Researchers discover traditional fluid flow observations may miss the big picture

June 21 2019

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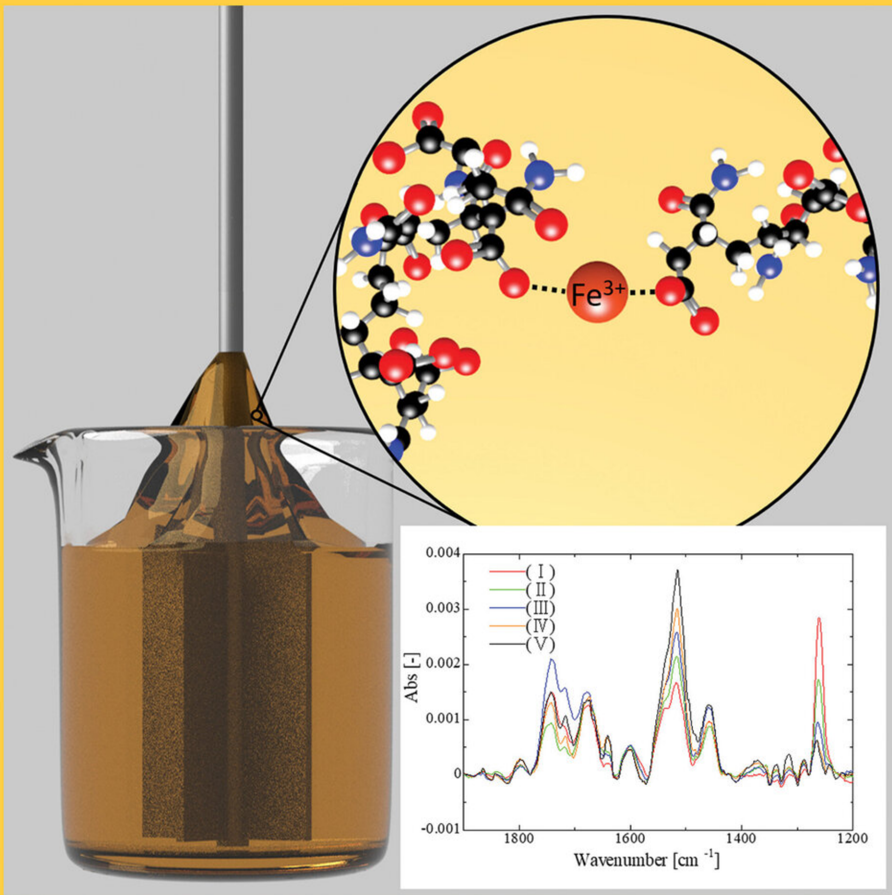
JPCBFK

MAY 30, 2019
VOLUME 123
NUMBER 21

pubs.acs.org/JPCB

THE JOURNAL OF PHYSICAL CHEMISTRY B



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A temporal reaction occurred during the flowing of fluids indicated a fundamental structural change in the fluids. Credit: Figure adapted with permission from the cover of *J. Phys. Chem. B* 2019, 123, 21, 4587-4593.

Before and after comparisons don't tell the full story of chemical reactions in flowing fluids, such as those in a chemical reactor, according to a new study from a collaboration based in Japan.

The researchers published their paper on May 6 in the *Journal of Physical Chemistry B*, a journal of the American Chemical Society. The results were featured on the journal's cover.

The team examined how a solution of dissolved polymers changed after the addition of Fe^{3+} solution. These types of solutions are used to better control variables in several fields, including manufacturing. In automobile manufacturing, for instance, the solutions help achieve a thorough evenness of paint coverage and control over how much a material expands or contracts under various temperatures.

Traditionally, researchers examine a solution before a reactant, such as Fe^{3+} solution, is added, and again after the reaction takes place.

"In other words, if a fluid property such as the viscosity of the solution is higher after the reaction than before, we would expect that an increase in viscosity occurs from the reaction during flow," said Yuichiro Nagatsu, corresponding author on the paper and an associate professor in the Department of Chemical Engineering at Tokyo University of Agriculture and Technology.

Nagatsu and the team discovered that the before and after comparison isn't as reliable as previously thought. They observed an increase in viscosity in the solution during a chemical reaction to Fe^{3+}, but the solution had thinned back out by the end of reaction. They confirmed their chemical observations with infrared spectroscopy, which allows researchers to examine microscopic interactions without extensive preparation that could further disturb the sample.

Flow dynamics account for microscopic changes within these chemical reactions—molecules stripping other molecules of electrons and the like—that fundamentally change the composition of the solution. However, viscosity is known as a macroscopic change—it describes the solution as a whole rather than the individual interactions on the microscopic level.

It's incredibly unusual for such a solution to shift through such macroscopic phases only to lose the characteristics by the end of a chemical reaction, according to Nagatsu. This understanding could have major implications across industrial, environmental, and biological fields.

"Our ultimate goal is to establish a new research area to understand chemically reacting flow involving the diagnosis of molecule structure," Nagatsu said. He also noted that the plans to develop a novel method to control fluid dynamics through their new understanding of interactions.

More information: Toshimasa Ueki et al, Unpredictable Dynamics of Polymeric Reacting Flow by Comparison between Pre- and Post-Reaction Fluid Properties: Hydrodynamics Involving Molecular Diagnosis via ATR–FTIR Spectroscopy, *The Journal of Physical Chemistry B* (2019). DOI: 10.1021/acs.jpcb.9b02057

Provided by Tokyo University of Agriculture and Technology