Continuum Simulations of Water Flow in Carbon Nanotube Membranes J.H. WALTHER, Technical University of Denmark, Denmark, A. POPADIC, National Institute of Chemistry, Ljubljana, Slovenia, P. KOUMOUT-SAKOS, ETH Zurich, Switzerland, M. PRAPROTNIK, National Institute of Chemistry, Ljubljana, Slovenia — We propose the use of the Navier-Stokes equations subject to partial-slip boundary conditions to simulate water flows in Carbon NanoTube (CNT) membranes. The finite volume discretisations of the Navier-Stokes equations are combined with slip lengths extracted from Molecular Dynamics (MD) simulations to predict the pressure losses at the CNT entrance as well as the enhancement of the flow rate in the CNT. The flow quantities calculated from the present hybrid approach are in excellent agreement with pure MD results while they are obtained at a fraction of the computational cost. The method enables simulations of system sizes and times well beyond the present capabilities of MD simulations. Our simulations provide an asymptotic flow rate enhancement and indicate that the pressure losses at the CNT ends can be reduced by reducing their curvature. More importantly, our results suggest that flows at nanoscale channels can be described by continuum solvers with proper boundary conditions that reflect the molecular interactions of the liquid with the walls of the nanochannel.

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