Pacific Northwest NATIONAL LABORATORY

Getting Your Molecule into the Movies

Computer simulations give insights into how carbon dioxide reacts with a sequestering liquid

"If we want to optimize gas sorption, we must understand the interface, because most of the chemical and physical processes usually occur at the interface."

Dr. Liem Dang
Pacific Northwest National Laboratory

RESULTS

Worse than toddlers on a sugar high, carbon dioxide molecules just don't like standing still. The tiny molecules, just three atoms, leap from place to place in less than a trillionth of a second. Yet, scientists at Pacific Northwest National Laboratory and the University of Wisconsin-Parkside found a way to get clear pictures. They used computer simulations to get detailed images of carbon dioxide reacting with an ionic liquid's surface. The images show that the surface's molecular strata increases the energy needed for the gas to move into the liquid. They also found that carbon dioxide and water molecules arrange themselves differently once these molecules get close to the surface, based on how the molecule's electrons are spaced.

This work by Dr. Liem X. Dang and Dr. Tsun-Mei Chang is featured in an invited perspectives article in *The Journal of Physical Chemistry Letters*. A perspective article provides state-of-the-art research on new and emerging areas by leaders in the field. An image from the team's study graced the journal's cover.

WHY IT MATTERS

While it might seem like an esoteric topic, useful only to those who inhabit ivory towers, understanding how gases interact with a liquid surface influences a lot, including the air we breathe and the energy we use. For example, coal-fired power plants produce large amounts of carbon dioxide. Scientists and industry leaders want to remove that dioxide and prevent its access to the environment. One option is to pump the gas through a liquid that traps only the carbon dioxide, and not other gases. But to do it, scientists must know how the gas interacts with the liquid's surface.

"If we want to optimize gas sorption, we must understand the interface, because most of the chemical and physical processes usually occur at the interface," said Dang.

This research appears on the cover of *The Journal of Physical Chemistry Letters*. ©American Chemical Society, 2012.

METHODS

When the reaction speed is measured in trillionths of a second and at scales measured in the width of atoms, scientists turn to powerful computer simulations to understand what is happening. The simulations allow them to freeze the action and gather accurate data. The researchers focused on

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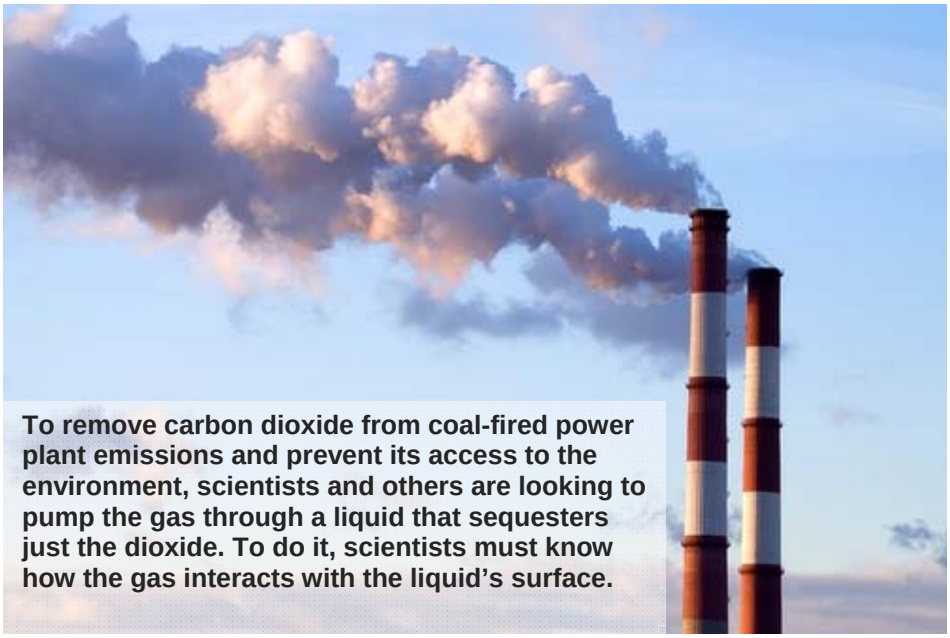


To remove carbon dioxide from coal-fired power plant emissions and prevent its access to the environment, scientists and others are looking to pump the gas through a liquid that sequesters just the dioxide. To do it, scientists must know how the gas interacts with the liquid's surface.

gaseous carbon dioxide and a more hydrophobic or water-fearing room-temperature ionic liquid (see sidebar) known as [bmim][Tf_2N].

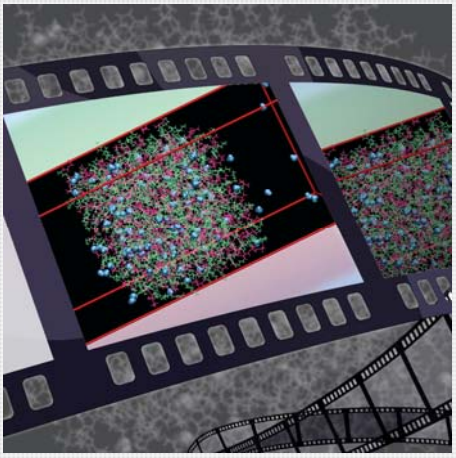
The accuracy of that data depends in part on how well the molecular interactions, molecular orientation and surface tension are described. The research duo began by thoroughly examining the models, creating accurate portrayals.

Then, the team ran a series of simulations and examined how the gas and the liquid interacted. They found the solubilities of gases are critically dependent on the type of anions or negatively charged ions used to construct the ionic liquids.

"Solubilities are an active research subject in the ionic liquids field," said Dang.

Not a Glass of Salt Water

The room temperature ionic liquids studied here are more complex than glass of warm water with table salt dissolved in it. Here, *room temperature ionic liquid* refers to a novel class of salts that are actually liquids at or near room temperature, or about 300 Kelvin. The salts are typically bulky and contain carbon, nitrogen and hydrogen atoms. These non-flammable liquids can be tweaked to have different properties, such as conducting electricity or absorbing large amounts of gas. The liquid's properties come into play in chemical processes such as creating nanosized catalysts.



WHAT'S NEXT?

The results raise questions about whether or not polarizable models are needed to simulate ionic liquids. This and questions about the influence of different charged particles in the liquid are being studied by the researchers.

ACKNOWLEDGMENTS

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Research Team: Liem X. Dang, PNNL; Tsun-Mei Chang, University of Wisconsin-Parkside

REFERENCE

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