH 7.0–8.0 (mV)	Pore radius (nm)	Contact angle (°)	References
NF270	Polypiperazine-based	Film Tec, Dow	0.46	>97	200–400	–	–	30.6	Higgins and Duranceau (2020)
			13.5	–	–	–	0.42	55	(Nghiem et al. 2004, 2005)
			17.8	–	300	−19	0.84	64.1	Lin et al. (2014)
			17.8	85–95	300	−24.7	0.42	63.2	Lin (2018)
			13.5	–	–	−24.7	0.84	32	Vogel et al. (2010)
			13.5	–	–	−24.7	0.84	–	Nghiem and Hawkes (2007)
			14.1	–	–	–	0.42	–	Azais et al. (2016)
			–	97	–	–	0.42	–	Shah et al. (2012)
			–	96	220	−82.1	0.258	35	Azaïs et al. (2014)
NF90	Composite polyamide	Film Tec, Dow	10.6	97	200	–	0.34	63.2	Lin et al. (2019)
			6.4	–	–	–	0.34	42.5	Nghiem et al. (2005)
			10.6	–	200	−24.9	0.68	63.2	Lin et al. (2014)
			17.8	85–95	200	−27	0.34	–	Lin et al. (2018)
			2.23	–	200	−32	0.34	–	Yangali-Quintanilla et al. (2010)
			6.4	–	–	−27.3	0.68	–	Nghiem and Hawkes (2007)
			6.6	–	150	–	0.34	–	Azais et al. (2016)
			–	97	–	–	0.34	–	Shah et al. (2012)
			–	98	102	−59.3	0.128	58.1	Azaïs et al. (2014)
SR2	Polyamide	Koch Membrane Systems (San Diego, CA)	15.4	–	–	−10.4	1.28	–	Nghiem and Hawkes (2007)
VNF1	Polyamide	Vontron Technology Co., Ltd.	–	96	–	−44.0	0.52	36.4	Xu et al. (2020)
VNF2	Polyamide	Vontron Technology Co., Ltd.	–	96	–	−52.0	0.48	79.4	Xu et al. (2020)
DF30	Polyamide	Beijing Origin Water Technology Co., Ltd.	7.56	–	400	−75.1	0.43	15.2	Xu et al. (2019)

rejection, screening, and steric resistance (Semiao et al., 2013). It has also been observed that the properties of NF membranes, including pore size, zeta potential, and the hydrophilicity or hydrophobicity of the membrane surface, can significantly influence the rejection of different MPs (Garcia-Ivars et al., 2017). Generally, the surface of the active layer of NF membranes is usually negatively charged. This can result in electrostatic repulsion between the active layer and negatively charged MPs as well as electrostatic adsorption towards positively charged MPs. Besides, MP adsorption onto NF membranes mainly occurs at the initial stage of the entire filtration process, while the mechanism of steric resistance plays a major role in MP rejection at later membrane filtration stages (Kim et al., 2018).

In this study, we investigated the effects of membrane pore size and zeta potential on MP rejection by different NF membranes. The results showed that the pore size of the NF membranes varied in the range 0.128–1.28 nm as reported in different studies (Fig. 1a). While different studies reported different pore sizes for the same NF membrane, for example, the pore size of the NF270 membrane was determined to be 0.258, 0.42, and 0.84 nm in different studies (Fig. 1a). In summary, the results indicated that MP rejection decreased with increasing NF membrane pore size, showing a general negative correlation ($r^2 = 0.21$, Fig. 1a).

The zeta potentials of the NF membranes investigated in this study were in the range of −82.1 to −10.4 mV (Fig. 1b). Specifically, different studies reported varied zeta potentials of the NF270 membrane, such as −82.1, −24.7, and −19.0 mV (Azaïs et al., 2014; Lin, 2018; Lin et al., 2014; Nghiem and Hawkes, 2007; Vogel et al., 2010). Similarly, the NF90 membrane also showed varied zeta potentials of −59.3, −32.0, −27.3, −27.0, and −24.9 mV in different studies (Lin et al. 2014, 2018; Nghiem and Hawkes, 2007; Yangali-Quintanilla et al., 2010). With a zeta potential of −27.3 mV, the NF90 membrane showed the highest MP rejection rate, with an average value of 98.88%. While the SR2 membrane, with a zeta potential of −10.4 mV, showed the lowest MP rejection rate, with an average value of 32.10%. The relationship between the zeta potential values of the NF membranes and MP rejection showed an inverted "U" type relationship with an r^2 value of 0.74, suggesting that the zeta potential of NF membrane should be in a reasonable range to achieve a high rejection rate to different charged MPs.

3.2. Effect of operation conditions on MP rejection

The operation conditions of the NF filtration process, including operation pressure, influent temperature, crossflow rate, and solution pH, can significantly influence MP rejection. With an increase in operation pressure, the interception effect on MPs is enhanced. One reason for this observation is that the contaminated layer on the membrane surface could be gradually compacted, resulting in a decrease in the number and diameter of membrane pores as well as an increase in the MP rejection rate by the NF membranes (Fig. 2). Moreover, according to the analysis based on the dissolution diffusion model, water flux increases with an increase in operation pressure, thereby leading to a relative decrease in the concentration of MPs in the permeate, while their concentration in the stock solution increases. Therefore, this analysis indicated that MP rejection by NF membranes increased with increasing operation pressure.

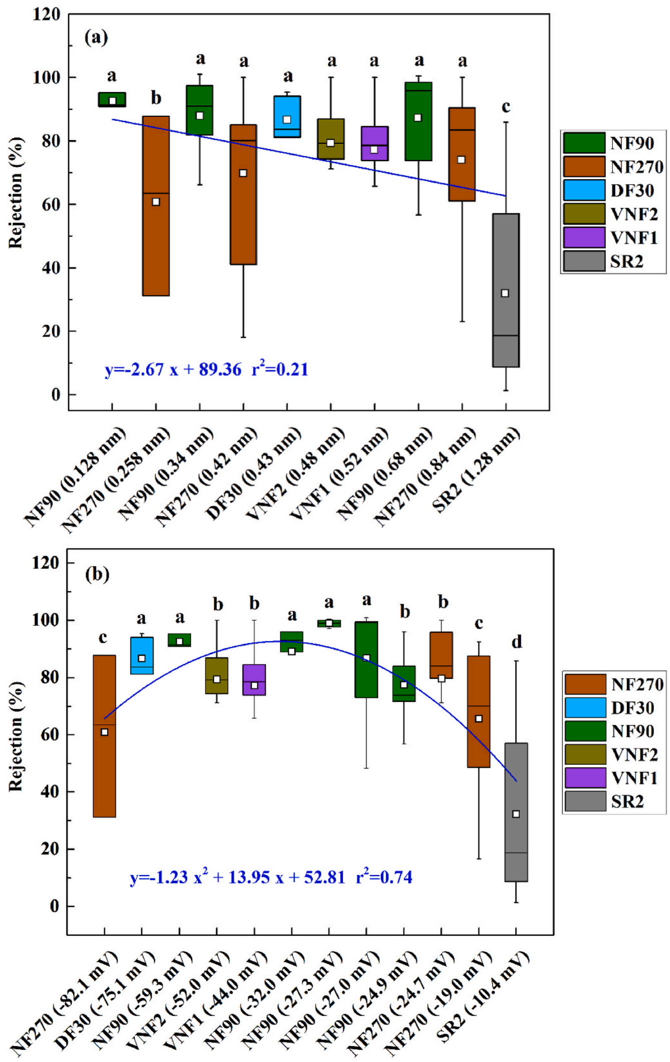

Fig. 1. Variation of micropollutant rejection rate with (a) Membrane pore size and (b) Membrane zeta potential. Statistically significant differences were assessed using SPASS version 19.0 ($p < 0.05$).

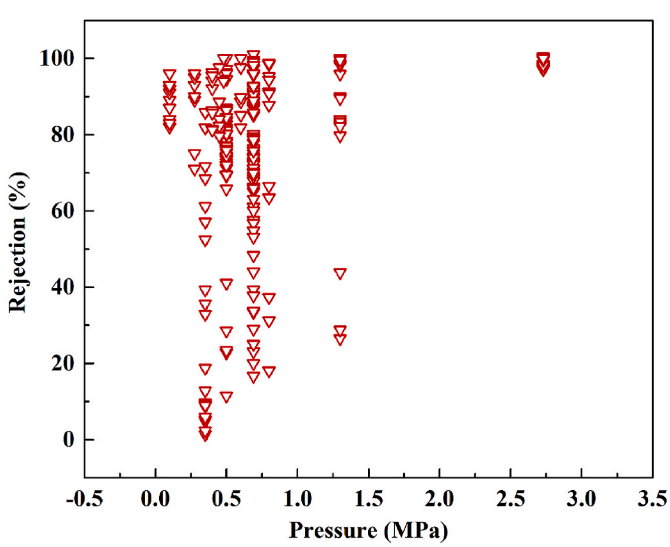

Fig. 2. Variation of micropollutant rejection rates with operation pressure.

The setting of the crossflow rate summarized in this study was relatively high, primarily at 0.08, 0.1, 0.304, and 0.5 m s^{-1} (Fig. S1). The sheer force of the water flow rate showed a positive correlation with the crossflow rate. On the one hand, a higher crossflow rate could exert a stronger stripping effect on the pollutants attached to the membrane surface; thus, leading to a better removal of pollutants from the membrane surface to reduce membrane pollution. On the other hand, it could lead to an increase in the degree of turbulence of the water, reduce the concentration polarization phenomenon near the membrane surface, and reduce the deposition of a high concentration pollutant layer on the NF membranes.

A change in solution pH will bring about a change in the surface charge of NF membranes and also induce the dissociation of the target MPs, possibly leading to a change in the electrostatic interaction between the membrane and the target MPs, thereby affecting MP rejection (Luo and Wan, 2013). It has been suggested that the charge density on the inner surface of the membrane pore increases with increasing pH or inorganic ion concentration so as to ensure the attraction of more counter ions. The results in stronger electrostatic repulsion, which brings about an increase in membrane pore size (Bouchoux et al., 2005; Mänttäri et al., 2006). The effect of pH on MP rejection was studied under pH conditions in the range 3–10 (Fig. S2). Thus, it was observed that for pH to affect MP rejection, the pH condition should be selected taking into account the electrical properties of the membrane surface charge as well as the nature of the MPs in aqueous solution (Hidalgo et al., 2014; Huang et al., 2019; Shah et al., 2012).

3.3. Effect of MP properties on their rejection

Previous studies have demonstrated that size exclusion is most often considered as the predominant mechanism for MP rejection, especially for NF membranes with small pore sizes (Fujioka et al., 2014). The properties of MPs, including molecular radius, molecular weight, hydrophilicity, hydrophobicity, ionization state, and molecular structure, could affect their rejection by NF membranes. Among these parameters, the molecular weight of MPs has been widely used to explain the size exclusion mechanism. In particular, the molecular radius of each MP plays an important role in its rejection efficiency when it is being transported across a given target NF membrane (Min et al., 2022). Several studies have shown positively correlations between MP rejection and the molecular radii of MPs (D'Haese et al., 2013). In this study, we investigated the relationship between MP rejection rate and molecular weight as well as that between MP rejection and molecular radius (Fig. 3). The results obtained showed scattered trends between MP rejection and molecular weight (Fig. 3a), which were consistent with previously reported results (Min et al., 2022). Further, given that the weight-related parameter does not include molecular structure and geometry, it implies that molecular weight might not be a reliable predictor for explaining the size exclusion mechanism (Agenson et al., 2003; Yang et al., 2017).

The relationship between the calculated MP radius and rejection rates was investigated to determine the effect of molecular radius on MP rejection. Compared with molecular weight, the relationship between the molecular radius and MP rejection showed a relatively strong correlation (Fig. 3b). However, previous studies have revealed a weak relationship between the Stokes diameter of MPs and their rejection rates (Min et al., 2022). This could be possibly attributed to the hypothesis on the basis of which the Stokes diameter is calculated; that the molecule exhibits a rigid and spherical structure, with a homogeneous surface without taking into consideration the actual molecular structure (Min et al., 2022). It has also been demonstrated that the ratio of MP radius (r_s) to membrane pore size (r_p), normalized molecular size ($\lambda = r_s/r_p$), plays an ultimately predominant role in size exclusion (Yang et al., 2017).

The relationship between λ and MP rejection is present in Fig. 3c. In previous studies, reliable equations indicating the influence of the size

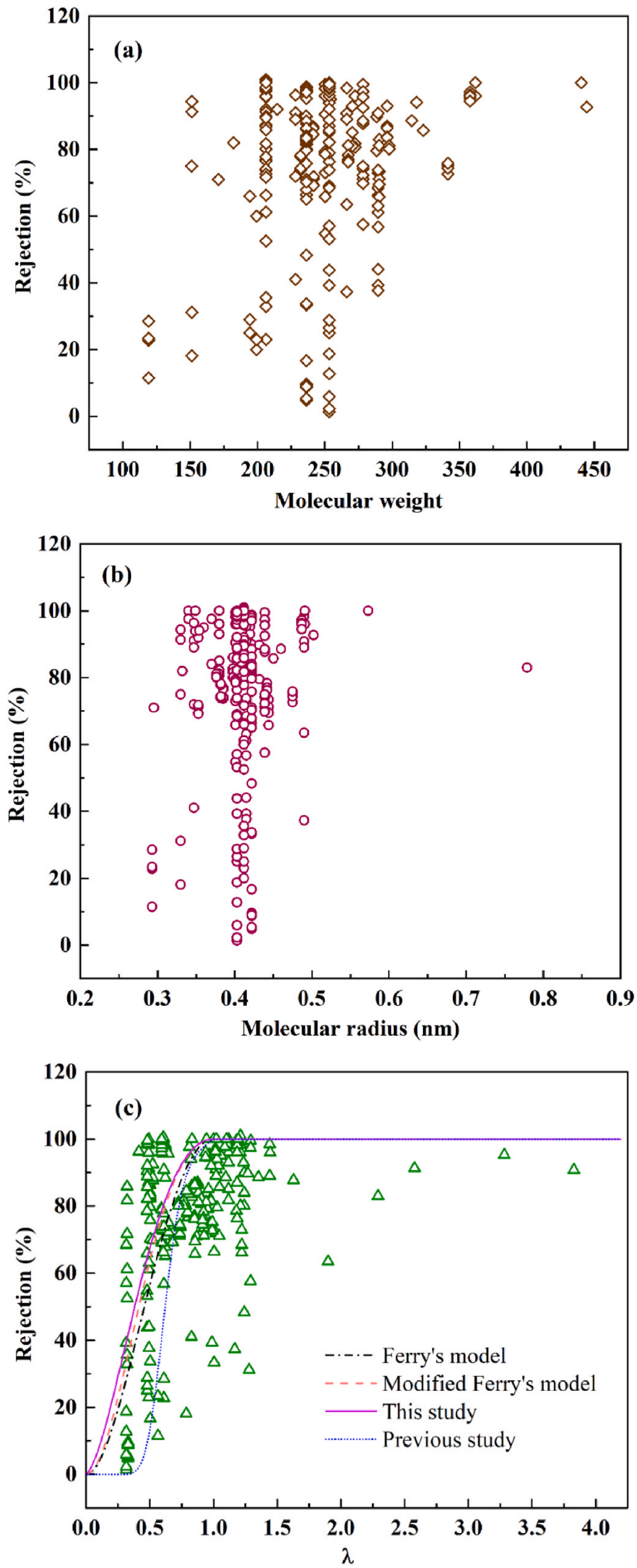

Fig. 3. Variation of Micropollutant rejection rate with (a) Molecular weight, (b) Molecular radius, and (c) Normalized molecular size.

exclusion mechanism on MP rejection, such as the Ferry's equation (Eq. 3), proposed by Ferry or its modified version (Eq. (4)), proposed by Werber, have been employed (Ferry and Douglass, 1935; Werber et al., 2016). Given that Ferry's model is derived depending on continuum fluid mechanics, empirical Eq. (5) was fitted, showing good correlation with the statistical data from published references (Fig. 3c). Further, Yang (Yang et al., 2017) optimized such a model for rejection prediction for nine haloacetic acids and seven surrogates by four RO/NF membranes (i.e., NF90, NF270, XLE, and SB50). Thus, a simple and rational strategy for treating the combined effects of size exclusion and electrostatic interaction was derived (Eq. (6)).

$$\text{Ferry's model}: R = \begin{cases} [\lambda(2-\lambda)]^2 & \lambda \le 1 \\ 1 & \lambda > 1 \end{cases} \tag{3}$$

$$\text{Modified Ferry's model}: R = \begin{cases} 1 - \left\{1 - [\lambda(2-\lambda)]^2\right\} exp\left(-0.7146\lambda^2\right) & \lambda \le 1 \\ 1 & \lambda > 1 \end{cases} \tag{4}$$

$$\text{This study}: R = \begin{cases} 1 - \left\{1 - [\lambda(2-\lambda)]^2\right\} exp\left(-0.648\lambda^{1.175}\right) & \lambda \le 1 \\ 1 & \lambda > 1 \end{cases} \tag{5}$$

$$\text{Previous study}: R = \begin{cases} \lambda^{0.3}\, exp\left[-36(1-\lambda)^{4.3}\right] & \lambda \le 1 \\ 1 & \lambda > 1 \end{cases} \tag{6}$$

3.4. Relative contribution rate of each impact factor to MP rejection

Since λ was calculated by r_s/r_p, the aforementioned ten parameters except λ were used in LMG analysis in order to avoid mutual influence. Among these properties, membrane pore size and zeta potential showed the first and third highest relative contribution rates to MP rejection with values of 32.11% and 10.15%, respectively (Fig. 4), suggesting that the property of membrane plays the maximum contributions to MP rejection. With respect to operation conditions, operation pressure and solution pH showed the second and fourth highest contribution rates to MP rejection, with relative contribution rates of 25.57% and 8.17%, respectively (Fig. 4). While for MP properties, the molecular radius showed a relative contribution rate of 7.83%, which was higher than those of MP charge, molecular weight, logKow, pKa and crossflow rate (5.36%, 5.13%, 2.15%, 2.05%, and 1.50%, respectively) (Fig. 4). The results showed that membrane pore size and operation pressure played the two highest relative contribution rates to MP rejection with a value of 32.11% and 25.57%, respectively, possibly suggesting that the

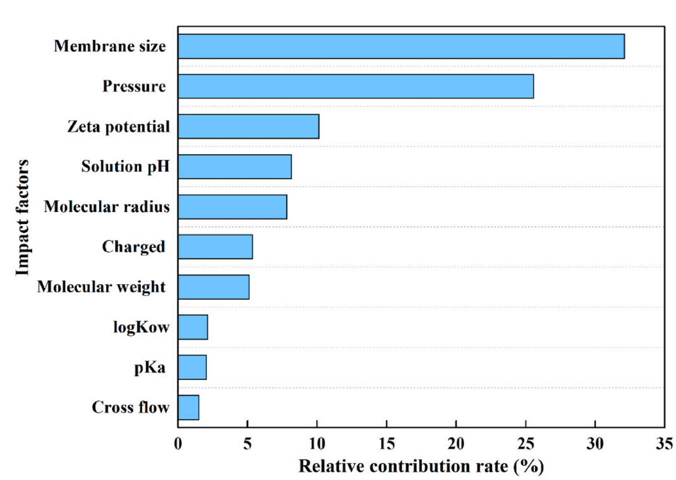

Fig. 4. The relative contribution rates of different impact factors on MP rejection.

predominant mechanism of size exclusion for MP rejection (Fujioka et al., 2014).

Based on the LMG analysis, the total relative contribution of membrane pore size, operation pressure, membrane zeta potential, solution pH, and molecular radius was 83.82% (Fig. 4), making the primary relative contribution to MP rejection. In order to simplify the modeling prediction process, the top five influencing factors for MP rejection were selected for prediction by the RFR model (Fig. 5). The results showed that the r^2 with a value of 0.73 indicates the degree of the model's interpretation of the data, showing a good prediction process. The value of *RMSE* was 12.22% in model prediction, which measures the magnitude of the error in the model prediction. And the value of *MAE* was only 6.92%, indicating a good average degree of model's prediction error.

3.5. Implications

In recent years, NF technology has been widely used in water and wastewater treatment, including advanced sewage treatment and reuse (Kang et al., 2020), seawater/brackish water desalination (Jrd et al., 2020; Sun et al., 2020), landfill leachate treatment (Almeida et al., 2020), industrial wastewater treatment (Garcia-Ivars et al., 2017), and drinking water treatment (Shen et al., 2020). This study demonstrated that membrane pore size, membrane zeta potential, and the normalized molecular size ($\lambda = r_s/r_p$) showed better individual relationships with MP rejection during NF membrane treatment. This individual relationship function in this study might contribute to MP rejection prediction under different experiment conditions. As membrane pore size plays a primary role in MP rejection, this observation might guide future NF membrane preparation and synthesis. Thus, further studies should focus on the preparation of NF membranes with different properties for different water treatment applications. Additionally, this study demonstrated that operation conditions, such as pressure, could considerably influence MP rejection, implying that it would be necessary to optimize the operational parameters in engineering applications. The machine learning-based model is a promising approach for understanding the membrane separation process, showing excellent prediction ability for MP rejection by NF membrane. Moreover, more research should be conducted to explore the impact of organic compounds on the rejection of MPs by NF membranes. For more complex situations, it will be better to explore new valuable models to adapt to more complicated data types for MP rejection.

4. Conclusions

This study summarized the data on the rejection/removal of 30 species of MPs by six types of NF membranes to investigate the impacts of different factors on MP rejection. Membrane pore size and membrane zeta potential showed relatively strong correlations with MP rejection, with r^2 values of 0.21 and 0.74, respectively. Quantitative assessment based on the LMG model revealed that membrane pore size and the operation pressure showed the highest relative contribution rates to MP rejection (32.11% and 25.57%, respectively), possibly suggesting that the predominant mechanism of size exclusion for MP rejection. The rejection prediction model of RFR with parameters of membrane pore size, operation pressure, membrane zeta potential, solution pH, and molecular radius showed high accurate with r^2, *RMSE* and *MAE* 0.73, 12.22% and 6.92%, respectively. These findings provide effective and efficient value for MP rejection prediction and future NF membrane design and operation.

CRediT authorship contribution statement

Rui Xu: Data curation, Investigation, Writing - original draft, Writing - review & editing, Formal analysis. **Zeqian Zhang:** Investigation. **Chenning Deng:** Visualization. **Chong Nie:** Formal analysis. **Lijing Wang:** Writing - review & editing. **Wenqing Shi:** Writing - review & editing. **Tao Lyu:** Conceptualization, Writing - review & editing. **Queping Yang:** Project administration, Supervision, Writing - review & editing.

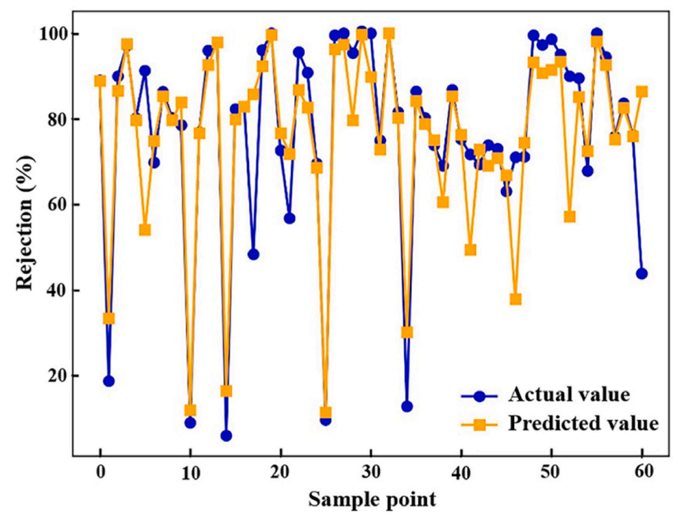

Fig. 5. The RFR model validation in testing samples.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envres.2023.117935.

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