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Selective Sorption of CO_2 and SO_2 in PEEK–Ionene Composite Membranes for Flue Gas Treatment

P. Stanovský[1], J. Škvára[2], K. Friess[3], J. E. Bara[4], P. Izák[3]

[1] Faculty of Science, Jan Evangelista Purkyně University in Ústí nad Labem, 400 96 Ústí nad Labem, Czech Republic
[2] Department of Physical Chemistry, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic
[3] Institute of Chemical Process Fundamentals of the Czech Academy of Sciences, Rozvojová 135, 165 00 Prague 6, Czech Republic; izak@icpf.cas.cz
[4] Department of Chemical & Biological Engineering, The University of Alabama, Tuscaloosa, AL 35487-0203, USA

This study integrates an innovative experimental sorption methodology with conventional Grand Canonical Monte Carlo (GCMC) and molecular dynamics (MD) simulations to deepen the understanding of gas sorption phenomena in materials developed for CO_2 and SO_2 removal from industrial flue gases. The advancement of efficient purification technologies for sour gas removal critically depends on the rational design of advanced materials and detailed insight into their physicochemical behavior.

Experimental measurements and molecular modeling were employed to investigate the sorption behavior of sour gases (CO_2 and SO_2), a sweet gas (CH_4), and SO_2/N_2 mixtures in advanced poly(ether ether ketone) (PEEK)–ionene composite membranes. These materials consist of PEEK backbones interconnected with imidazolium groups, featuring variations in imidazolium structure and different loadings of incorporated ionic liquids (ILs). The influence of both the imidazolium moiety and IL content on gas sorption performance was systematically evaluated.

The results demonstrate that SO_2 exhibits the highest sorption affinity, even at low concentrations (~5000 ppm) in N_2-rich mixtures. The sorption selectivity follows the order:

$SO_2 > CO_2 > CH_4 > N_2$

A PEEK–ionene variant lacking a methyl substituent on the imidazolium ring displayed enhanced CO_2/N_2 solubility selectivity compared to its methyl-substituted counterpart. However, increasing pressure reduced this selectivity difference by approximately fivefold. This behavior is attributed to restricted polymer chain mobility at elevated pressures, resulting in a dominant contribution of the free IL phase to gas transport within the composite membrane.

Molecular simulations further revealed that the polymer end-to-end distance reaches a maximum at an IL loading of two equivalents. Higher IL contents induce polymer chain contraction, accompanied by a decrease in polymer density. These findings provide valuable insight into the structure–property relationships governing gas sorption in PEEK–ionene composite membranes and support their promising application in flue gas purification.

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Reference

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