Membrane and Water Treatment, *Vol. 16, No. 6 (2025) 281-289*
https://doi.org/10.12989/mwt.2025.16.6.281

Development of composite index for predicting membrane fouling potential in SWRO pretreatment

Anton Dukhov*, Fahed Ebisi, Michael Themel and Sergey Agashichev

R&D Centre, Dubai Electricity and Water Authority, Dubai, P.O. Box 564, UAE

(Received November 21, 2024, Revised July 9, 2025, Accepted September 30, 2025)

Abstract. A model for water quality index is proposed. This index is based on the input quality variables such as concentration of turbidity, chlorophyll-a, ATP, absorbance at 260 nm and TOC. The index can be used for estimation of water quality before SWRO since the existing water quality metrics such as SDI and its derivatives do not provide reliable estimation for potential fouling. The impact of input variables was approximated by the second order function. The level of impact of input variables (such as concentration of chlorophyll-a; ATP; absorbance; TOC and turbidity) is characterized by weight factors. The target function – $Z(X_j)$ was assumed to be proportional to the probability of membrane fouling that, in turn, proportional to SDI. The target function implies cumulative-composite structure. It includes imbedded sub-models $f(X_j)$ for different fouling factors, $X_1 - X_5$. The proposed model can be applied in different characteristic locations such as seawater intake, the points before and after pretreatment. The developed model can represent mathematical background for the software for monitoring and management of feed water quality in desalination. Individual weight factors and target function in real time can be used as a component in the early warning system.

Keywords: desalination; modelling; reverse osmosis; water quality

1. Introduction

Quantification of water quality is a serious challenge for the water sector. There is a wide range of assessment characteristics of different hierarchy levels such as primary parameters, indicators, indexes, sub-indexes, criteria, etc. to be used for evaluation of water quality of different categories. It is essential both for quality estimation and for adjustment of operating parameters of the process. The concept of "water quality" covers various aspects and can have a broad meaning depending on the domain and target, particularly for surface water, seawater, potable water, effluents, etc.

Multiple studies cover different aspects of water quality depending upon the domain such as surface water, seawater, potable water, industrial discharge, etc. Review of water quality models for surface water, structure, components, weight factor and the principle of aggregation of sub-index was considered. Uddin *et al.* (2021) in their study have presented comparative discussion of the most commonly used water quality indexes and factors affecting model accuracy. The research indicated that although most water quality indexes have broadly similar structures, the intricate particulars of the four major components differ significantly. The focus was dedicated to parameterization of the models, defining the sub-indexes and their weighting values, sources of uncertainty, as well the functions for index aggregation. In similar study Uddin *et al.* (2023) developed a model for assessing water quality for coastal waterbodies in Ireland. The developed water quality index could be an efficient and reliable technique for the assessment of transitional and coastal water quality more accurately in any geospatial domain.

Real-time quantification of individual parameters of water quality index to adjust operation regime remains a challenge of desalination sector, especially for membrane desalination. To prevent Reverse Osmosis (RO) membrane fouling it requires site-specific customized pretreatment (Agashichev and Kumar 2017). Fouling phenomena can be caused by different types of foulants such as organic, inorganic, colloidal, suspended, combined etc and major factors such as membrane structure, the interaction between membrane, solute and solvent, the size of particle or solute (Badruzzaman *et al.* 2018). Continuous monitoring of water quality parameters is essential to quantify and to mitigate the probability of fouling. Seawater quality can be characterized by the wide spectrum of parameters, indexes, characteristics, criteria, etc. Multiple approaches for systemic development of the water quality parameters have been considered. The approaches including the following consecutive stages (1) selection of water quality parameter, (2) generation of sub-indexes, (3) calculation of the weighting factor and (4) aggregation of sub-indexes into composite quality index were presented in (Uddin *et al.* 2021, 2023). Depending upon the physical dimension and physical principle underlying the technique of characterization, the quality parameters can be subdivided into different hierarchy levels ranging from individual dissolved components (e.g. orthophosphates, dissolved organics, etc.) to composite indicators. The first group can be characterized just by the concentration of component. Another group includes composite and comprehensive indicators such as

---

*Corresponding author, M.Sc., Researcher
E-mail: anton.dukhov@dewa.gov.ae

http://www.techno-press.org/?journal=mwt&subpage=7
ISSN: 2005-8624 (Print), 2092-7037 (Online)

total suspended solids (TSS), absorbance at 254 nm, turbidity, SDI, etc. They include some groups of imbedded factors and cover groups of factors e.g. UV absorption intensity at 254 nm characterizes the presence of multiple forms of dissolved organics having specific functional groups. An absorbance of dissolved organic carbon (DOC) decreases with increasing wavelength. The range of 250 to 330 nm is widely recommended in some studies. At the wavelengths below 235 nm, nitrate forms can contribute to the total absorbance significantly. Different forms of water quality characteristics and indicators have been scrutinized in (Uddin *et al*. 2021, 2023, Yoo *et al*. 2021, ASTM 2014a, Rabie *et al*. 2001). Turbidity covers a wide group of colloidal forms characterized by light scattering.

Currently the most widespread water quality indicator to be used after Seawater Reverse Osmosis (SWRO) pretreatment is so called the Silt Density Index (SDI) (Alhadidi *et al*. 2011). It is widely used in different control points such as seawater intake, the points before and after pretreatment, etc. The SDI test is based on the quantitative evaluation of the decline of filtration rate through a standard filter (with 0.45μm pore size) under the applied pressure of 20.8 kPa (30 psi) (Yoo *et al*. 2021). The value of the index is estimated as follows (ASTM 2014a):

$$SDI_T = \frac{1}{T}\left[1 - \frac{t_1}{t_2}\right] \cdot 100 \quad (1)$$

where t_1 is the time required to collect the first 500 mL permeate and t_2 is the time required to the second 500 mL after total elapsed flow time T (usually 15 min).

There is a group of derivative indicators based on the SDI such as fouling index (FI), the modified fouling index (MFI), the plugging index (PI), etc. (Rabie *et al*. 2001). They have similar drawbacks since they do not reflect an impact of different potential fouling factors as well (Alhadidi *et al*. 2013).

There are some studies focusing on the relationship between SDI, rate of reagents injection and process characteristics. Fayaz *et al*. (2019) studied the relationship between SDI and the injection of calcium hypochlorite, by investigating correlations between oxidation reduction potential (ORP) and turbidity in various ranges. The findings suggest that the factors responsible for high SDI values may not always change even when all the water turbidity factors are removed. This implies that the SDI is greatly influenced by factors other than turbidity, such as organic and biological pollutants submicron particles. By adjusting ORP and turbidity in various ranges, favorable regression values were obtained. In another study, Mosset *et al*. (2008) recorded SDI values for seawater from the Arabian Gulf that had been pretreated, emphasizing a comparison with turbidity levels. The study highlighted that changes in SDI values are not always correlated with turbidity. The correlation between SDI and the deposition of contaminants has been analyzed by Kremen and Tanner (1998), whose studies indicated a geometric relationship between the values of the index and the weight of the particles collected. Iwahori (2013) further studied factors affecting SDI values such as pH and temperature. The case study noted higher temperatures resulted in higher SDI values, stating that SDI measurements at different temperatures cannot be comparable and may mislead operators. An increase of SDI values was also seen in conditions where pH is 8 or above due to higher scaling potential of $CaCO_3$ (Hchaichi *et al*. 2014). Other factors causing discrepancies in SDI measurements lay in the measurement practices taken by operators. SDI is a sensitive tool and therefore can be affected by air bubbles, particles from previous tests, air on membrane surface, membrane positioning and air leaks (Rachman *et al*. 2013). Recent commercialization of automatic SDI tools makes the operation less cumbersome and time-consuming and can reduce human errors in measurement. Despite all these alterations this index does not provide precise and reliable information regarding the water quality and the probability of potential fouling. It does not reflect the presence of some fractions of dissolved components such as dissolved organic carbon representing assimilable and biodegradable forms. Similar dissolved forms can represent the main factor for organic fouling and precursor for biofouling as well.

Many studies have emphasized the disadvantages of SDI-based methods such as the lack of precision and unreliability (Takeuchi *et al*. 2015, Koo *et al*. 2012, Abushaban *et al*. 2022). There are different reasons for its unreliability, it can be due to both manual operations of measurement and the fact that majority of potential factors remain outside the scope of detection of SDI method. In addition, this test must be accompanied by manual sampling and specific analysis in specialized labs. Such practice remains a cumbersome and time-consuming procedure. Relying upon existing experience and available published data, the preference can be given to continuous monitoring in real time followed by the development of multi-layer comprehensive water quality index. A similar approach was demonstrated in (Uddin *et al*. 2021, Uddin *et al*. 2023), where the components, hierarchical structure, weight factors, algorithms of aggregation of individual components within the structure of composite index are analyzed. It involves the following consecutive steps: (1) selection of individual water quality parameter; (2) generation of sub-indices for specific group of parameters; (3) calculation of the weighting factor, and (4) aggregation of individual sub-indices within composite water quality index.

In this regard the current study focuses on the development of the composite water quality index based on continuous monitoring in real time. The proposed index is expected to eliminate drawbacks and disadvantages inextricably linked to the existing SDI-based method. The proposed index is expected to provide more precise and reliable information. The index is expected to account for the fractions of dissolved high-molecular components as well.

2. Modelling composite index for estimation of water quality before SWRO

When we deal with a process evaluation (e.g. pretreatment before RO) the characteristics, can be represented in different physical dimension such as: (1) in the dimension of individual parameter of water quality e.g.

concentration, NTU, etc.; (2) as a degree of rejection for quantifying the effectiveness of the processes such as $R(X_i) = (X_{i+1} - X_i)/X_i$ and (3) in the format of indicators specifying the variation over time: $r = dX/d\tau$ (e.g. as a rate of deterioration, the growth of concentration over time).

2.1 Components and hierarchy structure of the composite index

The study focuses on the modelling of comprehensive index to quantify the water quality after the operations of seawater pretreatment before RO desalination in SWRO. Primary water quality parameters, the principles and techniques of aggregations of primary parameters and their weighting factors are analysed in this study. The development of the proposed index based on experimental data on water quality on the stage of seawater pretreatment (Malek *et al.* 2016, Okamoto *et al.* 2015). The following water quality characteristics were considered: X_1 is turbidity; X_2 is chlorophyll-a; X_3 is intracellular form of ATP; X_4 is absorbance at 260 nm; X_5 is TOC. These variables (X_1–X_5) represent input into the model. These variables were selected as the main inputs since they represent the main fouling groups and cover a wide spectrum of fouling factors contributing to SDI value. The target function in this case was assumed to be proportional to the probability of membrane fouling. Thus, SDI can be accepted as a reference value for the target function: $SDI \approx Z(X_1, X_2, X_3, X_4, X_5)$.

Turbidity (X_1) is an optical characteristic, it is a measure of relative transparency of the liquid sample and proportional to the intensity of light scattering, that, in turn, is proportional to the number particles in the sample.

Chlorophyll-a (X_2) is a light-absorbing pigment, is an important biomolecule produced through the metabolic way as other pigments. It gets its green color because it absorbs blue and red wavelengths of light. Since it is a light absorbing pigment, chlorophyll is called a photoreceptor. There are different forms that occur naturally, but the most widely distributed form in terrestrial plants is chlorophyll-a [$C_{55}H_{72}O_5Mg$]. In diethyl ether (Et_2O), chlorophyll-a has an approximate absorbance maximum of 430 nm and 662 nm, (while chlorophyll-b has approximate maxima of 453 and 642 nm. The absorption peaks of chlorophyll-a are at 665 nm and 465 nm. Chlorophyll-a fluoresces at 673 nm (maximum) and 726 nm (Crompton 2006).

Adenosine triphosphate (ATP), (X_3) is a nuclear triphosphate used in cells as a coenzyme often called the “molecular unit of currency” of intracellular energy transfer. ATP transports chemicals energy within cells for metabolism. One molecule of ATP contains three phosphate groups, and it is produced by a wide variety of enzymes. Metabolic processes that use ATP as an energy source convert it back into its precursors. Energy stored in ATP may be released upon hydrolysis of the anhydride bonds. Traditional indicators such as SDI or MFI do not give precise information about the biomass content that can be assumed as a measure of biofouling potential of seawater. In this regards adenosine triphosphate (ATP) is an indicator of biomass contents and bioaccumulation in seawater, therefore indicating biofouling potential.

Absorbance (X_4) is a measure of molecules to absorb light at different wavelengths. That makes it possible to determine if one type of molecule is in a large mixture of molecules. For example, proteins tend to absorb light with a wavelength of 280 nm (or we would say “absorb light at 280”). On the other hand, nucleic acids absorb light at 260 nm. The visible spectrum above ranges from about 380 nm to roughly 700 nm (260 nm and 280 nm are ultraviolet light UV). After all, ultra means more than and ultraviolet light has shorter wavelengths and thus more energy than violet light. Characterization of dissolved organic matter (DOM) of algal origin can be conducted at 390 nm. Mono-chromatic compounds and tryptophan peaks are located between 270 and 300 nm, two-considered ring systems between 310 and 370 nm, fulvic 370 and 400 nm and humic acids and other compounds at 470 nm and more (Crompton, 2006).

Total organic carbon (TOC), (X_5) includes the dissolved, particulate, and volatile organic fractions. The determination of dissolved organic carbon can be done by using different techniques, using oxidation methods or ultraviolet (UV) absorption. The methods of oxidation, in turn, can be subdivided into three main groups such as (1) wet chemical oxidation using oxidants such as persulphate; (2) high temperature combustion, or dry oxidation and (3) photo-oxidation of dissolved organic carbon. The advantages and limitations of these techniques were intensively scrutinized (Crompton 2006). UV absorption of seawater particularly in the wavelength between 250 and 300 nm, where the absorption is considered as a consequence of the presence of aromatic compounds. Some methods are based on the comparison of UV absorption intensity at two wavelengths, one less than 350 nm and greater than 400 nm. There are methods based on measurement of the ratio of the light transmitted by the sample at 254 nm in the ultraviolet that at 510 nm in the visible region.

Available published sources have somewhat disputable terminology. The term of “water quality” is widely used but this term has a multiple interpretation, and it can be misleading. It depends on the water type and site- specific water source. This paper deals with seawater as a source for desalination in the Gulf Area. Type of seawater pretreatment depends on seawater quality, in particular, the groups of fouling factors and their concentration. All the characteristics such as water quality, structure and groups of fouling factors, types of seawater pretreatment represent site-specific categories. Therefore, the structure of the index, in turn, is inextricably linked to the potential fouling factors as well. That’s why the structure of the index can be adjusted and modified as well. The current study focuses on the cases of seawater in the Gulf Area. That’s why this study covers mainly the components detected in this area. Special attention is due to chlorophyll as an indicator of algae concentration or ATP as an indication of cell activity. Those components are included into the index structure since algae bloom or red tide represents the one of phenomena hampering SWRO desalination in this area.

Some natural pollutants and potential anthropogenic components are outside the scope of this study. In the case if some chemical, pharmaceutical etc. pollutants can be detected in the water source the index structure can be altered. Those components can be inserted into the index depending on their functional behaviour or physical property (whether it is a dissolved component or it is colloid, suspended, etc. form with characteristic functional behaviour).

In this study we have utilized the three-hierarchy level structure to develop the composite water quality index. The lower level of hierarchy includes the individual water quality parameters which were used as input variables in the model and decrumbed above (X_1–X_5). The quantitative contribution of each individual fouling component represents the second hierarchy level of the comprehensive model. The target goal was assumed to be SDI value representing the target function (Z-variable).

2.2 Physical premises and assumptions

Alternative composite indicator is based on the following physical premises and assumptions:

- The following individual water quality input characteristics were considered (X_1 is turbidity; X_2 is chlorophyll-a; X_3 is intracellular form of ATP; X_4 is absorbance at 260 nm, and X_5 is TOC). These variables (X_1–X_5) represent input into the model. This study based on available experimental data on water quality after seawater pretreatment (Malek *et al*. 2016, Okamoto *et al*. 2015).
- For the mathematical treatment to simplify all the independent variables (x_1–x_5) and dependent variable (z) initially have physical dimensions must be converted into normalized dimensionless format:

$$X = \frac{x - x_{min}}{x_{max} - x_{min}} \tag{2}$$

where x is experimental readings in physical dimension, mg/L, mol/L, etc. It ranges from x_{min} to x_{max}; non-dimensional input variable ranges from $X_{min} = 0$ to $X_{max} = 1$ at boundary conditions.

- The impact of the concentration of individual factor was approximated by the function of the second order, $f(X_{i,j})$. The second order polynomial equation was selected since it demonstrates continuous and monotonous behavior corresponding to the physics of object and meets the required boundary conditions. Functional behavior of individual factor vs. concentration was approximated as follows:

$$f(X_{i,j}) = A_j\, X_{ij}^2 + B_j\, X_{ij} + C_j \tag{3}$$

- Boundary conditions

The contribution of any individual factor (X_1–X_5) was assumed to be ranged from 0 to 1 at the boundary conditions. Therefore,

At $X_i = 0$ we have:

$$f(X_{ij=0}) = 0 \tag{4}$$

At $X_i = 1$ we have:

$$f(X_{ij=1}) = 1 \tag{5}$$

- Estimation of coefficients A, B, C (see Eq. 3) can be done at the boundary conditions.

At $X_{ij} = 0$ we have $f(X_{ij=0}) = 0$.

Therefore, it gives $f(X_{ij}) = C,$ thus:

$$C = 0 \tag{6}$$

At $X_{ij} = 1$ $f(X_{ij=1}) = 1$ therefore

$$A = 1 - B \tag{7}$$

Inserting Eqs. (6) and (7) into Eq. (3) we get:

$$f(X_{i,j}) = A_j\, X_{ij}^2 + (1 - A_j) X_{ij} \tag{8}$$

$$f(X_{i,j}) = A_j\, (X_{ij}^2 - X_{ij}) + X_{ij} \tag{9}$$

- The target function (see Eq. 12) ranges from 0 to 1, therefore we can write:

$$Z_i(X_{i1}, X_{i2}, X_{i3}, X_{i4}, X_{i5} = 0) = 0 \tag{10}$$

$$Z_i(X_{i1}, X_{i2}, X_{i3}, X_{i4}, X_{i5} = 1) = 1 \tag{11}$$

2.3 Model development

The study focuses on the modelling of comprehensive water quality index to be used for estimation of water quality after pretreatment before SWRO. Traditionally SDI is assumed to be a key indicator of water quality before membrane operations, being assumed to be proportional to the probability of membrane fouling. As a result, we chose to use SDI as the target function in this study, $SDI \approx Z(X_1, X_2, X_3, X_4, X_5)$. Consequently, this work presents the development of quantitative correlation between the target function (Z) and independent variables (X_1–X_5).

The target function (Z-variable) represents cumulative-composite structure. In this study SDI was the reference indicator for the target function. The value of SDI is based on the deterioration of filtration rate through standard filter (the rate of filter plugging). Unlike the SDI value, the alternative Z-indicator represents a composition of the functions based on independent water quality characteristics. Eq. (3) is a mathematical formulation that can represent the indicator:

$$\begin{aligned} Z(X_1, X_2, X_3, X_4, X_5) &= N_1 f(X_1) + N_2 f(X_2) \\ &+ N_3 f(X_3) + N_4 f(X_4) + N_5 f(X_5) \end{aligned} \tag{12}$$

In this study the independence and lack of mutual coupling between individual factors (X_1–X_5) is assumed. The target function – $Z(X_1, X_2, X_3, X_4, X_5)$ does not contain any terms coupling the variables as well. Any quality parameter is characterized by individual weight factor – N_{j}. Any term on the right-hand side (Eq. 12) represents a product of the function depending upon the concentration of individual component – X_{j} and its weight factor – N_{j}. It can be rewritten as follows:

$$Z(X_1, X_2, X_3, X_4, X_5) = \sum_{j=1}^{j=5} N_j\, f(X_j) \tag{13}$$

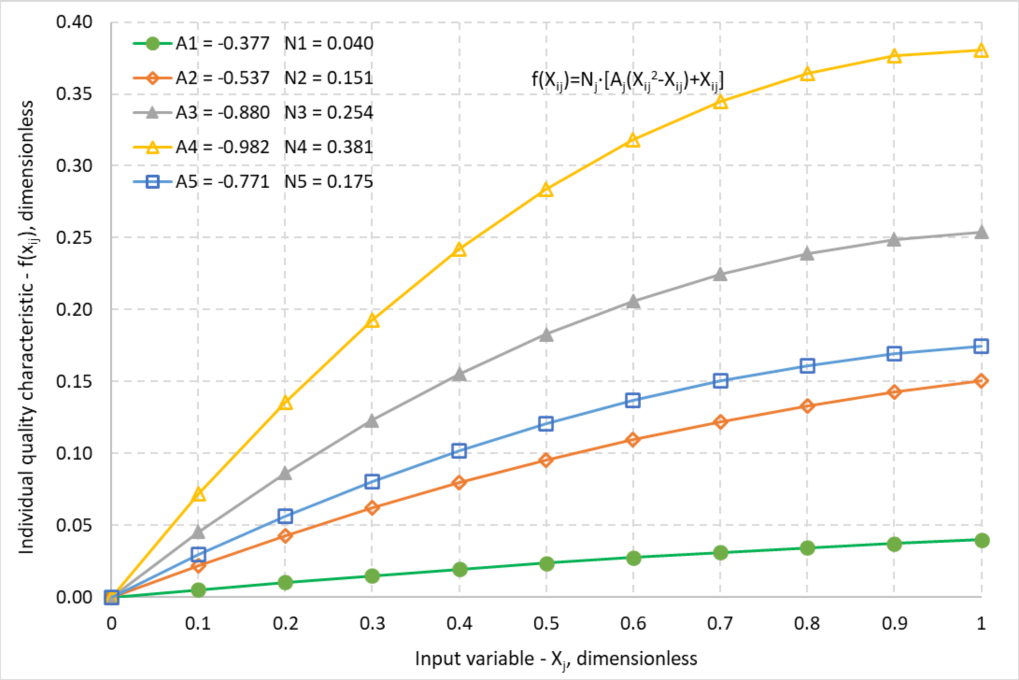

Fig. 1 Individual water quality characteristics corresponding to variables (X_1–X_5)

Combining Eqs. (13) and (3) we get:

$$Z_i(X_{i1},\dots,X_{i5}) = \sum_{j=1}^{j=n} N_j\,[A_j\,X_{ij}^2 + B_j\,X_{ij} + C_j] \qquad (14)$$

where n is number of individual factors.

Mathematical formulation $f(X_{ij})$ represents a quantitative contribution of individual fouling component into the target indicator $Z_i(X_{i1}, X_{i2}, X_{i3}, X_{i4}, X_{i5})$. Thus, on the right-hand side of Eq. (13) we get:

$$Z_i(X_{i1},\dots,X_{i5}) = \sum_{j=1}^{j=n} N_j\,[A_j\,(X_{ij}^2 - X_{ij}) + X_{ij}] \qquad (15)$$

where N_j is a weight factor of individual fouling component. It ranges from $N_j = 0$ to $N_j = 1$.

$$\sum_{j=1}^{j=n} N_j = 1 \qquad (16)$$

Optimization algorithm can be applied for estimation of the coefficients N_j and A_j (Eq. 15) corresponding to individual fouling factor such as turbidity (X_1), chlorophyll-a (X_2), ATP of intracellular form (X_3), absorbance at 260 nm (X_4) and TOC (X_5).

3. Application of the model

3.1 Estimation of the coefficients for individual components

This study is based on available experimental and pilot results (Malek *et al*. 2016, Okamoto *et al*. 2015). All data used in this work are shown in Appendix A. Data on turbidity, NTU (x_1), chlorophyll-a, mg/L (x_2), ATP (intracellular form), RLU (x_3), absorbance at 260 nm, Abs/m (x_4), TOC, mg/L (x_5) and SDI (z) were selected. The SDI value represents the output Z-variable. Input data represent an array including SDI value (Z-variable) at different values of independent variables (X_1–X_5).

All the used data were converted into non-dimensional format (see sub-section 2.2). All the independent variables (x_1–x_5) and dependent variable (z) being characterized by respective physical dimensions must be converted into dimensionless format as follows: $X = (x - x_{min})/(x_{max} - x_{min})$ where x is experimental readings ranging from x_{min} to x_{max}. The variable X is non-dimensional concentration. It ranges from $X_{min} = 0$ to $X_{max} = 1$ at boundary conditions. Appendix B presents the raw water quality parameters converted into dimensionless format.

Estimation of the coefficients N_j and A_j (Eq. 15) corresponding to individual factors such as turbidity (X_1); chlorophyll-a (X_2); intracellular form of ATP, (X_3); absorbance at 260 nm (X_4); total organic carbon (X_5) can be done using optimization algorithm. MS Excel embedded solver was used as a tool for optimization procedure. The program for selection of coefficients N_j and A_j in Eq. (16) at minimal deviation of the target function from experimental SDI values, $\sum(Z_{exp} - Z_{calc})^2 \rightarrow min$, was executed. The program is based on Generalized Reduced Gradient (GRG) nonlinear optimization algorithm. The coefficients A_j were restricted by the following constrains $-1 < A_j < 0$. The range [-1; 0] corresponds to the condition of the concave shape of the profile when the second derivative is negative. Weight factors N_j are restricted by the following imposed conditions: $N_j > 0$ and $\sum_{j=1}^{j=5} N_j = 1$.

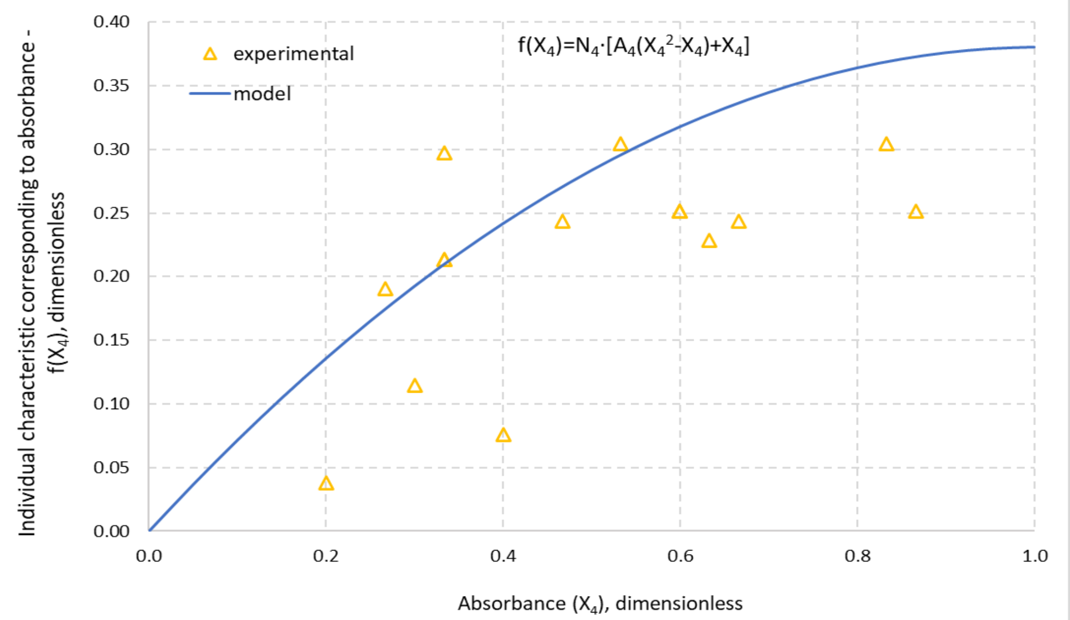

Fig. 2 Published experimental data and calculated values based on the proposed model ($N_4 = 0.381,\ A_4 = -0.982$) corresponding to absorbance at 260 nm (X_4)

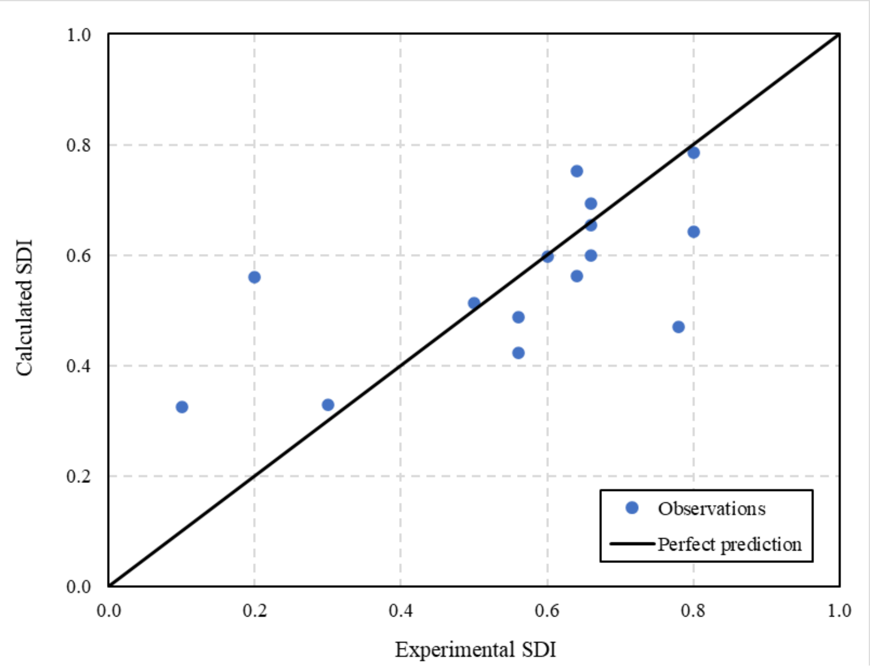

Fig. 3 Comparison between experimental data and calculated values based on the proposed model

Realization of the nonlinear optimization algorithm based on GRG (Generalized Reduced Gradient) gives minimum target function at the following values of coefficients N_j and A_j in Eq. 15. The objective target function can be expressed as follows:

$$\begin{aligned} Z = 0.04[-0.377\ (X_1^2 - X_1) + X_1] \\ +0.151[-0.537\ (X_2^2 - X_2) + X_2] \\ +0.254[-0.88\ (X_3^2 - X_3) + X_3] \\ +0.381[-0.982(X_4^2 - X_4) + X_4] \\ +0.175[-0.771\ (X_5^2 - X_5) + X_5] \end{aligned} \tag{17}$$

A set of calculated curves based on (Eq. 17) for different fouling variables are shown in Fig. 1. The plots show the impact of each input water quality characteristics on target function. Absorbance (X_4) shows the highest weight factor $N_j = 0.381$ in the target function compared to other individual factors. However, turbidity (X_1) demonstrates the lowest impact with the low weight coefficient ($N_j = 0.04$). This figure demonstrates that the implemented model has considered the physical assumptions and boundary conditions.

Calculated and experimental values for absorbance at 260 nm are shown in Fig. 2.

Table 1 Model validation values

X_1	X_2	X_3	X_4	X_5	Z_{exp}	Z_{calc}
0.56	0.55	0.06	0.12	0.73	0.45	0.56
0.70	0.50	0.36	0.34	0.43	0.37	0.59

Table 2 The first derivative (dZ_j/dX_j) at boundary conditions corresponding to estimated parameters A_j, N_j

	Turbidity		Chlorophyll-a		ATP intracell.		Absorbance at 260nm		TOC	
j	1		2		3		4		5	
N_j	0.04		0.151		0.254		0.381		0.175	
A_j	-0.377		-0.537		-0.880		-0.982		-0.771	
X_j	0	1	0	1	0	1	0	1	0	1
$^{dZ}/_{dX_j}$	0.06	0.02	0.23	0.07	0.48	0.03	0.75	0.01	0.31	0.04

3.2 Model performance results

The model performance was evaluated using regression statistical analysis. The common statistical measures were calculated for the developed model, which are root mean square error (RMSE); mean absolute error (MAE); and coefficient of determination (R^2). The results are shown below.

RSME	0.153
MAE	0.108
R^2	0.436

The R^2 for the regression analysis of the developed target function is shown in Fig. 3.

To validate the developed target indicator target function was calculated using the developed weights and coefficients. The results are presented in Table 1.

3.3 Sensitivity analysis of estimated target Z-function to independent variables

The first derivative of target Z-indicator (dZ/dX_j) represents an impact of individual estimated water quality characteristic to the composite cumulative target Z-function (see Table 2):

$$\frac{dZ}{dX_j} = N_j \frac{df_{X_j}}{dX_j} = N_j\left[2A_jX_j - A_j + 1\right] \tag{18}$$

At $X_j = 0$ we have:

$$\frac{dZ}{dX_j} = N_j\left(1 - A_j\right) \tag{19}$$

At $X_j = 1$ we have:

$$\frac{dZ}{dX_j} = N_j\left(1 + A_j\right) \tag{20}$$

4. Conclusions

Existing water quality metrics such as Silt Density Index (SDI) do not provide reliable estimation of water quality and fouling potential, so the preference must provide a real-time monitoring of multiple parameters to be converted into the comprehensive water quality index. In this regard the study covers the following:

1. Water quality index model $Z(X_1, X_2, X_3, X_4, X_5)$ for estimation of feed water quality after pretreatment in the membrane desalination is proposed. The target function is assumed to be proportional to the probability of membrane fouling, that in turn to be proportional to SDI: $SDI \approx Z(X_1, X_2, X_3, X_4, X_5)$.
2. The model is based on the primary quality input variables such as turbidity, concentration of chlorophyll-a, ATP, absorbance and TOC. Individual sub-model represents a product of individual water quality characteristic $f(X_{i,j})$ and weight factor N_j. An impact of individual variable was approximated by parabolic function: $f(X_{i,j}) = A_j X_{ij}^2 + B_j X_{ij} + C_j$. The coefficients were estimated using available published experimental data.
3. The level of impact of individual components such as concentration of chlorophyll-a; ATP; absorbance; TOC and turbidity is characterized by individual weight factor N_j. Turbidity demonstrated the lowest influence in the developed target function with the weight coefficient value $N_j = 0.04$. However, absorbance shows the highest impact in the proposed water quality model.
4. The proposed model is based on cumulative principle and includes a set of imbedded input sub-models of different hierarchy levels, $Z(X_1, X_2, X_3, X_4, X_5) = \sum_{j=1}^{j=5} N_j\, f(X_j)$.

The domains of application of the proposed model can include different locations (characterization points) such as seawater intake, the points before and after pretreatment. Evaluation of dynamics of behavior of individual weight factors in real time can be used as an input for the system of early warning. The developed model can be used as a mathematical background for the software for monitoring and management of feed water quality in desalination. It can be integrated as a component in the development of early warning systems.

References

Abushaban, A., Salinas-Rodriguez, S.G., Philibert, M., Léonie Le Bouille, Necibi, M.C., Chehbouni, A. (2022), "Biofouling potential indicators to assess pretreatment and mitigate biofouling in SWRO membranes: A short review", *Desalination*, **527**, 115543. https://doi.org/10.1016/j.desal.2021.115543.

Alhadidi, A., Blankert, B., Kemperman, A.J.B., Schurer, R., Schippers, J.C., Wessling, M., van der Meer, W.G.J. (2013), "Limitations, improvements and alternatives of the silt density index", *Desalin. Water Treat*., **52**(4-6), 1104-1113. https://doi.org/10.1080/19443994.2012.705049.

Alhadidi, A., Kemperman, A.J.B., Schippers, J.C., Wessling, M. and van der Meer, W.G.J. (2011), "The influence of membrane properties on the Silt Density Index", *J. Membr. Sci*., **384**(1-2), 205-218. https://doi.org/10.1016/j.memsci.2011.09.028.

American Society for Testing and Materials (ASTM) (2014a), "Standard test method for silt density index (SDI) of Water (D4189-07), D19.08 on membranes and ion exchange materials", *ASTM Int*., West Conshohocken.

Agashichev, S., Kumar, J. (2017), "UF pretreatment at elevated temperature within the scheme of hybrid desalination; Performance and environmental impact", *Membr. Water Treat*., **7**(3), 279-292. https://doi.org/10.12989/mwt.2017.8.3.279.

Badruzzaman, M., Voutchkov, N., Weinrich, L. and Jacangelo, J.G. (2019), "Selection of pretreatment technologies for seawater reverse osmosis plants: A review", *Desalination*, **449**, 78-91. https://doi.org/10.1016/j.desal.2018.10.006.

Crompton, T.R. (2006), *Analysis of Seawater: A Guide for The Analytical and Environmental Chemist*, Springer Science & Business Media, United Kingdom.

Fayaz, S.M.H., Mafigholami, R., Razavian, F. and Ghasemipanah, K. (2019), "Correlations between silt density index, turbidity and oxidation-reduction potential parameters in seawater reverse osmosis desalination", *Water Sci. Eng*., **12**(2), 115-120. https://doi.org/10.1016/j.wse.2019.05.006.

Hchaichi, H., Siwar, S., Elfil, H. and Hannachi, A. (2014), "Scaling predictions in seawater reverse osmosis desalination", *Water Sci. Eng*., **5**(3), 221-233. http://doi.org/10.12989/mwt.2014.5.3.221.

Iwahory, H., Jp, P.E. (2003), "Peculiar or unexpected behavior of Silt Density Index of pretreated seawater for RO desalination", *The Proceedings of the IDA World Congress at Bahamas*, Bahamas.

Koo, C.H., Mohammad, A.W., Suja, F. and Meor Talib, M.Z. (2012), "Review of the effect of selected physicochemical factors on membrane fouling propensity based on fouling indices", *Desalination*, **287**, 167-177. https://doi.org/10.1016/j.desal.2011.11.003.

Kremen, S.S. and Tanner, M. (1998), "Silt density indices (SDI), percent plugging factor (%PF): their relation to actual foulant deposition", *Desalination*, **119**(1-3), 259-262. https://doi.org/10.1016/S0011-9164(98)00167-2.

Mosset, A., Bonnelye, V., Petry, M. and Sanz, M.A. (2008), "The sensitivity of SDI analysis: from RO feed water to raw water", *Desalination*, **222**(1-3), 17-23. https://doi.org/10.1016/j.desal.2007.01.125.

Malek, S.A., Agashichev, S., Osman, E.F., Taher, M. (2016), "Pilot study of high-speed seabed infiltration system (HiSIS)", Technical report on joint pilot study between ADWEA and Hitachi Josen, Abu Dhabi, UAE.

Okamoto, Y., Almalek, S., Agashichev, S., Inoue, T., Nizato, H., Oiwa, T., Nishimura, T. (2015), "Field test of high-speed seabed infiltration system (HiSIS) with SWRO plant in Abu Dhabi", *The World Congress on Desalination and Water Reuse*, San Diego, CA, U.S.A.

Rabie, H.R., Cote, P. and Adams, N. (2001), A method for assessing membrane fouling in pilot-and full-scale systems, *Desalination*, **141**(3), 237-243. https://doi.org/10.1016/S0011-9164(01)85002-5.

Rachman, R.M., Ghaffour, N., Wali, F. and Amy, G.L. (2013), "Assessment of silt density index (SDI) as fouling propensity parameter in reverse osmosis (RO) desalination systems", *Desalin. Water Treat*., **51**(4-6), 1091-1103. https://doi.org/10.1080/19443994.2012.699448.

Takeuchi, K., Matsui, K., Ito, Y., Goda, Y., Hamano, I. and Ukawa, N. (2015), "Analysis of the filtration curve and the effect of temperature on silt density index (SDI)", *Desalin. Water Treat*., **57**(45), 21364-21376. https://doi.org/10.1080/19443994.2015.1123653.

Uddin, M.G., Nash, S. and Olbert, A.I. (2021), "A review of water quality index models and their use for assessing surface water quality", *Ecol. Indicat*., **122**, 107218. https://doi.org/10.1016/j.ecolind.2020.107218.

Uddin, M.G., Nash, S., Rahman, A. and Olbert, A.I. (2023), "A sophisticated model for rating water quality", *Sci. Total Environ*., **868**, 161614. https://doi.org/10.1016/j.scitotenv.2023.161614.

Yoo, H.Y., Lee, Y.S., Oh, H.K. and Kim, J.O. (2021), "Silt density index as a fouling propensity parameter of various membrane materials using dissolved organic matter", *J. Water Proc. Eng*., **44**, 102391. https://doi.org/10.1016/j.jwpe.2021.102391.

CC

Appendix A

The measured water quality characteristics before converting into dimensionless format

x_1 (turbidity, NTU)	x_2 (chlorophyll-a, mg/L)	x_3 (ATP, RLU)	x_4 (absorbance, Abs/m)	x_5 (TOC, mg/L)	z (SDI)
8	1.8	4.5E-10	0.13	2.03	15.5
12	1.5	1.7E-09	0.16	2.05	16
7	1.4	8.0E-10	0.145	1.8	16.5
6	3	1.8E-09	0.14	2.03	17.5
9	1.7	4.0E-10	0.15	2.17	17.8
8	3	1.2E-09	0.15	1.98	17.8
14	2.1	1.3E-09	0.195	1.95	18
6	3	1.5E-09	0.17	1.95	18.2
11	4.5	2.0E-09	0.2	2.15	18.2
10	3	1.8E-09	0.23	1.84	18.3
10	4	1.5E-09	0.19	2.2	18.3
10	3	1.5E-09	0.19	1.9	18.3
6	2	1.8E-09	0.15	1.85	18.9
16	6.5	2.5E-09	0.225	1.9	19
8	7	1.4E-09	0.18	1.94	19

Appendix B

The water quality characteristics in non-dimensional format

X_1	X_2	X_3	X_4	X_5	Z
0.24	0.07	0.07	0.20	0.55	0.10
0.38	0.05	0.39	0.40	0.58	0.20
0.21	0.04	0.16	0.30	0.17	0.30
0.17	0.18	0.42	0.27	0.55	0.50
0.28	0.06	0.05	0.33	0.78	0.56
0.24	0.18	0.26	0.33	0.47	0.56
0.45	0.10	0.29	0.63	0.42	0.60
0.17	0.18	0.34	0.47	0.42	0.64
0.34	0.32	0.47	0.67	0.75	0.64
0.31	0.18	0.42	0.87	0.23	0.66
0.31	0.27	0.34	0.60	0.83	0.66
0.31	0.18	0.34	0.60	0.33	0.66
0.17	0.09	0.42	0.33	0.25	0.78
0.52	0.50	0.61	0.83	0.33	0.80
0.24	0.55	0.32	0.53	0.40	0.80