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Nernst-Planck-Poisson modelling of properties and electrochemical response of sensing materials

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Abstract – Nernst-Planck-Poisson model (NPP) is a new theoretical approach for the description of time-dependent electro-diffusion processes in various materials. This model takes into consideration several parameters, which are neglected in simpler ones. The NPP model, because of its generality can be used in a wide range of cases such as transport of polyvalent ions, multi-component systems and for the description of transient states. The comparison between the NPP model and the Steady State Diffusion Model (SSDM) is shown and the limitations of SSDM are discussed.

In the field of ion selective electrodes (ISE) the steady state models are prevalently used for the description of the response of this type of electro-chemical sensors. This type of approach is burdened with several shortcomings [1]. The comparison of SSDM, which can be applied only for monovalent ions and steady state measurements, with the NPP model is discussed.

In the NPP model, processes of diffusion, migration and convection are taken into account. The changes of ion concentrations and electrical field in space and time lead to formation of a membrane potential. The time-dependency of the formation of the potential, is crucial for the description of the ISE response in low concentration ranges, and can give additional information for designing ISE materials (Figures 1 and 2).

The NPP model takes into account several materials specific parameters (neglected in other models) such as heterogeneous rate constants, dielectric permittivity and diffusion coefficients [2]. We use the full form of NPP problem, including explicitly the electric field as an unknown variable with no simplifications, such as electroneutrality or constant field assumption. The set of partial differential equations resulting from NPP problem is transformed to the set of ordinary differential equations using the Finite Difference Method and solved using integration procedure RADAU5 [3].

The NPP model is a general and powerful tool for modelling the properties and behaviour of wide range of materials, for example conducting polymers or liquid and solid membranes.

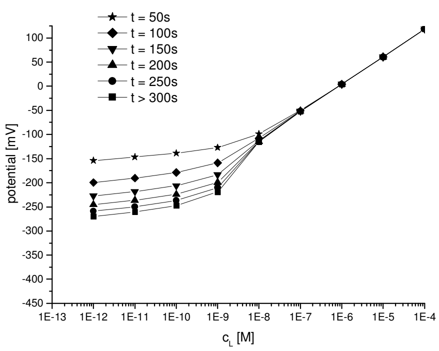

Figure 1: Influence of time of measurement for the ISE with primary ion inner solution concentaration 10^{-6}

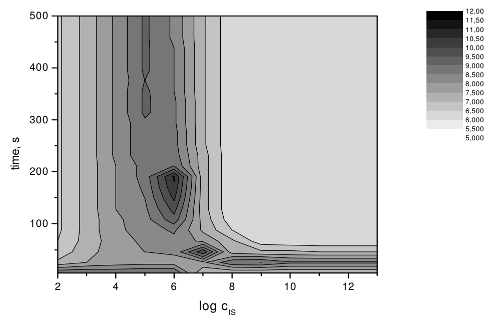

Figure 2: Time-concentration-detection limit maps obtained using NPP model

References

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