Mathematics Models in Reverse Osmosis Evaluation Processes

Subjects: Others

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An effective alternative for water purification is reverse osmosis (RO). Laboratory-scale RO modeling is widely applied worldwide, and allows the evaluation of the behavior of the system to find the most convenient operating variables to be applied in future industrial scale-ups. Statistical models provide a wide range of information that allows a statistical prediction of the operation of the plant, and allows people to obtain efficiency indices in its development; these are useful in the planning, operation and monitoring process in RO plants. The mathematical models describe the physical behavior of the membrane and allow the identification of optimal operating conditions, taking into account economic aspects, guaranteeing a greater implementation of RO technology in developing countries which have problems with water contaminated with toxic heavy metals. A comparative method is proposed to establish the advantages and selection criteria to apply the different models in IO.

reverse osmosis | mathematical model | statistical model

1. Introduction

Throughout the world, water scarcity is recognized as a present and future threat to humanity; as a consequence, the new trend is to recover water from wastewater or the sea through different technologies. Likewise, financial viability is often a concern in water reclamation projects [1]. Recent studies have shown membrane filtration technology to be a promising process for drinking water treatment and recovery [2][3][4][5]. One membrane filtration process that has drawn particular attention in the last few years is RO [6][7][8]. Feria-Díaz et al. [9] states that RO is the most advanced technology used for water desalination in the world, due to its high efficiency, flexibility, and ease of operation. In contrast, RO has become a tool with industrial applications, and its research is currently being deepened, with the aim of guiding this process towards sustainability [10]. In making reverse osmosis a more economically efficient technology, research has allowed advances in materials, better pumping efficiency, and the creation of energy recovery devices [11].

In order to understand the separation in a membrane process, it is necessary to build models. These models are especially useful when the transport coefficients are not functions of the driving forces, that is, pressure and concentration gradients [12]. The variables of the models are discussed by different authors seeking to reach an exact understanding of the process. For example, Sherwood et al. [13] define the coefficients in the solution—diffusion and solution-diffusion-imperfection models to be functions of both pressure and concentration, while the coefficients in the Kedem model [14] are relatively insensitive to pressure and concentration. On the other hand, Abbas [15] specifies two key variables that must be monitored and controlled for the correct performance of the RO system. One is product flow rate, and the second is conductivity (a measure of quality). However, there are many other variables that need to be monitored and/or controlled, including the feed rate, operating temperature, permeate pressure, and solute concentration.

Subramanni and Panda [16] state that steady-state statistical models in RO are built using flow, concentration, and pH data over a period of time. This indicates that statistical models are useful for the formulation of operational control strategies in real-time in the plant. On the other hand, laboratory-scale pilot plants are useful in order to understand the solute separation mechanism in water in an RO process. Mathematical models of the integrated process can be useful in the design and operation of plants at various levels. It should also be noted that phenomenological models derived from real-time plant data are useful for the calculation of the permeate and rejection characteristics that also incorporate concentration polarization [16]. However, the behavior of a real plant must be ascertained by analyzing its input and output data through statistical tools. Regression models were used to predict the performance index, which takes into account the consumption of energy depending on different variables.

2. Model Concentration Polarization

In membrane-based water treatment processes, membrane fouling is an unavoidable fact that can significantly affect the performance, operation, sustainability, and economic viability of the processes, with concentration by polarization being one of these mechanisms. There are several correlations for a quantitative description of this phenomenon [17].

The main research topic in mass transfer is the transfer process near the membrane, where concentration-polarization (CP) significantly affects this process. Therefore, the study of mass transfer to the outer membrane focuses on CP modeling to predict the RO separation process [5].

The phenomenon of concentration-polarization (CP) remains a challenge that generates problems in the operational process, such as increases in feed pressure, decreases in permeate, increases in energy consumption, and membrane fouling [8][18][19].

When a membrane separation process is carried out, as time progresses, solutes remain near the membrane on the feed side; they belong to dissolved salts that did not pass through the permeate. These solutes must be dragged by the rejection current; however, as this speed is almost zero, they can only pass into the rejection current by diffusion that is generated in the opposite direction to the *permeate flow*, which is also called retro diffusion. This causes a zone in the membrane called the boundary layer, where the concentration of the salt is greater than that of the rest of the solution. The explained phenomenon is called membrane polarization, and when the concentration of this solution in contact with the membrane increases, a concentration by polarization is generated [20][21].

Concentration polarization and the corresponding theory allow the simultaneous evaluation of the three characteristic parameters of the Spigler-Kedem [22] model: reflection coefficient σ, solute permeability Lp, and mass transfer coefficient K. In addition, the variable rate method gives quite good results, similar to those of the Spiegler-Kedem polarization model. The latter also provides information on the reflection and permeability of solutes [23].

Al-Obaidi et al. [24] show that a mathematical model applied in the processes of the separation of diluted aqueous solutions by RO can be used to predict and analyze the flow, pressure, concentration, and temperature in the membrane, in addition to facilitating the estimation of the behavior of the flow of water and the concentration of the solute.

Temperature is a very difficult parameter to control in a natural environment. However, in a plant operation process it is important to evaluate its effect on the operation of the RO [25]. Transport through dense films can be viewed as an activated process that can generally be represented by an Arrhenius-type equation. Temperature has an important effect on membrane permeability and solute transport, and the Arrhenius equation shows the temperature dependence of the membrane permeability in RO processes [26].

Alanod et al. [27] point out that the increase in pressure and temperature in a brackish water desalination process by RO allows better recovery but decreases when the feed flow increases. They also point out that lower energy consumption can be achieved with lower values of flow and pressures.

Ahmed et al. [28] point out that more than 60% of desalination processes installed in the world are operated by RO. New membrane materials, improved pretreatment methods, and novel process design have enabled the technology to operate near the theoretical energy limit. In turn, Lim and Elimelec [29] indicate that innovations in the system configuration, such as the use of multiple stages and/or passes, have been incorporated in large-scale RO plants to overcome the drawbacks of the RO process of a single stage in which the large, applied pressure results in avoidable energy dissipation and a high initial permeate flux.

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2.1. Mathematical Modeling

For Ersoy and Moscardini [32], a mathematical model is used to describe real problems as mathematical equations, and they are solved using different approaches. Sarker and Newton [33] indicate that the most frequently applied mathematical model is optimization or mathematical programming. This consists in maximizing or minimizing an objective function by systematically choosing input values within a set that stratifies some restrictions. They also point out that optimization is the way to find the best solution to a problem by analyzing several alternatives.

For Walker et al. [34], mathematical modeling and optimization in engineering allow the manipulation of design parameters to meet certain objectives and/or to help predict system performance. For their part, Yang and Koziel [35] state that the uncertainty of real systems and the costs involved in pilot experimental plants make mathematical models valuable, but more complex, such that they must be developed in a way that matches reality.

The development of a mathematical model that adequately expresses the performance of the RO process is essential in order for the final design of the system to be implemented to be optimal and efficient, whilst also allowing a reduction in costs during its implementation [36]. In this sense, several mathematical models have been proposed to describe mass transfer and hydrodynamic permeability in RO systems [5].

2.2. Membrane Modeling Approaches

Ahmed et al. [28] states that mathematical modeling techniques for membrane desalination processes have improved significantly in the last decade. Van der Bruggen [37] points out three benefits in modeling pressure-driven membrane separation processes. In the first instance, it helps to predict the behavior of the system and compare the different membranes. Secondly, the modeling allows a better understanding of the mechanisms that govern the permeate and rejection in the system. Thirdly, the models allow the generation of a monitoring process to find the factors that affect the performance of the process.

The modeling and optimization of solute separation processes by membranes has been critically studied in the last five years regarding the phenomena of transport and mass transfer, energy consumption, and fouling, etc. in technologies such as RO or multistage flash (MSF) [28].

2.3. Mathematical Modeling in Reverse Osmosis

In the 1960s, the solution diffusion model was developed, which—to date—continues to be the most widely used in RO separation processes. The model describes transport through a semi-permeable RO membrane [38]. In this model, the transfer of the solution (solute and solvent) through the membrane occurs in three steps: absorption to the membrane, diffusion through the membrane, and desorption from the membrane.

3. RO Optimization Modeling

Ahmed et al. and Zarzo and Prats [28][39] state that energy consumption in an RO system is between 50 and 60% of the total cost of the process, with this being the key factor for the use of any technology.

Between 1970 and 2022, the energy consumption in an RO system was reduced by 80% due to lower energy consumption in each of the components of the RO plant. Such is the case for the pretreatment system, high-pressure pumps, the material and configuration of the membrane, energy recovery devices, and post-treatment [39]. Initially, the energy consumption exceeded 15 kWh/m^3; today, and with the new advances in general, the consumption is in the order of 2.5 kWh/m^3 [39].

Ahmed et al. [28] point out that an adequate optimization of the system and greater energy reductions can be achieved with an adequate plant configuration, which can be achieved first through simulations before pilot-scale experimental tests. Geise et al. [40] state that the configuration of the membrane is fundamental for the reduction of energy consumption, where part of the driving force is the balance between the selectivity and permeability of the membrane.

In terms of energy consumption, several alternatives for the operation of the system were compared. Lin and Elimelech [41] compared two-stage reverse RO (SSRO) systems against a single-stage closed-loop (CC-RO). In the first case, the reject stream from the first stage is converted into feed for the second stage, while for the single-stage system, the reject is mixed with the feed stream that passes back through the membrane. The results show that the single-stage system in a closed circuit is less efficient than a two-stage system because it needs more energy to reduce the entropy generated by the mixture of the rejection to the feed flow [29].

In another investigation, Chong and Krantz [42] propose a low-consumption (EERO) system in which they seek to increase the overall water recovery by sending the retentate from one or more two-stage (SSRO) systems as feed to a countercurrent membrane cascade with recycling (CMCR). This consists in one or more low-salt-rejection RO stages (Stage 1) and high-salt-rejection stages (Stage 2). The results show a lower osmotic pressure differential and thus a lower net specific energy consumption [28].

King and Hong [43] propose a partial split single-pass system (SSO-RO) in which permeate from only the back RO elements in a pressure vessel is mixed with the RO feed to dilute the feed. This results in a high-quality permeate with lower energy demand. The modeling carried out shows that the energy efficiency is maximized for the process when the permeate of the last element is mixed with the feed. This modified process is up to 15% more efficient in permeate purity and energy efficiency than a normal two-step system [28].

An improvement to the RO system which is proposed to achieve a more uniform flow distribution throughout a pressure vessel is to use a hybrid membrane configuration known as internal staged design (ISD). This system involves the use of low-flux membranes in the front and high-flux membranes in the rear elements [44][45]. This system allows a significant reduction in permeate costs by requiring fewer pressure vessels and fewer membranes [46][47].

Han et al. [45] improved the system using three different types of RO membranes: high rejection, standard, and high flux. In an experimental boron rejection process, they showed that using three standard membranes at the front and four high-flow membranes at the back, energy savings of 0.41 kW/m^3 were achieved.

Jeong et al. [48] proposes a model based on a finite difference approximation that allows a better numerical optimization of the ISD system in the presence of colloidal fouling. Compared to conventional designs in which the same membrane is incorporated throughout the vessel, the ISD resulted in higher water flow and higher energy efficiency for long-term operation, without compromising the permeate quality (<400 mg/L).

Kotb et al. [49] point out that optimization studies require complex or highly non-linear models with many restrictions. They implemented a simple transport model to determine the operating parameters corresponding to the optimal structure of the RO system, that is, one-, two-, and three-stage arrangements with respect to the minimum cost of permeate production for a given *permeate flow* rate with the maximum total dissolved solids [28].

They suggest that the optimal permeate flow rate increases with the number of stages; while a single-stage RO system is suitable for up to 6 m^3/h, three-stage modules are suitable for production up to 20 m^3/h [28].

4. Statistical Modeling

The use of statistical models to analyze the separation process in RO is essential to knowing the behavior of an RO plant and analyzing the input and output data [16].

Subramanni and Panda [16], in their research carried out on a desalination process by RO, use statistical regression for the analysis of the experimental modeling. Among the most important conclusions, they point out that the statistical model allows a better understanding of the behavior of the plant's mechanism and the interaction between the input and output variables through the formulation of statistical models. The ANOVA analysis shows that the total dissolved solids of the permeate is affected by the change in the system recycle ratio. They also point out that the proposed statistical model is useful for the planning, monitoring, and analysis of the separation system.

Miyamoto et al. [50] statistically examined the performance of the sediment density index (SDI) and defined a new fouling index, defined as the "coefficient of permeation". The research was carried out in a desalination process under normal environmental conditions, where they statistically analyzed the relationships between the amount of filtered water, the elapsed time, and the environmental factors in order to obtain new knowledge about the performance and deficiencies of the use of SDI from a statistical point of view.

Khajet and Cojocaru [51] performed the modeling and optimization of the air-gap membrane distillation process using the response surface methodology. The optimization of a solar-powered desalination plant was evaluated through the response surface methodology [52].

Khajet et al. [52] investigated the optimization of an RO plant using solar-powered energy through statistical response surface modeling. They applied the orthogonal type methodology [53] for the design of the experiments and a minimum number of experimental runs—as proposed by Taguchi et al. [54]—with simultaneous temperature variations, which allowed them to develop a predictive model of salt rejection, permeate flux, and the RO specific performance index. The results obtained from the analysis of variance (ANOVA) confirm that the response surface models developed are statistically validated in order to simulate the OI process. They establish, for example, that for a drinking water production of 0.2 m^3/day they use an energy consumption of only 1.2 to 1.3 kWh/m^3.

In another investigation, Mohsen and Salen [55] evaluated the performance of an RO plant in Wadi Ma'in, Zara, and Mujib to present the state of the art of its operation and maintenance. They collected detailed information on plant design and engineering, water quality, plant personnel, and the cost of operation and maintenance since the plant was commissioned. They analyzed for 150 days the performance of the RO desalination process in terms of recovery, permeate flux, normalized permeate flux during the erratic period, normalized differential pressure throughout the RO system, and salt rejection, and obtained the state of the system operation and maintenance.

Khajet and Cojocaru [51] used the response surface methodology for the statistical design of the experiment, which allowed them to evaluate an air gap membrane desalination process. They developed and statistically validated two regression models, one for the performance index and one for the specific performance index that considers energy consumption. The temperature is the one that has the greatest positive effect on the performance index and the feed flow rate for the specific performance index.

De-wei et al. [56], meanwhile, used quadratic dynamic matrix control (QMDC), which is a model-based predictive control (MPC) strategy to evaluate and control an RO desalination system. For the QMDC controller, they installed a field-programmable gate array (FPGA) chip and operator using software developed for this purpose. The results showed that the proposed system performs better than the traditional proportional, integral and derivative (PID) controller systems.

Feo et al. [57] analyzed the production capacities and costs in production lines in small RO plants in the Canary Islands. For this purpose, they developed a mathematical model based on expressions related to costs based on production capacity. They collected and processed statistical data. They plotted all of the cost data on bar charts and box-and-whisker plots. They performed the study of outliers, as well as Kolmogorov-Smirnov and Shapiro-Wilk tests based on the Hubera M-wave, Tukey biweight, Hampel M, and Andrew's estimators. Subsequently, factorial analysis was performed using the Bartlett and Kaiser-Meyer-Olkin tests; they then analyzed the possible mathematical models.

The response surface model was proposed by Box and Wilson [58], and is very useful for the modeling and analysis of the results obtained in applications where the response of interest is influenced by different variables, and where the objective is to optimize said response. Its main advantage, compared to other models that relate a variable at three levels, is that it provides the minimum number of experimental runs. An economic design does so from the point of view of reagents, sample quantification, the payment of external checks, and energy, among others [59].

In order to form the MSR, it is necessary to consider several phases or steps, one of them being the exploration of the optimal response region, through 2k full factorial experiments or the option of 2k−p fractional factorial designs. This is necessary in order to determine a smaller number of experiments [60].

Taguchi contributed to the dissemination of the design of experiments because this, unlike what happens with classical design, does not require being an expert in the method in order to be able to apply it [54].

Taguchi's method manages to solve design of experiments problems in a practical way. The use of the classic design generally implies the allocation of more resources to experimentation (a greater number of experimental units, more personnel involved, more time, a special place may even be required for experimentation because there are more replicas, and efforts to maintain a homogeneous the experimental conditions, among others). In some cases, the Taguchi method constitutes the only possible way for companies to carry out experimentation [61].

Likewise, it should be pointed out that Taguchi's method would not be viable if its conclusions were not certain. The reliability of the results obtained through the design of experiments proposed by Taguchi [54] is given by the power of the AO, that is, the power of the ANOVA (ANalysis Of Variance).

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