Abstract

In the presented thesis we introduce a computational model that can be used for 2-D and 3-D computer simulations of experiments in electrophoresis. The simulations are carried out by the aid of the finite element method (FEM). In particular, commercially available program Comsol Multiphysics 3.3 is employed. A general shape of continuity equation is chosen to express the mass, electric charge, momentum and energy conservation law. Diffusion, migration and convection terms are taken into account when formulating the mass conservation law. Both external (driving voltage) and internal (diffusion currents) terms are considered in the electric charge conservation law. Both constant voltage mode and constant current mode can be handled. A solvent is regarded as an incompressible Newtonian fluid. Both pressure-driven and electroosmotic flows can be taken into consideration. The heat convection as well as the heat diffusion is governed by the energy conservation law. Both strong and weak electrolytes (of any attainable valency) may be regarded as system constituents. Furthermore, the model can handle the ionic strength correction if desired. A task may be assigned either in Cartesian or cylindrical coordinates. The presented model was employed to solve four particular tasks. The first one inspects the electromigration in the setup in the Agilent 3DCE electrophoresis equipment. Changes in the electrolyte composition due to the electrolysis are inspected. The electroosmosis is also considered. The second task focuses on the lab-on-a-chip analysis in a gel. The injection cross is of the main interest. The analysis is carried out in the constant current mode. Four model anionic species are considered as the analytes and their resolution is inspected under various conditions.

The third task deals with the free flow electrophoresis equipment. Both the electric field and the pressure-driven bulk flow are applied simultaneously. Three model cationic species are considered as analytes and their resolution is analyzed. The last task investigates the thermal effects in a capillary. The temperature rises in the capillary as the electric current passes through the electrolyte (Joule heating). Both air and water cooling efficiency are inspected. The coolant velocity field and the resulting temperature map are analyzed under various conditions.