

Abstract Submitted
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Mass transfer properties of nanoconfined fluids at solid-liquid interfaces: from atomistic simulations to continuum models MATTEO MORCIANO, MATTEO FASANO, Politecnico di Torino, ANDREAS NOLD, CARLOS CORREIA BRAGA, PETR YATSYSHIN, Imperial College London, DAVID SIBLEY, Loughborough University, BENJAMIN GODDARD, The University of Edinburgh, ELIODORO CHIAVAZZO, PIETRO ASINARI, Politecnico di Torino, SERAFIM KALLIADASIS, Imperial College London, MULTI-SCALE MODELING LABORATORY TEAM, COMPLEX MULTIPHASE SYSTEMS TEAM — At the nanoscale, traditional continuum models are not sufficient to describe fluid flow. For example, the no-slip assumption may not be valid for nanoscale flows, where interface effects dominate transport phenomena. Hence, classic boundary conditions should take into account possible interplays between fluid velocity, shear stress, surface chemistry and roughness. Unlike hydrodynamics, in molecular dynamics (MD), the boundary conditions are not specified a priori but arise naturally from computations. Here, mass transfer properties for a Lennard-Jones fluid confined in a nanochannel are studied by MD. Density, stress and velocity profiles within the fluid are evaluated with different nanoconfined conditions, shear rates and surface hydrophilicity. Our results show a strong anisotropic behavior of fluid properties along the channel section. Shear rates and velocity profiles allow calculating the spatial distribution of viscosity along the channel. We also observe that hydrophilic surfaces lead to increased viscosity. Our findings may have a potential impact on the design of nanofluidic devices for either engineering or biomedical applications.

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