# Electrochemical Simulation

Electrochemical reactions, also known as a typical type of redox reactions, involve transfers of electrons, which immediately suggest a link between this type of chemical reactivity and electricity. The main applications of electrochemistry are collectively known as electrochemical sensors.

In this section, our team is going to perform a simulation to design a successful model for our electrochemical sensor. In an electrochemical glucose sensor, the concentration of glucose in a sample is measured using amperometry; that is, the measurement of an electric current. An applied voltage causes the oxidation of glucose, and the current due to this oxidation is measured at the electrode. In a well-designed glucose sensor, there is a linear relationship between the glucose concentration and the current, enabling a calibrated measurement.

Our electrochemistry glucose sensor was programmed in the COMSOL Multiphysics®.

The model provides a sophisticated simulation of the multi-dimensional biophysical phenomena below:

The redox reaction of glucose is conducted on the working electrode surface within the chamber of the microfluidic chip.

$$glucose + ferri \leftrightarrow products + ferro$$
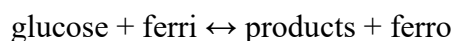
The rate of this equation could be calculated by this equation (Equ. 1):

$$R = \frac{C_{glucose} \times V_{max}}{1 + K_m \times C_{glucose}} \qquad \text{Equ.1}$$

Here, the parameter Vmax is the maximum rate of the enzyme-catalyzed reaction, depending on the quantity of enzyme available, and the parameter Km is a characteristic Michaelis-Menten coefficient. At large glucose concentration, the rate becomes independent of the glucose concentration and solely depends on the enzyme kinetics.

1, 2 and 3D versions of the models were developed allowing rapid solutions for more simplified symmetric geometries. 2 and 3D versions were employed where specific detail was required to capture the impact of geometric anomalies on the system.
Solutions were always time dependent due to the finite test times required from commercial biosensors.

The picture below (Fig.1) showed our 3-dimensional modeling of electrochemical sensor:
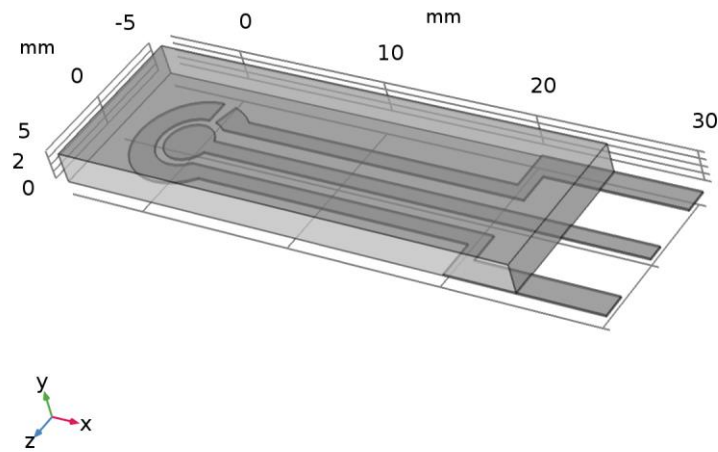

Fig.1 3-D modeling of the sensor

As the glucose redox reaction occurs on the surface of the work electrode, therefore, we used the Batteries & Fuel Cells Module for the electroanalysis of this model, the equation as shown in Equ.2:

$$\nabla \times (-D_i \nabla_{C_i}) = R_i$$

$$N_i = -D_i \nabla_{C_i} \qquad\qquad \text{Equ.2}$$

$$\Phi_I = 0$$

A large quantity of inert salt is added into the elctroanalytical experiments to increase the conductivity of electrolyte, which induced the low resistance of the solution. Therefore, the electric field is negligible, meaning we could assume a constant electrolyte potential $\Phi_I = 0$.

The Electroanalysis interface implements chemical species transport equations to describe the diffusion of the chemical species. The domain equation is the diffusion equation (also known as Fick's 2nd law). At steady-state, this reduces to:

$$\nabla \times (-D_i \nabla_{C_i}) = 0$$

for each species i.

In this model three species are modeled: the active redox couple-ferricyanide and ferrocyanide anions-as well as the concentration of the glucose analyte.

In this model, Ri=0.

The current density for this reaction is given by the electroanalytical Butler–Volmer

equation (Equ.3) for an oxidation:

$$I_{loc} = I_0(C_R \exp(\frac{\alpha cF\eta}{RT}) - C_0 \exp(\frac{-\alpha cF\eta}{RT}))$$

Equ.3

Here I_0 is the electrode-redox couple exchange current density, CR is the concentration of reduced species, C0 is the concentration of oxidized species, R is the universal gas constant, F is Faraday's constant, T is the temperature in kelvin, α is the transfer coefficient, η is the over-potential.

According to Faraday's laws of electrolysis, the flux of the reactant and product species are proportional to the current density drawn (Equ.4):

$$-n \times N_i = \frac{V_i \times i_{loc}}{nF}$$

Equ.4

An Integration Component Coupling is used to define an electrode current variable according to (Equ.5):

$$I_{el} = \int i_{loc} dA$$

Equ.5

Results

Concentration (elan)

Fig.1 showed a concentration profile for the ferrocyanide ion in the unit cell. Ferrocyanide was generated in the solution between the electrodes and bulk by the enzyme-catalyzed oxidation of glucose. It reacts at the anode in the center of the unit cell to provide the working electrode current used to measure the concentration of glucose. Ferrocyanide was regenerated at the cathode counter electrodes at the left and right of the cell.
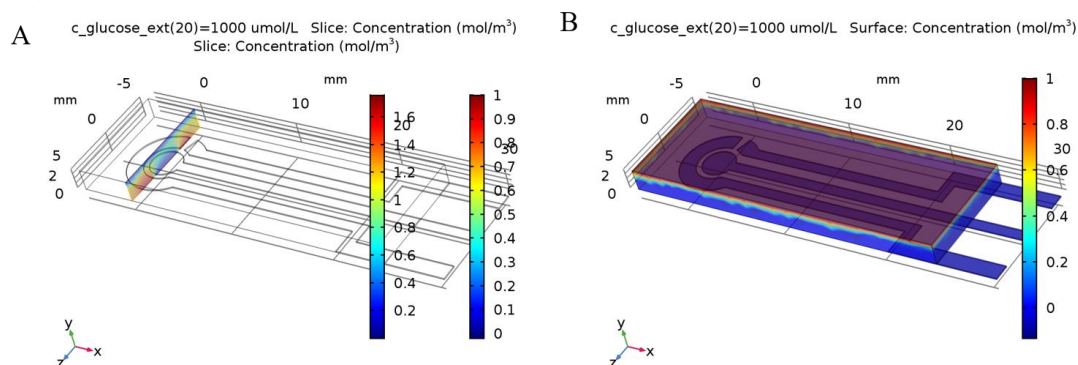

Fig.2 Ferrocyanide concentration for an external glucose concentration of 1 mol/m^3.

Average Current Density

This model tested the concentrations of glucose from 50 to 1000 umol/L, and we've acquired excellent linear relationship and strong current density. This illustrates a good performance of our electrochemical sensor. Our result is shown in Fig.3.
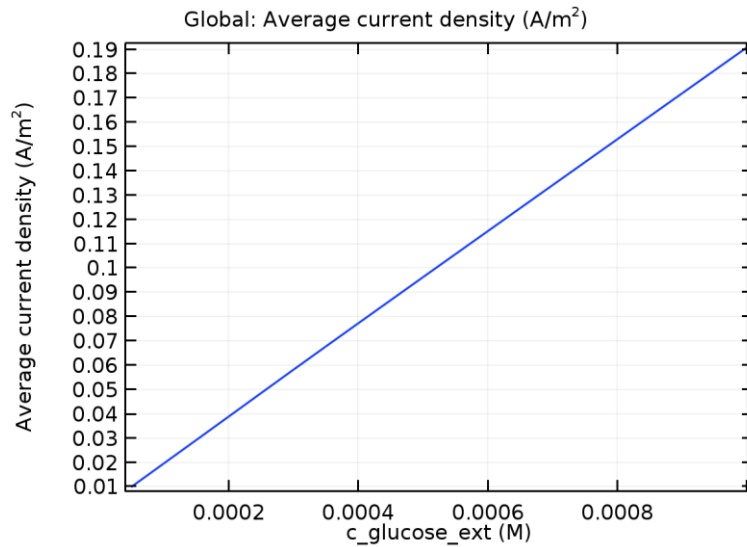
Fig.3 Current density versus glucose concentration

Conclusion

Using COMSOL to establish and simulate the 3D glucose-enzyme electrochemical sensor model designed by this project, we have learned and understood the finite element analysis method. At the same time, the model theoretically analyzed and verified the sensor we designed, and directed the sensor's further improvements in its performance. Through the results of the model, we will further adjust the sensor design parameters in the next step to improve the current density for better signal-to-noise ratio (SNR) and higher sensitivity.