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NUMERICAL SIMULATIONS OF PAPER-BASED ELECTROMIGRATIVE SEPARATIONS

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Abstract. Microfluidic paper-based analytical devices is nowadays a well established technology. Nevertheless, several aspects related to the transport of chemical species in the porous substrate are still to be improved to reach higher levels of analytical precision, efficiency, and portability. In this context, numerical simulations of fluid and mass transport in microfluidic paper-based analytical devices are essential for better understanding the different phenomena that are relevant in this particular porous matrix. Among these transport phenomena, advective, diffusive and dispersive mechanisms have been already addressed in previous works. This work focuses on the electrophoretic transport of species and the fluid transport associated to electroosmotic flow in paper substrates. Consequently, we present a transport model for ionic and ionizable compounds under the effect of an externally applied electric field. The model includes the effects of porosity, tortuosity, and permeability of the paper substrates over the fluxes of ionic compounds and the solvent velocity profile due to the electroosmotic flow. The model was implemented and validated with experimental data from literature, and then tested with several numerical prototypes running different eletrophoretic techniques for the separation of analytes of bioanalytical interest. Numerical prototypes were implemented using an upgrade of *electroMicroTransport*, an open source toolbox for the well known finite volume library OpenFOAM®. This upgraded version enables us to evaluate all the particular effects related to the properties of the paper substrates, according to the proposed mathematical model. The results obtained indicate that the proposed model and the code upgrade for *electroMicroTransport* configure a suitable tool for numerical prototyping of electrophoretic paper-based analytical devices.