

AN AVERAGE PORE GRADIENT APPROACH
FOR MODELING REJECTION OF
ELECTROLYTE SOLUTIONS USING
NANOFILTRATION: MODEL DEVELOPMENT
AND ASSESSMENT

(SUPPORTING INFORMATION)

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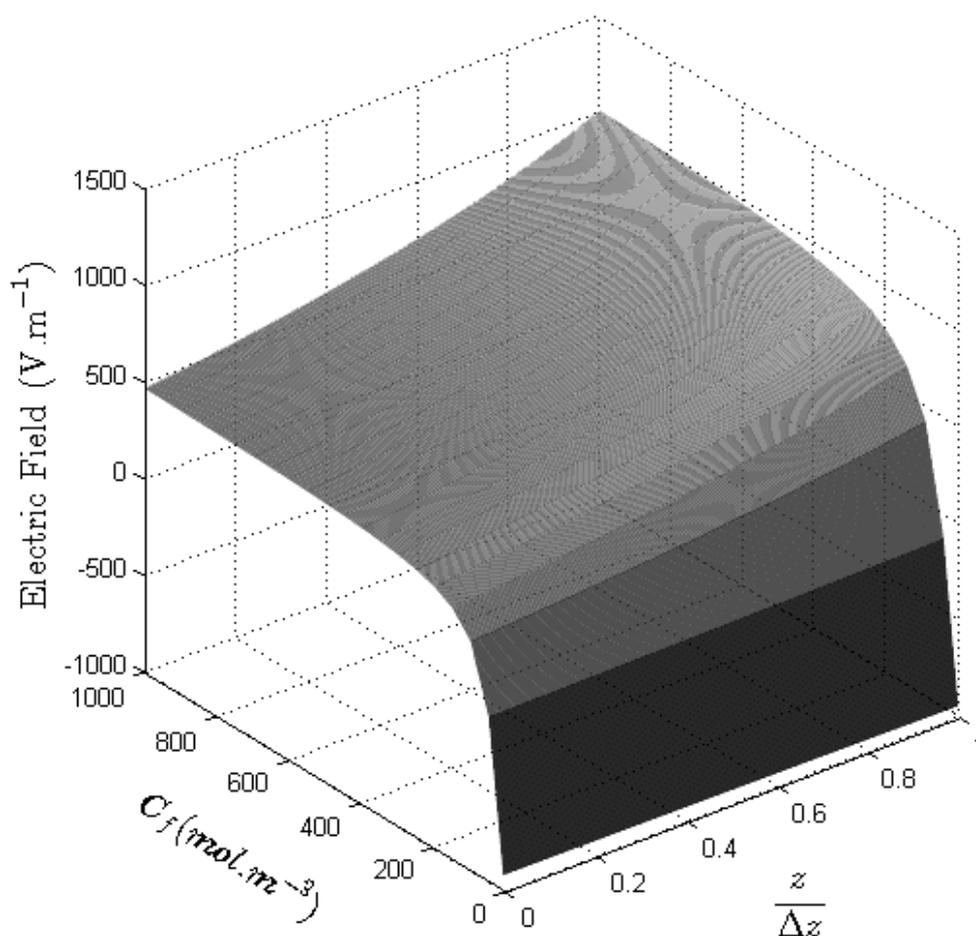
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1. Influence of pore radius and charge density on the electric field along the pore

1.1. Pore radius

The membrane considered in the main text for the study of the electric field along the pore can be considered as having a relatively small pore radius. Indeed the typical range for pore radius of nanofiltration membranes is between 0.5 and 2 nm. Therefore it is relevant to further investigate the behaviour of the electric field for larger pore sizes. Fig. S1 presents plots of the electric field considering a pore radius of 1.5nm all else being equal to the membrane considered in the main text.



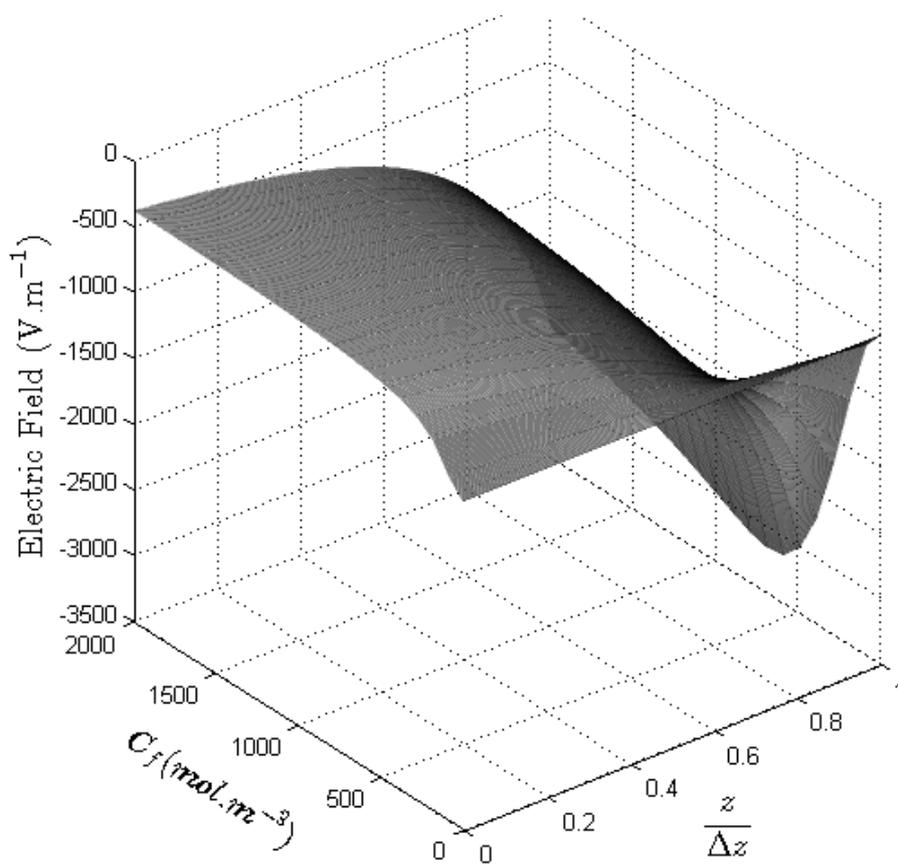
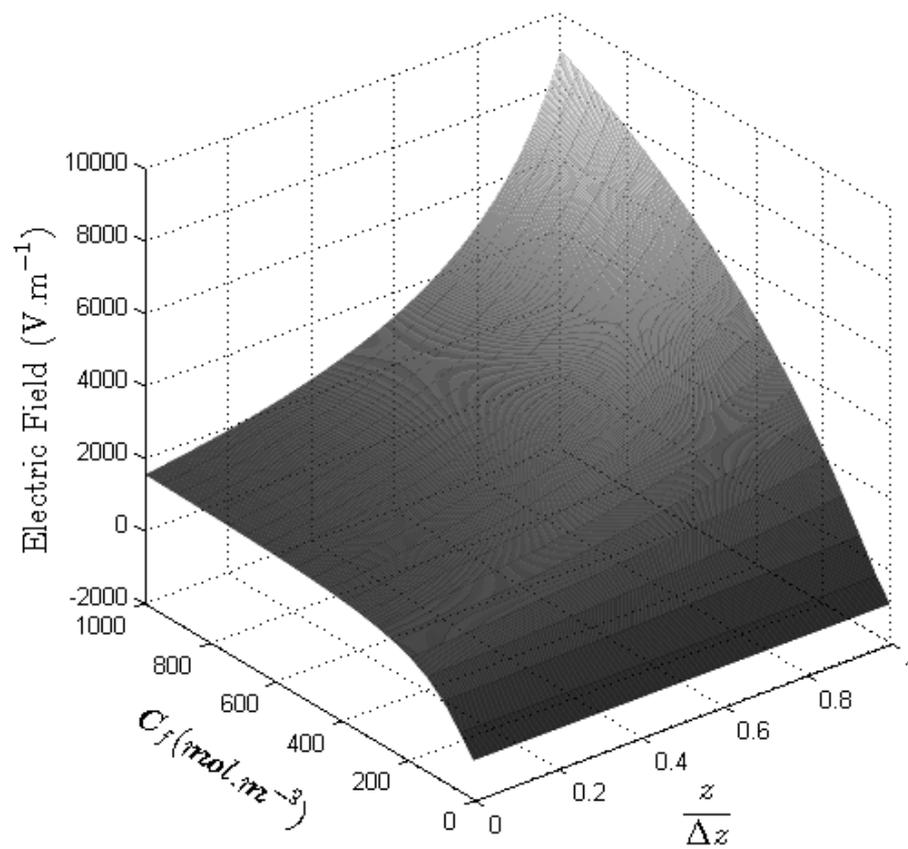


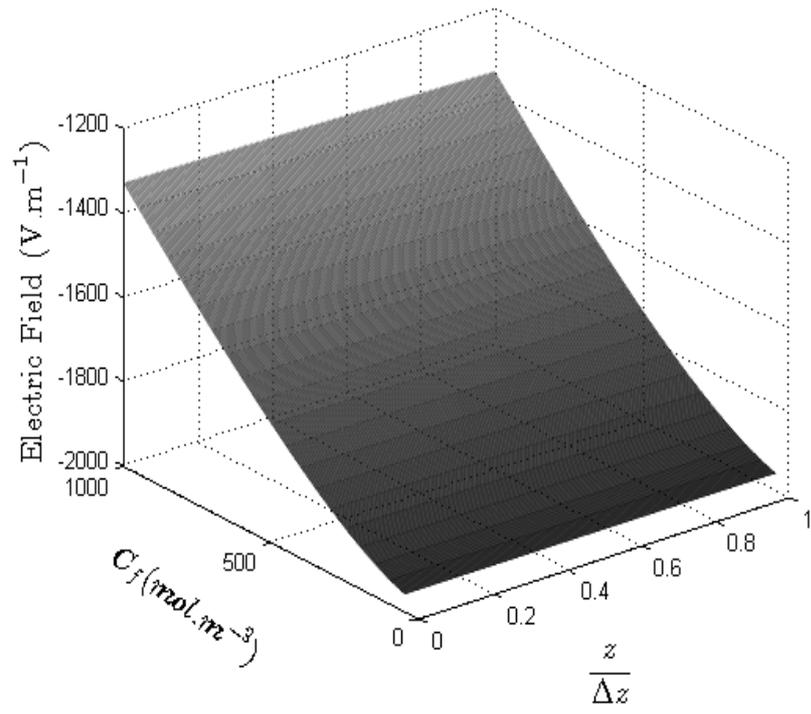
Figure S1. Representation of the electric field along the pore as a function of the concentration for different simple salt solutions. Figures (i), (ii) and (iii) respectively represents the electric field for NaCl, CaCl₂ and Na₂SO₄. The parameters chosen for the membrane are a pore radius of 1.5nm, a thickness over porosity ratio of 5μm, a dielectric constant inside the pore of 40 and a charge density of -10 mmol.L⁻¹. The volumetric flux is

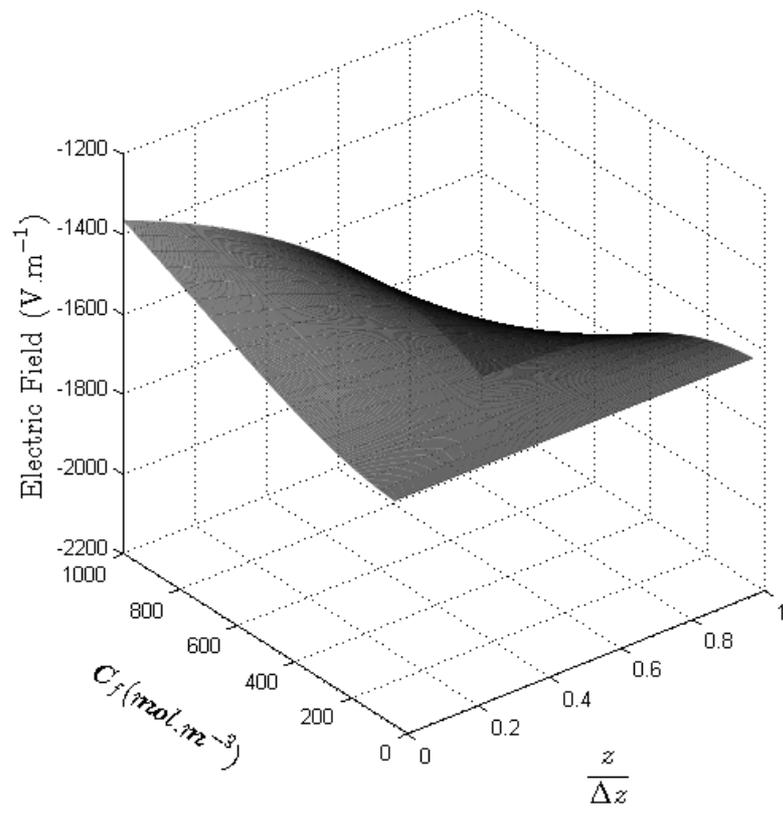
$$J_v = 3.9 \times 10^{-5} \text{ m.s}^{-1}.$$

These plots are to be compared with the Fig. 2 in the main text. Indeed, the variation along the pore of the electric field in the case of larger pore are smaller than in the case of smaller pore. Therefore if the average potential gradient approximation is valid for smaller pore, then it should also be valid for larger pores.

1.2. Charge density

Another parameter which is decisive for the evolution of the electric field along the pore is of course the membrane fixed charge density. The charge density chosen in the model development (-10 mmol.L⁻¹) is relatively small, and it seems legitimate to question the effect of a lower charge value on the electric field. Fig. S2 presents plots of the electric field considering a charge density of -200mmol.L⁻¹ all else being equal to the membrane considered in the main text.





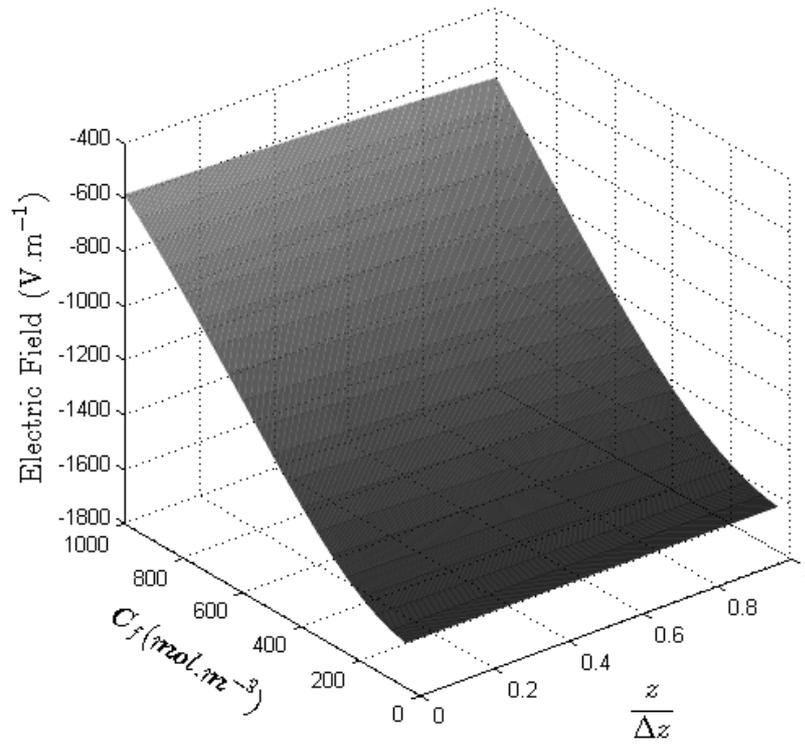


Figure S2. Representation of the electric field along the pore as a function of the concentration for different simple salt solutions. Figures (i), (ii) and (iii) respectively represents the electric field for NaCl, CaCl₂ and Na₂SO₄. The parameters chosen for the membrane are a pore radius of 0.43nm, a thickness over porosity ratio of 5μm, a dielectric constant inside the pore of 40 and a charge density of -200 mmol.L⁻¹. The volumetric flux is

$$J_v = 3.9 \times 10^{-5} \text{ m.s}^{-1}.$$

A considerably smaller variation along the pore of the electric field along the pore is observed for every electrolyte solution. Therefore if the average potential approximation is successfully applied at lower charge density it will most likely be valid for higher charge densities.

2. Validity of the SEDE-APG at high concentration

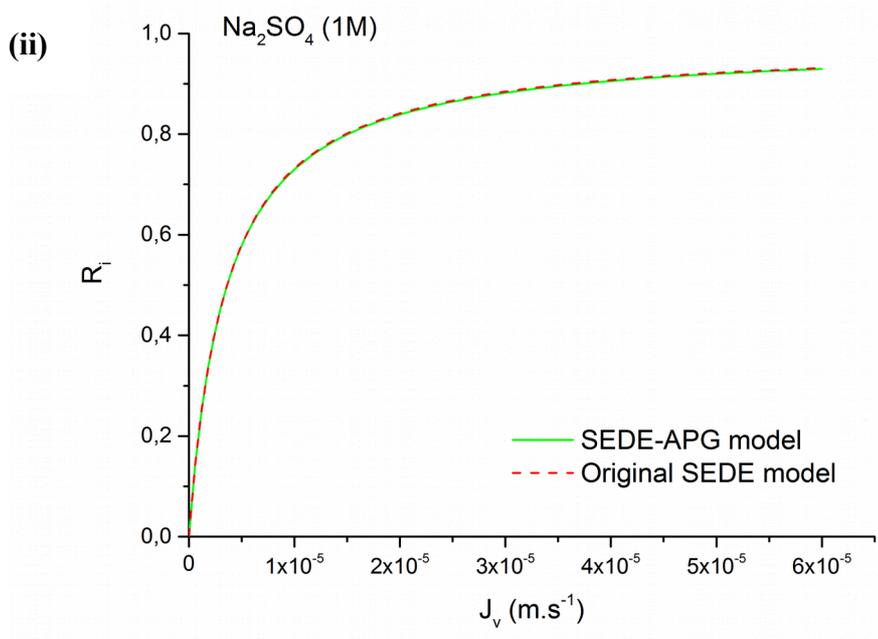
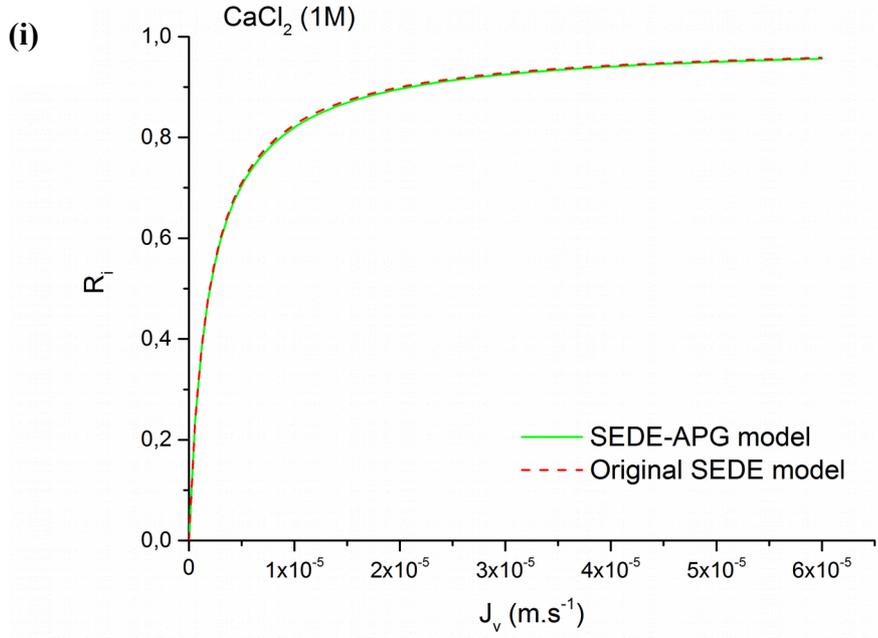
The evolution of the electrical field along the pore with increasing concentration predicted by the original SEDE model can roughly be decomposed in two phases:

- At lower concentration its variation is driven by the charge density along the pore;
- At higher concentration the diffusion potential – resulting from the difference in ion

mobility – is dominant.

Thus Fig. 2 and 3 in the main text exhibit seemingly non-negligible variations of the electric field along the pore at higher concentration. Hence the question is whether the prediction obtained using the average potential gradient approximation are on a par with those obtained through the original SEDE model.

Fig. S3 and S4 below compare the predicted rejection of the two models at high concentration for simple electrolytes solutions and electrolytes mixtures respectively.



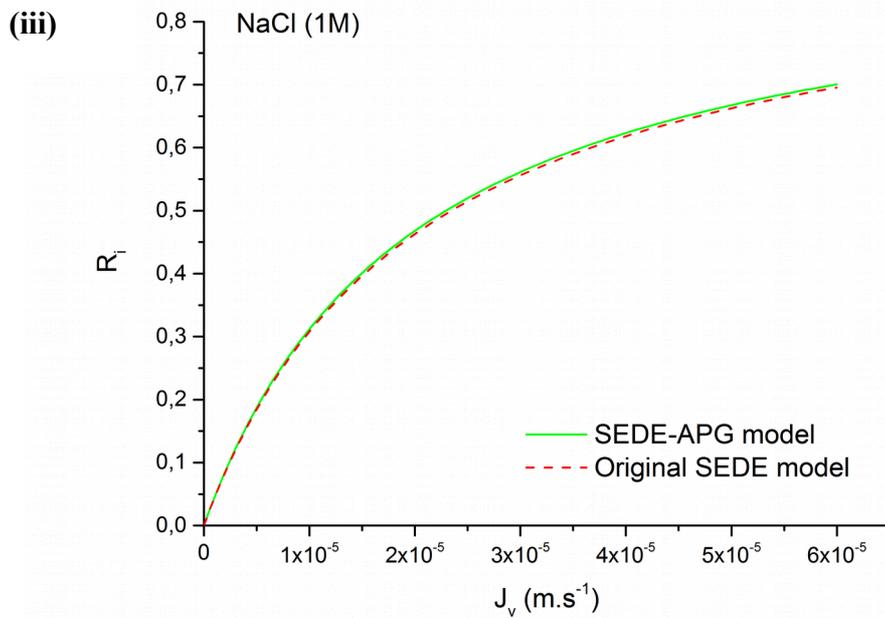
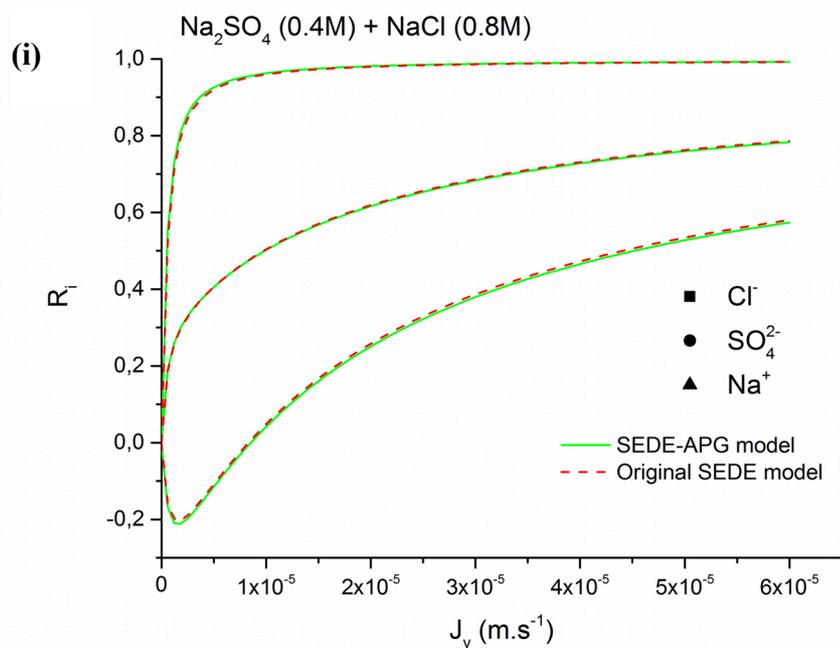


Figure S3. Comparison of the rejection rate against the volume flux using SEDE-APG and the original SEDE model for high concentration. Figures (i), (ii) and (iii) respectively correspond to the rejections of CaCl_2 , Na_2SO_4 and NaCl . Each of the solution is concentrated at $1000 \text{ mmol}\cdot\text{L}^{-1}$. The membrane parameters are as described in the main text in 2.3.



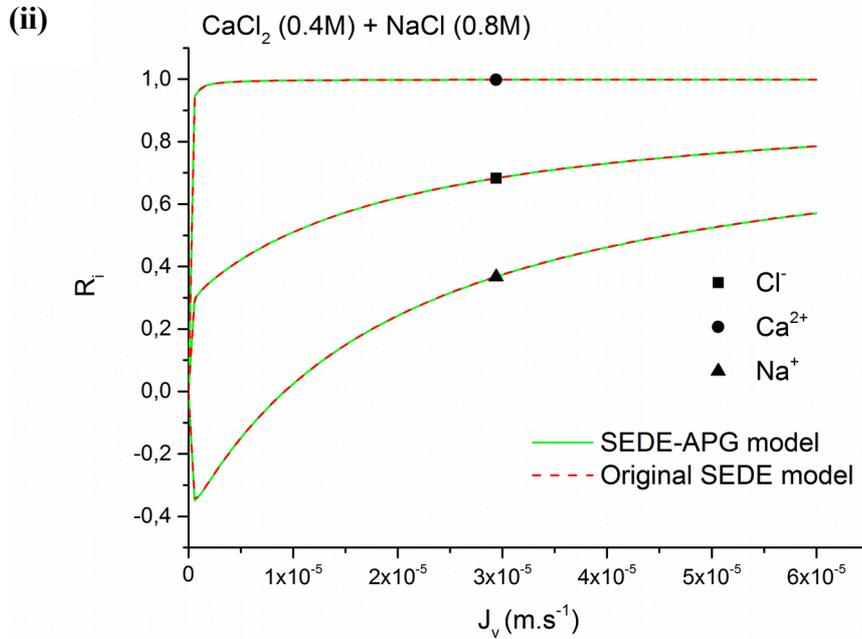


Figure S4. Comparison of the rejection rate against the volume flux using SEDE-APG and the original SEDE model for high concentration. Figure (i) correspond to an electrolyte solution of 400 mol.L⁻¹ Na₂SO₄ and 800 mol.L⁻¹ NaCl. Figure (ii) correspond to an electrolyte solution of 400 mol.L⁻¹ CaCl₂ and 800mol.L⁻¹ NaCl.

Very good agreement is maintained between the two models, even at high concentration. This is likely to mean that the variations of the electric field along the pore are small enough to be averaged. This is also confirmed by the good results obtained on the application at high concentration in the main text (Section 3).