Jestin Baby Mandumpal, Int J Petrochem Res. 2018
http://dx.doi.org/10.18689/2638-1974.a2.006

Can DMSO Preclude Formation of Gas Hydrates in Oil Pipeline?

Jestin Baby Mandumpal
Khazar University, Baku

Gas hydrates are crystals that are formed around gas molecules such as methane and ethane in extreme conditions, low temperature and high pressure. Smooth oil transportation can be hindered when these gas hydrates are present in the oil pipe lines. One of the assumptionsto bypass this problem is to inject some chemicals that can preclude crystallisation in water such that the formation of gas hydrates can altogether be avoided. These solvents can preferentially interact with water, thereby reducing the chances of gas hydrate production. Systematic experimental study of low temperature products such as gas hydrates is complicated due to the formation of ice crystals. However, with the aid of atomistic computer simulations one can effectively investigate the problem using effective atomic potentials. In order to unlock the mechanism of interactions of small organic molecules with water, performing extensive molecular dynamics simulations are envisaged. The systems are studied in a wide range of temperatures, going from normal temperatures to super cooled regime. As a starting step, a comparative study of aqueous Dimethyl Sulfoxide (DMSO) and acetone solutions using widely used TIP4P/OPLS combination potentials have been performed to see whether this organic solvent has got anti-crystallising property. The choice of acetone is made because the principal difference between acetone and DMSO lies only in the central atom of these molecules. The principal site- site correlations and degree of structure of both aqueous systems have been investigated, which suggests that sulfinyl group of DMSO interacts more strongly with water than carbonyl group in acetone does. Stronger interaction of sulfinyl group than carbonyl group with water is also reflected in quantitative hydrogen bonding analysis. Density calculations across a wide range of temperatures were also made, in order to investigate its dependence with respect to temperatures. Analysis indicates that the solute-solvent separation does not exist at higher concentrations studies, implying weakening of thermodynamic anomalies.

The present study reveals the quantitative and qualitative aspects of interactions that exist between amphiphile solutes like DMSO and acetone and water. Analyses indicate existence of three dimensional DMSO-water complexes by which DMSO molecules can avoid crystallisation. Such complexes cannot exist in aqueous acetone solutions due to planarity of acetone molecule. Occurrence of the three dimensional structures can trap more water molecules, thereby inhibiting water from nucleation and subsequent crystallisation. Stronger interactions of DMSO with water that are observed across a wide range of temperature have profound impact on petroleum industry because stronger interactions of DMSO with water resulting in larger three dimensional complexes that can prevent water nucleation, prologue to crystallisation which reduces oil transporting efficiency by preventing the formation of gas hydrates.

Biography:

Dr Jestin Mandumpal, obtained a PhD from Curtin University, Australia, currently is a lecturer in Chemistry at Khazar University Baku. His academic activities are focused on three themes: development in novel education methods in Chemistry, development and application of novel computing methods for physics of liquids and solutions, & teaching various chemistry courses to undergraduates and pre-university students. He has procured vital teaching research experience in chemistry from four continents. Recently, he has been awarded chartered chemist status by the Royal Society of Chemistry, UK. He is the author of “A Journey through Water: Scientific Explorations of The Most Anomalous Liquid on Earth”