

Electronic Supporting Information

Study of mixed matrix membranes with in-situ synthesized zeolite imidazolate frameworks (ZIF-8, ZIF-67) in polyethersulfone polymer for CO₂/CH₄ separation

Aditya Jonnalagedda, Bhanu Vardhan Reddy Kuncharam *

Department of Chemical Engineering,
Birla Institute of Technology & Science, Pilani, Pilani Campus
Rajasthan, 333031, India

*Corresponding author:

Dr. Bhanu Vardhan Reddy Kuncharam,
Associate Professor, Department of Chemical Engineering,
Birla Institute of Technology and Science, Pilani, Pilani, Rajasthan, India
Phone: +91-1596255839
Email: bhanu.vardhan@pilani.bits-pilani.ac.in

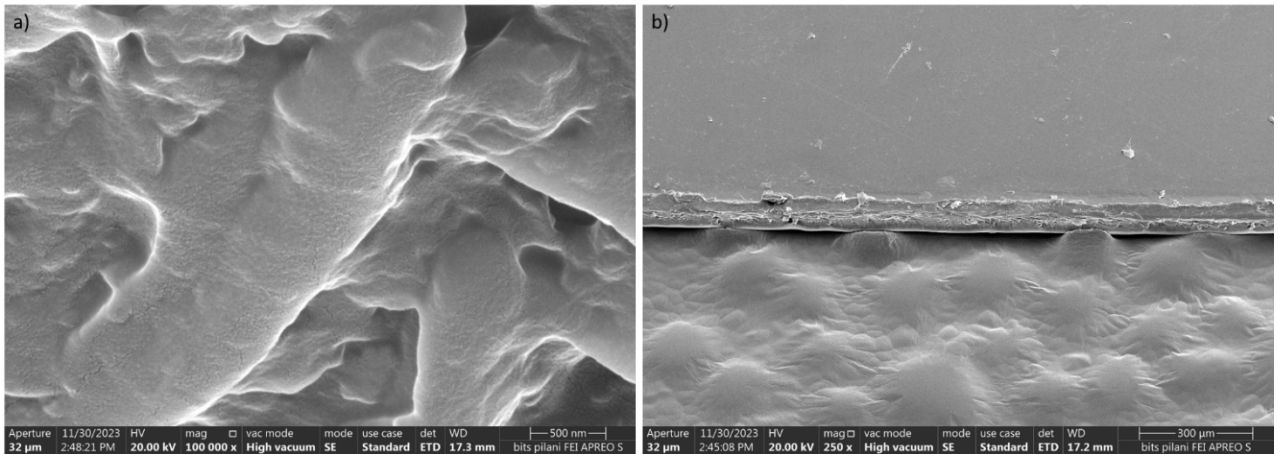


Fig S1. (a, b) Cross-section FESEM images of pure polyether sulfone (PES) membrane

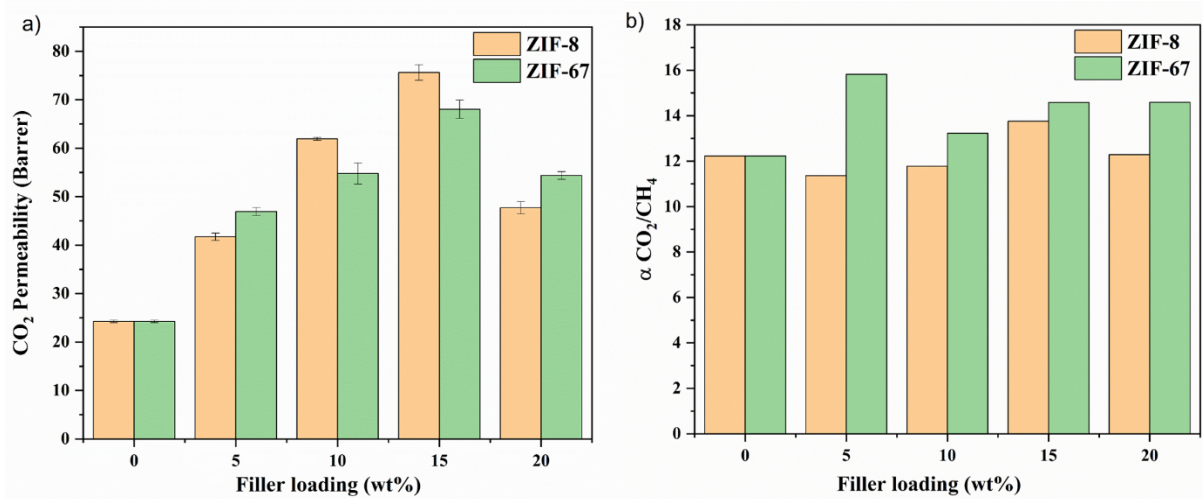


Fig. S2 Comparison plot of a) CO₂ permeability and b) CO₂/CH₄ Selectivity for ZIF-8/PES and ZIF-67/PES MMMs at 0.5 bar

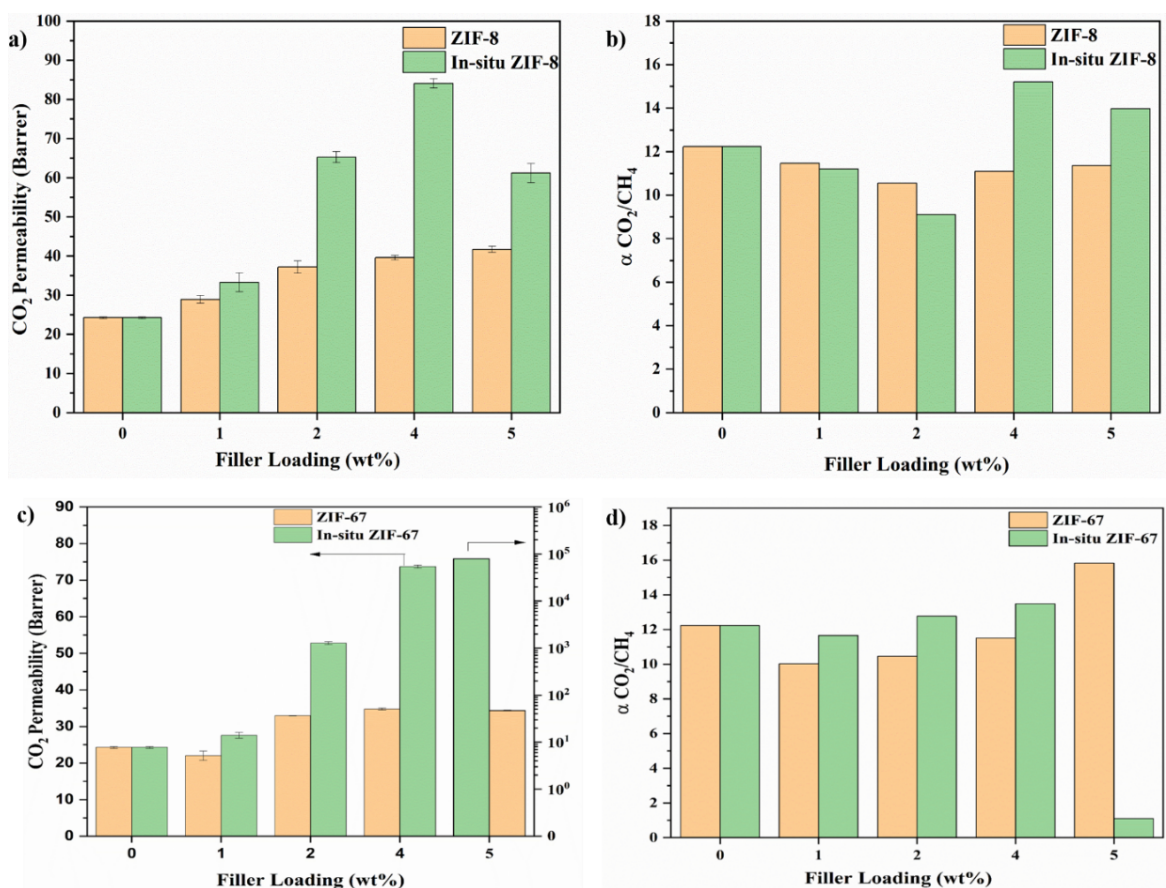


Fig. S3 Comparison plot of (a, c) CO₂ permeability and (b, d) CO₂/CH₄ Selectivity for in-situ and non-in-situ MMMs at 0.5 bar

Effect of unreacted species (metal ions and linkers)

We have used gas permeation data of in-situ membranes to study the effect of unreacted metal ions (Zn^{+2}/Co^{+2}) and imidazole linkers. In Fig.S3, we can see the CO₂ permeability of in-situ ZIF-8 membranes is increased until 4 wt.% ZIF-8 and decreased at 5 wt.% ZIF-8, this decrease is possibly associated with unreacted Zn^{+2} ions hindering the CO₂ passage through the membrane,¹ the unreacted Zn^{+2} ions in PES polymer functioned as a gas barrier without causing any significant structural defects² and also some literature studies show significant decrease in CO₂ permeability at high Zn^{+2} ions concentration.^{3,4} The presence of unreacted 2-methyl imidazole linkers should enhance CO₂/CH₄ selectivity exponentially,¹ but when we observe the in-situ MMMs selectivity it has decreased for 2 wt.% in-situ ZIF-8, 5 wt.% ZIF-8 and 5 wt.% in-situ MMMs despite the increase of CO₂ permeability in some cases. The CO₂ permeability of in-situ ZIF-67 MMMs has not dropped, this might indicate the low presence of Co^{+2} ions in PES polymer chains (possibility of higher conversion of ZIF-67). A detailed

experimental investigations need to be conducted in future studies to get the full idea of this phenomenon.

References

- 1 M. S. Maleh and A. Raisi, *Colloids Surfaces A Physicochem. Eng. Asp.*, 2023, **659**, 130747.
- 2 C. S. Lee, N. U. Kim, B. J. Park and J. H. Kim, *Sep. Purif. Technol.*, 2020, **253**, 117514.
- 3 D. Peng, S. Wang, Z. Tian, X. Wu, Y. Wu, H. Wu, Q. Xin, J. Chen, X. Cao and Z. Jiang, *J. Memb. Sci.*, 2017, **522**, 351–362.
- 4 T. Hou, L. Shu, K. Guo, X.-F. Zhang, S. Zhou, M. He and J. Yao, *Cellulose*, 2020, **27**, 3277–3286.