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COUPLING THE TRANSPORT OF WATER AND AQUEOUS SPECIES IN FINITE ELEMENT MODELING OF ELECTROKINETICS

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The electrokinetic transport of ionic and non-ionic species through a porous media under the effect of an external electric field can be mathematically described by the Nernst-Planck-Poisson (NPP) system of equations. The Nernst-Planck mass balance equation describes the transport of aqueous species by a combination of the diffusion and electromigration terms. Since the ions themselves contribute to the local electric potential, Poisson's equation of electrostatics, that relates the electrostatic potential to local ion concentrations, is solved simultaneously to describe this effect. This strongly coupled non-linear system has been satisfactory solved by finite element integration, and combined to additional physicochemical aspects such as the electrode processes and the chemical interaction between the species in the system for modeling of electrokinetic transport processes.

Proper models of the electrokinetic phenomena have to take into account the transport of the pore solution itself. Water is suggested to electroosmotic flow under electric fields. Electroosmotic advection is of mayor importance when considering the transport of non-charged particles such as organic contaminants from soil. The transport of water may dry the material at the anode surroundings, what may interrupt the ionic current and stop the process. Capillary forces and hydraulic gradient, between others, can also affects to the transport of water in the porous media.

In the present work, the NPP system has been extended in order to include the water transport equation, and to calculate the advective flow contribution on the ionic transport. In this model, the transport of water is assumed to be a combination of hydraulic gradient, capillary suction forces and electroosmotic flow. In the model presented here, the advective term has been implicitly included in the Nernst-Planck equation of each individual aqueous species. Thus, this coupling strategy between the water and the ionic transport together with a numerical procedure for solving the non-linearity character, allows a simplified finite element analysis.

References

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