Membrane Modeling for Simulation and Control of Reverse Osmosis in Desalination Plants

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Abstract: A mathematical model of Reverse Osmosis membranes is proposed for use in the testing and comparison of control strategies in Reverse Osmosis plants. The model has been developed so that it can be used within off-the-shelf software and the parameters are simple to obtain from available plant measurements. Some simulations of the proposed model show that it correctly reproduces the expected process responses and can be used for testing different control strategies.

Keywords: Reverse Osmosis, Desalination, Modeling for Control.

1. INTRODUCTION

Nowadays, desalination activities based on Reverse Osmosis (RO) are being intensively introduced to combat water scarcity, as they provide a cost-effective solution to produce drinkable water from underground and sea water (Baker, 2004; Wilf, 2007). In recent years, significant advances in membrane technology have brought about an improvement in the filtering quality and a general reduction of costs (For a short review of the process see Fritzmann *et al.,* 2007). Hence, RO plants today need less energy, investment cost, space requirements and maintenance than other desalination processes (Gambier *et al.*, 2007), so they are being extensively implanted in fresh-water depleted areas.

Unfortunately, cost reduction and energy saving in RO plants have, until now, been undertaken almost exclusively from the point of view of the technological improvement of the basic components of the plant: membranes and pumps (See, for example, Geislera, 2001; Seibert *et al.*, 2004). However, the RO process is by nature energy intensive, so good control is basic to maintain water-production costs at acceptable levels and to raise the plant availability. Nonetheless, there are few applications of advanced control to this kind of processes (we can just mention Mindler, 1986; Robertson *et al.*, 1996; Jafar *et al.*, 2002). We believe that this lack of applications of advanced control in RO plants is partly due to the lack of adequate simulation tools to compare different designs. The availability of precise simulation tools for this complex systems would make it possible to show plant designers how an adequate controller design can save energy and increase plant availability. There are several simulation tools commercially available, usually provided by membrane manufacturers. However, these tools represent only static simulations, so they are very useful for design (sizing, configuration, layout, etc), but cannot be used for controller design or testing.

The fact that the lack of dynamic models and simulation tools limits the application of advanced control in RO plants has been pointed out by Robertson *et al.* (1996) and Gambier and Badreddin (2004). Thus, it is crucial to have dynamic simulation tools available to be able to apply advanced techniques of model-based control. Some efforts in this direction have been carried out by Alatiki (1999) and Gambier *et al.* (2007).

The approach used in this paper is based on developing models adequate for use within modern object-oriented simulation software with automatic selection of causality. This makes it possible to concentrate on modeling issues rather than on implementation problems, as the mathematical model that describes the system behaviour can be given directly in terms of algebraic and differential equations, which can be organized and solved automatically by the software. In particular, this makes it possible to reuse software for approximating Partial Differential Equations in a simple way. In our case, EcoSimPro (Perez-Vara *et al.*, 2000) has been used, as it has been proven to efficiently simulate problems of a similar level of complexity (Acebes *et al.*, 1995; Vilas *et al.*, 2007). A Library of components developed following the models discussed in this paper is presented elsewhere (Palacin *et al.*, 2008).

2. REVERSE OSMOSIS PLANTS

The salinity of potable water recommended by the World Health Organization is 500 mg/L, but the salinity of brackish water pumped from wells is usually between 2000 and 10000 mg/L, so 90% of the salt must be removed from these feeds. A similar situation appears when treating seawater, the main difference is the higher concentration of salts, which requires higher pressures. The basic components of the RO process are now discussed.

2.1 Reverse Osmosis Membranes

Osmosis is the net movement of a solvent (water) across a partially permeable membrane from a region of high solvent potential to an area of low solvent potential down a concentration gradient. Roughly speaking, Reverse Osmosis (RO) is the reverse of the normal osmosis: If a hydrostatic pressure greater than the *osmotic pressure* (hydrostatic pressure that stops the water flow, $\Delta\pi$) is applied, then water flows from the salt solution through the membrane, giving a stream of pure water (called *permeate*). The salt solution (called *retentate*) is continuously removed, following the scheme in Fig. 1.

Thus, RO can be defined as a separation process that uses pressure to force a solvent through a semipermeable membrane that retains the solute on one side and allows the pure solvent to pass to the other side. This process requires a high pressure to be exerted on the *feed* side of the membrane, that can reach even 70 bar (1000 psi) for seawater.

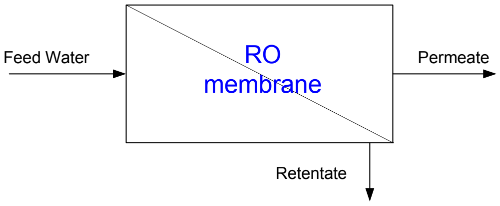

Fig. 1: RO membrane schematic used for modeling.

2.2 Pretreatment

Although this paper concentrates on modeling the membranes themselves, it is important to understand the whole RO process: For the membrane in the RO process to have a long life, the feed water must be pretreated before it passes through the membrane, as the main cause of permeate flux decline and loss of product quality in RO systems is membrane fouling. Prevention of fouling requires adequate control procedures for each plant. This pretreatment may represent as much as one-third of the operating and capital cost of the plant, but is essential for reliable long-term operation. The usual processes for pretreatment of brackish water are shown in Fig. 2.

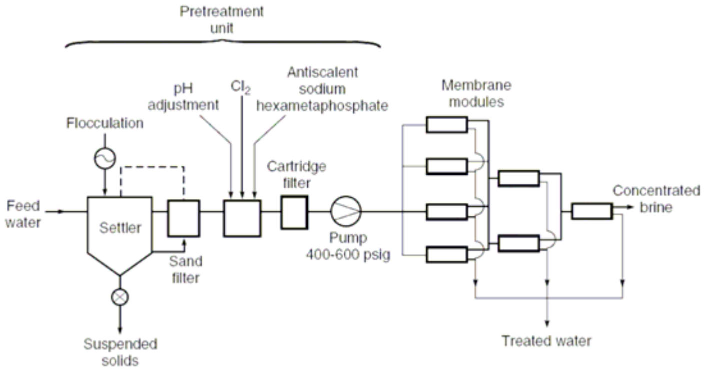

Fig. 2. Reverse osmosis plant (Baker, 2004).

Thus, pre-treatment has the objective of reducing the effect on the membranes of the following components in the feed water:

- *Silt,* that is formed by suspended particulates of all types that accumulate on the membrane surface (organic colloids, iron corrosion products, precipitated iron hydroxide, algae, and fine particulate matter). To avoid fouling, reverse osmosis units are usually fitted with 0.45-μm cartridge filters before the high-pressure pump, but a sand filter, sometimes supplemented by the addition of a flocculating chemical such as alum or a cationic polymer, is also required.

- *Scale*, which is caused by the precipitation of dissolved metal salts in the feed water on the membrane surface. Scale control is complex: the particular procedure depends on the composition of the feed water. For example, calcium carbonate scale can be controlled by acidifying the feed, using an ion exchange water softener or adding an antiscalant chemical such as sodium hexametaphosphate can be added; Silica can be a particularly troublesome scalant because no effective antiscalant or dispersant is available.

- *Biological* fouling, which is the growth of bacteria on the membrane surface. The susceptibility of membranes to biological fouling is a strong function of the membrane composition. For example, Cellulose Acetate membranes are an ideal nutrient for bacteria and can be completely destroyed by a few weeks of uncontrolled bacterial attack. Therefore, feed water to cellulose acetate membranes must always be sterilized. Polyamide Hollow Fiber membranes are also somewhat susceptible to bacterial attack, but Thin-film Composite membranes are generally quite resistant. Periodic treatment of such membranes with a bactericide usually controls biological fouling. Thus, control of bacteria is essential for cellulose acetate membranes and desirable for polyamides and composite membranes. Unfortunately, membranes are very sensitive to oxidizing compounds: cellulose acetate cannot tolerate more than 1ppm of chlorine, but residual chlorine must be almost completely removed in polyamide and interfacial composite membranes, as they are chlorine-sensitive. This dechlorination is generally achieved by adding sodium metabisulphate just before the membranes, which means that chlorination must completely destroy all biological components before the water is fed to the membranes.

2.3 Modeling variables

Based on the previous discussion, the variables used to model the membranes are the following:

1. Density of Flow J.
2. Pressure P.
3. Salt concentration C_S (salts that give osmotic pressure: Na^+, Cl^-, etc.).
4. pH.
5. Concentration of undesirable products:

    a. Bacteria C_b (includes other microorganisms that clog filters).
    b. Scale-causing salts C_{sc} (dissolved metal salts: $CaCO_3$, salts of aluminum, iron, copper, etc).
    c. Silt-causing C_{ss} (fine particulate matter).
    d. Oxidizing ions C_{Cl} (Chlorine).
    e. Organic components.
6. Concentration in the water of cleaning products:
    a. Anti-scale agents C_{as} (Sodiumhexameta-phosphate or others).
    b. Dechlorination agents C_m (metabisulphite).
7. Temperature, to reproduce the effect of water temperature in membrane efficiency and cleaning.

3. REVERSE OSMOSIS MEMBRANE MODELING

The model that is proposed in this section to represent dynamic behaviour of RO membranes is derived from basic knowledge of the process acquired from different sources in the literature. This information has been adapted to take into account that the objective of the simulation is the testing of control strategies and that the parameters should be easily obtained from input/output experiments on the RO plant.

It must be pointed out that there are a few more detailed dynamical models in the literature that can be easily included in the proposed approach: for example, Alexiadis *et al.* (2005) give detailed models of step changes in pressure. However, the time constants involved in these dynamics are so fast (in terms of seconds), compared with flow dynamic throughout the plant (in terms of minutes), that from a control point of view the effect of these dynamics is negligible, so they are not included in the proposed model. This allows a faster simulation of the control algorithms throughout the life span of the membranes (membranes last a couple of years). These elimination of fast dynamics make possible to reduce the number of experiments needed to obtain the parameters: parameterization of the proposed model can be carried out by measuring flow, pressure and concentration (at different temperatures), chloride concentration, and inlet concentrations of salts causing osmotic pressure or silt.

To develop the model it is assumed that RO membranes separate flows, affecting concentration and pressure, but having no effect on temperature, or pH. The proposed approach is based on the fact that RO membranes have a wide surface, with flow in one of the main directions; so for modeling, it is assumed that they can be divided in N sections following the flow direction (see Fig. 3). In each of these sections (denoted by $[i]$), the variables on both sides of the membrane are assumed to be constant, subject to the same input and output pressures (respectively, P_{in} and P_{out}).

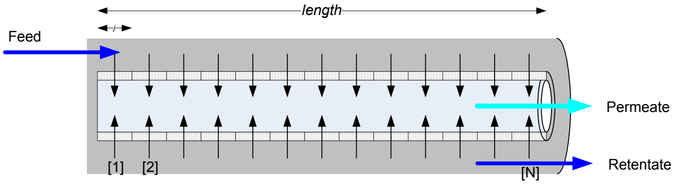

Fig. 3: Division of the membrane in N sections for modelling.

For each of these sections, Fick's law for water flow (J_w) across the membrane is related with the pressure and concentration gradients by the following equation:

$$J_{w[i]} = A[i]\left(\Delta p - \Delta\pi[i]\right), \tag{1}$$

where A is the *water permeability constant* (which depends on the composition of the membrane, amount of scaling, aging, temperature, etc), Δp is the pressure difference across the membrane and $\Delta\pi$ is the osmotic pressure, calculated as follows:

$$\Delta\pi[i] = \gamma M[i] RT, \tag{2}$$

where γ is the van't Hoff factor (average number of moles of solute actually in solution per mole of solid salt), M is the average molar concentration of the dissolved salts, R is 8.314 J/K/mol and T is the temperature (K).

Similarly, the flow of salt across a section of the RO membrane J_s, is described as:

$$J_s[i] = B[i]\left(C_S^P - C_S[i]\right), \tag{3}$$

where B is the *salt permeability constant* (which depends on the composition of the membrane, amount of scaling, aging, etc) and $C_S[i]$ and C_S^P are, respectively, the salt concentration on the feed and permeate sides of the membrane.

The water permeability and salt permeability constants in (1) and (3) are usually determined experimentally (Fritzman *et al.*, 2007). They are assumed to depend on temperature and fouling through the following equation:

$$A[i] = A_0 A_t[i] \exp\left(a_T \frac{T - T_0}{T}\right), \tag{4}$$

$$B[i] = B_0 B_t[i] \exp\left(b_T \frac{T - T_0}{T}\right), \tag{5}$$

where A_0 and B_0 are membrane coefficients at the reference temperature T_0=291K; the A_t and B_t coefficients correspond to membrane fouling (affected by aging and scaling, following (8) and (9), respectively); finally a_T and b_T are dimensionless empirical constants.

The *membrane selectivity* S, which corresponds to the percentage of salt rejection, is then given by:

$$S = \left[1 - \frac{C_S^P}{C_S^{in}}\right] \times 100\%. \tag{6}$$

The salt concentration on the permeate side of the membrane can be related to the membrane flows by the expression:

$$C_S^P = \frac{\sum J_s[i]}{\sum J_{W[i]}} \rho_w, \tag{7}$$

where ρ_w is water density.

It must be pointed out that, assuming that the water permeability constant is constant throughout the membrane (that is, that membrane fouling and aging is uniform) and a hollow cylinder shape (usual in RO membranes), the alternative model proposed by Gambier *et al.* (2007) can be obtained.

3.1 Modeling Fouling and Cleaning of Membranes

A major impediment in the application of RO membrane technology for desalinating brackish water is membrane fouling. For the RO membrane to have a long life, a good pretreatment is essential. Nonetheless, pretreatment must be backed up by an appropriate cleaning process. The specific RO membrane cleaning procedure is a function of the feed water chemistry, the type of membrane, and the type of fouling. In most cases, the cleaning regimen is based on flushing membrane modules by recirculating the cleaning solution at high speed through the module, followed by a soaking period. This process is repeated several times (Baker, 2004).

Typically, chemical cleaning agents used are acids, alkalis, chelatants, detergents, formulated products, and sterilizers. When the membrane module performance deteriorates with operating time, it can be restored with effective cleaning. However, after prolonged exposure to fouling conditions, performance restoration through membrane cleaning is less effective, and the limits of the system performance are exceeded. Then, replacing old membranes with new elements is the only way to restore system performance.

Following Lu *et al.* (2006), membrane fouling is modeled assuming an exponential decay in water permeability over time, with incomplete recovery:

$$A_t[i] = \left(1 - \Psi_1[i] t_2\right)\exp\left(-\frac{t_1}{\Gamma_1[i]}\right), \tag{8}$$

$$B_t[i] = \left(1 + \Psi_2[i] t_2\right)\exp\left(\frac{t_1}{\Gamma_2[i]}\right), \tag{9}$$

where t_1 is the length of time since the last cleaning and t_2 is the length of time since the last replacement. The constants Ψ_1 and Ψ_2 denote the extent to which the membrane has become degraded (see (12) and (13)); Γ_1 and Γ_2 are membrane performance decay constants (see (10) and (11)).

It must be pointed out that the model proposed so far in (1) to (9) reproduces the usual models in RO literature when a single section is used. Thus, for N=1 it is thoroughly validated and the constants are frequently known. The proposal that the membrane is divided in sections with different parameters comes from the fact that the "constants" A, B, M, Ψ_1, Ψ_2, Γ_1 and Γ_2 are experimentally known to depend on the amount of scaling, which is different in different parts of the membrane.

Thus, to include the effect of scaling (and aging by hydrolysis, explained in section 3.2), it is proposed in this paper that these constants are empirically obtained from a simple linear model, as it can be easily fitted from experimental data:

$$\Psi_1[i] = \Psi_{10} - k_{xs1}\left(C_{sc}[i] - C_{scnom}\right) + k_{xh1}h \tag{10}$$

$$\Psi_2[i] = \Psi_{20} - k_{xs2}\left(C_{sc}[i] - C_{scnom}\right) + k_{xh2}h \tag{11}$$

$$\Gamma_1[i] = \Gamma_{10} - k_{gs1}\left(C_{sc}[i] - C_{scnom}\right) + k_{gh1}h \tag{12}$$

$$\Gamma_2[i] = \Gamma_{20} - k_{gs2}\left(C_{sc}[i] - C_{scnom}\right) + k_{gh2}h \tag{13}$$

where Ψ_{10} and Ψ_{20} correspond to the mean value of the degradation of the membrane by scaling in new membranes in the absence of hydrolysis, when the concentration of scaling salts is C_{scnom}, and h corresponds to the degree of hydrolysis, defined in (14). This model represents the fact that the concentration of scaling salts C_{sc} is different at each section, so scaling will be different: the concentration of salts causing scaling increases near the outlet due to the loss of water through the membrane.

3.2 Modeling Aging of Membranes

Membrane filtration characteristics degrade with time, in a process called *aging*. Among other factors, chemical degradation is important. For example, cellulose acetate membranes for an RO process deteriorate by hydrolysis in a fast process under acidic or alkaline conditions, as shown in Fig. 4. Thus, for pH 4 - 5, membrane lifetimes can easily reach up to 4 years, while for pH 1 or 9 membrane lifetime is just days. Therefore, for a cellulose acetate membrane, it is critical to monitor and control the pH of the feed.

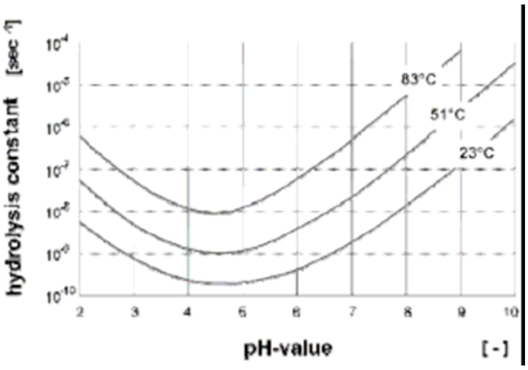

Fig. 4. Effect of pH and Temperature on Hydrolysis constant [Fritzmann, *et al.*, 2007]

For modeling, a single hydrolysis constant is extrapolated directly from temperature and pH measurements of the inlet flow (following Fig. 4), through the equation:

$$h = h_0 T\left(pH - pH_0\right)^2 . \tag{14}$$

The effect is also included in an aging-by-hydrolysis parameter that gives the expected lifetime of the membrane:

$$\frac{d(life)}{dt} = l_0 T\left(e^{\left|pH - pH_0\right|} - 1\right) + \kappa C_{Cl}, \tag{15}$$

where κ is a constant (default value κ=36000m^{3}kg^{-1}), and C_{Cl} is the concentration of oxidants (chlorine).

Of course, the model in (14) could be extended to include variations of pH throughout the membrane, but these variations are usually very small.

4. VALIDATION

The model proposed in Equations (1) to (15) was expressed directly using EcoSimPro, as this professional simulation software offers an efficient object-oriented solution to industrial problems, generating directly C++ code that can be used to simulate the plant, or even interfaced with control software for on-line model-based control and validation. The model was then validated and refined reproducing results in the literature and using the expected responses of the process.

Some experiments are presented to show the validity of the proposed approach. The default parameters, obtained from the literature, are the following: A_0=5.501x10^{-7} kg/m^2 s bar B_0=1.82x10^{-5} kg/m^{2}sbar, a_T=3.0, b_T=3.08, $\Psi_{10}=\Psi_{20}=3\times10^{-5}h^{-1}$, Γ_{10}=328h, Γ_{20}=650h, $k_{xs1}=k_{xs2}$=1.9m^{3}kg^{-1}h^{-1}, $k_{xh1}=k_{xh2}$=3700, $k_{gs1}=k_{gs2}$=128hm^{3}kg^{-1} and $k_{gh1}=k_{gh2}$=300h.

For example, Figures 5 to 7 show some result in a period of 7 days for step changes in inlet pressure with no cleaning. The results agree with the expected responses: For example, Fig. 5 shows the evolution of the concentration of salts that cause osmotic pressures at different point in the membrane: the concentration increases along the membrane until the osmotic pressure is reached. The concentration of salts that cause scaling is shown in Fig. 6: scaling will be more serious near the permeate outlet, as concentration also increases along the membrane. The consumed power is shown in Fig. 7: it can be seen that to maintain the pressure more power is consumed as time passes if the membrane is not cleaned, due to the deposition of scaling salts in the membrane.

To highlight the effect of cleanings, simulations were carried out using a high concentration of scale-causing salts, together with infrequent cleanings: the flow of retentate and permeates are shown in Fig. 8. The flows at different points of the membrane are depicted in Fig. 9. Finally, the consumed power is depicted in Fig. 10, which shows how important it is to schedule cleaning times correctly: cleaning consumes energy without producing water, but reduces the global energy consumption and increases the global water production, by increasing the permeability.

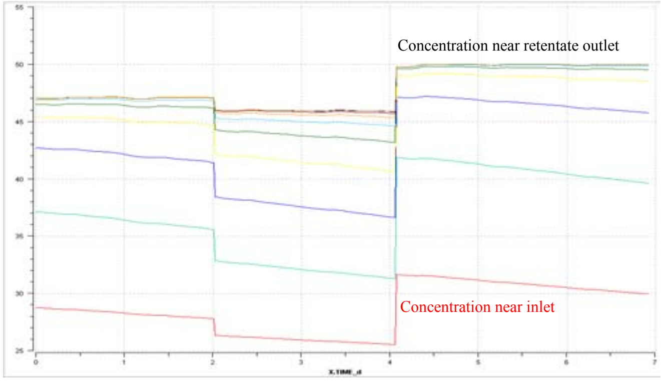

Fig. 5: Effect on Salt Concentrations.

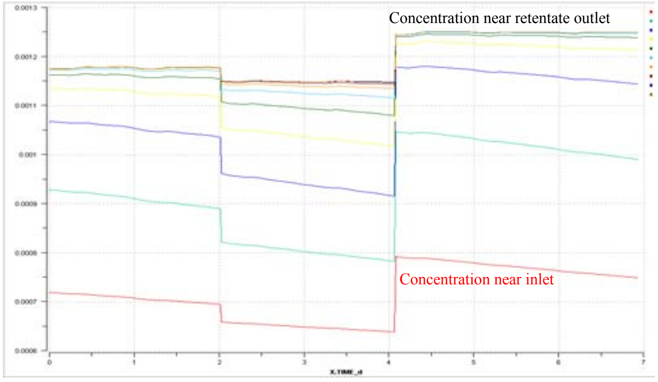

Fig. 6: Effect on Concentration of Scaling Salts.

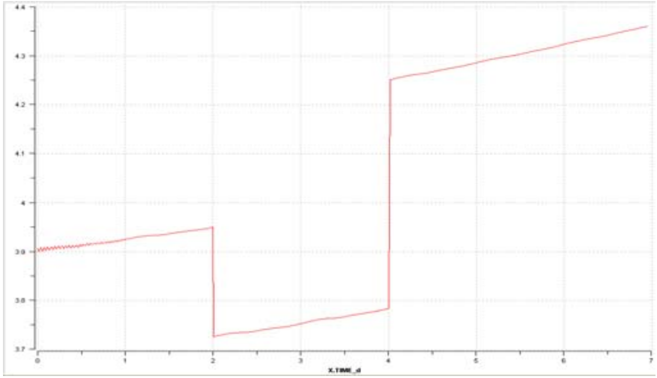

Fig. 7: Consumed Power with step changes in Feed Pressure.

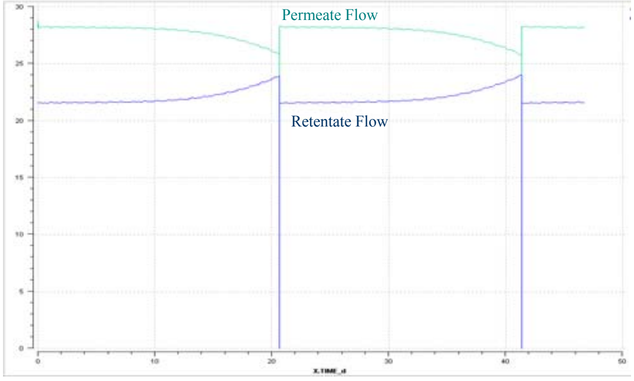

Fig. 8: Effect of cleanings on Permeate and Retentate flows.

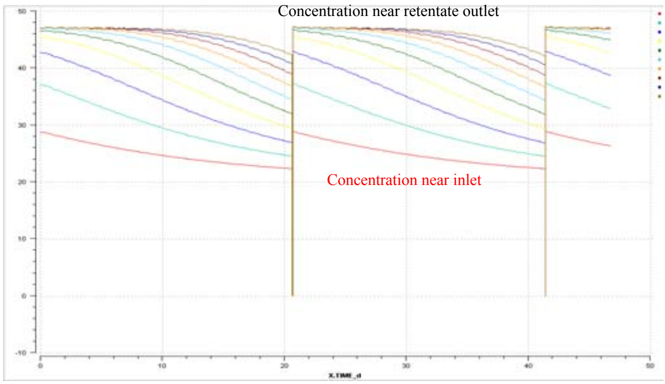

Fig. 9: Effect of cleanings on Salt Concentrations throughout the membrane.

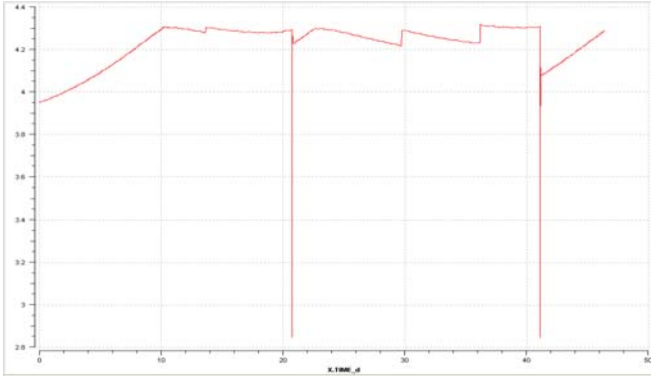

Fig. 10: Effect of cleanings on total Consumed Power.

5. CONCLUSIONS

This paper has discussed the importance of developing adequate models of Reverse Osmosis plants to optimize efficiency through an adequate design of the control software. For this, a membrane model has been derived, suitable for testing and comparing controllers in simulation. Compared with previous models the emphasize is in the dynamic simulation of the system for controller testing in the presence of fouling agents. For this, the membrane is considered to be divided in several sections with different fouling characteristics. It has been shown that the proposed model reproduces the expected behaviour of the plant in a very efficient way, so it can be used for rapid testing of control algorithms for this kind of processes.

Some control algorithms are know being developed using the implementation in software of the proposed models (Palacin *et al.*, 2008): these algorithms are based on regulating the high-pressure pump in the feed side and scheduling cleaning times based on predicting the water consumption and energy availability in a 24 hours basis.

ACKNOWLEDGEMENTS

This work has been funded by the European Commission (Reference FP6-2004-INCO-MPC-3). We would like to thank SETA, S.L. and the rest of the groups of “OPEN-GAIN” for feedback and comments.

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