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Membrane-based SWRO pretreatment: Knowledge discovery in databases using principal component analysis regression

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ABSTRACT

At the time being there are several technological designs of membrane-based seawater reverse osmosis (SWRO) pretreatment systems on the desalination market. The abundance of different membrane materials and configurations (pressurized/submerged/inside-out/outside-in etc.) combined with site specific conditions make the unbiased assessment of their general performance a difficult task. In this paper we suggest a data mining method based on the principal component analysis (PCA) to serve as a more systematically logical regression tool on currently available literature data. PCA is a multivariate statistical method that uses a linear transformation for dimension reduction and pattern recognition. The results show how this method can be used effectively in the case of SWRO membrane based pretreatment for both literature data reconciliation and reconstruction, as well as for future data prediction.

Keywords: Desalination; Pretreatment; Ultrafiltration; Principal component analysis; Data mining

1. Introduction

The use of porous membranes for the pretreatment of seawater in the reverse osmosis desalination industry has been on the rise since the beginning of the century. Membrane pretreatment involves removing seawater borne fouling inducing substances such as suspended solids, colloids, organics and bacteria. This step is essential if the reverse osmosis (RO) process is to be operated in an efficient manner with as little (fouling induced) RO membrane performance reduction as possible. There are currently several companies supplying membrane technology for seawater treatment but there is neither an official nor unofficial industry standard for the design or operation of this technology [1]. This is a typical characteristic of a still-immature technology that has not yet found its optimal point. RO desalination, on the other hand, can already be considered a well-established, well-proven membrane technology utilizing cross flow operation of unofficially standardized 4 or 8 inch spiral wound composite polyamide elements aligned in a row inside a horizontal pressure vessel. It is still constantly improving and changing, but that is mostly due to development of better membrane chemistry (increasing water flux and salt rejection) or some process operation optimization, and not so much due to changes of the mechanical, geometrical and physical design of the unit operations' core technology.

When comparing that with the current state of the art in membrane pretreatment technology one sees a com-

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pletely different picture. Although most solutions today deploy dead-end filtration through hollow fibers of an ultrafiltration membrane (usually having a molecular weight cut off of around 100 kDa), the physical design of the units themselves as well as their operation modes have a large spectrum of variance. Some use inside-out filtration while others use outside-in filtration. Some use pressurized vessels (either horizontal or vertical) while others prefer submerged membrane tanks with the filtrate being sucked out under vacuum. The membrane elements' geometry, materials (most common ones are polyvinylidiene fluoride (PVDF), polyether sulfone (PES) and polysulfone (PS)) and packing are also inconsistent when comparing products of different companies (some of the main suppliers and their technology are listed in Table 1). This in turn affects the different operation parameters: filtration fluxes, trans-membrane pressures, backwash fluxes and frequency, chemical use for coagulation as well as for membrane cleaning, air scouring and others all make the membrane pretreatment process design and operation question not only site specific but also vendor specific. Furthermore, unlike the RO systems, using different elements in the same skid is currently not possible, making membrane pretreatment systems proprietary ones [2]. As a result, not only the over-all plant flexibility and sustainability are impaired [3], but also the unbiased assessment and comparison of the general performance of different membrane plants becomes a difficult task. For example if certain process parameters of an existing plant are documented in the literature, how can one estimate the value of a different parameter of the same plant when it is not given? Furthermore, how can one make a prediction regarding theoretical non existing plants regardless of the membrane vendor? Consider a known seawater intake water quality and desired filtrate flow rate: How can one forecast the expected chemical demand of an ultrafiltration plant regardless of its configuration? This could prove to be especially important when trying to generally assess entire processes regarding aspects such as economical feasibility or environmental impacts. Relying on published literature and guessing the values of process parameters which are not documented could be a necessary and yet very inexact process. Usually, one has to use some kinds of inaccurate rules of thumb, semi-educated guesses or pure averages to prospectively estimate certain process parameters. Based on multivariate statistics, the method proposed in the next section does that in a more mathematically and logically sound manner.

2. Materials and methods

Multivariate analysis is a field in statistics that searches to study and explain the behavior of more than one statistical variable at a time. PCA is one of the multivariable analysis methods that can be used on a data set in order to investigate it for existing patterns and internal behaviors.

The covariance is a two dimensional size that tells us how much two variables' dimensions vary from their statistical mean with respect to each other. For a two variable (x, y) sample the covariance estimator is calculated using:

$$\operatorname{cov}(x,y)=\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y}) \tag{1}$$

where $\bar{x},\bar{y}$ are the means, n the number of samples and i their indexes. When the covariance is positive, the two samples have a positive linear connection between them. When the covariance is close or equal to zero, the two groups have no linear connection between them and no prediction can be made from one group to the other. In a k-dimensional data set one can compute

$$\frac{k!}{2(k-2)!}$$

different covariances and put them all in a matrix called the covariance matrix. For example:

$$C=\begin{pmatrix}\operatorname{cov}(x,x) & \operatorname{cov}(x,y)\\ \operatorname{cov}(y,x) & \operatorname{cov}(y,y)\end{pmatrix} \tag{2}$$

The main diagonal of the covariance matrix contains

Table 1
Common types of membrane pretreatment solutions for SWRO

Manufacturer	Product	Material	Pore size (μm)	Configuration
Dow	SFP	PVDF	0.03	Outside–in
Hydranautics	Hydracap	PES	0.02–0.025	Inside–out
Inge	Multibore	PES	0.01–0.025	Inside–out
Koch	PMPW	PS	0.01–0.02	Inside–out
Siemens	Memcor	PVDF	0.04	Submerged
Norit	Seaguard	PES	0.02–0.025	Inside–out
Pall	Microza	PVDF	0.01	Outside–in
Zenon	Zeeweed	PES	0.01–0.025	Submerged

the one dimensional variance: A measure of how much each variable is spread around its own mean.

Every matrix can be seen as a linear transformation over a specific basis in vector space. It takes vectors from one defined space into the other. Whenever a linear transformation, implemented as multiplication by a matrix, is imposed on an arbitrary vector, the result is a new vector spread in a new vector space belonging to that matrix. This new vector usually has different length and different direction, which represent the same information in another spanned vector space. There are however, special vectors that do not change their direction when transformed by a matrix, rather only their size (Fig. 1). These are the eigenvectors of that matrix and they can be understood as the ones spanning the new space connected with that matrix/linear transformation. They can be found using Eq. (3). The degrees to which these eigenvectors ($\vec{v}$) change their size are often referred to as eigenvalues (λ).

$$\mathbf{A}\vec{v} - \lambda\mathbf{I}\vec{v} = \vec{0} \tag{3}$$

Eigenvectors are orthogonal and linearly independent. As a result, one can express all of the information in the matrix's space (known as eigenspace) using a linear combination of the eigenvectors.

The principal components can be understood as none other than the eigenvectors of the covariance matrix. Due to linear algebra properties, the trace of the covariance matrix is exactly equal to the sum of its eigenvalues, meaning that the eigenvalues can be treated as variance components. By dividing each eigenvalue with the sum of all eigenvalues one can determine what part of the variance in the original data is being accounted for by this specific eigenvalue and its corresponding eigenvector. By finding the eigenvalues and eigenvectors of the covariance matrix, one can use only the most significant eigenvectors, corresponding to the biggest eigenvalues, in order to express the data in a new space which has fewer dimensions than the original space of the covariance matrix. This can be understood as compressing the data, keeping only the important information or patterns in it, and getting rid of the unwanted parts such as noises or unimportant dynamics. Generally speaking, principal component analysis can be seen as an orthogonal linear transformation, transforming the data to a new coordinate system in which the first axis projects the biggest variance in the data (Karl Pearson, inventor of PCA, called it "line of best fit"), the second axis the second biggest variance and so on [4].

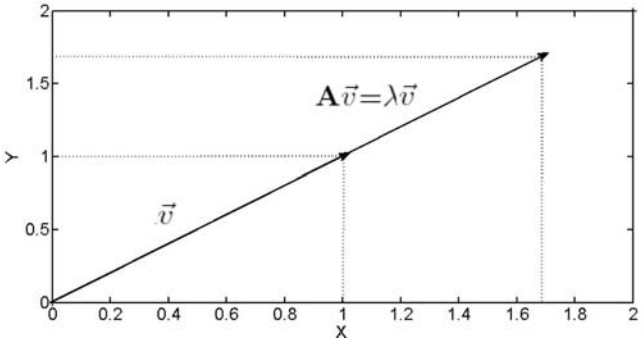

Fig. 1. Eigenvector in a two-dimensional system.

At this point a large amount of statistical data should be collected in order to form a sound representation of the covariances and linear relations between different process parameters. The statistical data set used in this work is process information taken from 20 different pilot or industrial plants that was gathered by extensive literature research. These 20 publications describe different SWRO plants around the world, all utilizing different ultrafiltration membrane technology as pretreatment under different conditions. Since the membrane technology is constantly evolving, we have focused our search on information published in the last 5 years. The 16 gathered parameters either refer to inlet seawater quality (temperature, TSS, SDI, turbidity, TOC, TSS), membrane operation (flux, transmembrane pressure, cleaning regime), chemical use (Fe coagulation, NaOCl concentration in chemically enhanced backwashes) or over-all process information (production rates, recovery, UF configuration, energy demand). In the case a certain parameter was not given, an average value from all of the other publications was used (not always resulting in logical values but considered a common way of handling missing data in PCA [4]). For the UF configuration the following markers were used: 1 = pressurized outside-in, 2 = pressurized inside-out, 3 = submerged outside-in. The data is shown in Table 2 with the arithmetic average values highlighted. A ' | ' or a ';' sign mean several parameters were given or tested in one reference (as they were in this analysis). The bracketed numbers on the first row correspond to the reference numbers.

Before applying the principal component analysis the data must be transformed into a 16×16 covariance matrix. In this case, because the different variables have very different units and variances, a more prudent approach would be to use the correlation matrix instead. The correlation matrix is nothing else but the covariance matrix normalized to the different variables' standard deviation. This makes sure that there is no over significance given to large numbers in the data.

3. Results and discussion

After building the correlation matrix (including mean centration and standard deviation scaling), the 16 principal components and their respective eigenvalues (the variances) were found. A depiction of the first 12 PCs' relative contribution to the overall correlation in the data set is shown in the Pareto diagram in Fig. 2.

As it implies from this analysis, 8 principal components can be used to explain 83.78% of the data's variance. This means we can shrink down the dimension size of

Table 2
SWRO membrane pretreatment literature data. Highlighted cells are arithmetic averages

	[5]	[6]	[7]	[8]	[9]	[10]	[11]	[12]	[13]	[14]	[15]	[16]	[17]	[18]	[19]	[20]	[21]	[22]	[23]	[24]
Feed Temp	18	21.64	20	30	40	14	15	20	21.64|28.3	15.5	17	27	21|15	21.64	25.5	21.64	18	19.5	24	21.64
Feed TSS [mg/l]	28.47	28.47	5	28.47	28.47	60	28.47	28.47	28.47	70	40	28.47	28.47	8.29|28.47	28.47	28.47	2	28.47	28.47	2.5
Feed SDI	17.57	17.57	17.57	4	17	17.57	17.57	17.57	17.57	17.57	17.57	17.57	17.57	17.57	19	17.57	14.63	19.8	17.57	31
Feed NTU	4.50	3|2	5	0.15	5.89	4.3	25.55	5.89	3.7|7	5.4	9.9	6.5	5.89	0.12|7.11	5.89	5.89	0.16	0.3	8	5
Feed TOC	3.75	3.75	3.75	3.75	2.7	3.6	3.75	3.75	7.8|4.5	7.5	4	7.4	3.75	3.75	3.75	3.75	0.75	1.2	3.75	1.6
UF flux [lmh]	80	65.43|35	65.43	70	65.43	25	54.42	51|51;68|51	61|61	60	102|85	81.6	75|81	102|68	70	67.5	37	50	60|75|85	60
UF TMP [bar]	0.105	0.54	0.35	0.11	0.54	0.9	0.65	0.51|0.41;0.18|0.34	0.2|0.2	0.75	0.16|0.54	1.38	0.55	0.83|1.38	0.25	0.54	0.22	0.813	0.5|0.7|0.575	0.3
Fe dose [ppm]	1.31	1.31|0	1.31	0	1.31	0	10	5|0;5|0	1.5|1.5	0	0.175|0	1.75	0.75	0|0.375	0.25	0	0	0	2.25|2.6|0.75	1.31
BW freq [1/hr]	1.33	2.10	2	1.33	2.10	1	2	2.10	3	2	2	4	2	1|2	3	2	1.6	2	3|2|2	2.10
CEB freq [1/d]	2	3.03	3.03	2	3.03	24	1	0|1;0|1	1.33|3	2	2	1	6	0|1	9.6	1	3.03	1	1|3.42|3.42	3.03
CEB conc [NaOCl ppm]	20	143.42	143.42	10	143.42	15	200	0|500;0|200	143.42	500	200	500	50	0|30	50	100	143.42	100	143.42	143.42
UF Recovery [%]	92	92.59	90	92.59	88.46	95	94	92.59	92.59	93	91|93.5	95	97	90	92.59	90	93	92.59	92|92.8|92.8	92.59
SWRO Production [m³/d]	8700	76800|20222	20222	14000	64000	8000	20222	109	43.71	100000	43.9	20222	20222	20222	20222	75000	20222	20222	20222	20222
UF Production [m³/d]	23500	34560|32681	28000	25500	184000	32681	32681	32681	265.15	32681	32681	32681	5280|8640	32681	32681	32681	32681	32681	32681	16800
UF type	2	3|3	2	2	2	1	3	3;2	2	1	2	1	2	2	2	1	3	1	3|2|2	2
Energy [kWh/m³ UF filtrate]	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.05	0.092	0.07	0.07	0.07	0.07

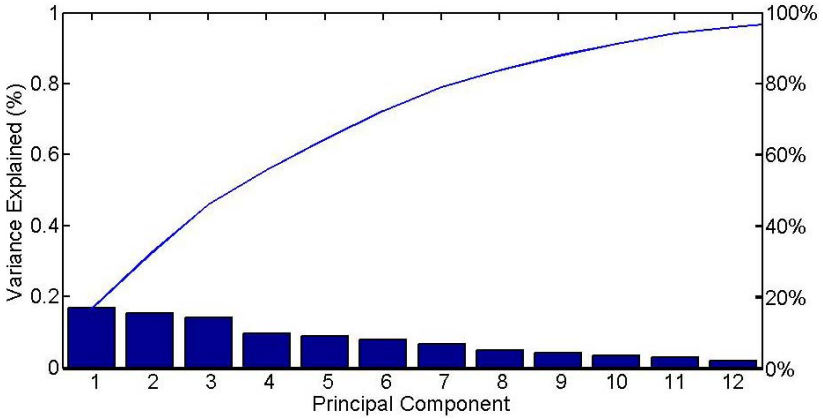

Fig. 2. Pareto diagram of the first 12 principal components.

the problem in half (from 16 to 8), while still retaining a greater part of the information regarding the correlation between the variables. The eight normalized vectors are the columns of the following **V** matrix going left to right in order of significance:

$$\mathbf{V} = \begin{pmatrix} 0.176 & -0.424 & 0.167 & -0.175 & 0.371 & -0.073 & 0.091 & -0.269 \\ -0.436 & -0.036 & -0.210 & 0.165 & 0.137 & -0.335 & -0.011 & 0.263 \\ -0.045 & 0.093 & 0.094 & 0.129 & -0.033 & 0.769 & 0.189 & -0.308 \\ -0.193 & 0.194 & 0.310 & 0.391 & 0.010 & -0.141 & 0.257 & 0.129 \\ -0.464 & -0.102 & 0.139 & -0.254 & -0.047 & -0.241 & -0.049 & 0.013 \\ -0.022 & -0.153 & 0.165 & -0.310 & -0.334 & -0.161 & 0.610 & 0.270 \\ -0.304 & -0.158 & -0.053 & 0.208 & 0.007 & 0.230 & 0.252 & -0.555 \\ -0.021 & 0.241 & 0.437 & 0.381 & 0.037 & -0.169 & 0.134 & -0.189 \\ -0.255 & -0.074 & 0.387 & -0.317 & 0.243 & 0.238 & -0.082 & -0.213 \\ -0.117 & 0.184 & -0.450 & 0.129 & 0.402 & 0.025 & 0.181 & 0.009 \\ -0.375 & -0.159 & 0.206 & -0.035 & 0.022 & 0.167 & -0.419 & 0.255 \\ -0.287 & 0.408 & -0.105 & -0.102 & 0.092 & -0.006 & -0.044 & -0.214 \\ -0.142 & -0.400 & -0.082 & 0.307 & -0.065 & 0.053 & -0.175 & 0.201 \\ 0.144 & -0.422 & 0.061 & 0.334 & 0.370 & -0.063 & 0.114 & 0.117 \\ 0.296 & 0.277 & 0.317 & 0.078 & 0.133 & -0.116 & -0.362 & 0.087 \\ 0.02 & -0.188 & -0.057 & 0.287 & -0.582 & -0.018 & -0.207 & -0.335 \end{pmatrix} \quad (4)$$

The regression method for data prediction or reconciliation proceeds as follows: since every point in the 16 dimensional correlation space can be described as a linear combination of the principal components and since we chose only 8 components to reproduce and downscale that space, any point in the 16 dimensional space can be fully described in the 8 dimensional space by knowing only 8 of its coordinates. In other words, in order to fully define one point of information, *k*, one needs to solve Eq. (5):

$$\mathbf{V} \cdot \vec{a} = \mathbf{V} \cdot \left(a_1, a_2, \ldots, a_8\right)^T = \left(k_1, k_2, \ldots, k_8\right)^T = \vec{k} \quad (5)$$

by knowing 8 of *k*'s 16 coordinates and fully determining $\vec{a}$. As an example, let us presume we know the first five entries of an imaginary data point applying to the feed water's quality: temperature = 22°C, TSS = 30 mg/l, SDI = 20, NTU = 7 and TOC = 5 mg/l. Now only three more entries are needed in order to solve the problem. Let us assume we are planning a 10,000 t/d SWRO plant with a 20,000 t/d inside-out UF system as a pre-treatment. What would be some of the UF operation parameters we can predict from the PCA? At first we need to center our data around the mean and normalize with the standard deviation of each variable (as we did with the original data). This makes sure our data is placed in the correct area of

the principal components' vector space. Next we simply use this data to solve Eq. (5), first by finding the vector $\vec{a}$ and then figuring out the other entries of k. These entries correspond to the data we are looking for but since they still need to be translated back to the units of the original parameters, we first have to multiply each one of them with the appropriate standard deviation and add the mean. The result is:

$$\vec{k} = \begin{pmatrix} k_1 = \text{temp} = 22 \\ k_2 = \text{TSS} = 30 \\ k_3 = \text{SDI} = 20 \\ k_4 = \text{NTU} = 7 \\ k_5 = \text{TOC} = 5 \\ k_6 = ? \\ k_7 = ? \\ k_8 = ? \\ k_9 = ? \\ k_{10} = ? \\ k_{11} = ? \\ k_{12} = ? \\ k_{13} = \text{RO cap} = 10000 \\ k_{14} = \text{UF cap} = 20000 \\ k_{15} = \text{UF type} = 2 \\ k_{16} = ? \end{pmatrix} \rightarrow \text{PCA regression} \rightarrow \begin{pmatrix} k_1 = \text{temp} = 22 \\ k_2 = \text{TSS} = 30 \\ k_3 = \text{SDI} = 20 \\ k_4 = \text{NTU} = 7 \\ k_5 = \text{TOC} = 5 \\ k_6 = \text{flux} = 108.8 \\ k_7 = \text{TMP} = 0.76 \\ k_8 = \text{Fe} = 0.46 \\ k_9 = \text{BW} = 2.31 \\ k_{10} = \text{CEB} = 3.53 \\ k_{11} = \text{CEB conc} = 69.87 \\ k_{12} = \text{recovery} = 92.69 \\ k_{13} = \text{RO cap} = 10000 \\ k_{14} = \text{UF cap} = 20000 \\ k_{15} = \text{UF type} = 2 \\ k_{16} = \text{energy} = 0.07 \end{pmatrix} \quad (6)$$

which makes sense as a high flux and (relatively) high pressure operation utilizing relatively frequent NaOCl chemically enhanced backwashes.

Other estimations are made possible using any 8 of the 16 starting parameters but one has to take the following into consideration:

Choose reasonable starting parameter values (within the ranges provided in Table 2).

Be critical in handling and interpretating parameters which are not well documented by the literature data. These are easy to identify in Table 2 as the rows having the most highlighted cells (such as energy demand or SDI).

A failure in doing so can give faulty results which may make no sense in reality (such as negative or very large numbers). One should keep in mind that PCA assumes linear connections between variables and that high signal-to-noise ratios exist within the data. This is not always the real life case when handling process related statistics, but as a basic approximation, PCA can give useful results which are often more reasonable than using thumb-ruled based estimations. This enables the user to perform general assessments of SWRO membrane pretreatment systems without conforming to a specific vendor assumption. Currently, the amount of data collected for this analysis is only sufficient for a basic, rough prediction. For better accuracy, one should increase the size of the sampled data set by collecting more documented information from the literature.

4. Conclusions

This paper has introduced the PCA-Regression method for the systematic retrieval of undocumented data and estimation of membrane technology performance in SWRO pretreatment. For the first time, such a multivariate statistical method was applied to large data collected from recent literature. The method is very helpful when one is looking to generally analyze proprietary, location-dependent UF technology for SWRO pretreatment (for example for economic or environmental assessment). Since the method includes the use of orthogonal regression (based on the principal components), the estimation can be made from any variable to another even when all variables contain inaccuracies (an advantage over normal regression which assumes inaccuracies only in the predicted variables).

Future work would include increasing the accuracy of the analysis by collecting more data.

The next step would be using this method for a general analysis of membrane based SWRO pretreatment for the sake of either comparing different manufacturers or comparing the technology as a whole with that of conventional rapid filtration.

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