

Nanofiltration modeling based on the Extended Nernst-Planck equation under different physical modes



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Introduction

Nanofiltration (NF) is a pressure-driven membrane process. NF membranes have pores of nanometric scale and fixed charges and are able to separate ions [1]. NF models aim at obtaining permeate concentrations for specific operating conditions. The Donnan Steric-partitioning Pore Model (DSPM) based on the Extended Nernst-Planck equation is the basis of modern NF models [2]. Nowadays, solution procedures of DSPM-like models use finite differences or Runge-Kutta and are iterative (as permeate concentrations appear in the differential equations of the model). Convergence problems is the main drawback of these procedures [3].

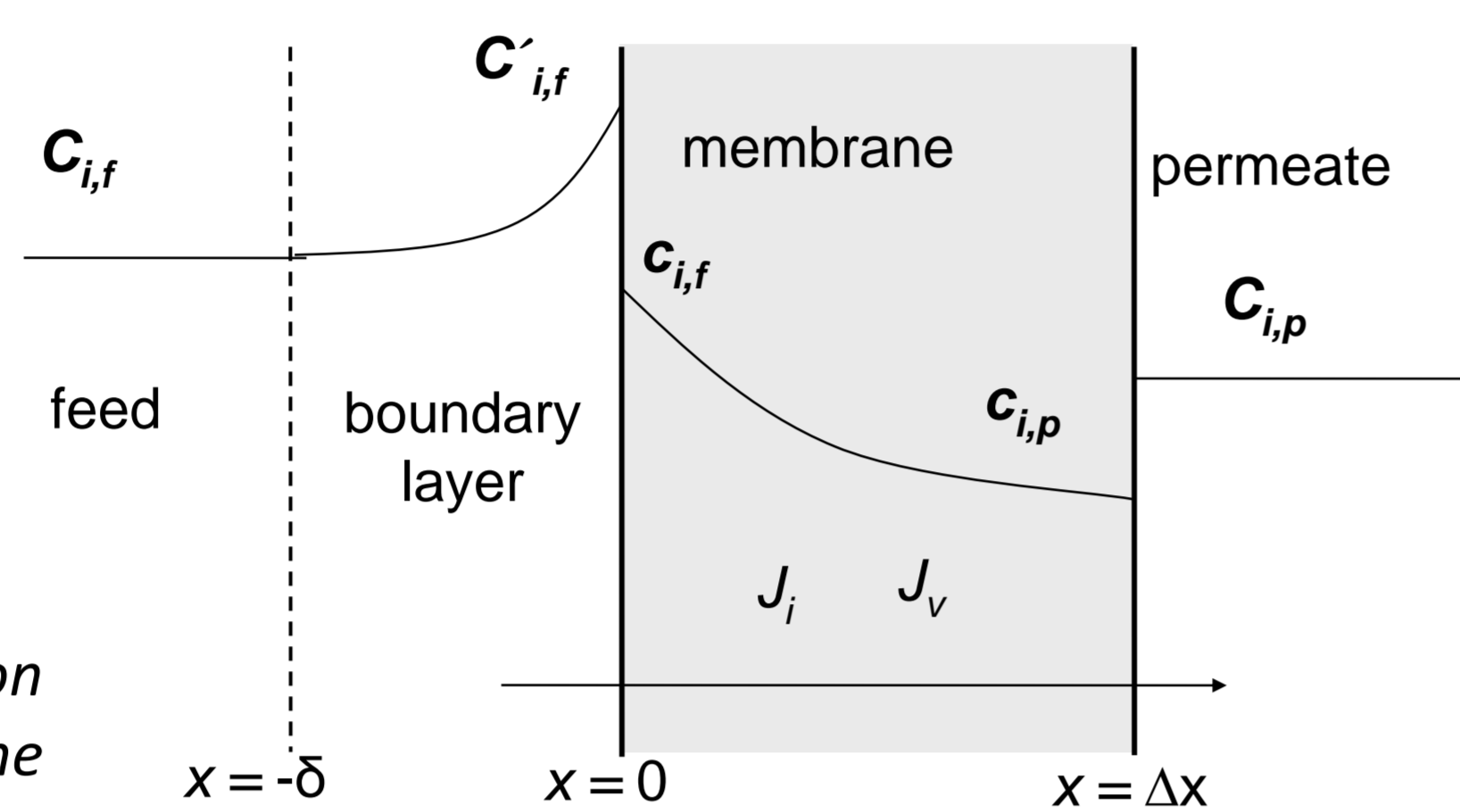


Fig. 1. Concentration profiles in a membrane

Aim

To develop a procedure of solution of DSPM-like models using a finite element software looking for good convergence properties and an easy implementation of the coupling between transport in the membrane and the feed boundary layer.

Method of solution

The solution required the coupling of two one-dimensional subdomains (boundary layer and membrane).

The permeate does not need to be defined as subdomain (concentrations calculable from the right-hand membrane boundary)

Governing equations and subdomain definition

- **Boundary layer:** Nernst-Planck equation (NP) and electroneutrality condition
- **Membrane:** Extended NP and electroneutrality condition

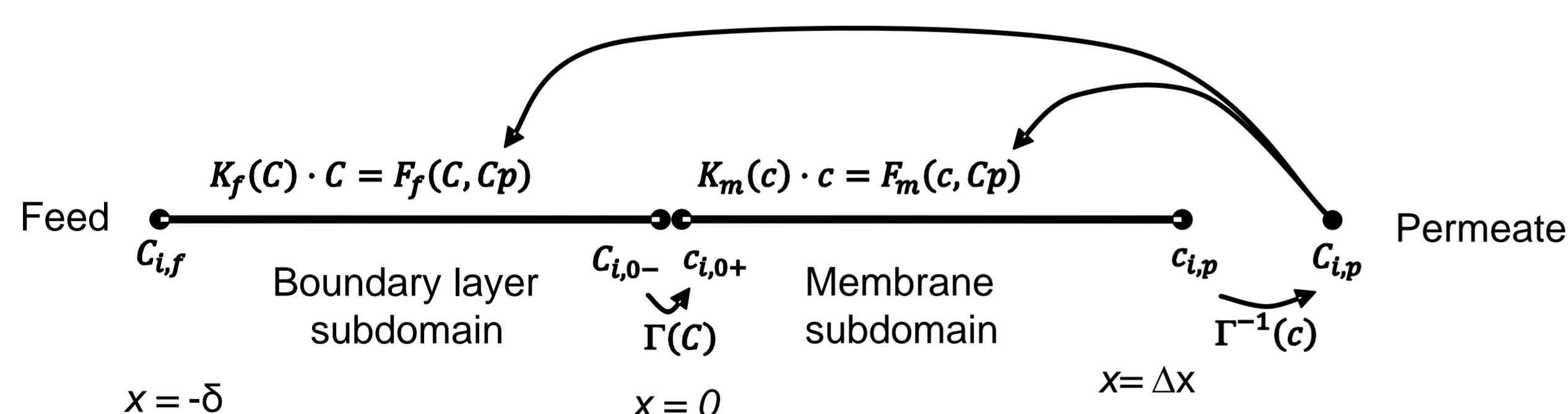
These equations were combined to obtain the concentration gradients in each membrane subdomain.

Boundary definition

Left-hand boundary of the boundary layer subdomain = Feed concentrations

Right-hand boundary of the membrane subdomain = subdomain concentrations ($c_{i,p}$)

Internal boundary = Donnan-steric condition.



The permeate concentrations $C_{i,p}$ are calculated from $c_{i,p}$ using Donnan-steric condition and sent to each subdomain as a boundary extrusion variable.

Solver used

A direct solver (UMFPACK) was used. For cases of difficult convergence a parametric solver had to be used.

Literature

1. Schaeffer et al., *Nanofiltration. Principles and applications*, (2005)
2. W.R. Bowen, H. Mukhtar, Characterisation and prediction of separation performance of nanofiltration membranes, *J. Membr. Sci.*, **112**, 263-274 (1996)
3. A. Santafé-Moros, J.M. Gozávez-Zafrilla, Applicability of the DSPM with dielectric exclusion to a high rejection NF membrane in the separation of nitrate solutions, *Desalination*, **221**, 268-276 (2008)

Conclusions

- ⇒ Both “Convection and diffusion” and “PDE coefficient form” modes could be used to develop a modeling procedure of the DSPM model.
- ⇒ A better convergence was obtained compared with traditional methods, but lower speed.
- ⇒ The procedure can greatly simplify the study and development of nanofiltration models (smaller time of implementation, post-processing tools) .
- ⇒ Possibility of extending the procedure to systems of more ions including concentrations as additional states.

Results

The DSPM was successfully implemented either using the “Convection and diffusion” or the “PDE coefficient form” modes. However, for the “Nernst-Planck” mode this could be done only approximately.

The successful implementations gave the same results than a DSPM code in MATLAB with the classical solution procedure [3]. Computation time using the FEM approach was slightly higher, but there were less convergence problems.

Meshing with 32 elements or more in each subdomain gave a satisfactory solution (less than 0.05% relative error was observed in a benchmark case).

The solver used showed to be very efficient for most problems. For high absolute values of membrane charge, a parametric continuation technique based on the variation of membrane charge had to be used to make the solution to converge.

The prediction capabilities of the model allow us to perform different studies. For example:

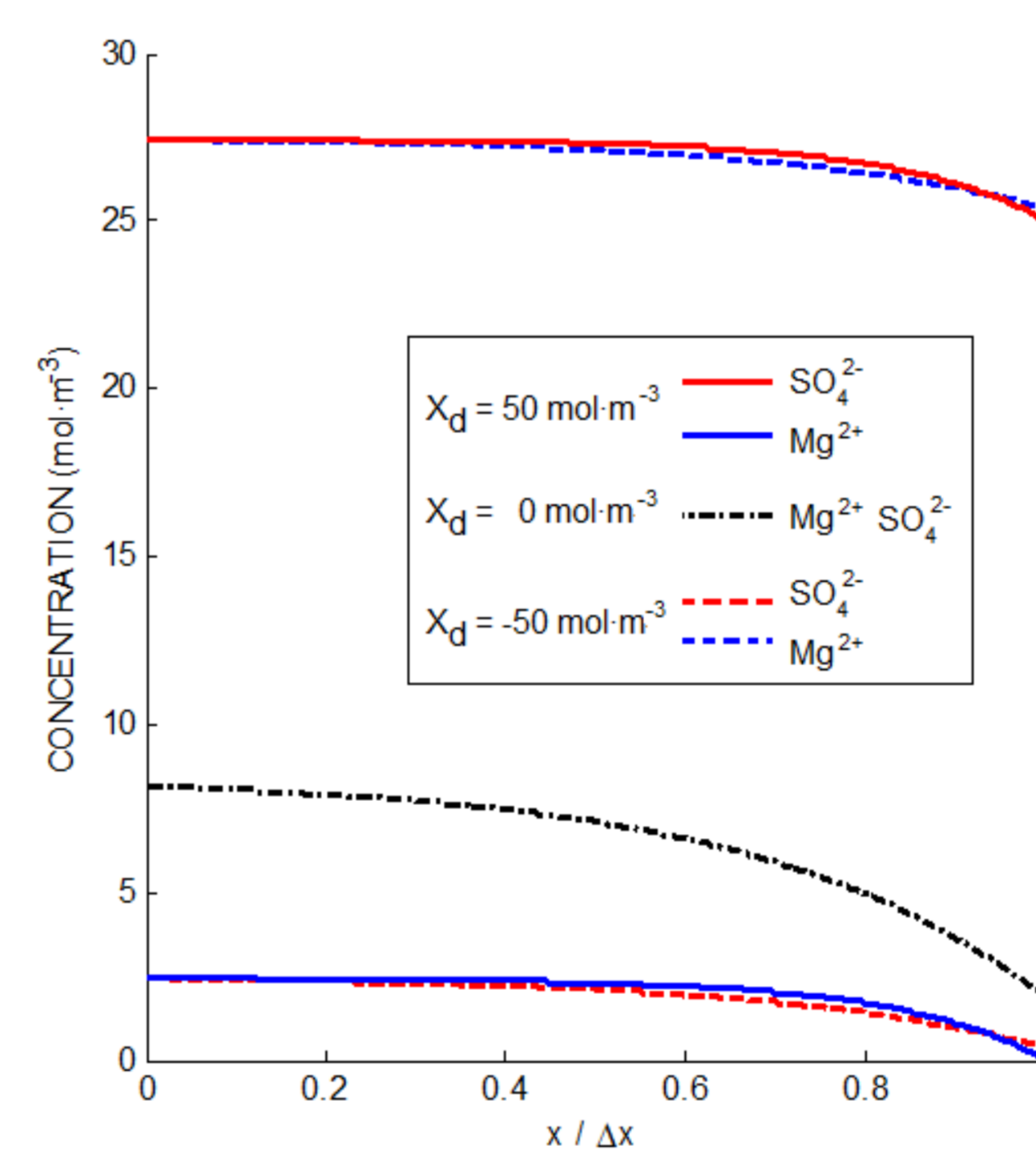


Fig. 2

- Fig. 2 shows the concentration profiles in a NF membrane treating a $MgSO_4$ solution. This result is useful to interpret how the change of a membrane parameter affects the ionic transport.

- Fig. 3 shows a parametric study of the membrane charge useful to maximize the retention of a specific ion.

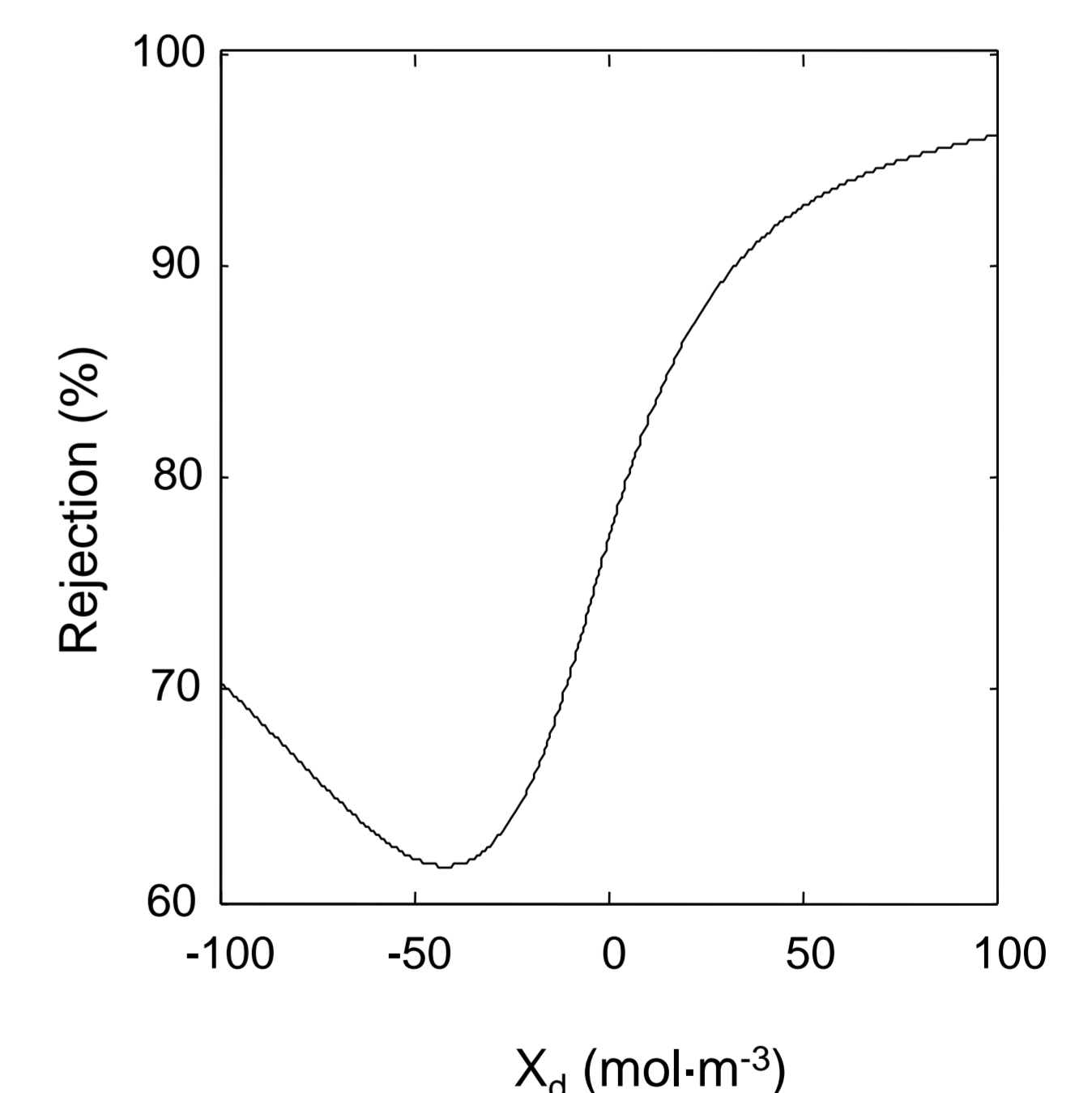


Fig. 3

Acknowledgements

Authors wish to thank to the project GV/2007/197 of the Conselleria d'Educació (Generalitat Valenciana) for the financial support to this study.

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