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**Spatial Diffusion of Water in Carbon Nanotubes**[1] AMIR BARATI FARIMANI, N.R. ALURU, Department of Mechanical Science and Engineering, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana — Water desalination and transport are the great applications of carbon nanotubes (CNTs). Understanding the dynamics of water molecules in carbon nanotubes can shed light on the physics of transport, diffusion and other thermodynamic properties of water. Among all these properties, diffusion is of great importance as it affects most of other key properties. In this article, the spatial variation of the axial, radial, and tangential diffusion coefficients in carbon nanotubes (CNTs) of various diameters were computed. Based on the spatial variation of the diffusion coefficient, the diffusion mechanisms in different regions of the nanotube are defined. The effect of confinement and CNT wall on the diffusion coefficient is studied and discussed. The dependence of the diffusion coefficient on the carbon water interaction parameter is investigated. The average diffusion coefficient in the nanotube as a function of the nanotube diameter is calculated, and the diffusion mechanisms, including the transition regimes, are identified. It has been shown that the axial diffusion coefficient is enhanced in the adjacent water layer to the wall. The results are explained via hydrogen bond network and water orientations.

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