Contribution ID: **243** Type: **Poster (+) Presentation**

Bulk and interfacial properties of alkanes in the presence of carbon dioxide, methane, and their mixture

Wednesday, 2 June 2021 09:00 (1 hour)

Currently, more than 30 Gt of anthropogenic CO2 is emitted per year, mainly from combustions of fossil fuels. The emissions of CO2 into the atmosphere play an important role in global warming and lead to key environmental problems. Interestingly, enhanced oil recovery (EOR) methods have been employed for CO2 storage and improving oil recovery. For example, in 2019, CO2-EOR delivered about 2.5% of the United States crude oil supply. Traditionally in the United States, CO2 from natural sources is employed for approximately 84% of CO2-EOR supply. However, CO2-EOR utilizing anthropogenic emissions would be required to attain the desired environmental benefits. Usually impurities such as CH4 are present along with the CO2 removed from exhaust gases of power plants and industrial processes. In this work, molecular dynamics simulations are performed to study the bulk and interfacial properties of systems containing alkanes (our model oil), CH4, and CO2 under geological conditions. Linear, branched, and cyclic alkanes (C7-C19) are considered for this work. We found preferential dissolution in the alkane-rich phase and accumulation in the interfacial region of CO2 from the CH4/CO2 mixture. The solubility of CH4 and CO2 generally decreased with the number of carbon atoms in the alkane molecule n and was relatively lower in the presence of cycloalkanes. The interfacial tension (IFT) values of the CO2+alkane system increased with the addition of CH4 which is in good agreement with experimental results. This can be explained by the higher enrichment of the interface in CO2 than CH4. These IFTs increased with n and are relatively higher in the presence of cycloalkanes. Furthermore, the simulation results were in good agreement with the theoretical calculations based on the predictive Peng-Robinson equation of state and density gradient theory.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

1) Choudhary, N., Nair, A. K. N., Ruslan, M. F. A. C., & Sun, S. (2019). Bulk and interfacial properties of decane in the presence of carbon dioxide, methane, and their mixture. Scientific reports, 9(1), 1-10.
2) Choudhary, N., Ruslan, M. F. A. C., Nair, A. K. N., & Sun, S. (2021). Bulk and interfacial properties of alkanes in the presence of carbon dioxide, methane, and their mixture. Ind. Eng. Chem. Res., 60(1), 729-738.

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Primary author: Dr NARAYANAN NAIR, Arun Kumar (King Abdullah University of Science and Technology (KAUST), Saudi Arabia)

Co-author: SUN, Shuyu (King Abdullah University of Science and Technology (KAUST))

Presenter: Dr NARAYANAN NAIR, Arun Kumar (King Abdullah University of Science and Technology (KAUST), Saudi Arabia)

Session Classification: Poster +

Track Classification: (MS6-B) Interfacial phenomena in multiphase systems