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Polymeric Membrane Materials For Gas Separation: opportunities of phase design

V.V.Teplyakov[1] and I.N.Beckman[2]

[1] *A.V.Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Leninskii pr., 29, Moscow, 117912, Russia*
[2] *Moscow State University, Chemistry Department, Russia*
FAX 7(095)230-2224; E-mail: TIPS@tips.aha.ru

INTRODUCTION

The gas permeability parameters of polymers are varied in the range of ten orders of magnitude. So, there is a great potential for design at least of two phase polymeric medium with required gas permeability and selectivity due to physical and chemical organization of heterogeneous materials.

THEORY, SIMULATION AND EXPERIMENT

The theoretical approach to the description of gas diffusion in heterogeneous medium (dispersion media, percolation-type structure) with consideration of the number of components in the medium, the medium topology (layers, inclusion, dispersion of inclusions, etc), the transport properties of the constituents, the isotherm type of diffusant for each polymeric components, the nature of interface between components is developed.
The mathematical modeling includes the analytical approaches, the numerical methods and the Monte Carlo method. The concentration profiles, permeabilities and separation of gases were calculated depending on the medium composition and structure.
The gas permeability, diffusivity and solubility of H_2, He, O_2, N_2, CO_2, CH_4, Ar, Kr, and Xe were measured for PVTMS-PDMS block copolymers in the range of 5-75 vol.% of "soft" component.

RESULTS AND DISCUSSION

It is shown that calculated permeability parameters are varied as non-linear monotone function depending on the medium composition. However, the extremal permeability can be obtained due to the interface defects creation. The extremal selectivity can be expected in the range of percolation threshold. The experimental permeability parameters obtained for PVTMS-PDMS block copolymers confirmed the above mentioned calculation. It is particularly noted that permeability is very sensitive to shape of dispersed particles.

CONCLUSION

The suggested approaches give an opportunities to select an optimal structure of heterogeneous gas separation membrane.