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Implementation of membrane models on a CAPE-OPEN tool to simulate a process including RO membranes

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ABSTRACT

Process simulators are a useful tool for evaluating different configurations of chemical processes and developing new ones. Although these programs include many standard units like reactor or distillation towers, membrane units are not usually included. In this paper, it is shown the possibility to implement a reverse osmosis (RO) membrane unit in the free process simulator COCO, using input membrane parameters. The RO modeling is based on the coupling of the solution–diffusion model with a model for concentration polarization. The model was implemented as a Matlab CAPE-OPEN unit operation. In order to show the functionality of the developed application, a rinsing process adapted from literature was implemented to test different configurations. In this way, the combined use of the COCO simulator and the model of a reverse osmosis unit proved to be a useful tool for comparing the performance of different process configurations.

Keywords: Reverse osmosis; CAPE-OPEN; Rinsing; Process simulation; Modeling

1. Introduction

Process simulators are a cheap and safe way to analyze and optimize process performance. They can be used to design and improve processes without taking any risks and can reduce investing in pilot plant tests. For this reason, many authors have worked in this area, not only analyzing processes using these tools, but also improving them by implementing their own functionalities [1,2].

Membrane units are not usually included in process simulators as built-in units because of the diversity of existing membrane materials and module characteristics. Besides, as Karabelas et al. remarked [3], the use of commercial software available from membrane manufacturers is not practical because these tools are inflexible to perform detailed parametric studies. To work out this problem, some authors have focused their efforts on developing custom-made membrane units for specific purposes. As an example, Peshev and Livingston [4] implemented a nanofiltration unit in various simulators and proved that the simulation results agree with the experimental results.

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Commercial process simulators allow to implement custom unit operations, usually, requiring model coding in a specific framework. However, a CAPE-OPEN environment offers an alternative to this approach, since it allows the interoperability between process simulators, user-defined unit operation models, and thermodynamic servers [5]. Other examples of the use of CAPE-OPEN tools can be found in [6,7].

In this paper, a free-of-charge CAPE-OPEN simulator (COCO) was used to simulate a water regeneration process using reverse osmosis (RO) membranes. The RO model coupled with concentration polarization was implemented as a CAPE-OPEN compliant unit operation in Matlab script using the tool developed by AmsterCHEM for unit prototyping in the COCO simulator. Besides the Matlab tool, other generic modeling tools are available for Scilab and Excel [8] to develop custom-made units that can interact with the ones included in the simulator.

As an example of application, the regeneration process of the rinsing waters of a metal-finishing plant was chosen. In these plants, large amounts of water are consumed in the rinsing operation to remove heavy metals from work pieces. Therefore, it is suitable to apply membrane technologies, as permeate and concentrate streams can be recycled to the process. The results obtained with the process simulator were used to analyze alternative configurations and to set suitable operating conditions. This task would have been more difficult using commercial membrane design software because of the impossibility to interact with a process simulator.

2. Modeling

Membranes stages are not standard units of the COCO simulator. To have the possibility to simulate processes including reverse osmosis units, a reverse osmosis model was previously implemented in Matlab. The model gives the stationary values of the exiting stream variables as a function of the input streams and the operating conditions. Then, the model was included in the COCO simulation environment (COFE) to relate the input and output ports of a reverse osmosis user unit.

Fig. 1 shows a schematic drawing of the module with the main variables. In the figure, it is indicated the position of a generic differential element placed at a coordinate z from the input position. Plug flow is assumed for the stream that goes from feed ($z = 0$) to retentate ($z = L_{mod}$). For the permeate stream, it is assumed that the permeate flow to the permeate collector is high enough to discard diffusional effects between the permeate bulk and the permeate exiting the membrane.

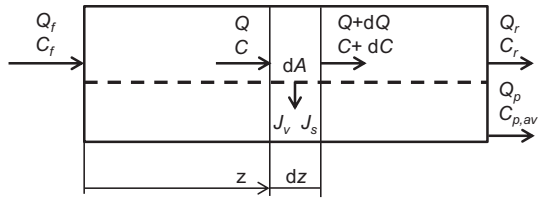

Fig. 1. Scheme of the module and main variables.

The RO model at differential scale is based on the combination of the solution–diffusion model with film layer theory. The driving force for permeate flux is the difference between applied pressure and osmotic pressure (Eq. (1)). The osmotic pressure is calculated according to the Van't Hoff law in terms of liquid concentration at the membrane wall, C_w, and permeate concentration, C_p (Eq. (2)). The driving force for solute flux is the difference between the wall liquid concentration and the permeate concentration (Eq. (3)). The wall liquid concentration, the bulk concentration C, and the permeate concentration are related by Eq. (5) that accounts for concentration polarization [9] which causes an concentration increase from the bulk solution to the membrane wall. The mass transfer coefficient, k_s, of this equation was calculated according to [10].

$$J_v = A_w \cdot (\Delta P - \Delta\pi) \quad (1)$$

$$\Delta\pi = b_\pi \cdot (C_w - C_p) \quad (2)$$

$$J_s = B_s \cdot (C_w - C_p) \quad (3)$$

$$C_p = \frac{J_s}{J_v} \quad (4)$$

$$J_v = k_s \cdot \ln\frac{C_w - C_p}{C - C_p} \quad (5)$$

For each membrane position, it is necessary to determine the volumetric and solute flux that correspond to the flow inside the membrane module Q, concentration inside the bulk of the membrane channel C, and transmembrane pressure ΔP. In order to do that, the set of Eqs. ((1)–(5)) was carried out iteratively as follows:

(1) Start with guessed values of C_w (greater than C) and C_p.
(2) J_v and J_s are calculated using Eqs. (1) and (3), respectively.

(3) C_p is calculated using Eq. (4).
(4) A new value of C_w is obtained from Eq. (5).
(5) If the absolute relative error between the guessed value and the calculated value of C_w is greater than a pre-specified tolerance, a new guessed value is obtained using a damping factor β (Eq. (6)).

$$C_w^o = \beta \cdot C_w + (1-\beta) \cdot C_w^o \tag{6}$$

The damping factor is necessary to improve convergence. In our case, an initial value $\beta = 0.5$ was used. In the next iterations, the parameter value was calculated using the Wegstein method. An error tolerance of 10^{-4} was used as a stopping criterion.

The iteration procedure previously described gives flux values to be used in the differential balance equations for flow and concentration with respect to the coordinate, z (Eqs. (7) and (8)). These equations are derived from flow and solute balances under the assumption of incompressibility and constant density. The equations use the following parameters related to module geometry: the effective cross-section module S_{mod} and the ratio of the membrane area to the internal volume $(A/V)_{mod}$.

$$\frac{dQ}{dz} = -J_v \cdot (A/V)_{mod} \cdot S_{mod} \tag{7}$$

$$\frac{dC}{dz} = \frac{J_v \cdot C - J_s}{Q} \cdot (A/V)_{mod} \cdot S_{mod} \tag{8}$$

Besides, the loss of charge along the system was taken into account (Eq. (9)) [10]:

$$\frac{d\Delta P}{dz} = -k_0 \cdot \left(\frac{Q}{S_{mod}}\right)^{k_n} \tag{9}$$

These equations were integrated using a Matlab solver based on the Runge–Kutta method to the whole length of the membrane stage L using the feed variables (Q_f, C_f, and P_f) as boundary conditions at $z = 0$. It was considered a gauge pressure of zero for the permeate stream, therefore, the transmembrane pressure coincides with the gauge pressure at the feed side.

Once the retentate stream is calculated, the permeate stream is obtained by applying a global mass balance under the assumption of constant density.

$$Q_p = Q_f - Q_r \tag{10}$$

$$C_{p,av} = \frac{Q_f \cdot C_f - Q_r \cdot C_r}{Q_{p,out}} \tag{11}$$

3. Case study

The process selected to illustrate the use of the RO unit is adapted from one studied by Chilyumova and Thöming [11]. These authors simulated the dynamic behavior of a rinsing process with a regeneration stage based on high-pressure RO. They stated that the performance of the RO unit is critical to the system functionality.

The original process (Fig. 2) consists of: (i) a cascade of seven rinsing baths operating in countercurrent mode, (ii) a RO membrane unit using a disc–tube module, and (iii) an ionic exchange unit (IX).

The main part of the process is the rinsing cascade in which the nickel concentration of the drag-out stream must be reduced from the input drag-out concentration of $210\,g\,L^{-1}$ to a value under $0.21\,g\,L^{-1}$. The membrane unit operates in such a way that the nickel concentration of the retentate is close to that of the process, and then it is recycled back to the nickel-plating process. The permeate stream is recycled to the sixth bath in order to decrease fresh water consumption. The rinsing water coming out from the seventh bath is partially treated in the IX unit and then recycled back to this bath.

Fig. 3 shows the flow sheet for a modified process including a different type of RO modules. In this process, the RO unit of the process was changed by a pressure vessel containing six spiral wound modules in series. The membrane unit works intermittently, so to guarantee a suitable feed flow through the membrane unit, the regeneration system is completed

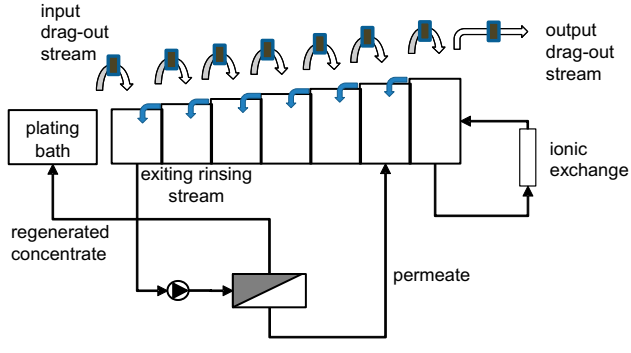

Fig. 2. Rinsing process with RO regeneration.

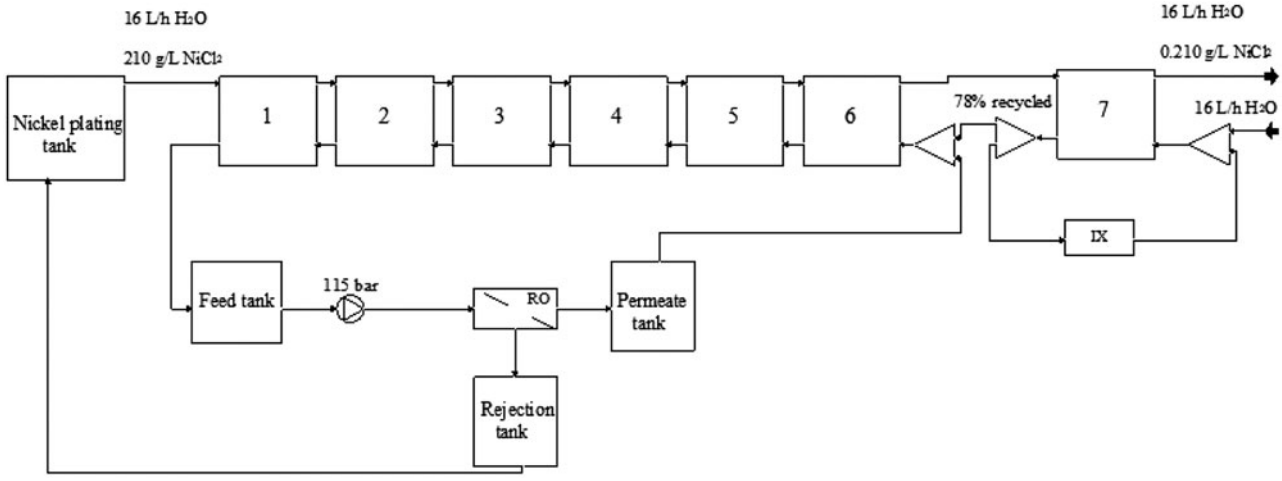

Fig. 3. Case of study process configuration.

Table 1
Membrane properties (T = 298 K) and module parameters

Variable	Value
A_w	6.90×10^{-4} m^3 m^{-2} h^{-1} bar^{-1}
B_S	1.26×10^{-4} m h^{-1}
b_π	0.57 bar m^3 kg^{-1}
k_0	0.5 bar m$^{-2.6}$ h$^{1.6}$
k_n	1.6
S_{mod}	3.0×10^{-3} m^2
$(A/V)_{mod}$	1,000 m^{-1}
k_S	$0.081 \times (Q/S_{mod})^{0.5}$ m h^{-1}

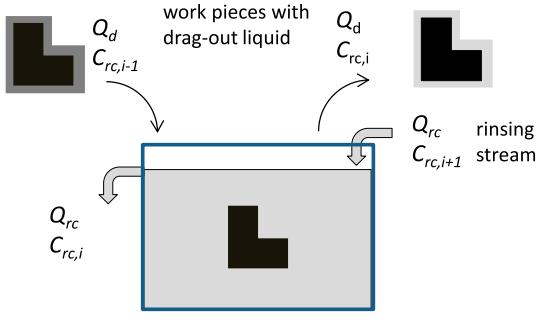

Fig. 4. Input and output streams for a tank in the rinsing cascade.

with three storage tanks (feed tank to the membrane unit, retentate, and permeate tanks). The membrane properties and module parameters used in the simulation are shown in Table 1. These properties were similar to those of a SW30-2540 module (Dow-Filmtec).

To build the rinsing tank models, stationary conditions were considered. Fig. 4 shows the situation for a tank in a generic position i of the rinsing cascade. The work pieces coming from the preceding tank i enter with a certain volume of drag-out liquid at concentration $C_{rc,i-1}$ and exit from the tank with the same drag-out volume and concentration $C_{rc,i}$. The rinsing flow Q_{rc} comes from the tank in the next position of the rinsing cascade. For specific positions this flow includes also a regenerated stream. It is assumed that the input rate of pieces is high enough that the drag-out liquid can be considered as a continuous flow Q_d. It is assumed perfect mixing in each tank so, both the exiting drag-out and liquid streams reach the same concentration, therefore, we have:

$$C_{rc,i} = \frac{Q_d \cdot C_{rc,i-1} + Q_{rc} \cdot C_{rc,i+1}}{Q_d + Q_{rc}} \quad (12)$$

The IX unit recycles water with a nickel concentration under 0.01 g L^{-1} assuring that the concentration specification required for the drag-out water exiting the rinsing process is obtained.

Additionally, in order to prove the effectiveness of the process simulation, several modifications of the above configuration were analyzed.

4. Simulation results

Fig. 5 shows the results obtained for the initial configuration of the rinsing process using six RO spiral wound modules in series. Feed pressure was adjusted to reach the bath concentration in the retentate stream. Although the rising criterion is accomplished, it is not achieved in the most efficient way. In this case, the

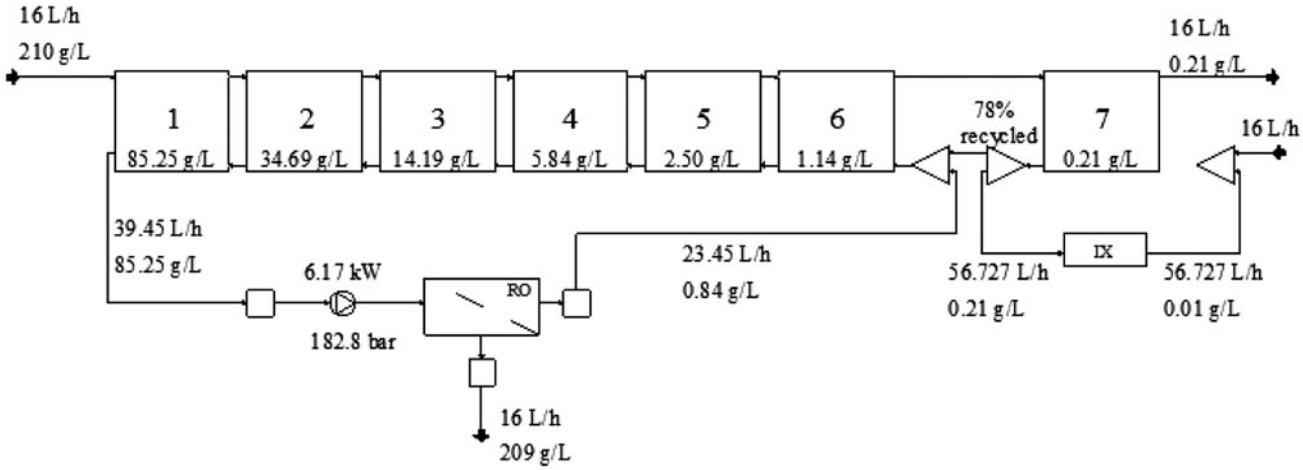

Fig. 5. Simulation results for the case study configuration.

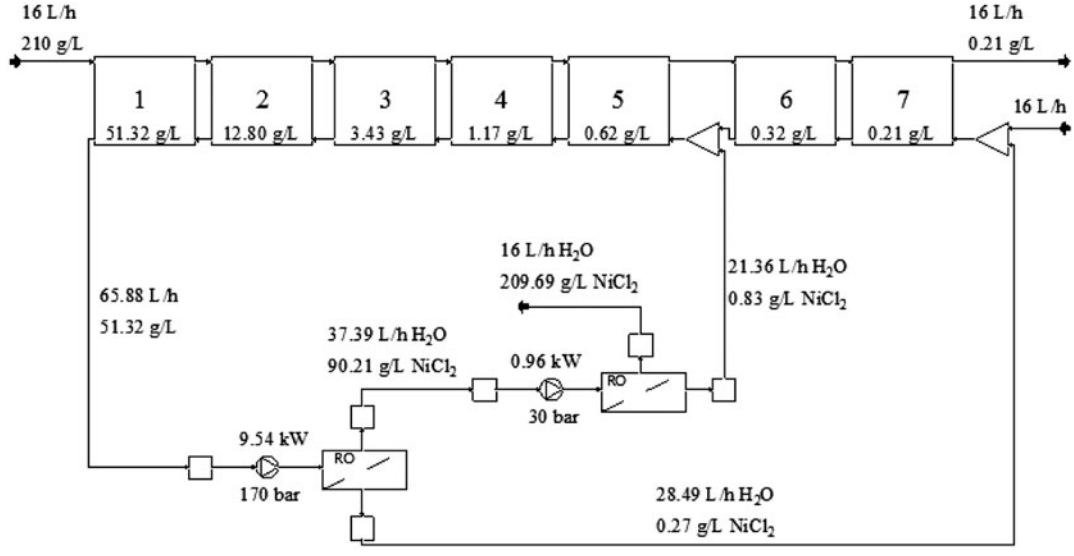

Fig. 6. Simulation results for a two-stage configuration.

regenerated permeate is obtained from an only stage and the corresponding concentration is $0.84\,g\,L^{-1}$. Therefore, it is necessary to have an ionic exchange unit to achieve the target concentration of $0.21\,g\,L^{-1}$.

As an alternative to the use of a single permeate, it was considered the use of two membrane stages. Fig. 6 shows the results obtained for a configuration of five modules in the first stage and four modules in the second stage. It can be seen that a permeate stream with lower concentration than that of the previous configuration is obtained. This permeate has the enough quality to be used directly in the last tank. The second stage unit allows achieving the bath concentration. The permeate stream exiting from the second stage has higher concentration, so it was recycled to a previous position of the rinsing cascade.

In this new configuration, there is an energetic consumption of 10.50 kW by the system pumps, which is greater than that of the original process. However, the rinsing criterion is accomplished without using the ionic exchange unit.

It was studied the possibility to achieve the concentration criteria with a lower energetic consumption by using a double pass (Fig. 7). In this configuration

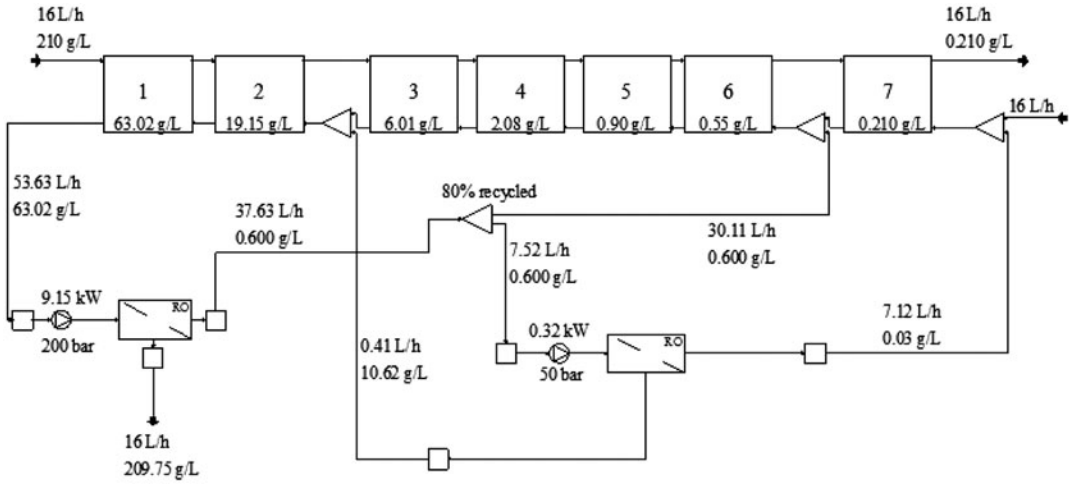

Fig. 7. Simulation results for double pass configuration.

the first stage has seven modules to the aim of concentrating the bath liquor. The permeate stream is divided into two streams and one of them is treated in the second pass stage which has two membrane modules. In this way, three streams are obtained, which can be introduced in suitable positions of the rinsing cascade according to their concentration level. The recycling of a higher number of streams has allowed to obtaining a process more efficient as the power consumed is smaller 9.47 kW. Besides, like in the previous solution, it is not necessary the use of the ionic exchange unit.

5. Conclusions

This work shows the use of a free simulator able to interact with a user model as an alternative to design and study chemical processes including membranes. For a sequential process including membrane process, commercial membrane software can be used to calculate the membrane stages. However, for recycling processes that include loops in their configuration, the membranes units and other unit operations must be calculated together.

The Matlab CAPE-OPEN unit of the process simulator allowed the implementation of an RO model including concentration polarization to build a membrane user unit. This unit allowed testing with the simulator different alternatives of the process configuration in a fast way.

The process configuration was gradually improved. In the end, it was found a process that meets the quality requirements without the need of an ionic exchange unit and with low energetic consumption.

Acknowledgments

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Symbols

$(A/V)_{mod}$	—	ratio of the membrane active area to the internal volume of the module, m^{-1}
A_w	—	water permeability, m bar^{-1} h^{-1}
B_S	—	solute permeability, m h^{-1}
b_π	—	osmotic coefficient, bar m^3 kg^{-1}
C	—	bulk concentration in the membrane stage, kg m^{-3}
C_f	—	feed concentration to the membrane stage, kg m^{-3}
C_{tank}	—	concentration in the stream exiting from rinsing tank i, kg m^{-3}
C_p	—	permeate concentration at each membrane position, kg m^{-3}
$C_{p,av}$	—	average permeate concentration of the system, kg m^{-3}
C_r	—	retentate concentration, kg m^{-3}
C_{rc}	—	concentration of the rinsing cascade, kg m^{-3}
C_w	—	membrane surface concentration, kg m^{-3}
Q	—	flow inside the membrane channel from feed to retentate, m^3 h^{-1}
Q_{rc}	—	flow of rinsing streams, m^3 h^{-1}
Q_d	—	flow dragged out by work pieces, m^3 h^{-1}
J_s	—	solute flux, kg m^{-2} h^{-1}
J_v	—	volumetric flux, m^3 m^{-2} h^{-1}
k_0	—	proportional loss coefficient, bar $m^{-(1+kn)}$ h^{kn}
k_n	—	potential loss coefficient
k_s	—	mass transfer coefficient, m h^{-1}

L_{mod} — module length, m
L — system length, m
ΔP — pressure difference, bar
P — gauge pressure in the stream from feed to retentate, bar
P_f — feed gauge pressure, bar
Q_f — feed flow to membrane stage, $m^3 h^{-1}$
Q_p — total permeate flow, $m^3 h^{-1}$
Q_r — rejection flow, $m^3 h^{-1}$
S_{mod} — module cross section, m^2
$\Delta\pi$ — osmotic pressure difference, bar

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