ABSTRACT

Nanofiltration modelling requires a deep understanding of the different separation mechanisms involved and their importance in nanofiltration performance for different solutions. In this context, the first part of the thesis approaches the characterization of the commercial membrane ESNA1-LF2 through the study of the experimental results for synthetic ionic solutions in the range of brackish waters and, more specifically, the natural brackish groundwaters of the Valencian Community. The effect of the feed composition and concentration, and pressure on the results obtained with the membrane was studied at a laboratory scale working with a flat module. Variations in permeate flux and rejection due to fouling phenomena were also studied with synthetic solutions of organic compounds, confirming the classification of the ESNA1-LF2 membrane within the low fouling membranes.

In order to predict the membrane perfomances with nanofiltration models, it is necessary to determine the characteristic parameters of the models for a given feed and operating conditions. Thus, the second part of the thesis is focused on the application of the Donnan Steric-Partitioning Pore Model (DSPM) with dielectric exclusion to the results obtained with the different ionic solutions and on the determination of the five characteristic parameters of this model: pore radius (r_p), effective membrane thickness ($\Delta x/A_k$), membrane charge density (Xdq and XdS) and pore dielectric constant (ε_p).

Firstly, a first-order sensitivity analysis was performed with results obtained by simulation, evaluating the changes of the output model variables (permeate flux and rejection) with the variation of each parameter. Only r_p and $\Delta x/A_k$ have influence on the permeate flux results while r_p and ε_p resulted the key parameters for rejection calculation.

Model parameters can be determined directly or indirect by fitting the model with experimental results. In the present thesis, two indirect methodologies for the model parameters determination were used with the ESNA1-LF2 membrane results for the different ionic solutions studied. Thus, an individually determination of each parameter and a simultaneous determination of all parameters by fitting the model with a single set of experimental results were performed. To determine the best set of experiments for this simultaneous determination, a methodology based on simulation results is proposed which allow to evaluate a large number of combinations of experiments. The two groups of parameters obtained by both methodologies were validated by comparing the experimental results and those predicted by the model, obtaining unequal results for different feed compositions.

The time validity for the values of the parameters for a continuous use of the membrane was verified by its determination before and after the fouling tests with organic compounds, obtaining only a significant variation of the parameter $\Delta x/Ak$ due to the observed decrease in membrane permeability.