Engineers discover predictor of mobility for fluids at nano-scale

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Chemical engineers at The University of Texas at Austin have discovered a new way to predict the mobility of confined fluids at nanometer scales. At these scales, often just a few molecules across, fluids exhibit significantly different properties than at the macroscopic level.

The ability to predict these changes has applications in fields such as cell biology and geophysics, as well as important implications for the design of nanoscale devices.

The research by graduate student Jeetain Mittal and Dr. Thomas Truskett, assistant professor in the Department of Chemical Engineering at The University of Texas at Austin, along with Dr. Jeffrey Errington of the University at Buffalo, SUNY, appears in the May 5 issue of *Physical Review Letters*.

These results will help engineers understand how a variety of confined fluid systems function, from the performance of new materials for chemical separation and environmental remediation to transport processes in biological membranes. The discovery also provides a way to study the behavior of fluids in nanodevices, such as miniaturized “lab on a chip” tools for biomedical and analytical chemistry applications.

Confining fluids in very small, nanometer-scale channels can affect how the molecules pack together, how they withstand compression, and their ability to rapidly mix or flow. Changes to the first two properties are

relatively well understood, but predicting the third, which is connected to the mobility of the molecules, has proven elusive.

“One of the most dramatic changes you see going from macroscopic scales to nanometer scales is that materials can actually change their state,” Truskett said. “A solid may become liquid upon confinement. If that solid material is a bonding agent and it turns into a runny fluid, it doesn’t do its job. Likewise, a liquid can become a solid when confined to small scales. If it is a lubricant, it fails. So in the engineering of nanoscale devices, these kinds of changes can have potentially catastrophic effects.”

In a bulk fluid, such as a glass of water, fluid molecules interact primarily with other fluid molecules. Relatively few are in contact with the surface of the container. At nanometer scales, however, a much higher proportion of molecules come in contact with the confining material. This surface interaction can significantly alter fluid properties, including molecular mobility.

The key to successfully predicting changes to mobility in a confined fluid, the researchers discovered, is the relationship between mobility and excess entropy.

“One way to think about how mobility relates to entropy is to think of entropy as measuring a sort of randomness at the molecular level,” Truskett said. “In a gas, where the molecules are randomly distributed, entropy is high and the gas mixes readily. In a solid, the molecules are aligned in a regular spatial pattern; there is little randomness and the solid barely mixes at all. Our discovery is that while both excess entropy and mobility of a fluid are affected by confinement, the relationship between the two quantities essentially remains the same down to very small scales.”

Because scientists already have reliable methods for predicting how confinement will affect excess entropy, they can now use this information together with the group's findings to predict how confinement will affect fluid mobility.

The group performed computer simulations to study the behavior of fluids in highly restrictive channels with different shapes and boundary interactions. They were able to successfully model changes to fluid mobility and entropy in these conditions, a critical breakthrough that will allow engineers to learn how these changes occur while avoiding the difficult task of gathering experimental data on such small scales.

Source: University of Texas at Austin