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Optimization of a Water Purification System in Real Time

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This work considers the problem of the optimal control of a water treatment plant. It examines the existing mathematical models of reverse osmosis membranes and the need for developing own mathematical model of these elements. Moreover, it mentions existing systems of automatic control for reverse osmosis elements. Finally, it presents the results of the comparison between the control efficiency achieved with PID-controllers and using the MPC on the reverse osmosis facility.

1. Introduction

Water resources are used in industry for a variety of purposes, such as cooling devices and products production, washing machines and finished products, the production of solutions and others. After using water resources in a production process, they contain different impurities, which can be harmful to humans and the environment. One of the problems in modern industry is to reduce water consumption and lower the release of pollutants to the environment. This problem can be solved by applying a closed water cycle. In this way, the issue of the treatment of industrial waste pollutants arises.
The variety of products used and produced in industrial plants cause industrial effluents to be contaminated with all sorts of inorganic substances. Modern water treatment plants are configured as a sequential multistage process where the removal of impurities from wastewater is addressed step by step.
Recently, very popular purification methods for water and wastewater, based on the process of reverse osmosis, have been broached. This is because, unlike bulk filters, aeration and chemical treatment, membrane systems have the following advantages: their operation is low-energy demanding, chemical-resistant membranes are available, they are able to obtain high-quality filtering in one step water treatments.
In the literature there are more and more works devoted to the development of mathematical models of reverse osmosis membranes. Article Gambier et al. (2007) is devoted to analysis of existing mathematical models of reverse osmosis membranes, as well as the creation of a reverse osmosis membrane model based on physical laws. Article Absar et al. (2008) deals with the development of a simplified model of a reverse osmosis membrane which will be used to investigate the effectiveness of the hollow fiber. All these works are focused on the creation of models that are suitable for the synthesis of control systems. Indeed, several authors are dedicating to the development of automated control systems for reverse osmosis plants. Article Bartman et al. (2009) is devoted to the development of nonlinear control system based on the model of a reverse osmosis membrane obtained from experimental data. Article Sobana et al. (2014) is devoted to the development of management systems based on models of reverse osmosis membranes. Researchers are also trying to apply different methods for the control of desalination plants, e.g. (Riverol et al., 2005) in paper outlines the computer simulation using real data of a decoupled control system for a desalination unit. The aim of this work is to create a model of a reverse osmosis membrane allows us to describe a wide range of membranes, rather than any particular. And to show the possible solutions in the control of the reverse osmosis membrane.

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2. Mathematical model of a reverse osmosis membrane

A typical technological layout of a water purification process is shown in Figure 1. The structure of the technological scheme includes several purification steps. First step mechanical filtration involves the separation of small heavy particles by precipitation. After the precipitation step, there comes the second stage that is the chemical-driven coagulation. These reagents interact with the dissolved impurities of water and form a precipitate, which can be easily removed Won et al. (2012).

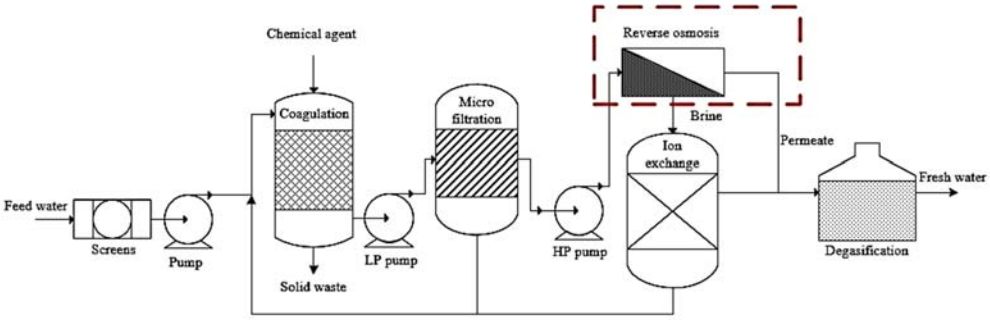

Figure 1: Typical technological scheme of a water purification process

Next step microfiltration permeate is then fed to a reverse osmosis unit. After the reverse osmosis, there is a stage of ionic exchange. This stage of ionic exchange relies on ion-exchange resins. The following one is the degassing stage. Degassing is necessary for removing carbon dioxide and restoration of the pH level Subramani et al. (2014). Of course, it is not necessary to use all of the aforementioned steps for a specific wastewater. Depending on the kind of impurities that are contained in the polluted water, some of the steps shown in Figure 1 may be skipped.
A nowadays key, problem is that of creating a mathematical description and mathematical models for closed water systems and wastewater systems These models must reflect their dynamic behavior and their intrinsic physical and chemical laws. This is necessary for solving problems of optimization and predictive control. Since the water treatment process is a multistep process, it is suitable to use predictive control for quality control and system stability. Article Rossi et al. (2014) devoted to the development of a new optimization algorithm using dynamic optimization and control of transients in real time. Article Abbas (2006) is devoted to the study of dynamic matrix control (DMC) algorithm for the management model based on reverse osmosis membranes of the hollow fibers. As mentioned earlier, reverse osmosis modules are very functional and effective nodes of water treatment plants, thus this work is devoted to the development of a mathematical model of the membrane used in a step of reverse osmosis of a water treatment unit.
There are many scientific papers on the development of mathematical models for reverse osmosis membranes. Dynamic models of reverse osmosis can be found in Gambier et al. (2007). In Alatiqi et al. (1989), the model was obtained by identification with a second-order transfer function of the form:

$$G(s) = \frac{K \cdot (\tau \cdot s + 1)}{\tau^2 \cdot s^2 + 2 \cdot \varsigma \cdot \tau \cdot s + 1} \quad (1)$$

A similar membrane model was used in Robertson et al. (1996).These models were obtained via identification for a specific treatment plant. These models were used to develop control algorithms, such as: Alatiqi et al. (1989) - CMPC (Constrained Model Predictive Control), Robertson et al. (1996) - DMC (Dynamic Matrix Control). In the latter work DMC is also compared with the standard PID controller. However, the models reported in the literature show different dynamic characteristics. Thus, there is a need for a mathematical model of reverse osmosis membranes. The novelty being developed of the model will be that in models with acceptable accuracy to describe the existing reverse osmosis membranes.
In papers like Alatiqi et al. (1989), which are devoted to the modeling of reverse osmosis membranes, the transverse flow rate of permeate through the membrane is determined by a modified Fick's law as follows:

$$V_p = A \cdot \left[\Delta P - \sigma \cdot \Delta \pi \right] \quad (2)$$

In Eq.(2), V_p is the transverse flow rate of permeate through the membrane, m/s, A is the pure water permeability constant [$m^3/(m^2 \cdot Pa \cdot s)$], σ is the reflection coefficient, ΔP is the pressure drop across the membrane [Pa] and $\Delta \pi$ is the osmotic pressure [Pa].

The value of the osmotic pressure in a solution depends on the amount, but not the chemical nature, of the substances dissolved in it. The greater the concentration of substances in a solution, the greater the osmotic pressure. This rule, called the osmotic pressure law, is expressed by the simple formula reported in Eq.(3). Notice that the $\Delta\pi$ is linearly related to the concentration.

$$\Delta\pi = \alpha \cdot \Delta C = \alpha \cdot \left(C_f - C_p\right) \tag{3}$$

In Eq.(3), C_f is the concentration of the solute in the feed water [mol/m^3] and C_p is the concentration of solute in the permeate [mol/m^3], α is osmotic pressure proportionality parameter and is determined from the following expression:

$$\alpha = iz \cdot T \cdot R_{\Gamma\Pi} \tag{4}$$

In Eq.(4), *iz* is the isotonic coefficient and is calculated from the ratio of the total number of particles in a solution to the number of molecules. Since its final value is rather difficult to compute, it is often set to 2. Moreover, T is the solution temperature [K], R_{GC} = 8.31 is the Boltzmann constant [J/(mol·K)].
The expression for the transverse velocity of the permeate through the membrane takes the form:

$$V_p = A \cdot \left[\Delta P - \sigma \cdot \phi \cdot \alpha \cdot \left(C_f - C_p\right)\right] \tag{5}$$

Accumulation of solute at the membrane surface leads to a polarization layer formation. The equation describing the polarization effect is the following one Assef et al. (1995):

$$\phi = \left(C_m - C_p\right) / \left(C_f - C_p\right) = \exp\left(V_p / k\right) \tag{6}$$

In Eq.(6), C_m is the concentration of substance on the surface of the membrane [mol/m^3] and k is the mass transfer coefficient [m/s]. The concentration of the solute in the permeate is determined from the following expression Alatiqi et al. (1989):

$$C_p = B \cdot \phi \cdot C_f / V_p + B \cdot \phi \tag{7}$$

In Eq.(7), B is the permeability coefficient of solute [m/s].
The coefficients A and B are dependent on the temperature of the solution supplied to the input of the membrane element. The temperature dependence of these coefficients has been determined by Rautenbach and Albrecht (1981). As a result, Eq.(8) was obtained:

$$A = A_0 \cdot \exp\left(\alpha_T \cdot (T - T)_0 / T_0\right) \;\; u \quad B = B_0 \cdot \exp\left(\beta_T \cdot (T - T)_0 / T_0\right) \tag{8}$$

In Eq.(8), T_0 equals 293 K, A_0 equals 5.501·10^{-7} m/(Pa*s), B_0 equals 1.82·10^{-5} m/(Pa*s), α_T is 7.08 and β_T is 3. Eq.(8) is valid for the temperature range from 4 to 95 C. Temperature dependency shown in the article Gambier et al. (2007).
The pressure distribution on the membrane is determined from the expression:

$$\begin{aligned} &P(x_i) = P(x_{i-1}) + \left(P_I(t) \cdot sh(\sqrt{a} \cdot (x_i - L)) - P_F(t) \cdot sh(\sqrt{a} \cdot x_i) / sh(\sqrt{a} \cdot L)\right) \\ &a = R^3 / 3 \cdot \mu \end{aligned} \tag{9}$$

In Eq.(9), $P_I(t)$ is the pressure at X = 0 [Pa], $P_F(t)$ is the pressure at $X = L$ [Pa], R is the half-height of the intermembrane channel [m], μ is the dynamic viscosity [Pa·s] and L is the membrane length [m].
Finally, the expression to evaluate the volumetric flow through the membrane is taken from Senthilmurugan et al. (2005):

$$Q_{pt} = V_p \cdot S \tag{10}$$

In Eq.(10), S is the membrane area [m^2].
The abovementioned equations, which describe the physical and chemical phenomena occurring in the membrane, have been implemented in Matlab / Simulink. As a result, the charts in Figure 2 were obtained.
The achieved simulation results show the change in the volumetric flow of the permeate of the reverse osmosis membrane and the impurity concentration in the permeate. In the simulation, the solution to be treated was fed to the membrane at 0.15 h with the pressure at the inlet of the membrane that was set to 2 MPa. As it can be seen from the results, at the initial time the output stream increases dramatically.

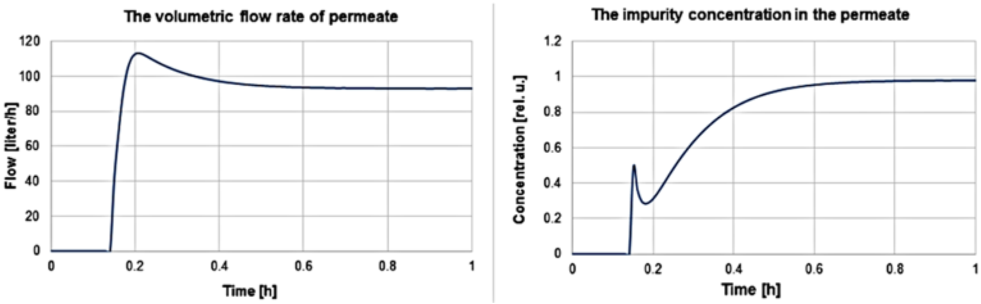

Figure 2: The simulation results

Then there is a decline in the output stream and its value settles to a certain constant value. This is due to the polarization effect, i.e. the increase in concentration of substances near the membrane, which leads to a decrease in the permeate flow. In addition, the membrane concentration polarization effect increases the concentration of harmful impurities in the permeate stream (chart on the right in Figure 2).

3. Control systems for a reverse osmosis module

The main goal of the control system of a membrane module is to maintain a certain flowrate of permeate with the lowest possible value of the operating pressure at the inlet membrane side. This will reduce the operation costs (electric power consumed by the pump) and extend the life of the membrane element. The external perturbations effect typically consists of a change in the concentration of harmful substances in the membrane module inlet feed water. Figure 3 presents the simulation results concerning the dynamic behavior of a reverse osmosis membrane when a stepwise change in the concentration of pollutants in the inlet solution is performed.

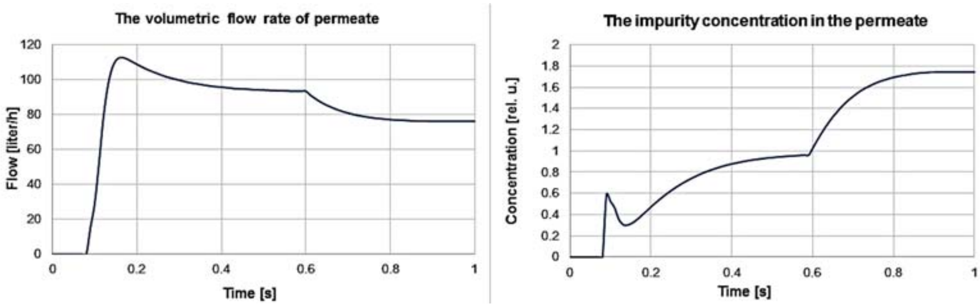

Figure 3: Open loop dynamics of the membrane

At time 0.6 h filed disturbance, the concentration of pollutants in the feed water has increased by 60%. It caused decreased the volumetric flow rate of the permeate outlet of the membrane module and increased the concentration of impurities in the resultant filtrate. In order to stabilize the volumetric flowrate of the permeate, it is proposed to synthesize an automatic control system. Both a PID controller and a MPC control schemes are considered. The control performance achieved with both of these strategies is analyzed in order to choose the one that provides the best control quality. The proposed control system is shown in Figure 4. As the regulator proposed to use the PID or MPC controller.

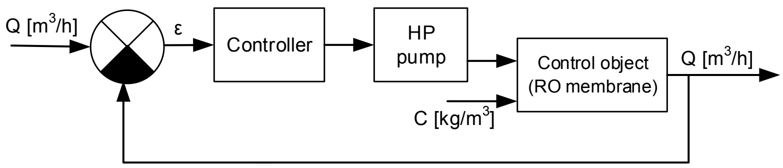

Figure 4: The automatic control system of reverse osmosis module

In order to use a standard PID controller, it is necessary to calculate its tuning coefficients by means of a tuning procedure (optimum module aperiodic stability, etc.), thus it is necessary to describe the transfer function of the controlled system (the membrane in this case). The dependence of the volumetric flow of the permeate on the operating pressure at the inlet membrane side can be described by a second order transfer function. By applying the aforementioned first-principles model, a transient response is achieved. Using this transient response, the coefficients of the transfer function describing the membrane were obtained Eq.(11).

$$W_{ob}(s) = K_{ob}/T_{ob} \cdot s + 1 = 0.06/12 \cdot s + 1 \qquad (11)$$

Using the optimal module method, the best tuning coefficients of the PID controller were calculated for the controlled system described by the transfer function presented in Eq.(11). A PID control law with the following parameters is obtained:

$$W_R(s) = K_R \cdot \left(1 + 1/T_i \cdot s + T_d \cdot s\right) = 322 \cdot \left(1 + 1/9.6 \cdot s + 1.5 \cdot s\right) \qquad (12)$$

By using the previously described model of the reverse osmosis membrane, it has also been implemented a regulator based on model predictive control. The next step was the simulation of the transition process, when incorporated in a system disturbance. Disturbance is an abrupt change in the impurity concentration in the feed water. At entering the disturbance, the controller must keep the permeate flow rate (Q) at the desired level. At this stage, the control and regulation of the impurities in the permeate is not performed. Figure 5 presents the results of this closed-loop simulation (PID controller and MPC controller). The transient processes obtained at different values the set point and of different disturbing influences.

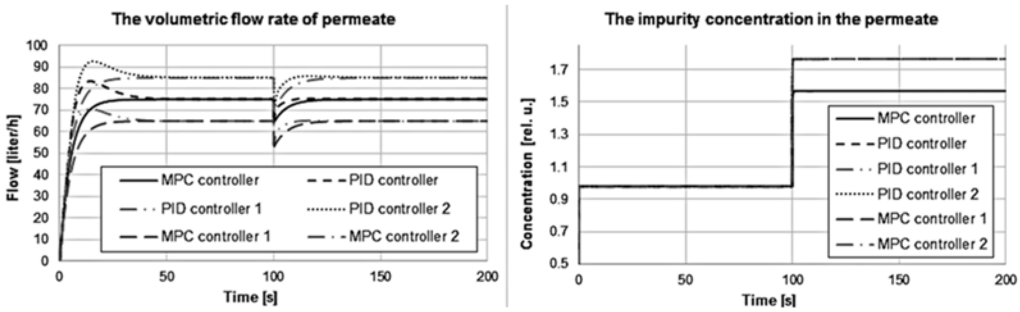

Figure 5: Closed-loop dynamic behavior of the membrane using both a PID controller and a MPC scheme

The presented charts (Figure 5) show that the membrane equipped with the MPC controller reaches the permeate flow set point without overshoot while the system equipped with the PID controller presents an overshoot. Quality indicators transient processes are presented in Table 1.

Table 1: Quality indicators

		PID controller	PID controller 1	PID controller 2	MPC controller	MPC controller 1	MPC controller 2
Settling time	control	25 s	23 s	24.5 s	15.4 s	15.4 s	15.6 s
	the perturbation	1.8 s	2.8 s	3.4 s	6.5 s	8.3 s	8.3 s
Overshoot		11 %	8.9 %	8.8 %	-	-	-
Integral quality indicators	control	8000	982	1760	8000	271	702
	the perturbation	6.31	7.4	16.7	34.6	45.1	77.1

For choosing the best regulator, one should consider the features of the provided control actions (Figure 6). The manipulated variable corresponds to the pressure at the inlet membrane side. The pressure at the inlet of the membrane is limited inside a feasible range. Indeed, it can vary from 0.1 MPa to 2.5 MPa. Limiting the pressure at the inlet of the membrane module is connected with the technical characteristics of the membrane element. As it can be seen from the transients presented in Figure 6, MPC controller, unlike the PID controller, generates control actions that are not reaching the maximum allowed value. As a consequence, the membrane is exposed to less stress as well as lower power consumptions in the pump are obtained. Based on the ensured control quality and comparing the control actions, it is advisable to use the MPC controller to control the reverse osmosis module.

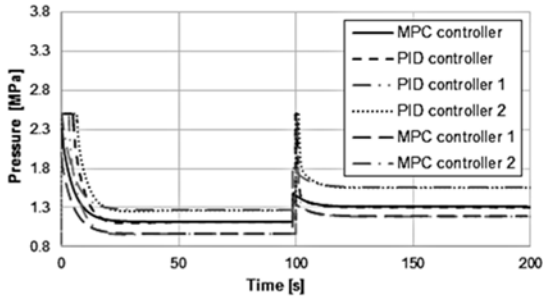

Figure 6: The control action on the reverse osmosis pressure

4. Conclusions

The paper discusses some existing works devoted to the modeling of reverse osmosis membranes and the development of control systems for the same units. From the review of existing models, it is observed that there is a need for developing mathematical models for reverse osmosis membranes. As a result, in this work a model for reverse osmosis membranes is developed, which is based on existing work and takes into account the disadvantages of the other existing models. In addition, in this work automatic control systems based on conventional (PID) and MPC algorithms are investigated. By comparing the control performances ensured by the two investigated control solutions, the conclusion is that it is preferable to use the MPC controllers since they ensure the best compromise between low settling times and smoothness of the control actions.

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References

Abbas A., 2006, Model predictive control of a reverse osmosis desalination unit, Desalination, 194, 268–280.

Absar B., Lamine Kadi S.El M., Belhamiti O., 2008, Mathematical modeling of Reverse Osmosis Process by the orthogonal collocation on finite element method, Asian Journal of Applied Sciences, 1, 1-18.

Alatiqi I., Ghabris A., Ebrahim S., 1989, Measurement and control in reverse osmosis desalination, Desalination, 75, 119–140.

Assef J.Z., Watters J.C., Desphande P.B., Alatiqi I.M., 1995, Advanced Control of a Reverse Osmosis Desalination Unit, Proc. International Desalination Association (IDA) World Congress, Vol. V, 174-188.

Bartman A.R., Christofides P.D., Cohen Y., 2009, Nonlinear Model-Based Control of an Experimental Reverse-Osmosis Water Desalination System, Ind. Eng. Chem. Res., 48, 6126–6136.

Gambier A., Krasnik A., Badreddin E., 2007, Dynamic Modeling of a Simple Reverse Osmosis Desalination Plant for Advanced Control Purposes, Proceedings of the 2007 American Control Conference July 11-13.

Rautenbach R.; Albrecht R.; 1981, Membrantrennverfahren, Otto Salle Verlag.

Riverol C., Pilipovik V., 2005, Mathematical Modeling of Perfect Decoupled Control Systemand Its Application: A Reverse Osmosis Desalination Industrial-Scale Unit, Journal of Automated Methods & Management in Chemistry, 2, 50–54.

Robertson M.W., Watters J.C., Desphande P.B., Assef J.Z., Alatiqi I.M., 1996, Model based control for reverse osmosis desalination processes, Desalination, 104, 59-68.

Rossi F., Manenti F., Kozin K.A., Goryunov A.G., 2014, Defeating the sustainability challenge in batch processes through low-cost utilities usage reduction, Chemical Engineering Transactions, Vol. 39 (Special Issue), 697-702.

Senthilmurugan S., Ahluwalia A., Gupta S. K., 2005, Modeling of a spiral-wound module and estimation of model parameters using numerical techniques, Desalination, 173, 269–286.

Sobana S., Panda R.C., 2014, Modeling and control of reverse osmosis desalination process using centralized and decentralized techniques, Desalination, 344, 243–251.

Subramani A., Jacangelo J.G., 2014, Treatment technologies for reverse osmosis concentrate volume minimization: A review, Separation and Purification Technology, 122, 472–489.

Won C.H., Choi J., Chung J., 2012, Evaluation of optimal reuse system for hydrofluoric acid wastewater, Journal of Hazardous Materials, 240, 110– 117.