VALIDATION OF A REVERSE OSMOSIS DYNAMIC SIMULATOR

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ABSTRACT
Reverse Osmosis (RO) is the most common technique to produce drinkable water in arid and semi arid regions, from brackish and sea water. However, these plants are usually not optimally designed and operated, because only a short number of constant operation points is considered and not a changeable control strategy. Dynamic tools of design and simulation of RO plants will help to improve the design and operation of this kind of desalination plants. In order to do this, a new dynamic simulation library of RO plants was previously presented and a hydraulic validation shown elsewhere. Now, the present paper deals with the chemical validation of that library, using experimental data from a real RO plant.

Keywords: desalination plants, reverse osmosis, dynamic simulator, validation, parameter estimation.

1. INTRODUCTION

Reverse Osmosis (RO) is known to be an effective technique to produce drinkable water from brackish and sea water, (Fritzmann et al. 2007). This is because RO plants need less energy, investment cost, space and maintenance than other alternative desalination processes, (Gambier et al. 2007), hence, it is the preferred desalination technique worldwide, (Baker 2004; Wilf 2007). In the particular case of water supply of villages and small settlements, small to medium-size RO plants are successfully used. In this case, energy consumption is commonly fulfilled by renewable energy sources, such as solar or wind, while diesel generators are needed in order to keep it operating when no renewable sources are available, (Tadeo et al. 2009).

ROSA© and TorayDS© are perhaps the most common software for design of RO plants. They have been developed by two important membrane manufactures (Dow Chemical and Toray respectively) and are very powerful tools for static simulation of RO membranes. First, the user defines the characteristic of the feed water (solutes concentration, pH, temperature, etc.) and the required characteristic of the permeate (flow, TDS, Boron concentration, etc.). Next, the software helps to choose the best membrane model and configuration for the plant: number of pressure vessels, number of membranes per pressure vessel, possibility of a second pass, feed pressure, etc.

This software responds to the typical methodology of operation of RO plants. These plants, specially the high productions ones (50,000 - 200,000 m3/day of permeate), operate usually at a constant operation point, (Palacin et al. 2009a). However, this operation method looks incoherent if it is taken into account that consumed water varies along a day and along a year. Figure 1 shows a typical water demand curve of a population of 300 inhabitants over two days. It can be seen that during the night, the water consumption reaches its minimum value. Water demand curves are slightly different for each day of the week, and especially, for each month of the year.

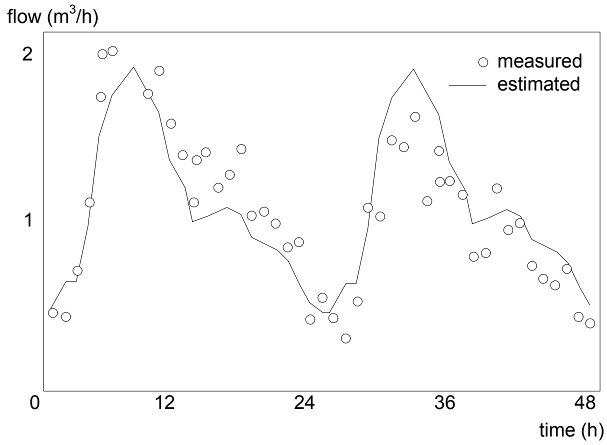

Figure 1: Typical water demand curve along two days.

Typical RO plants solve the daily variation of water demand by using big freshwater tanks at the end of the production line, and the annual variation by switching on/off membrane banks. It is easily understood that a priori this operation methodology is not optimal. On the other hand, using a variable operation point, producing more potable water when more is consumed, it will be possible to decrease the size of supply tanks, reducing the evaporation and minimizing the consumption of chemical products and the cost of equipments, (Palacin et al. 2009b). From an energy consumption point of view, a variable operation point looks more adequate too. It is very common that the availability and cost of electric energy varies along a day. This looks that producing more permeate water when energy cost is cheaper, the water total prize will decrease, (Salazar et al. 2010). In order to find the better operation point curve, both effects must be taken into account: the variation of the water demand and the energy cost. Advanced control design techniques, which take into account a changeable operation point, improve efficiency of the RO plant, extend the life of the components and reduce installation and operation costs, (Palacin et al. 2010a). Several interesting and advantageous applications of advanced control techniques in desalination plants can be seen in (Bacelli et al. 2009; Bartman et al. 2009a; Bartman et al. 2009b; McFall et al. 2008; Palacin et al. 2009c; Zafra-Cabeza et al. 2009).

Unfortunately, using static simulation tools, as ROSA© or TorayDS©, it is not possible to design a RO plant with a variable operation point and better performance, (Gambier et al. 2004). In order to solve this, a complete tool for the dynamic simulation of RO plants was developed and presented elsewhere (Palacin et al. 2008), and upgraded in (Palacin et al. 2009a). This software is a dynamic and modular library, which is developed in EcosimPro© simulation environment, and it is based on using first-principles and correlations from the literature and requires the typical system parameters in a RO plant (quality of feed water, salinity, scale concentration, pH, temperature, pump characteristic curves, type of the filters, characteristic of the membranes, etc.). A description of the math model can be consulted in (Syafiie et al. 2008). An initial validation of the hydraulic part of this dynamic library (pressures and flows) was shown previously (Palacin et al. 2010b). Now, the present paper deals with the chemical validation (salinity, feed water quality...) of the library. Initially, the values of the different parameters of the math models of the library had been taken from the specialized bibliography. It is now shown how these parameters can be directly estimated from simple experiments on real RO plants.

This paper is organized as follows: Section 2 shows the pilot plant used for validation and section 3 presents a brief description of the dynamic library. Finally, methodology and results of the validation are shown in section 4, followed by Conclusions and References.

2. REVERSE OSMOSIS PILOT PLANT

The RO pilot plant used for validation of the library is shown in Fig. 2, and a simplified diagram of the plant is shown in Fig. 3. First, a pump (B1) pumps brackish water from a well to the supply tank (T1). From this tank, water is pumped to a set of filters and chemical additions. The high pressure pump (B2) increases its pressure to a value above the osmotic pressure so that the pressurized water can pass then through the RO membrane rack. The difference in pressure between each side of the membranes produces a flow of clean water through the membranes. Finally, this clean water is stored in other tank (T2), which supplies water to the consumers.

Figure 2: RO plant for testing.

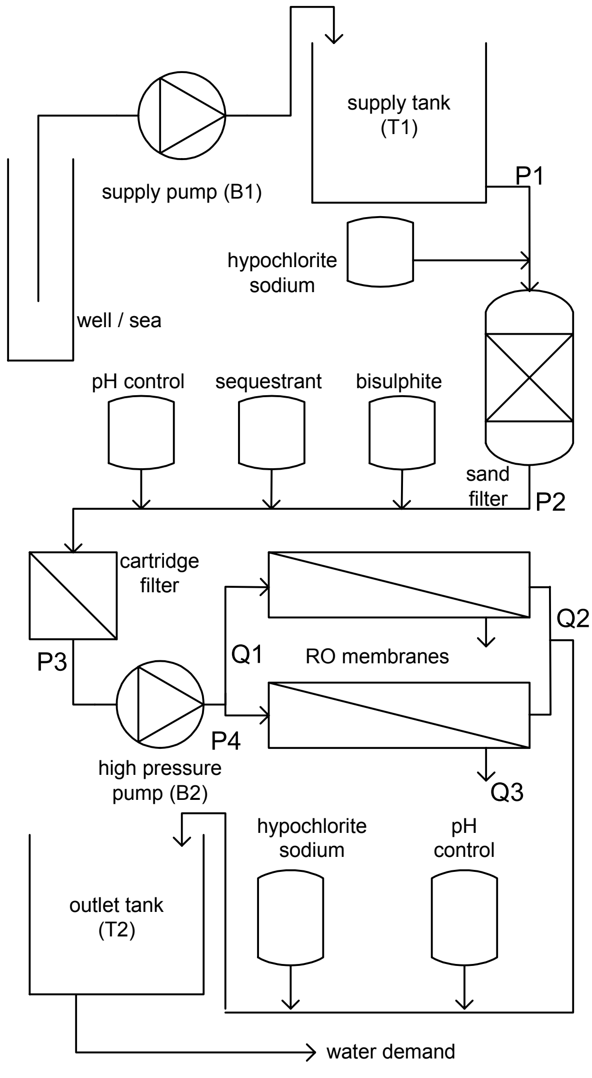

Figure 3: Diagram of the pilot plant.

Reverse osmosis is a separation process that uses high pressure to force a solvent (water) through a semi permeable membrane that retains the solute (salt) on one side. The clean water flow is called “permeate” and needs a remineralization before consumed, and the

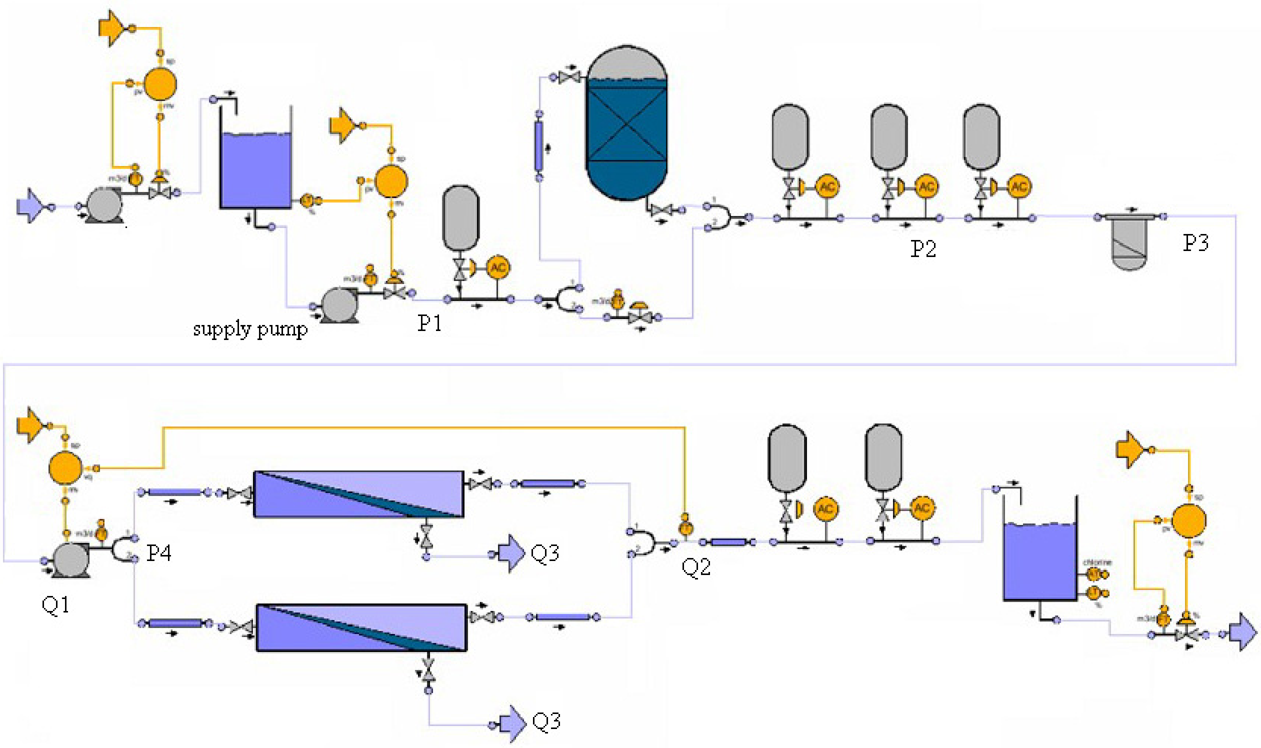

Figure 4: Graphical simulator of the pilot plant, made with the dynamic library.

rejected water flow is called “retentate” or “concentrate”. The ratio between retentate and feed is called recovery. Typical values of recovery are 45% for sea water and until 80% for brackish water. An in-depth description of the components of an RO plant could be seen in (Al-Bastaki et al. 1999).

The RO plant which is utilized in this paper has been design to produce 800 L/h of permeate water from a flow of 2000 L/h of brackish water. A central problem during operation is the decrease in performance of the membranes, due to deposits (silt, scale, organic components, etc). Thus, in order to prevent precipitation and eliminate microorganisms, a pretreatment is needed. It normally consists of filtration and the addition of chemical products. In addition, periodic cleanings are scheduled to reduce the amount of deposits. The final part of the process is a post-treatment, to make the water drinkable, by the addition of chlorine and a remineralization.

The RO process requires a high pressure on the feed side of the membrane: close to 30bar bar for the plant utilized in this validation (and up to 80 bar for extreme cases with very salty seawater). This pressure is generated by the high pressure pump (B2), (that, in this case, it is a positive displacement pump), that consumes most of the electrical energy needed by the plant.

The permeate flow is controlled by a PID, which manipulates the velocity of the high pressure pump, using a variable-frequency drive. The recovery of the system is controlled manually by a back pressure valve in the outlet the concentrate.

3. DYNAMIC LIBRARY OF RO PLANTS

The dynamic library of RO plants has been developed in the simulation environment EcosimPro©. EcosimPro© is a powerful modeling and simulation tool that follows advanced methodology for modeling and dynamic simulation. It provides an object oriented and non causal approach that allows creating new simulations interconnecting reusable component libraries. EcosimPro© is based on very powerful symbolic and numerical methods capable of processing complex systems represented by DAE equations and discrete events. Moreover, free versions are available for research and teaching (http://www.ecosimpro.com).

The dynamic library of RO plants is based on a set of components representing the different units of a RO plant. As sand filters, cartridge filters, different types of pumps, RO membranes, storage tanks, exchanger energy recoveries, valves, control systems (such as PIDs or PLCs), etc.Every component has been modeled using first principles and correlations from literature: Mass balances, energy balances, and physic-chemist equations are in the core of the models. Complex elements, such as sand filters or RO membranes, have been discretized by using the finite volume method. Fig. 4 corresponds to the graphical simulator of the real plant (shown in Fig. 1.), than is validated in the present paper. The simulator consists of two parallel membranes, one high pressure positive displacement pump, one sand filter, one cartridge filter, the addition of several chemical components (hypochlorite, bisulphite, sequestrant, chloride acid, etc.), supply centrifugal pumps and storage tanks.

4. VALIDATION

The evolution of all important variables in RO plants (flows, pressure, salt concentration, solids concentration, pH, temperature, etc.) is calculated by the dynamic library. However, the present paper only deals with the validation of the chemical part (salinity and quality of the feed water). The hydraulic part (pressure and flow) of the validation was shown elsewhere (Palacin et al. 2010b). The pilot plant was specially designed for testing and experimentation and has a huge number of sensors, bigger than in a typical RO plant. All the main parameters in the RO plant can be measured in different points of the plant. Sensors are managed from an OMRON PLC, and the data loading is carried out by the use of OPC protocol. In order to realize correctly the parameter estimation, several experiments were carried out changing the quality of the feed water and covering all the range of pressures and flows allowed in the plant. Once enough experiments have been done and data have been filtered and treated, it is possible to do the parameter estimation and the validation of the library. This is done by the minimization of a certain objective function that penalizes the different between the value of the measured variables, y, and the value of the calculated, by the math model, variables, $\hat{y}$, for each sample time and for each variable, and modifying the value of the parameters to be identified.

$$objective\ function = \sum_{variable}\sum_{sample\ time}(y-\hat{y})^2 \qquad (1)$$

The minimization of the single objective function can be solved by any non linear optimization algorithm, such as Sequential Quadratic Programming (SQP). This algorithm is available directly in the own EcosimPro©. For the calculation of the variables of the system, the simulator of the pilot plant needs to know the value of some variables, or boundary conditions. The typical boundary conditions are the input and output conditions of the system. In particularly, the simulator requires to know the value of the inlet pressure of the system (P1), the outlet pressure of the system (atmospheric pressure in this case), the quality of the feed flow and the setpoint of the different PID controllers. Figure 5 and 6 show the profile of the setpoint of the permeate flow realized in experimentation. Measured data from the pilot plant obtained with the profile of the figure 5 are used for parameter estimation, and data from the profile of the figure 6 are used for validation. The setpoints profiles are repeated three times, with different values of the salinity of the feed water (15, 17 and 19 g/L). Figure 7 shows the velocity of the high pressure pump, automatically manipulated in order to get the permeate flow fixed in the setpoints profile of the figure 6. The relation between velocity of the pump and flow is calculated by the simulator using the characteristic curve of the pump, which, in this case, is a positive displacement pump. Figure 8 shows the estimated values of the curve of the pump, as well as the measured data. Notice how both curves coincide in the most part of cases. The coefficient of determination, R^2, for the characteristic curve of the pump gets the 0.92, which is reasonably good.

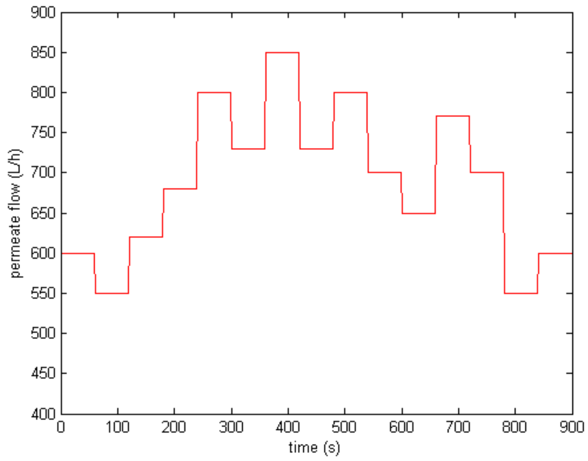

Figure 5: Profile of setpoint of permeate flow, used for parameter estimation.

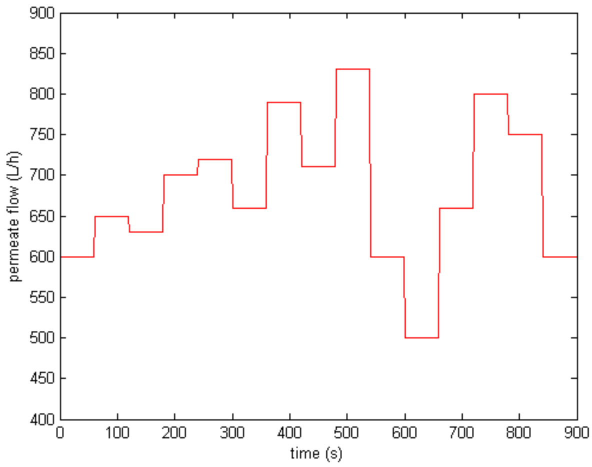

Figure 6: Profile of setpoint of permeate flow, used for validation.

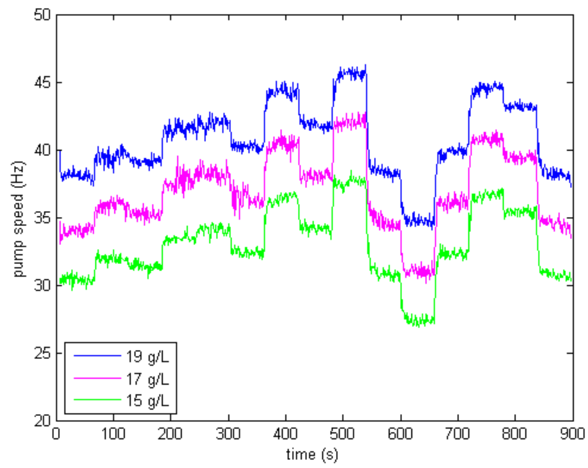

Figure 7: Velocity of the high pressure pump, the manipulated variable of the control of permeate flow.

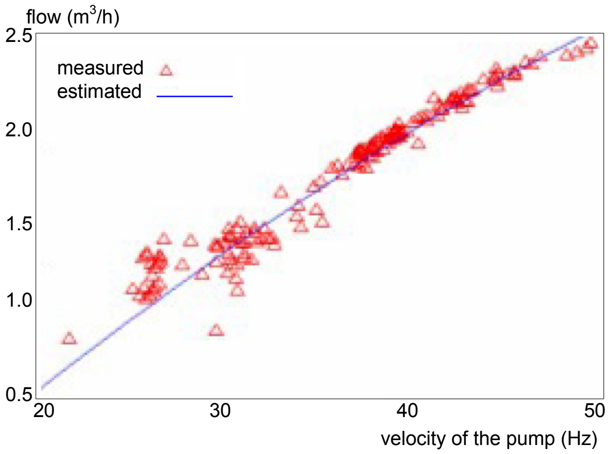

Figure 8: High pressure pump curve.

The permeate flow, which is the critical variable in the system, is typically calculated depending of the difference between the drop pressure (*ΔP*) and the osmotic pressure (*ΔΠ*) through the membrane. As it can be seen in equation 2, where *A* is the area of the membrane and *L* is the permeability. *A* and *L* are two parameters fulfilled by the membrane manufacturer.

$$permeate\ flow = L \cdot A \cdot (\Delta P - \Delta \Pi) = L^{*} \cdot (\Delta P - \Delta \Pi) \qquad (2)$$

However, permeability is not a constant value, and depends dynamically on the inevitable and unwanted fouling. As it was mentioned before, in order to avoid this, different types of cleanings should be periodically realized. Figure 9 shows the evolution of the permeability during one experiment. The permeability was correctly estimated using the equation 3. Data from experimentation in the pilot plant were used to estimate the parameters of this equation for this particular case: L_o ~ 230 L/(h·bar) and Ψ ~ 1100 s.

$$L^{*} = L_o \cdot exp(-t/\Psi) \qquad (3)$$

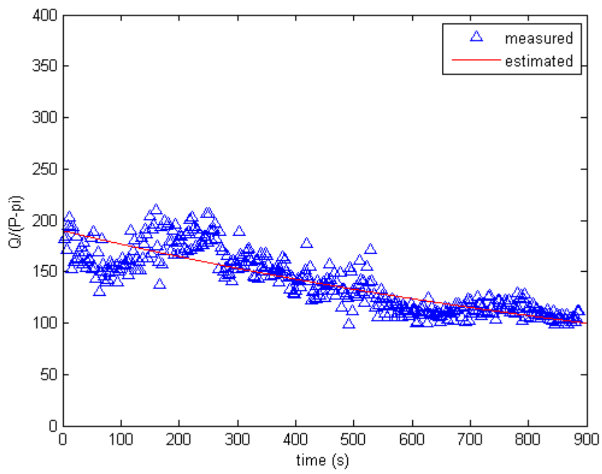

Figure 9: Fouling affecting the permeability.

On the other hand, the salt flow that is able to cross along the membrane is typically calculated depending on the difference of concentration through the membrane (*ΔC*). As is can be seen in the following equation, where L_s is the salt permeability:

$$salt\ flow = L_s \cdot A \cdot (\Delta C) = L_s^{*} \cdot (\Delta C) \qquad (4)$$

Salt flow is not a measured variable in a typical RO system. The important variable is the salt concentration of the permeate flow, which is easily calculated dividing equations 4 and 2:

$$salt\ concentration = L_s^{*}/L^{*} \cdot (\Delta C)/(\Delta P - \Delta \Pi) \qquad (5)$$

Figure 10 shows the salt concentration of the permeate vs. the term *(ΔC)/(ΔP-ΔΠ)* for different experiments. This curve corresponds to a straight line, whose slope is L_s^{*}/L^{*}. Data from experimentation in the pilot plant were used to estimate this slope, and then, the salt permeability of the membrane, L_s^{*} ~ 360 L/h.

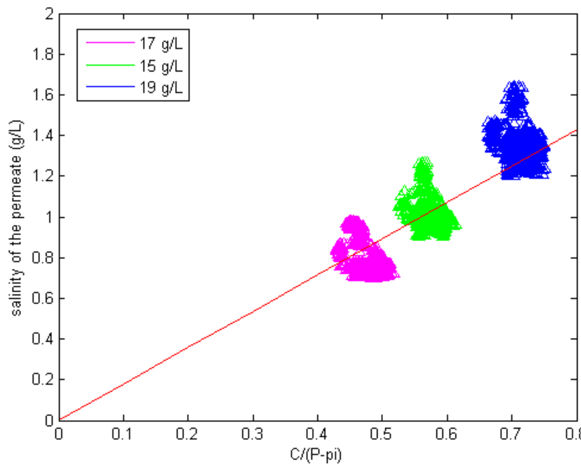

Figure 10: Salinity of the permeate vs. *(ΔC)/(ΔP-ΔΠ)*.

Once the parameter estimation has been completed, it is possible to do the validation of the library. Figures 11-13 show the estimated profile of the permeate flow and the real one, which has been measured in the pilot plant. Notice how both curves roughly coincide, which validate this part of the library. The average error between the estimated curve and the real one is around 3%. Figures 11, 12 and 13 correspond to the permeate flow with a salinity of the feed flow of 15, 17 and 19 g/L respectively.

CONCLUSIONS

The importance of dynamic simulation tools for the design of RO plants has been discussed. In order to improve the design and control of this kind of plants, a dynamic library of RO plants previously developed, has been checked, and initial results for a preliminary validation based on experiments carried out on the real plant are presented here. More precisely, tests of the chemical part of the simulator are presented, confirming the validity of this part of the dynamic library.

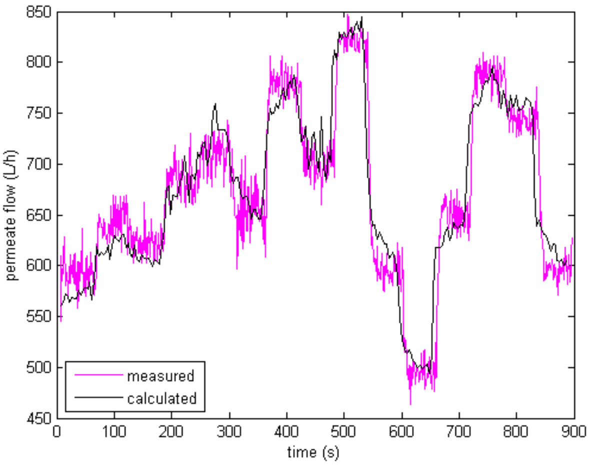

Figure 11: Permeate flow, estimated and measured, with a feed salinity of 15 g/L.

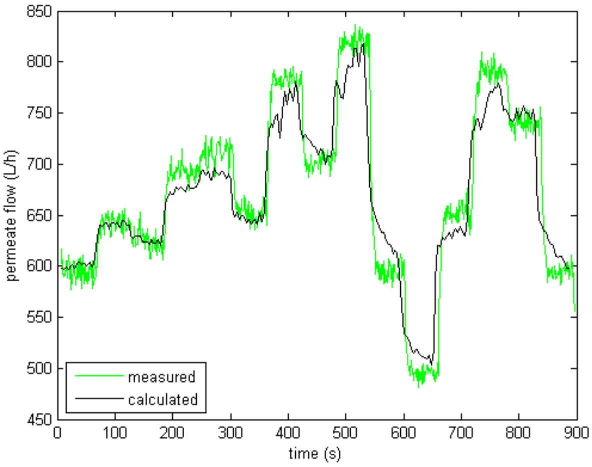

Figure 12: Permeate flow, estimated and measured, with a feed salinity of 17 g/L.

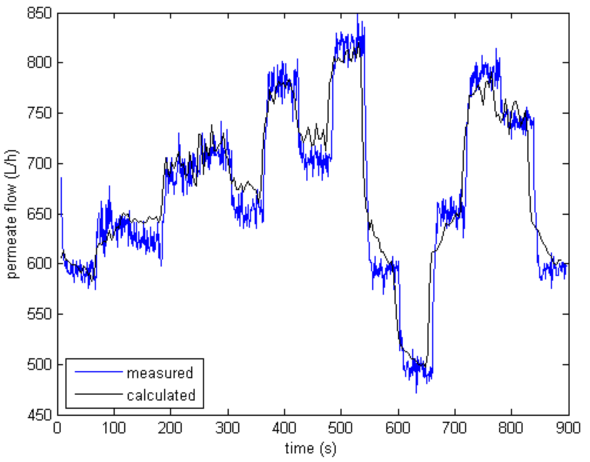

Figure 13: Permeate flow, estimated and measured, with a feed salinity of 19 g/L.

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