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APPENDIX

Assumptions, definitions, and calculations.

To facilitate the calculations in this work, some assumptions were made as follows:

1. All the gaseous behaviors obey the ideal gas law.
2. Pressure drop across the system is very small and can be negligible.
3. The pressure in the system equals to the atmospheric pressure.

1. Catalyst Preparation

1.1 Amount of Ni loading

Prepared 0.2 g of 8wt%Ni/KH Zeolite

- To prepare 0.2 g of catalyst with 8wt%Ni (MW=58.69 g/mole) need to have

  0.2* 8/100 = 0.016 g of Ni

- Amount of $Ni(NO_3)_2{\bullet}6H_2O$ (MW=290.81 g/mole)

  0.016*290.81/58.69 = 0.07928 g

- Amount of KH Zeolite

  0.2-0.016= 0.184 g

2. Conversion and Selectivity

2.1 Methane Conversion

$$CH_4 \text{ conversion} = \frac{CH_{4,in} - CH_{4,out}}{CH_{4,in}} \times 100$$

Where $CH_{4,in}$ = CH_4 fed to the reactor

$CH_{4,out}$ = CH_4 left the reactor

2.2 Carbon Dioxide Conversion

$$CO_2 \text{ conversion} = \frac{CO_{2,in} - CO_{2,out}}{CO_{2,in}} \times 100$$

Where $CO_{2,in}$ = CO_2 fed to the reactor

$CO_{2,out}$ = CO_2 left the reactor

2.3 Hydrogen Selectivity

Calculation H_2 selectivity vs CO selectivity:

$$CH_4 + CO_2 \longrightarrow 2H_2 + 2\,CO$$

$$H_2\text{ selectivity} = \frac{\frac{1}{2} * F_{,out} * y_{(H_2,out)}}{F_{,in} * y_{(CH_4,in)} - F_{,out} * y_{(CH_4,out)}} * 100$$

$$CO\text{ selectivity} = \frac{\frac{1}{2} * F_{,out} * y_{(CO,out)}}{F_{,in} * y_{(CH_4,in)} - F_{,out} * y_{(CH_4,out)}} * 100$$

$$\text{Therefore, selectivity of } H_2 \text{ vs CO} = \frac{H_2 selectivity}{CO selectivity + H_2 selectivity} * 100$$

$$= \frac{\frac{1}{2} * y_{(H_2,out)}}{(\frac{1}{2} * y_{(H_2,out)}) + (\frac{1}{2} * y_{(CO,out)})} * 100$$

$$= \frac{y_{(H_2,out)}}{y_{(H_2,out)} + y_{(CO,out)}} * 100$$

Where $F_{,in}$ = Total flow rate of feed stream that fed to the reactor

$F_{,out}$ = Total flow rate that left the reactor

$y_{(H_2,out)}$ = Mole fraction of H_2 in the effluent stream

$y_{(CO,out)}$ = Mole fraction of CO in the effluent stream

$y_{(CH_4,in)}$ = Mole fraction of CH_4 in the feed stream

$y_{(CH_4,out)}$ = Mole fraction of CH_4 in the effluent stream

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