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Atomistic Simulations of Fluid Flow through Graphene Channels and Carbon Nanotubes[1] HARVEY A. ZAMBRANO, Universidad de Concepcion, JENS H. WALTHER[2], Technical University of Denmark, ELTON E. OYARZUA , ENRIQUE WAGEMANN, Universidad de Concepcion — The transport of aqueous solutions in artificial nanopores is of both fundamental and technological interest. Recently, carbon nano-structured materials (fullerenes) have attracted a great deal of attention in nanotechnology. In fact, due to their large specific surface area, high thermal conductivity, extremely low surface friction and superior mechanical properties, graphene channels and carbon nanotubes (CNTs) are promising candidates to be implemented as fluid conduits in nanosystems. Performing Non-equilibrium Molecular Dynamics simulations, we study the transport of water-eletrolyte solutions inside single and multi-wall graphene channels and inside zig-zag and armchair CNTs of similar cross sectional area. In order to calibrate the force fields, we use dedicated criteria relevant to the hydrodynamics of the systems of interest. Different fluid driving mechanisms such as pressure fields, electro-osmosis and thermal gradients are evaluated. We conduct a detailed analysis of the transport efficiency of each system to impose similar volumetric flow rates. From the simulations, we extract density and velocity profiles to study the liquid structure, wall slippage and flow enhancement in order to compare the hydrodynamic performance of these two novel materials.

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