Fractal-like microreactor for hydrogen production

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Introduction

The purpose of this project was to explore the use of a novel design for a microreactor. The reaction modeled was one for conversion of methanol into hydrogen via steam. This is known as steam reformation. Ideally, the produced hydrogen would be fed into a fuel cell for energy production.

The channels were arranged in a branched pattern. The geometry of the branching network was produced via allometric scaling laws; the same that dictate how veins and arteries bifurcate.

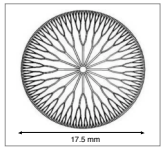


Figure 1. The branched channel microreactor

This efficacy of this design was benchmarked against another micro-reactor that had a simple array of straight channels. The yields, on a per channel basis, were compared.

The channels were modeled as being coated with catalyst. The catalyst used was a mix of Copper-Alumina, or Cu/Al_2O_3. This catalyst was chosen for its well documented kinetics. The assumption was made that the thickness of the catalyst coating was accounted for in the channel heights and widths.

Model and kinetics

For the methanol steam reformation reaction there were four reactions to be considered, they are as follows.

$CH_3OH + H_2O \Leftrightarrow CO_2 + 3H_2$	*Steam Reformation*
$CH_3OH \Leftrightarrow CO + 2H_2$	*Methanol Decomposition*
$CO + H_2O \Leftrightarrow CO_2 + H_2$	*Water Gas Shift*
$2CH_3OH \Leftrightarrow CH_3OCH_3 + H_2O$	*Dimethyl Ether Formation*

Dynamic mole balances were preformed on the system to give the following design equations

$$\frac{dF_i}{dz} = 2^{(m+1)} \gamma_i \cdot P \cdot \rho_{cat}$$

F_i is the molar flow rate of species i
γ_i is the rate of reaction for species i
P is the parameter of the channel in
r_{cat} is the density of the catalyst per unit suface area
m is the branching level

The Hagan-Pousielle relation was used to determine the following pressure drop along the length of the reactor

$$\frac{dP}{dz} = -\frac{1}{2} \cdot c_f \cdot \frac{4\rho \overline{v}^2}{d_h}$$

ρ is the density of fluid
$\overline{v}^2$ is the bulk fluid velocity
d_h is the hydraulic diameter
c_f is the coefficient of skin friction

These relations were then modeled in MATLAB judge the reactor's performance

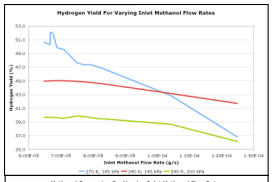
Results

The reactor's performance was modeled at varying operating conditions to optimize hydrogen yield. Methanol conversion, hydrogen production, and carbon monoxide were all studied to gauge how the operating conditions affected the competing reactions.

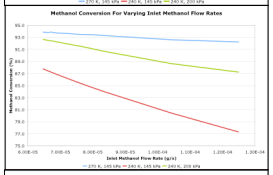
This was then compared to the straight channeled reactor to highlight differences between the two designs.

Hydrogen yields of branched channel design

(a)



(b)



(c)

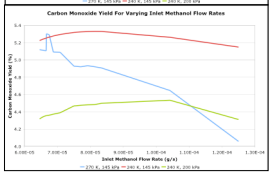


Figure 2 Reactor performance with varying operating conditions

Methanol conversion in *Figure 2a* shows linear decline with increasing flowrates. This result is to be expected; as the flowrates are increased the amount of time the reactants spend in the reactor decreases. *Figure 2a* also indicates that higher methanol conversion is accomplished at higher temperatures and pressures.

While methanol conversion is increased when the temperature and pressure is increased, *Figure 2b* shows that the increased pressure actually decreases hydrogen yield. This can also be see in *Figure 2c* for carbon monoxide. This can be attributed to the formation of dimethyl ether; at these conditions this reaction is faster than the others, and therefore less hydrogen is produced.

Comparison of straight and branched channels

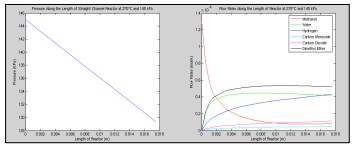


Figure 3 Pressure drop along the straight channels

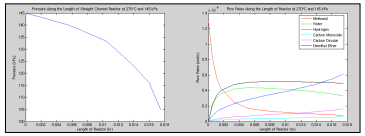


Figure 4 Pressure drop along the branched channels

Figures 3 and *4* show an observable difference in pressure drop. An accelerating pressure drop can be seen in *Figure 4*, which coincides with the bifurcation of the channels. It is also clear that the increased pressure drop increases the hydrogen yield.

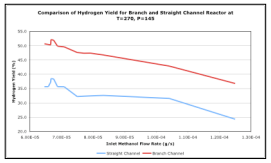


Fig. 5 Hydrogen yield comparison

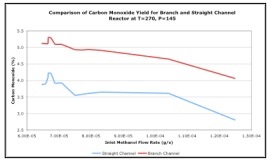


Fig. 6 Carbon monoxide yield comparison

With the increased pressure drop in the branched channel the production of both species is higher. The increased pressure drop suppresses the dimethyl ether formation (black line) within the branched channel design, as this prefers higher pressures. Hydrogen and carbon monoxide follow a similar pattern.

Conclusions

One can see from *Figures 5* and *6* that yield of hydrogen for the branched channel configuration was higher than for the straight channel configuration. It also visible in *Figures 3*, and *4* that the pressure drop is higher across the branched channel design.

It is hypothesized that the increased pressure drop in the reactor contributes to the higher conversion for two reasons. The first being that from the analysis of *Figures 2b* and *2c*, the decrease in pressure helps to suppress the dimethyl ether formation reaction, as this does not contribute to hydrogen production.

The second reason being that the increased pressure drop helps to forward the reactions' equilibrium to favour the products. The decrease of pressure reduces the partial pressures of all species in the reaction mixture which keeps the equilibrium constant, K_{eq}, high.

This is significant as this implies that other reactions which have similar kinetics, (i.e. multiple reactions of which desirable reactions favor lower pressures), or reactions that require lower pressures near the end of the reactor, will attain higher yields.

Future work will entail removing the isothermality from the model, as well as a more detailed analysis of hydro and thermodynamics of the system. Additionally, optimizing the network of branches so as to favour a specific product for a given reaction will be explored.

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For further information

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