

## Separation Based on Molecular Level Using Zeolitic Membranes

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### Introduction

Much effort has been directed towards the development of advanced membrane-based separation technologies to facilitate the deployment of sustainability into industrial production processes. By supporting sustainable development through knowledge and creation of dissemination, innovation goals can be revisited and new targets can be set. Currently, an integrated approach towards sustainable process design strongly emphasises the use of membrane separation processes. Zeolite membranes in particular are very attractive alternatives by offering exceptionally high selectivities, which can be used in separation processes based on their ability for molecular sized exclusion and their adsorption and diffusion properties.

### Aims

In situ removal of small process molecules (e.g.  $H_2O$ ,  $NH_3$  and  $H_2S$ ) at high temperatures using zeolite membranes is aimed where they lead to:

- Unwanted side reactions
- Equilibrium limited conversions
- Catalyst deactivation

Amongst several processes, Fischer-Tropsch synthesis, Knoevenagel condensation and esterification reactions are the most attractive ones.

Furthermore, we aim to predict membrane performances and therewith facilitate the design of efficient membrane processes. The transport mechanisms in zeolite membranes will be investigated in close interplay between experimental and theoretical studies by means of linking molecular modelling to macroscopic transport modelling.

### Tools

Sodalite will be used primarily as the adsorptive membrane. It complies particularly well with the process conditions adopted in Fischer-Tropsch synthesis. Eventually the flow behaviour of permeating molecules through the membrane will be modelled and based on the diffusion properties and reaction conditions, an appropriate reactor (on pilot-scale), which can house the membrane, will be designed.

### Preliminary Results

An explorative study has been carried out in which water was successfully separated from a Fischer-Tropsch mixture containing octane. The separation was carried out under

Fischer-Tropsch reaction conditions ( $T$ : 250-350 °C;  $P$ : 20 bar). Flow rates were achieved in the range of  $4 \text{ kg}\cdot\text{m}^{-2}\cdot\text{h}^{-1}$  and separation factors as high as  $10^6$  were obtained using sodalite as the selective membrane. [1]

### **Outlooks**

The main focus of this research project will be put on:

- Synthesis of a thin defect free zeolite layer using novel techniques [2]
- Investigation of diffusion of water in zeolites by means of molecular dynamics simulations

Based on the experimental findings and modelling results, a catalytic membrane reactor will be designed and made applicable for operation.

### **Literature**

[1] Jansen, J.C.; Kapteijn, F.; Strous, S. Chemical reaction and separation method, European Patent (03078287.4)

[2] McLeary, E.E.; Jansen, J.C. Basic views on the preparation of porous ceramic membrane layers, Topics in Catalysis 29 (2004)