O39

Behavior of Weak Electrolytes in the Diffuse Layer of the Double Layer

Bohuslav Gas

Faculty of Science, Charles University, Prague, Czech Republic, bohuslav.gas@natur.cuni.cz

Summary

The structure of the double layer on the boundary between solid and liquid phases is described by various models. We have proposed a mathematical model of diffusion and electromigration in the diffuse layer of the double layer considering the high deviation from electroneutrality. The liquid phase is allowed to be a solution of weak multivalent electrolytes of any valence and any complexity. The mathematical model joins together the Poisson equation, the continuity equation for electric charge, the mass continuity equations, and the modified G-function [1].

In the present paper we have additionally implemented the Navier-Stokes equation into the model to describe the electroosmotic flow (EOF) acting inevitably in electromigration separation methods. The model is solved by the numerical simulation software COMSOL and allows to calculate (i) the velocity profiles of liquid, (ii) volume charge density, (iii) electric potential, (iv) deviation from electroneutrality and (v) concentration profiles of all ionic forms of all electrolytes in the diffuse part of the double layer.

The model can depict, e.g., a pH drop in the solution of a multivalent weak electrolyte, here the phosphate buffer, in the diffuse layer in the vicinity of a silica wall, see Fig.1.

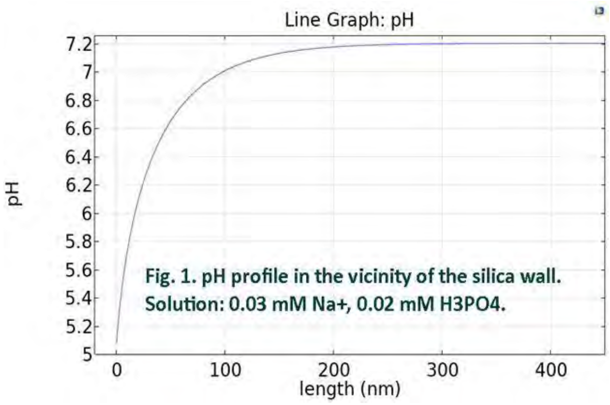

Fig. 1. pH profile in the vicinity of the silica wall. Solution: 0.03 mM Na+, 0.02 mM H3PO4.

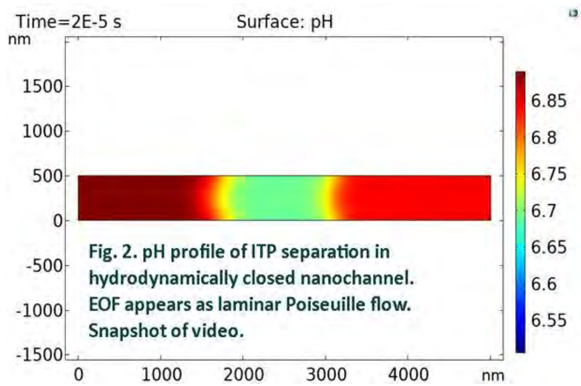

Fig. 2. pH profile of ITP separation in hydrodynamically closed nanochannel. EOF appears as laminar Poiseuille flow. Snapshot of video.

When a tangential electric field is applied, as it is in channels of electromigration methods, we can calculate spatial profiles of all significant parameters of electromigration, such as, e.g., pH profiles, as demonstrated in Fig. 2.

Due to the electrical double layer the composition of electrolyte solutions near surfaces is different when compared with the rest of the solution. Practical examples and video sequences are presented to demonstrate behavior of the diffuse layer. The presented model is applicable in complex biological systems for the calculation of all quantities of solutions in the vicinity of cell membranes or tissues.

References

[1] T. Novotný, B. Gaš, Mathematical model of electromigration allowing the deviation from electroneutrality, Electrophoresis 42 (2021) 881–889.