Abstract Submitted
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Temperature and viscosity effects on the velocity profile of a nanochannel electro-osmotic flow[1] BOHUMIR JELINEK, SERGIO D. FELICELLI, Mississippi State University, PAUL F. MLAKAR, JOHN F. PETERS, ERDC, Vicksburg MS — Significant temperature and viscosity effects on the electrokinetic transport in a nanochannel with a slab geometry are demonstrated using a molecular dynamics (MD) model. A previously studied system consisting of Na^+ and Cl^- ions dissolved in water and confined between fixed crystalline silicon walls with negatively charged inner surfaces in an external electric field was investigated. Lennard-Jones (LJ) force fields and Coulomb electrostatic interactions with Simple Point Charge Extended (SPC/E) model were used to represent the interactions between ions, water molecules, and channel wall atoms. Dependence of the flow of water and ions on the temperature was examined. The magnitude of the water flux and even its direction are shown to be significantly affected by temperature. Temperature dependence of the flux was attributed to the charge redistribution and to the changes in viscosity of water. Using a simple inverse power approximation for water viscosity profile across the channel instead of constant viscosity, an improved prediction of MD electro-osmotic velocity profile from charge density by Stokes equation is demonstrated.

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