Nongnuch Artrith 2008: Structure and Dynamics of Water Confined in Single-Walled Nanotubes: A Molecular Dynamics Study. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Assistant Professor Piboon Pantu, Ph.D. 78 pages.

Structures and dynamics of water molecules in nanoporous media exhibit interesting characteristics different from their ordinary bulk properties and may lead to potential applications in sophisticated nanofludic devices. In this study, molecular dynamics simulations were performed to investigate water molecules confined in single-walled carbon nanotubes (SWCNTs) and boron nitride nanotubes (SWBNNTs). Water density of 1.00 g cm^{-3} was placed inside the models of (*n*,*n*)-armchair nanotubes with different diameterrs (*n* = 9, 10, 12, 14, 16 and 20) and the simulations were performed in the canonical *NVT* ensemble at 298 K by using the Nosé-Hoover thermostat in DL_POLY program package. The wall-water interactions were varied within reasonable limits by changing the strength of the Lennard-Jones (LJ) parameters. Distribution functions were reported for the water in the tubes in spherical and cylindrical coordinates and the single-molecule dynamics, in particular self-diffusion, were monitored. While this motion was very much slowed down in narrow tubes, in keeping with previous findings (Mashl, R.J. *et al*. 2003 Nano Lett. 3(5):589-592.), bulk-water like self-diffusion coefficients were found in wider tubes. Axial diffusion coefficient increased with increasing tube diameter and reached its bulk value in the widest tubes with diameters of about 24 Å. The convergence was faster for smaller wall-water interactions. An anomaly is, however, found for the SWBNNTs where the convergence was not monotonous.

_____ _____ ___ / ___ / ___

Student's signature Thesis Advisor's signature