Concentration and Electric Potential Profile In a Solution of Electrolytes Under Redox Reaction

Professor: PhD. Enrique Muñoz

Student: Agustín Escobar Blanc

Introduction

Copper electro-refining is the process of obtaining highly pure copper by applying a voltage to a solution of electrolytes. Our work aims to obtain the concentration of these electrolytes from one of the electrodes and the corresponding electric field screening due to these ions. This allows to measure the bulk concentration by obtaining the electric field at the electrode, measuring the spectrum of an NV-Center based sensor.

Mathematical Model

The system can be modeled as a diffusion reaction problem coupled with a local electric field which depends on the concentration of the charged electrolytes. The electric potential is determined by the Poisson-Boltzmann Equation

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

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

$$\nabla^2\Psi = -\kappa^2 \left(C_+ - C_-\right). \quad (3)$$

$\Psi = \frac{zF}{RT}\phi$	Dimensionless Potential	$C_\pm$	Electrolyte concentration
$D_\pm$	Diffusivities	$\kappa = \sqrt{\frac{2(zF)^2 C_b}{\epsilon RT}}$	Ionic Strength
C_b	Bulk Concentration		
R	Ideal Gas Constant	ϵ	Water Permittivity
T	Temperature	F	Faraday's Constant

The chemical reaction rate r is included as a border condition at the interface.

Steady state solution

We used Runge-Kutta method to obtain the numerical solution to the problem, to see how profiles change at different reaction rates..

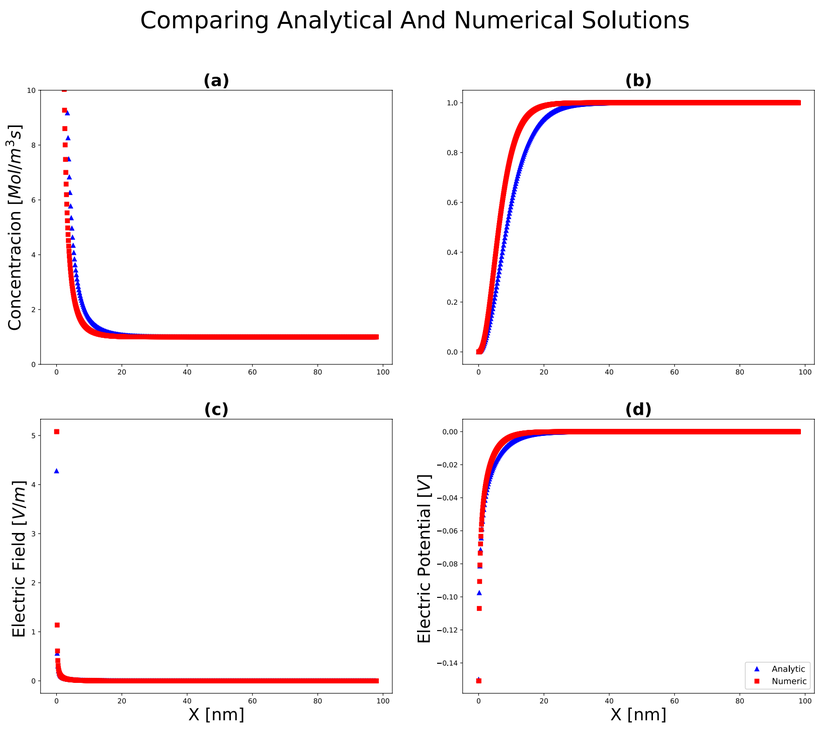

Fig. 1 Concentration of positive (a) and negative (b) electrolytes. Electric field (c) and electric potential (d). Interface is located at x=0.

Conclusion

Our model predicts the local concentration of each species, and in particular at the surface of the electrode when a voltage is applied. The measurement of the bulk concentration can be measured by sensing the electric noise produced by the electrolyte concentration at the surface.

Further Work

1. Obtain a numerical simulation of the dynamics system (that is, where the concentration of each species changes in time).

2. Couple electric noise to NV-Center to retrieve sensible information from measurements.