Solubility study could impact energy, biology, environment

September 5 2017

Rice University chemical engineers have used the most realistic computer model yet devised to simulate the precise atomic and molecular interactions that come into play when water mixes with alkanes, a family of hydrocarbons that includes methane, propane and other products refined from petroleum and natural gas, such as paraffin.

In a new study published this month in the *Journal of Chemical Physics*, Rice researchers Dilipkumar Asthagiri, Arjun Valiya Parambathu and Walter Chapman, as well as former graduate student Deepti Ballal of Ames Laboratory, offered new answers to a puzzle that has long stymied chemists: When calculating the expected attraction between water and alkane molecules in an alkane-rich solution, scientists find that their answers don't jibe with experimental results.

Asthagiri and colleagues demonstrated that underlying electrostatic and polarization effects—things considered inconsequential in conventional approaches—are critical for accurate simulation of water-alkane solubility.

Chapman, the William W. Akers Professor of Chemical and Biomolecular Engineering and associate dean of engineering for energy, said the research could have far-reaching impacts in fields as diverse as biology, environmental systems and energy and chemical production.

"Simulations are increasingly used to understand, and potentially to manipulate, processes at the nanoscale," Chapman said. "For example,

our results could offer new insight to those who study free-energy surfaces related to protein folding and protein denaturation. They could be helpful in better interpreting MRI scans and in predicting the fate of contaminants in the environment. In energy production, insights from this work could be useful for improving flow assurance, preventing corrosion and improving processes in other ways that reduce costs and environmental impacts."

Chapman said his group hopes to build upon the work with future models that incorporate quantum corrections to both the movement of the particles and in assessing interatomic interactions, something that's only become feasible through recent advances in both parallel computing and linear-scaling quantum chemical calculations.

More information: D. Asthagiri et al, Electrostatic and induction effects in the solubility of water in alkanes, *The Journal of Chemical Physics* (2017). DOI: 10.1063/1.4997916

Provided by Rice University