Contribution ID : **206** Type : **Oral Presentation**

Interpretable Models for Targeted CO_2 Membrane Design

The design of polymer membranes with high CO_2 selectivity is essential for advancing gas separation technologies and carbon capture [1]. In this work, we develop highly interpretable machine learning models to predict the permeability of polymer membranes—particularly towards CO_2 and N_2—based on the chemical structure of their repeat units. A key challenge in this field is the scarcity and incompleteness of available permeability data[2][3]. To address this, we implemented data imputation strategies that significantly reduced error, especially when including crucial experimental parameters such as measurement temperature and pressure. The models were trained on permeability data for six gases (He, H_2, O_2, N_2, CH_4, CO_2), and achieved good predictive performance for CO_2 and N_2 permeability.

As molecular descriptors, we employed MACCS keys, which yielded promising results despite their simplicity. The machine learning models are based on decision tree architectures, with the XGBoost regressor standing out due to its high accuracy and computational efficiency. We are currently evaluating the integration of more complex molecular fingerprints and plan to apply feature selection to retain only the most informative descriptors. In parallel, we are expanding our dataset by incorporating additional polymer entries to enhance the applicability domain of the models. Overall, this work supports a data-driven and interpretable approach to targeted membrane design for efficient CO_2 capture.

Acknowledgements: This project has received funding from the European Union's Horizon Europe research and innovation program under grant agreement No 101115488. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or European Innovation Council and SMEs Executive Agency (EISMEA). Neither the European Union nor the granting authority can be held responsible for them.

[1] G. Hazarika et al, Advances in Separation Sciences. Elsevier, 2025. 191-210. [2] R. Dangayach et al, Environ. Sci. Technol. 2025, 59, 2, 993−1012 [3] G. Ignacz et al, J. Membr. Sci. 2025, 713, 123256

Primary author(s) : Dr. VIGNA, Vincenzo (CNR-ITM)

Co-author(s) : Dr. FUOCO, Alessio (CNR-ITM); Dr. TOCCI, Elena (CNR-ITM)

Presenter(s) : Dr. VIGNA, Vincenzo (CNR-ITM)