Molecular Dynamics Simulation of Liquid Behavior When Under SiO_2 Nanoscale Channel Confinement

MCM-41 (Mobil Crystalline Material), a silicate containing uniformly aligned, hexagonal nanochannel arrays, was discovered in the 1992 by Mobil Research scientists. As nanochannel diameter decreases (approaching molecular diameter), properties of liquid in the channels such as criticality, liquid-liquid equilibrium, and self-diffusivity change. The dual purpose of this project is to investigate the property of diffusivity of Cl^- ions in solution over time while confined within nanoscale channels and to perform molecular dynamics simulations to obtain values for comparison with bulk diffusivity. Films with various channel diameters were utilized. A two-fold approach was utilized in order to accomplish the project goals. Experimental work was done in a laboratory setting to produce silica films of uniformly aligned, hexagonally shaped nanotube arrays. Once the films were successfully produced and characterized, a 0.0297M aqueous NaCl solution was introduced on one side of the film. Using an ion-specific electrode, the concentration of the Cl^- ions was measured in the solution that subsequently diffused through the film. The experiment was performed over a six-hour period in order to ensure an acceptable number of data points were taken. Using Fick's law of diffusion, calculations were then made based on this experimental data to determine the diffusivity coefficients of Cl^- ions in solution within the channels. Comparisons of the standard diffusivity value for Cl- with the experimental results were then made. The second part of this research project involves performing molecular dynamics simulations in order to model liquid behavior in nanoscale tubes of varying diameters. These simulations are to be performed by utilizing the Fortran programming language from a UNIX platform. Upon completion of these simulations, comparisons will then be made between the values obtained by experimental procedures and the theoretical results obtained by the molecular dynamics simulations. Relatively close correlation was found between standard bulk diffusivity values and the values calculated from experimental data. Molecular dynamics simulations have not yet been performed, but will be in the near future to obtain comparative values. Further research must be done to insure valid confirmation of experimental results. Important progress will also be made when the simulation code is properly modified and run to fit experimental parameters.

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