# Numerical Simulations of Methane Aromatization with and Without a Ceramic Hydrogen Separation Membrane

Zuoan Li[1], Christian Kjølseth[2], Reidar Haugsrud[1], S. Hernandez Morejudo[3]

[1]University of Oslo, Department of Chemistry, FERMiO, Oslo, Norway
[2]Protia, Oslo, Norway
[3]University of Oslo, Department of Chemistry, InGAP, Oslo, Norway

## Abstract

Nowadays, oxygen-free methane aromatization has been receiving growing attention from the industry due to a potential means for producing high valuable products such as aromatics and hydrogen via the reaction 6CH4=9H2+C6H6 [1]. Many investigations with respect to this process have been focused on catalysts' characterizations and elementary thermodynamic steps of the reaction. However, little attention has been paid to fluid dynamics including velocity and temperature fields, which are important for an industrial application. In the present investigation, 2D 'Transport of Concentrated Species' and 'Free and Porous Flow' interfaces in COMSOL were applied to a fixed bed reactor, which contains two free flow regions and one porous catalyst bed where the methane aromatization takes place (see Figure 1). The effect of various parameters such as temperature, pressure, and flow on the reaction has been simulated, indicating that high pressure and fast flow lead to lower conversion of methane while increasing temperature results in higher one. To increase the yield of benzene, a ceramic membrane based on Ln6-xWO12-d (Ln = rare earths) [2] has been applied to remove hydrogen. Figure 2 compares the concentration distribution along the center of the reactor with and without a hydrogen separation membrane. A significant increase in the production of benzene has been observed through the removal of hydrogen. The effect of hydrogen permeability of the membrane on the yield of benzene has also been explored. The 'Heat Transfer' interface will be utilized to study temperature effect and energy utilization. Meanwhile, 'coking' effect will be studied in combination with the effect of hydrogen removal. Finally a thorough image of this process including temperature, flow, yield of benzene, and 'coking' effect will be demonstrated, and a series of optimal parameters may be presented depending on the purpose of applications.

## Reference

[1] Z.R. Ismagilov, E.V. Matus, and L.T. Tsikoza, Energy Environ. Sci. 1 (2008) 526.
[2] R. Haugsrud, and C. Kjoelseth, J. Phys. Chem. Solids 69 (2008) 1758.

## Figures used in the abstract

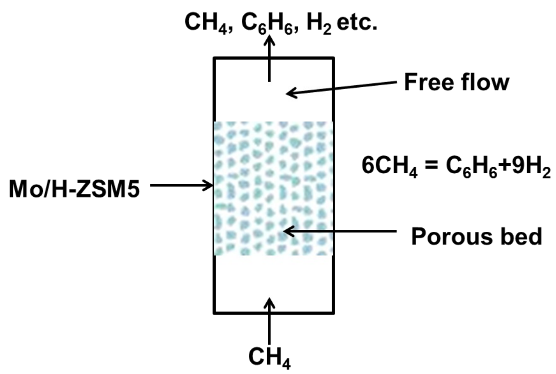


**Figure 1**: Schematic illustration of a catalytic reactor for the methane aromatization.

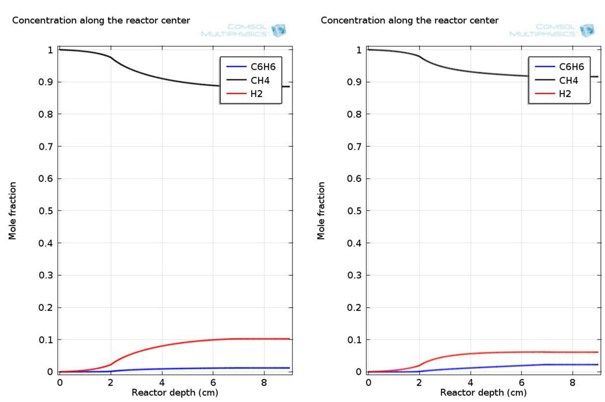


**Figure 2**: Comparison of the concentration distribution between a reactor without (left) and with (right) a hydrogen separation membrane.