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Molecular traffic jam makes water move faster through nanochannels

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Cars inch forward slowly in traffic jams, but molecules, when jammed up, can move extremely fast.

New research by Northwestern University researchers finds that water molecules traveling through tiny carbon nanotube pipes do not flow continuously but rather intermittently, like stop-and-go traffic, with unexpected results.

"Previous molecular dynamics simulations suggested that water molecules coursing through carbon nanotubes are evenly spaced and move in lockstep with one another," said Seth Lichter, professor of mechanical engineering at Northwestern's McCormick School of Engineering and Applied Science. "But our model shows that they actually move intermittently, enabling surprisingly high flow rates of 10 billion molecules per second or more."

The research is described in an Editor's Choice paper, "Solitons Transport Water through Narrow Carbon Nanotubes," published January 27 in the journal *Physical Review Letters*.

The findings could resolve a quandary that has baffled fluid dynamics experts for years. In 2005, researchers—working under the assumption that water molecules move through channels in a constant stream—made a surprising discovery: water in carbon nanotubes traveled 10,000 times faster than predicted.

The phenomenon was attributed to a supposed smoothness of the carbon nanotubes' surface, but further investigation uncovered the counterintuitive role of their inherently rough interior.

Lichter and post-doctoral researcher Thomas Sisan performed new simulations with greater time resolution, revealing localized variations in the distribution of water along the nanotube. The variations occur where the water molecules do not line up perfectly with the spacing between carbon atoms—creating regions in which the water molecules are unstable and so propagate exceedingly easily and rapidly through the nanotube.

Nanochannels are found in all of our cells, where they regulate fluid flow across cell membranes. They also have promising industrial applications for desalinating water. Using the newly discovered fluid dynamics principles could enable other applications such as chemical separations, carbon nanotube-powered batteries, and the fabrication of quantum dots, nanocrystals with potential applications in electronics.

More information: prl.aps.org/abstract/PRL/v112/i4/e044501

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