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Direct numerical simulation of current-induced convection near an ion-selective surface CLARA DRUZGALSKI, MATHIAS B. ANDERSEN, ALI MANI, Stanford University — Understanding fundamentals of electrokinetic transport and fluid flow phenomena near ion-selective surfaces provides insight to improve systems such as electrodialysis for water deionization. The work of Rubinstein and Zaltzman [e.g. Phys Rev E 62, 2238 (2000)] have clarified qualitative aspects of how development of current-induced space-charge layers near ion-selective surfaces can lead to the onset of electro-osmotic instabilities. We expand on this work through multidimensional numerical simulation of the full nonlinear Poisson-Nernst-Planck and Navier-Stokes equations with ideally selective membrane boundary conditions. Our numerical scheme is optimized by exploiting the periodicity in the system parallel to the ion-selective surface, using a spectral method in these coordinates. In the wall normal direction a finite difference approach accurately captures the strongly nonlinear nested boundary layer structure. Our numerical scheme fully resolves the concentration profiles throughout the system including the numerically stiff electric double layer and extended space charge layer. Our simulations enable prediction of the full continuous current versus voltage curves showing overlimiting current without resorting to any adjustable parameter.

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