



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 CO<sub>2</sub> is emitted per year, mainly from combustions of fossil fuels. The emissions of CO<sub>2</sub> 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 CO<sub>2</sub> storage and improving oil recovery. For example, in 2019, CO<sub>2</sub>-EOR delivered about 2.5% of the United States crude oil supply. Traditionally in the United States, CO<sub>2</sub> from natural sources is employed for approximately 84% of CO<sub>2</sub>-EOR supply. However, CO<sub>2</sub>-EOR utilizing anthropogenic emissions would be required to attain the desired environmental benefits. Usually impurities such as CH<sub>4</sub> are present along with the CO<sub>2</sub> 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), CH<sub>4</sub>, and CO<sub>2</sub> under geological conditions. Linear, branched, and cyclic alkanes (C<sub>7</sub>-C<sub>19</sub>) are considered for this work. We found preferential dissolution in the alkane-rich phase and accumulation in the interfacial region of CO<sub>2</sub> from the CH<sub>4</sub>/CO<sub>2</sub> mixture. The solubility of CH<sub>4</sub> and CO<sub>2</sub> 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 CO<sub>2</sub>+alkane system increased with the addition of CH<sub>4</sub> which is in good agreement with experimental results. This can be explained by the higher enrichment of the interface in CO<sub>2</sub> than CH<sub>4</sub>. 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.

### Acceptance of Terms and Conditions

[Click here to agree](#)

### Newsletter

I do not want to receive the InterPore newsletter

## **Student Poster Award**

**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