Orienting Flow in Carbon Nanotubes

September 2 2008, By Miranda Marquit

(PhysOrg.com) -- Carbon nanotubes provide some of the most interesting possibilities for future technology. One of the more intriguing possibilities – with a variety of practical applications – is using carbon nanotubes for water transport. In the past, experiments have suggested that extremely fast water transport can be attained through carbon nanotubes as small as two nanometers in diameter by applying a pressure gradient.

Professor N.R. Aluru at the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign, and Sony Joseph, who defended his Ph.D. thesis recently, have used computer simulations to explore a method by which water transport through smaller carbon nanotubes could be further enhanced. Some of the results of their work appears in *Physical Review Letters*: "Pumping of Confined Water in Carbon Nanotubes by Rotation-Translation Coupling."

"Until now," Sony Joseph tells *PhysOrg.com*, "previous simulations had shown that single file water movement in short carbon nanotubes have net transport in both directions. But if you could get the water to orient in one direction, in a long tube, you could have net transport along that direction. This would further increase the flow rate when a pressure gradient is applied and be useful in many ways, including to allow us to mimic biological protein channels."

Joseph and Aluru used molecular dynamics simulation in long carbon nanotubes (around 10 nanometers long) to show the relationship between the flow direction of the water and the dipole orientation. “In order to maintain the direction,” professor Aluru explains, “we need either local electrical fields or chemical functional groups at the ends of the nanotubes. These orient the water and keep it flowing in one direction.” The two scientists point out that in order to change the direction of the water flowing through the carbon nanotube, one has only to reverse the direction of the electrical field.

Focusing on using an external electrical field, Joseph and Aluru modeled how the field interacts with the water molecules. The molecules have a net zero charge, and interact with the field through torques. These torques are applied to the rotational degrees of freedom of the molecules. Changes to translational degrees of freedom in this water transport system, the scientists point out, are mostly due to how rotational and translational motions couple with each other.

Some of the applications considered for carbon nanotube membranes include such items as drug delivery, desalination, and selective ion transport. Joseph and Aluru, however, are especially interested in using this technology for water purification and nanofiltration. “We are trying to show how this would aid the process of reverse osmosis,” Aluru says.

Joseph and Aluru emphasize that, right now, this work is largely based on computer simulations with theoretical models. Joseph explains that right now water transport through nanotube membranes of two nanometers have been achieved, but that scientists are working toward pumping water through membranes that are less than one nanometer.

“We’ve shown that it is theoretically possible to get this sort of water transport,” Joseph points out. “The next step is getting to the point where this could be tested.”