

Abstract Submitted
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Toward predicting the electrokinetic zeta potential in slit micro/nanochannels with nanoscale surface features: Continuum and molecular dynamics analysis.¹ TROY SINGLETARY, AMIR RAHMANI, SIJIA HUANG, GERARD MILES, CARLOS COLOSQUI, State Univ of NY - Stony Brook — We present a recently developed continuum description of electrokinetic flows for predicting the zeta potential in the case of slit channels with nanoscale surface features of dimensions comparable to the Debye length. The proposed analytical model considers the average effects that such nanoscopic features commonly found on macroscopically smooth surfaces have on the streamwise-averaged fluid velocity and ion density by solving a unidirectional Navier-Stokes and Poisson-Boltzmann equation for such variables. The proposed analytical model is simple and compact and quantitatively accounts for results from molecular dynamics simulations that consider the finite size of ionic species as well as the presence of ion solvation shells and hydration layers on the channel surface. Our theoretical and computational analysis indicates that under conditions for which the Onsager symmetry holds, a simultaneous knowledge of the electroosmotic flow rate and the pressure-driven flow rate or streaming current is instrumental to unambiguously determine the zeta potential and the effective height of the nanoscale surface features.

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