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Single-file flows in carbon nanotubes: A simplified molecular dynamics model[1] THOMAS SISAN, SETH LICHTER, Northwestern University — Carbon nanotubes (CNT) are ideal systems for the study of nanofluidics and hold promise for diverse applications, such as desalination and power generation. Sub-nanometer CNTs adsorb single-file chains of water that transport at high speeds– equal to that measured in aquaporin channels. Molecular dynamics (MD) simulations of these fast-moving single-file water chains suggest simultaneous hopping of the whole chain and the invariance of water transport properties to CNT length. We investigate these claims using simplified one-dimensional MD with appropriate boundary conditions, thus achieving a highly-reduced system size and rapid simulations. The model is verified by comparison with full MD simulations. We find that simultaneous hopping of water molecules is an invalid approximation for very long channels where the transit time for a kink in the one-dimensional chain becomes important. Finally, our rapid prototyping capability is used to investigate the effects of chemical and geometric changes to the nanotube wall in order to enhance water transport through CNTs.

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