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Effect of Velocity-Slip in Nanoscale Electroosmotic Flows: Molecular and Continuum Transport Perspectives

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Abstract : Electroosmotic (EO) slip flows in nanochannels are investigated using non-equilibrium molecular dynamics (MD) simulations, and the results are compared with analytical solution of Poisson-Boltzmann and Stokes (PB-S) equations with slip contribution. The ultimate objective of this study is to show that well-known continuum flow model can accurately predict the EO velocity profiles in nanochannels using the slip lengths and apparent viscosities obtained from force-driven flow simulations performed at various liquid-wall interaction strengths. EO flow of aqueous NaCl solution in silicon nanochannels are simulated under realistic electrochemical conditions within the validity region of Poisson-Boltzmann theory. A physical surface charge density is determined for nanochannels based on dissociations of silanol functional groups on channel surfaces at known salt concentration, temperature and local pH. First, we present results of density profiles and ion distributions by equilibrium MD simulations, ensuring that the desired thermodynamic state and ionic conditions are satisfied. Next, force-driven nanochannel flow simulations are performed to predict the apparent viscosity of ionic solution between charged surfaces and slip lengths. Parabolic velocity profiles obtained from force-driven flow simulations are fitted to a second-order polynomial equation, where viscosity and slip lengths are quantified by comparing the coefficients of the fitted equation with continuum flow model. Presence of charged surface increases the viscosity of ionic solution while the velocity-slip at wall decreases. Afterwards, EO flow simulations are carried out under uniform electric field for different liquid-wall interaction strengths. Velocity profiles present finite slips near walls, followed with a conventional viscous flow profile in the electrical double layer that reaches a bulk flow region in the center of the channel. The EO flow enhances with increased slip at the walls, which depends on wall-liquid interaction strength and the surface charge. MD velocity profiles are compared with the predictions from analytical solutions of the slip modified PB-S equation, where the slip length and apparent viscosity values are obtained from force-driven flow simulations in charged silicon nano-channels. Our MD results show good agreements with the analytical solutions at various slip conditions, verifying the validity of PB-S equation in nanochannels as small as 3.5 nm. In addition, the continuum model normalizes slip length with the Debye length instead of the channel height, which implies that enhancement in EO flows is independent of the channel height. Further MD simulations performed at different channel heights also shows that the flow enhancement due to slip is independent of the channel height. This is important because slip enhanced EO flow is observable even in micro-channels experiments by using a hydrophobic channel with large slip and high conductivity solutions with small Debye length. The present study provides an advanced understanding of EO flows in nanochannels. Correct characterization of nanoscale EO slip flow is crucial to discover the extent of well-known continuum models, which is required for various applications spanning from ion separation to drug delivery and bio-fluidic analysis.

Keywords : electroosmotic flow, molecular dynamics, slip length, velocity-slip
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