Modeling Ionic Transport through Ion-Exchange Membranes

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Introduction

Electrodialysis (ED) is a membrane separation process in which ions are transferred through selective ion-exchange membranes (IEMs) from one solution to another using an electric field asthe driving force. ED is a mature technology in the field of brackish water desalination, but in thelast decades, the development of new membranes has allowed to extend its application in the food, drug, and chemical process industry, as well as in the environmental engineering field.

The effectiveness of ED separation depends on numerous variables, including cell properties membranes properties and operational parameters (electric current; electrical resistance of IEMsand electrolyte; pH and concentration). All these parameters are interrelated between them, and the study of their effect is important to design and optimize the process. A key factor to understandthe process is the ions transport through the IEMs, together with the concentration and potential profile create in the boundary layer between the electrolyte and the membrane charged surface.

Use of COMSOL Multiphysics

The ternary current distribution physics block, from the Electrochemistry Module of COMSOL Multiphysics, has been used to study the migration of ions through an IEM. The Nerst-Plank-Poisson (NPP) system of equations has been used, which includes the effects of diffusion, electromigration and convection[1].

This system of equations allows the analysis of the electric double layer formed at the interface between the membranes and the surrounding free electrolytes. The model is completed with chemical reactions between the involved species [2].

Results

Two studies were carried out: First, a stationary study aiming to compute the equilibrium concentration and electric potential profiles of membranes under an acid soaking pre-treatment. The second study uses the results of the previous step as initial values for a time-dependent simulation of cobalt selective separation from an e-waste recycling stream.

Figure 1.a shows the pH and voltage profile in the membrane and the surrounding electrolyte afterthe pre-treatment. **Figure 1.b** illustrates the details of the electrical double layer between the electrolyte and the membrane charge surface.

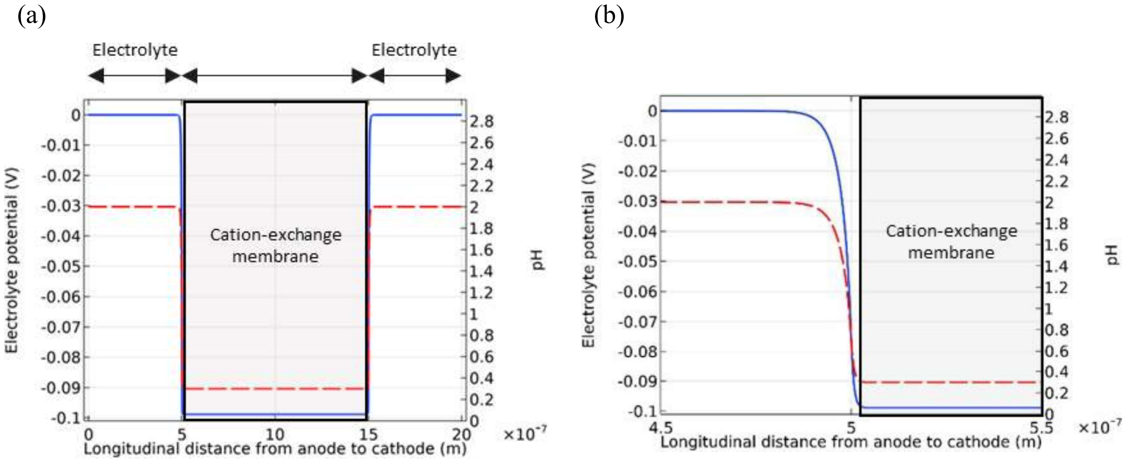

Figure 1: pH and voltage profile in: (a) membrane (b) electrical double layer.

Conclusion

The NPP system of equations including chemical reactions is a strongly coupled non-linear and stiff system, which requires extremely fine mesh and short time steps for its numerical solution. However, COMSOL Multiphysics allows the accurate simulation of this type of electrochemicalproblems.

References

1. Paz-García, J. M., Johannesson, B., Ottosen, L. M., Ribeiro, A. B. & Rodríguez-Maroto, J. M. Modeling of electrokinetic processes by finite element integration of the Nernst-Planck-Poisson system of equations. *Sep. Purif. Technol.* **79**, 183–192 (2011).
2. Paz-Garcia, J. M., Johannesson, B., Ottosen, L. M., Ribeiro, A. B. & Rodriguez-Maroto, J. M. Modeling of Electric Double-Layers Including Chemical Reaction Effects. *Electrochim. Acta* **150**, 263–268 (2014).