diffusion-fundamentals

The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Zeolite Membranes: Separations Based on Specific Molecular Interactions

J. Kuhn, J. Gross, J.C. Jansen**, P.J. Jansens**

Delft University of Technology
* Laboratory for Process Equipment
Leeghwaterstraat 44, 2628 CA, Delft
** Ceramic Membrane Centre, The Pore
Julianalaan 136, 2628 BL, Delft

INTRODUCTION

The removal of process water from an organic product stream is one of the most frequently encountered unit operations in the process industry. Membrane separation processes such as pervaporation and vapor permeation can perform such operations in a very energy efficient manner. Zeolites are microporous crystalline aluminosilicates which have uniform, molecular-sized pores. Zeolites can be used as membrane material to separate gaseous or liquid mixtures based on difference in molecular size and/or adsorption and diffusion properties.

AIMS

We aim to predict membrane performances and therewith facilitate the design of efficient membrane processes. The transport mechanism of water in a zeolite membrane will be studied using Molecular Dynamics simulations (MD) the simulation data will be used to predict the membrane performance.

THEORY

In vapour permeation and pervaporation the driving force is the chemical potential difference over the membrane. The chemical potential profile over the cross section of a membrane is often assumed to be linear. Using MD simulation we aim to determine the actual potential gradient. This information facilitates a more reliable prediction of the mass transport.

Zeolites are build-up of TO_4 tetrahedra, where T is a silicon or aluminium atom. One of the tuneable parameters in zeolite synthesis is the silicon to aluminium ratio (Si/Al). Due to the tetravalancy of the aluminium atom, the zeolite framework will no longer be charge neutral. To compensate for the net negative charge of the framework, charge-compensating cations (e.g. H^+, Na^+, Ca^{2+}) will be present in the zeolite. The Si/Al ratio is

a measure for the polarity of the zeolite, the higher this number, the less aluminium is present and the less polar the framework will be.

Highly polar zeolites have strong interaction with polar substances, such as water. However the strong interaction also inhibits the diffusive movement of permeating molecules. Thus, there is a trade-off between strong adsorption and fast diffusion. This means that in membrane synthesis, there has to be an optimum framework polarity at which the zeolite membrane shows maximum performance. The influence of zeolite polarity on transport properties will be investigated by means of MD as well as experimentally, i.e. through synthesis of zeolite membranes with varying polarity and subsequent permeation measurements.

OUTLOOK

Using MD simulation combined with macroscopic modelling and experimental work will be used to determine the chemical potential gradient over a membrane and systematically investigating the influence of framework polarity. We eventually aim to predict membrane performance and facilitate the membrane process design.