Mathematical model for the concentration and electric potential profiles in a solution of electrolytes under a redox reaction

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Copper electro-refining is the process of obtaining highly pure copper by applying a voltage to a solution of electrolytes. In its natural state, Copper is bounded to other minerals, typically in the form of Copper Sulfate Cu_2SO_4. Our work aims to predict the local concentration of the electrolytes which make up this salt when a voltage is applied through an electrode, and the corresponding electric field screening due to these ions in solution. This allows us to measure the bulk concentration of electrolytes by detecting the electric field at the surface of the electrode, by means of an NV-Center based sensor.

The configuration is modeled as a system of diffusion-reaction equations, coupled with a local electric field which depends on the concentration of charged electrolytes. The electric potential is determined by the Poisson-Boltzmann equation

$$\frac{\partial C_+}{\partial t} = D_+[\nabla^2 C_+ - \nabla \cdot (C_+ \nabla \Psi)], \tag{1}$$

$$\frac{\partial C_-}{\partial t} = D_-[\nabla^2 C_- + \nabla \cdot (C_- \nabla \Psi)], \tag{2}$$

$$\nabla^2 \Psi = -\kappa^2 (C_+ - C_-). \tag{3}$$

Here, $\Psi = \dfrac{z\mathcal{F}}{RT}\phi$ is the dimensionless electric potential, where ϕ is the actual potential and z is the valence of each electrolyte (+2 in the case of copper), $\mathcal{F}$ is the Faraday constant, R the universal gas constant and T the temperature. $C_\pm$ and $\mathcal{D}_\pm$ are the concentration and the diffusion coefficients of each species of the binary salt. κ is a constant known as the ionic strength, which is given by $\kappa = \sqrt{\dfrac{2(z\mathcal{F})^2 C_b}{\epsilon RT}}$ where ϵ is the relative water permittivity and C_b is the bulk concentration of the salt.

The electro-chemical reaction rate r is included as a boundary condition, since it only occurs at the surface of the electrode, i.e. at the liquid/solid interface.

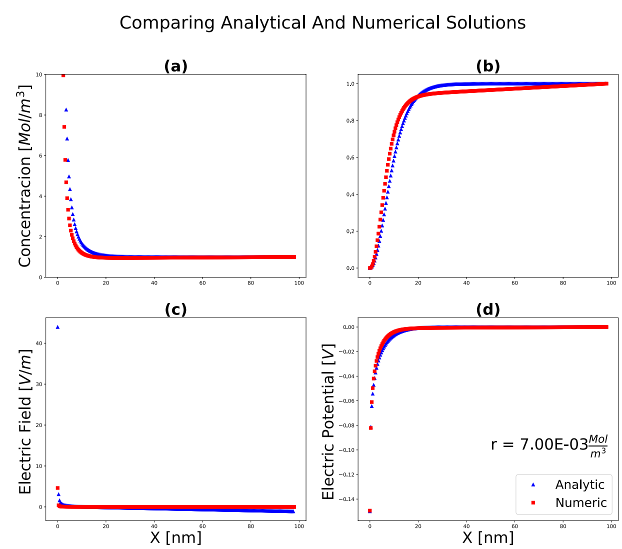

Figure 1. *Concentration of positive (a) and negative (b) electrolytes. Electric field (c) and electric potential (d). Interface is located at x=0.*

The bulk concentration can be measured by sensing the electric noise produced by the electrolyte concentration at the surface.

References

[1] E. L. Cussler, Diffusion and Mass Transfer (2009).

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