# Prediction of Permeate Flux and Rejection Rate in RO and NF Membrane Processes: Numerical Modelling of Hydrodynamics and Mass Transfer Coupling

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# Prediction of permeate flux and rejection rate in RO and NF membrane processes: Numerical modelling of hydrodynamics and mass transfer coupling

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## 1. Introduction

Modelling membrane separation processes and well predicting process variables can reduce the amount of tests, the costs and time usually consumed in pilot scale experiments. For these purposes, numerical simulation is very convenient as it combines rapidity, low cost and relatively easy implementation. The current work consists on developing a predictive numerical model for applications ranging from reverse osmosis to nanofiltration. The model does not use empirical correlations or experimental transfer coefficients: it depends only on solution physical properties, membrane characteristics and operating conditions. Validation is made by comparison to results found in scientific publications.

## 2. Methods

The present model considers a two-dimensional steady laminar Newtonian flow commonly encountered in plane channels of membrane modules operating in the cross-flow filtration mode. It follows the analytical works performed by Haldenwang et al. [1, 2] on the hydrodynamics combined with solute transfer (concentration polarization) for a flow in a channel presenting a leakage through its permeable walls. In addition to these phenomena, this numerical model considers osmotic pressure effects and a variable rejection rate along the membrane surface. The solvent flux through the membrane follows Darcy law and the solute transport within the membrane is considered to follow the solution-diffusion model [3]. The coupled Navier-Stokes and solute conservation equations are all conveniently rewritten in terms of non-dimensional parameters under the assumption of Prandtl hypothesis (axial diffusion negligible compared with transverse diffusion) and simultaneously solved by a second order finite difference scheme.

## 3. Results

Main results concern the prediction of permeate fluxes, intrinsic rejection rates and transverse concentration profiles.

Geraldes et al. [4] experimentally validated a predictive model using aqueous solutions and commercial nanofiltration membranes in a plane channel module. When applied to the same conditions, the model presented in this work exhibits a good agreement with experimental results for permeate fluxes as a function of transmembrane pressure as shown in Fig. 1, particularly in the case where other osmotic pressure laws are employed instead of van't Hoff law [4]. Comparisons with all polyethylene glycol (1000 $g.mol^{-1}$) experimental values in [4] yield a maximal relative error of 23% with a third-degree polynomial osmotic pressure law and of 70% with van't Hoff law. For sucrose, 5,9% and 12,3% respectively. Finally, for $Na_2SO_4$, errors are of the order of 7,5% for a power law and of 18,5% for van't Hoff law. Pure water flux is estimated at a 6,2% maximal error.


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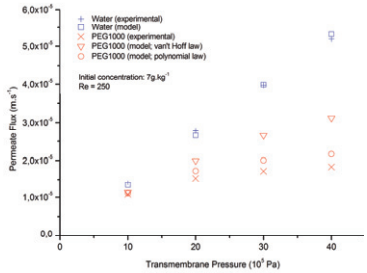


Fig. 1. Comparison of predicted and experimental permeate fluxes [4] as a function of the operating pressure for a polyethylene glycol (1000g.mol$^{-1}$) aqueous solution.

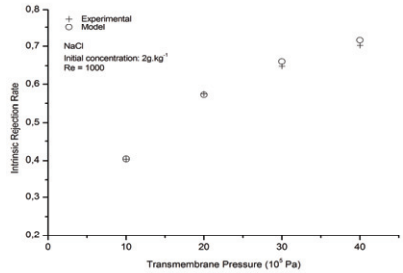


Fig. 2. Comparison of predicted and experimental intrinsic rejection rates [7] as a function of the operating pressure for a NaCl aqueous solution.

A good qualitative agreement is found with the experimental observations of permeate flux made by Zhou et al. [5] in the RO treatment of a NaCl solution in a spiral-wound module. From this finding, we also infer that a spiral-wound module channel may indeed be likened to a plane channel.

Fernandez-Sempere et al. [6] visualized and quantified the concentration polarization layer in a plane channel module during RO treatment of aqueous salt solutions through Digital Holographic Interferometry. For this case too, the model reproduces with considerable agreement the transverse concentration profile.

Geraldes et al. [7] calculated intrinsic rejection rates as functions of transmembrane pressure by CFD by making use of experimental apparent rejection coefficients and permeation rates in a plane channel configuration. As shown in Fig. 2, the present model well fits these results (maximum relative error of 2%). For $Na_2SO_4$, sucrose and polyethylene glycol (1000 g.mol$^{-1}$), the model yields a rejection rate of near 100% (as in [7]). In all these simulations, osmotic pressure was considered to follow a power law.

## 4. Discussion

Using a well defined set of easily accessible parameters, the current model proves to be able to well predict permeate fluxes, concentration polarization profiles and intrinsic rejection rates in reverse osmosis and nanofiltration.

It is also an adaptable model. Any theoretical or empirical osmotic pressure law may be employed, broadening the model's range of applicability to more specific solutes and yielding better results. This represents an important advantage given that the classical van't Hoff law is primarily valid for dilute solutions.

The model may also be regarded as a practical tool for membrane selection with respect to its expected performance as it allows to readily evaluate and quantify the impact of solute (and solvent) permeability over virtually all process variables.

Lastly, applications for which the reduction in the amount of experimental tests is a critical constraint could particularly benefit from this predictive model, as it may be the case for dangerous, scarce or expensive solutions.

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