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Metal-Based Deep Eutectic Solvents for Extractive Desulfurization of Fuels: Analysis from Molecular Dynamics Simulations

Authors : Aibek Kukpayev, Dhawal Shah

Abstract : Combustion of sour fuels containing high amount of sulfur leads to the formation of sulfur oxides, which adversely harm the environment and has a negative impact on human health. Considering this, several legislations have been imposed to bring down the sulfur content in fuel to less than 10 ppm. In recent years, novel deep eutectic solvents (DESs) have been developed to achieve deep desulfurization, particularly to extract thiophenic compounds from liquid fuels. These novel DESs, considered as analogous to ionic liquids are green, eco-friendly, inexpensive, and sustainable. We herein, using molecular dynamic simulation, analyze the interactions of metal-based DESs with model oil consisting of thiophenic compounds. The DES used consists of polyethylene glycol (PEG-200) as a hydrogen bond donor, choline chloride (ChCl) or tetrabutyl ammonium chloride (TBAC) as a hydrogen bond acceptor, and cobalt chloride ($CoCl_2$) as metal salt. In particular, the combination of ChCl: PEG-200:$CoCl_2$ at a ratio 1:2:1 and the combination of TBAC:PEG-200:$CoCl_2$ at a ratio 1:2:0.25 were simulated, separately, with model oil consisting of octane and thiophenes at 25^{o}C and 1 bar. The results of molecular dynamics simulations were analyzed in terms of interaction energies between different components. The simulations revealed a stronger interaction between DESs/thiophenes as compared with octane/thiophenes, suggestive of an efficient desulfurization process. In addition, our analysis suggests that the choice of hydrogen bond acceptor strongly influences the efficiency of the desulfurization process. Taken together, the results also show the importance of the metal ion, although present in small amount, in the process, and the role of the polymer in desulfurization of the model fuel.

Keywords : deep eutectic solvents, desulfurization, molecular dynamics simulations, thiophenes
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