Modeling Reactor for the Synthesis of Dimethyl Ether

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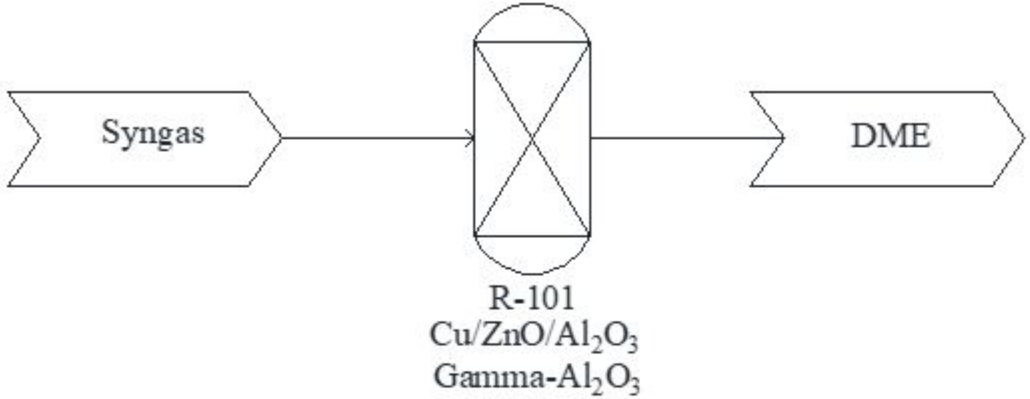
Introduction

Applications

- ❖ Diesel engine fuel.
- ❖ Petroleum liquid gas (PLG) complement (substitute).
- ❖ Cosmetic industry.
- ❖ Chemical industry (Synthesis of acetic acid).



Introduction

Methanol Production

Catalyst:
$Cu/Zn/Al_2O_3$

$$CO + 2H_2 \leftrightarrow CH_3OH \quad (1)$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O \quad (2)$$

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \quad (3)$$

Methanol Dehydration

Catalyst:
γ-Al_2O_3

$$2CH_3OH \leftrightarrow CH_3OCH_3 + H_2O \quad (4)$$

Model

Assumptions

- ❖ Ideal gas equation describes gas behavior.
- ❖ Pressure drop is negligible.
- ❖ Reactor is isothermal due to the presence of a cooling jacket.
- ❖ Gas phase reaction

Mass Balance

$$\frac{dF_i}{dW} = r_i'$$

$$r'_{DME} = \frac{R_4}{2}$$

$$r'_{MetOH} = R_1 + R_3 - R_4$$

$$r'_{H_2O} = R_2 + R_3 + \frac{R_4}{2}$$

$$r'_{H_2} = -2R_1 - R_2 - 3R_3$$

$$r'_{CO_2} = -R_2 - R_3$$

$$r'_{CO} = -R_1 + R_2$$

Reaction Kinetics

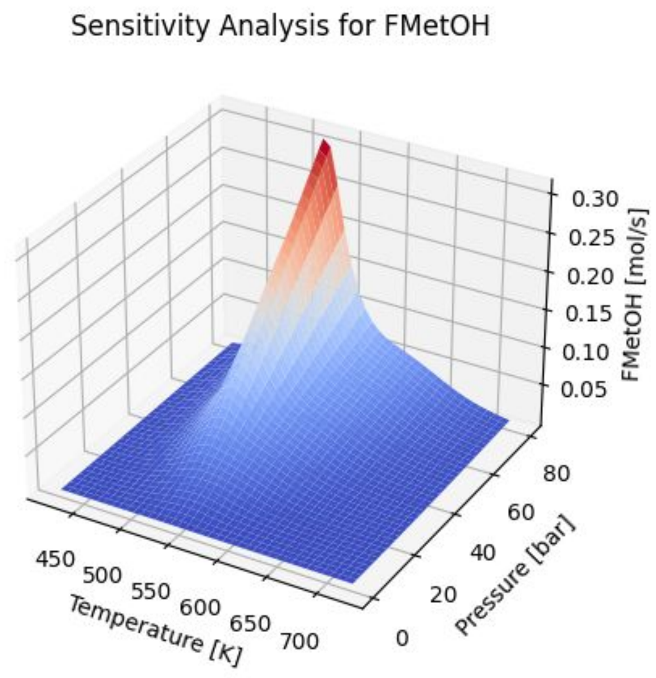
$$R_1 = k_1 \frac{K_{CO}\left(f_{CO} f_{H_2}^{3/2} - f_{CH_3OH} / \left(f_{H_2}^{1/2} K_{eq,1}\right)\right)}{\left(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}\right)\left(f_{H_2}^{1/2} + K_{H_2O/H_2} f_{H_2O}\right)}$$

$$R_2 = k_2 \frac{K_{CO_2}\left(f_{CO_2} f_{H_2} - f_{H_2O} f_{CO} / K_{eq,2}\right)}{\left(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}\right)\left(f_{H_2}^{1/2} + K_{H_2O/H_2} f_{H_2O}\right)}$$

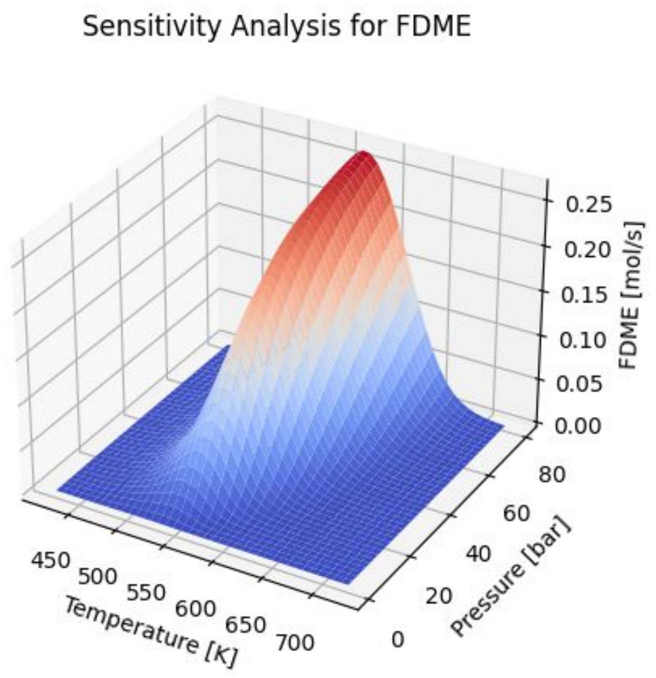
$$R_3 = k_3 \frac{K_{CO_2}\left(f_{CO_2} f_{H_2}^{3/2} - f_{CH_3OH} f_{H_2O} / \left(f_{H_2}^{3/2} K_{eq,3}\right)\right)}{\left(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}\right)\left(f_{H_2}^{1/2} + K_{H_2O/H_2} f_{H_2O}\right)}$$

$$R_4 = k_4 \frac{K_{CH_3OH}^2 C_{CH_3OH}^2 \left(1 - C_{H_2O} C_{CH_3OCH_3} / \left(C_{CH_3OH}^2 K_{eq,4}\right)\right)}{\left(1 + 2\sqrt{K_{CH_3OH} C_{CH_3OH}} + K_{H_2O} C_{H_2O}\right)^4}$$

Analysis



Sensitivity Analysis for FMetOH
0.30
0.25
0.20
0.15
0.10
0.05
FMetOH [mol/s]
450
500
550
600
650
700
Temperature [K]
0
20
40
60
80
Pressure [bar]



Sensitivity Analysis for FDME
0.25
0.20
0.15
0.10
0.05
0.00
FDME [mol/s]
450
500
550
600
650
700
Temperature [K]
0
20
40
60
80
Pressure [bar]

Optimization

- Maximize Dimethyl Ether Final concentration *10000
- Dcost = 3
- Increase iterations for gekko to converge
- Upper and lower bounds were very important for convergence

Concentrations

```
FDME0=   0 #[mol/s]
FMetOH0= 0 #[mol/s]
FH2O0=   0 #[mol/s]
FH20=    3 #[mol/s]
FCO20=   1 #[mol/s]
FCO0=    1 #[mol/s]
```

l_1−norm Objective

The l_1-norm objective is like an absolute value objective but also includes a dead-band to reject measurement error and stabilize the parameter estimates.

$$\min_{x,y,p} \Phi = w_x^T (e_U + e_L) + w_m^T (c_U + c_L) + w_{\Delta p}^T (\Delta p_U + \Delta p_L)$$

$$\text{subject to}$$

$$0 = f\left(\frac{dx}{dt}, x, y, p\right)$$

$$0 \leq g\left(\frac{dx}{dt}, x, y, p\right)$$

$$e_U \geq y - y_x - \frac{db}{2}$$

$$e_L \geq y_x - y - \frac{db}{2}$$

$$c_U \geq y - \hat{y}$$

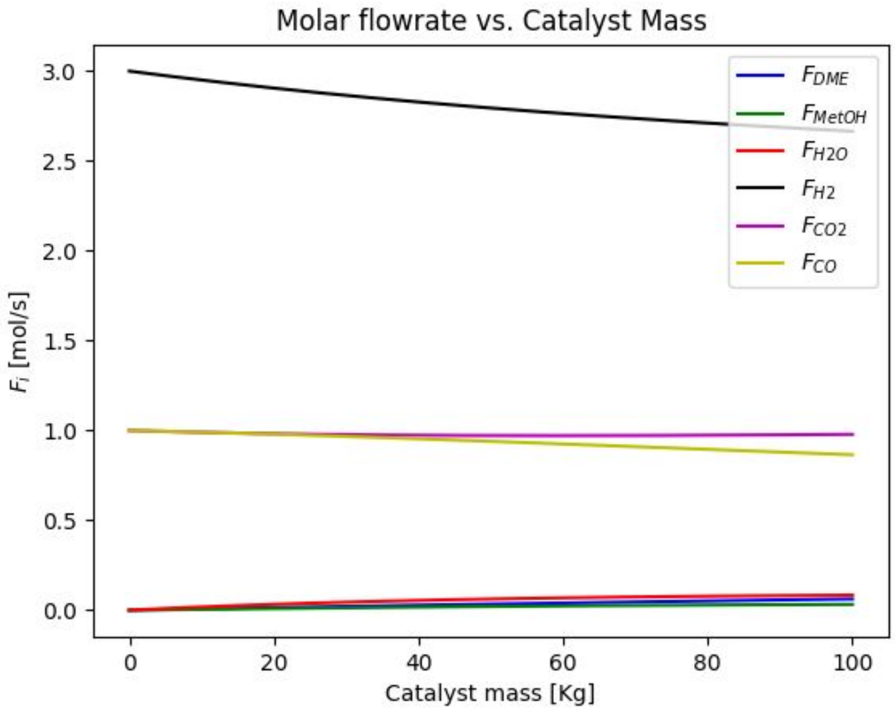
$$c_L \geq \hat{y} - y$$

$$\Delta p_U \geq p_i - p_{i-1}$$

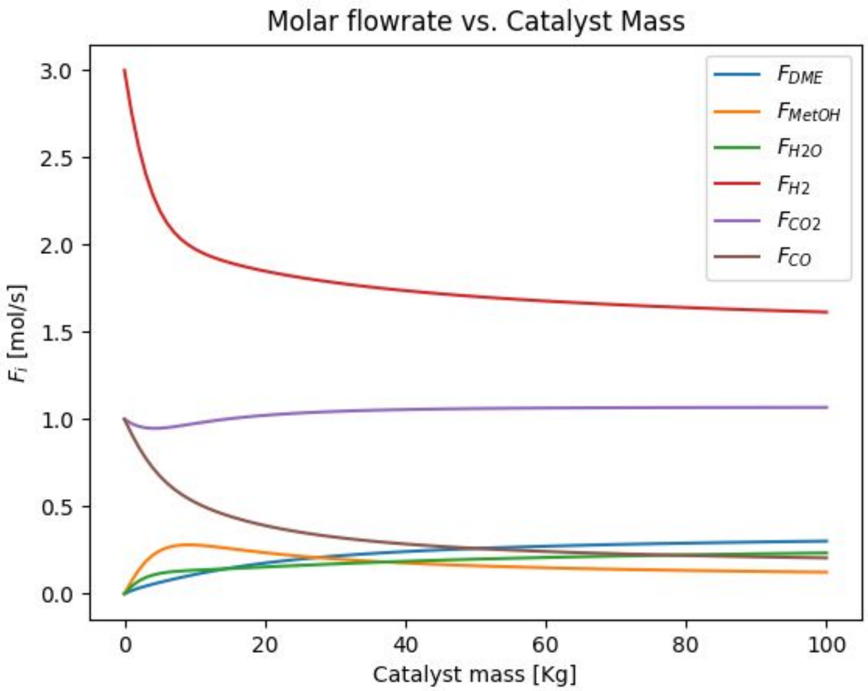
$$\Delta p_L \geq p_{i-1} - p_i$$

$$e_U, e_L, c_U, c_L, \Delta p_U, \Delta p_L \geq 0$$

Results



Molar flowrate vs. Catalyst Mass
F_{DME}
F_{MetOH}
F_{H2O}
F_{H2}
F_{CO2}
F_{CO}
F_i [mol/s]
Catalyst mass [Kg]



Molar flowrate vs. Catalyst Mass
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F_{MetOH}
F_{H2O}
F_{H2}
F_{CO2}
F_{CO}
F_i [mol/s]
Catalyst mass [Kg]

Conclusion

- This worked as a proof on concept for the modeling of the dimethyl ether reactor and it serves as a good starting point to improve on

- For this project we only optimized with respect to one desired output, but we would like to be able to formulate a dynamic optimization of one or the other desired products

- Additionally, it would be good to have quantifiable benefits (profit, use of materials, eco-friendly, etc.) of this reaction as part of our analysis to motivate the benefits of this process

Thank you for your time

Questions?