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Implementation and Simulation of drift-diffusion models for organic mixed conductor devices

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Abstract

In the past years, organic electrochemical transistors (OECTs) have emerged as potential transducers in applications that require the conversion of ion fluxes to electronic current. In order to deepen the understanding and optimization of the fundamentals of OECTs and OECT-based applications, however, it is essential to have theoretical models capable to predict the experimental data[1]. Mostly, in the OECT models available in the literature, the ion flux from the electrolyte into the organic semiconducting layer takes place only due to an electrical field. These models are efficient to describe the steady-state operations of OECTs, but are rather limited for the predictions of transient behaviors. In order to improve the existing approaches, recent models take into account the diffusion processes. Analytical attempts to solve the respective equations are limited to specific boundary conditions that not describe properly the devices of interest. In our work, we therefore employ numerical approaches to solve those equations. This allows to go beyond the standard boundary conditions and add some extensions like non-uniform electric field, chemical potential, among others.

Keywords: OECT, Drift-diffusion, Numerical, Modeling.

Introduction

In the nature, biological systems function via ion fluxes. In order to imitate these processes, it is necessary to develop devices capable to transduce and therefore support both electronic and ionic current efficiently[2]. Due the capacity to transport charge along the conjugated backbones while allowing ionic transport in the course of redox reactions, the semiconducting polymers represent an optimal choice to be used for this purpose[3]. One important application of these materials is the organic electrochemical transistor[4-6].

Organic electrochemical transistors (OECTs): In an OECT, the organic semiconductor is in direct contact with an electrolyte, in which an electrode called the gate is immersed. Two further electrodes (source and drain) are bridged by the organic semiconductor, defining the channel through which electric current flows. The ion migration from the electrolyte to the organic film is controlled by the gate voltage (V_G), which cause variations in the doping state of the polymers and hence its conductivity[7]. The fundamentals of how these devices function, however, is still not fully understood. Therefore, to improve the performance of these devices, the better understanding of the internal functioning is necessary. Hence, in addition to further experimental characterizations, theoretical models[8-10] are needed to explain the underlying mechanisms.

Methods and implementation

Drift-diffusion model: Most models available in the literature, only consider the ion flux coming from the electrolyte to the organic semiconductor as consequence of the electric field due to the gate voltage. Drift-diffusion based models, on the other hand, also take contributions due to diffusion. In a one-dimensional model, the temporal evolution of the concentration is given by the Nernst-Planck equation[10].

$$\frac{\partial c(x,t)}{\partial t} = -\nabla J(x,t) = D\nabla\left(\nabla c(x,t) - \frac{zF}{RT}E(x)c(x,t)\right) \qquad (1)$$

where D is the diffusion coefficient, c(x,t) the time dependent concentration, z the charge number of the ion, F the Faraday constant, R the universal gas constant, T the temperature of the system and E(x) the electric field at one point.

Transient Current: The Bernards-Malliaras model defines the value of the electric current flowing through the semiconducting channel in an OECT[11]:

$$I(t) = G\left(1 - \frac{Q(t)}{ep_0V}\right)V_D - f\frac{\partial Q(t)}{\partial t} \qquad (2)$$

In the equation (2) $G=e\mu p_0V/L^2$, is the conductance of the organic semiconductor film, μ is the hole mobility, p_0 is the initial hole density, V is the volume of the semiconductor material, V_D the constant drain voltage, f a correction factor and Q(t) the amount of charge injected from the electrolyte to the channel[19].

Simulation approach: By solving the equation (1) numerically, it is possible to overcome some limitations of the analytical solution. In the numerical formulation, a set of discrete points x_i in space is considered. The finite difference method (FD) is used to approximate the solution by turning the Nernst-Planck expression into an algebraic system of linear equations that have to be solved (**Equation 3**).

$$\psi(x,t_i+\Delta t) = A\psi(x,t_i) \qquad (3)$$

Then, concentration at any time can be calculated by the product of a matrix and the concentration vector of the previous time step. The errors that are made by the discretization in space and time can be reduced by considering smaller intervals Δx and Δt. However, this results in increased computational efforts. Consequently, it is necessary to define the proper limits in order to reduce the numerical errors but maintaining the computation times affordable.

Results and Discussion

In order to investigate the accuracy of the model, a comparison of the open boundaries case was made with the analytical solution[22] (**Figure 1**).

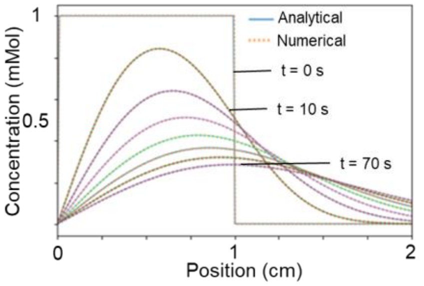

Figure 1: Agreement of the model (dotted line) with the the analytical solutions (solid line) [10].

Using a constant field E=0.005 Vcm^{-1} and a diffusion coefficient $D=5\times10^{-7}m^2s^{-1}$ in the electrolyte as well as in the semiconductor region is obtained a good agreement between the solutions at different times.

The numerical approach allows solving the problem at any time when some extensions are added to the analytical model. In difference to the open boundaries situation, the closed boundary case considers that the fluxes at the limits of the device are zero. In this case, a convergence of the solution into a steady state is obtained (**Figure 2a**). The comparison of the steady state solutions (analytical and numerical) makes visible the similarity of the results (**Figure 2b**). Further, it is possible to simulate a system in which the electric field acts only in the electrolyte (**Figure 3**). In this situation, a marked

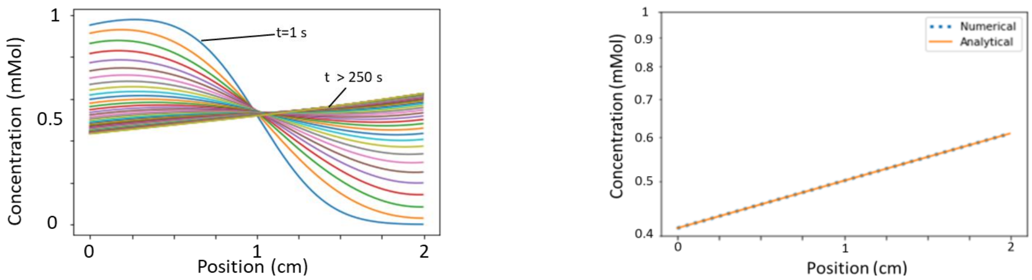

Figure 2: (a) Time evolution of the concentration in the closed boundary case. (b) Comparison between the analytical and numerical steady state solutions.

difference in the concentration distribution for each region is obtained.

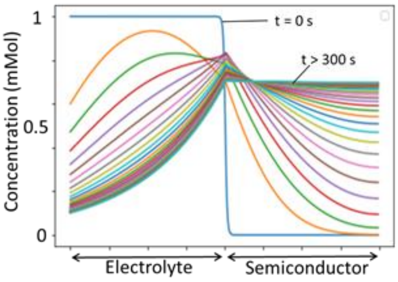

Figure 3: Concentration profiles with an electric field $E^{*}= (10\times E)\ Vm^{-1}$ applied in the electrolyte region.

In addition, the model allows to investigate the impact of each extension on the drain current (**Figure 4**), allowing a complete study on the OECTs.

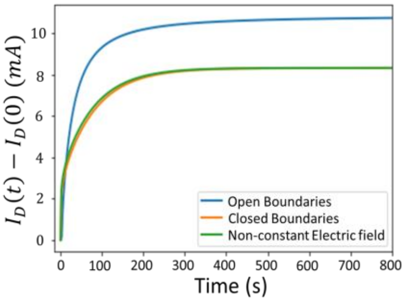

Figure 4: Drain current for different cases studied.

Conclusions

The solution of the Nernst-Planck equation provides a way to simulate the functioning of the OECTs. In order to solve the problem analytically, some simplifications must be considered, which usually results in a limited solution. On the other hand, the numerical approach allows extending the analytical model. When open boundaries are considered, the numerical method provides a solution which is in a good agreement with the analytic result. Besides, the numerical implementation makes viable to investigate situations like closed boundaries, a non-constant electric field, among others. The impact of these considerations are studied by examining the impact in the time evolution of the concentration, the flux at the interface and the drain current. The correct theoretical modeling will allow us to deepen the understanding of the OECTs functioning and look for possible optimizations in these devices.

References

[1] Colucci, R, *et al*. Flex. & Print. Elec. 5(1): 013001, 2020.
[2] Rivnay J, *et al*. Chem. Mater. 26, 679, 2014.
[3] Malliaras, G. *et al*. Nat. Commun. 8, 1767, 2017.
[4] Colucci, R., *et al*. Synth. Met. 241, 47, 2018.
[5] Amanchukwu, C.V., *et al*. J. Phys Chem. L, 7, 3770-3775, 2016.
[6] Gkoupidenis, P., *et al*. Appl. Phys. 107,263302, 2015.
[7] Bernards, D.A, *et al*. Adv. Func. Mat, 17, 3538, 2007.
[8] Shirinskaya, A., *et al*. Biosensors, 8, 103, 2018.
[9] Elschner, A., *et al*., CRC press, 2010.
[10] Coppede, N., *et al*. Sci. Rep, 4, 1, 2014.
[11] Bernards, D.A, *et al*. Adv. Func. Mat, 17, 3538, 2007.