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

UNIGARRO, A. D. P.¹; GÜNTHER, F.¹; FARIA, G.¹

ap.unigarro@ifsc.usp.br

¹Instituto de Física de São Carlos - USP

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. For the rational optimization and understanding of the fundamentals of OECTs and OECT-based applications, however, it is essential to have theoretical models that can predict the experimental data. (1) The OECT models, which have majorly been discussed during the past decade, mostly originate from Ohm's law where 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. More recent models take a diffusion term into account in order to improve the existing approaches. For example, Coppedè *et al.* (2) developed a model for which the analytical solution of the Nernst-Planck equation in one dimension with standard boundary conditions was used. In doing so, the diffusion coefficients of different metal cations could be fitted to experimental transient measurement with a very good agreement. In their work, however, only metal cations of the electrolyte were considered. In our work, we intend to solve the equations numerically to overcome the limitations of the analytical solution. This allows us to go beyond the standard boundary conditions and also to analyze the impact of other alterations, such the existence of anion, variations in the diffusion coefficient between electrolyte and polymer film, etc.

Palavras-chave: OECT. Finite differences. Simulation.

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- 2 COPPEDÈ, N.; VILLANI, M.; GENTILE, F. Diffusion driven selectivity in organic electrochemical transistors. **Scientific Reports** v. 4, p. 4297-1-4297-7, 2014. DOI 10.1038/srep04297.