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Direct numerical simulation of electrokinetic chaos driven by ion concentration polarization next to an ion-selective membrane[1] CLARA DRUZGALSKI, MATHIAS ANDERSEN, ALI MANI, Stanford University — We present a three-dimensional direct numerical simulation (DNS) of electrokinetic instability and hydrodynamic chaos near an ion-selective membrane subject to normal electric current. We employ a non-dissipative computational algorithm to numerically solve the full Poisson-Nernst-Planck and Navier-Stokes equations for a symmetric binary electrolyte in a gap between an ion-selective surface and a stationary reservoir. In our simulation the numerically stiff electric double layer (EDL) and extended space charge (ESC) regions are resolved without resorting to asymptotic models. Our 3D results enable visualization of the onset of instability and detailed flow structures over a wide range of scales and distances to the membrane. We present the time-averaged statistics from this simulation and its comparison to an otherwise identical 2D calculation. These simulations demonstrate transport phenomena that are crucial for accurate prediction of charge and mass transport in various electrochemical systems such as flow batteries and electrodialysis and electrolysis cells.

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