catalysts

Supplementary material: The effect of potassium on cobalt-based Fischer-Tropsch catalysts with different cobalt particle sizes

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Calculation procedures

1.1. Site time yield

The site-time yield (STY) was calculated as follows:

First, equation (1) was used to calculate the CO conversion:

$$X_{CO} = \frac{F_{in} - F_{out}}{F_{in}} = 1 - \frac{(\frac{A_{CO}}{A_{N2}})_x}{(\frac{A_{CO}}{A_{N2}})_{feed}} \quad (1)$$

Where X_{CO} (%) is the CO conversion, F_{in}, F_{out} are inlet and outlet flow of the CO, respectively; A_{CO}, A_{N2} are GC areas of CO and N_2, respectively; $(\frac{A_{CO}}{A_{N2}})_x$ is the ratio of the GC areas at the hour x, while $(\frac{A_{CO}}{A_{N2}})_{feed}$ is the ratio of the GC areas of the feed.

Then, the equation (2) is used to calculate the reaction rate:

$$r = \frac{F_{tot} * Y_{CO} * X_{Co}}{W} \quad (2)$$

Where $r\ (\frac{ml}{g_{cat}*s})$ is the reaction rate; F_{tot} is the total syngas flow; Y_{CO} is the procentage of the CO in the gas; X_{Co} is the conversion of the CO; W is the catalyst mass. The STY is then calculated using equation (3):

$$STY = \frac{r * M_{CO}}{V_m * 3600 * \frac{x_m}{100} * \frac{D}{100}} \quad (3)$$

Where STY $(\frac{mol_{CO}}{mol_{cat}*s})$ is the site time yield; $r\ (\frac{ml}{g_{cat}*s})$ is the reaction rate; $M_{CO}\ (\frac{g_{CO}}{mol_{CO}})$ is the molecular mass of CO; $V_m(\frac{ml}{mol})$ is the volumetric flow per mole of syngas; $x_m(\frac{g_{CO}}{g_{cat}})$ is the metal loading; D (%) is catalyst dispersion.

1.2. Selectivities.

In order to calculate the methane selectivity(S_{CH_4}), a methane flow needs to be found (4):

$$F_{CH_4} = \frac{F_{N2} * RRF_{CH_4} * A_{CH_4}}{A_{N2}} \quad (4)$$

Where $F_{CH_4}(\frac{ml}{min})$ is the methane flow; $F_{N2}(\frac{ml}{min})$ is the nitrogen flow; $RRF_{CH_4}$is relative response factor of methane obtained from the calibration data; $A_{CH_4}$and A_{N2} are GC areas for methane and nitrogen, respectively. Then, the methane selectivity is calculated using equation (5):

$$S_{CH_4} = \frac{F_{CH_4}}{F_{CO} * X_{CO}} \quad (5)$$

Where S_{CH_4}(%) is the methane selectivity; $F_{CH_4}(\frac{ml}{min})$ is the methane flow; $F_{CO}(\frac{ml}{min})$ is the CO flow; X_{CO}(%) is the CO conversion.

The same procedure is used to calculate CO_2 selectivity (S_{CO_2}) using equation (6):

$$F_{CO_2} = \frac{F_{N2} * RRF_{CO_2} * A_{CO_2}}{A_{N2}} \tag{6}$$

Where $F_{CO_2}(\frac{ml}{min})$ is the CO_2 flow; $F_{N2}(\frac{ml}{min})$ is the nitrogen flow; $RRF_{CO_2}$is relative response of CO_2 factor obtained from the calibration data; $A_{CO_2}$and A_{N2} are GC areas for CO_2 and nitrogen, respectively. Then, the CO_2 selectivity is calculated using equation (7):

$$S_{CO_2} = \frac{F_{CO_2}}{F_{CO} * X_{CO}} \tag{7}$$

Where $S_{CO_2}(\%)$ is CO_2 selectivity; $F_{CO_2}(\frac{ml}{min})$ is the CO_2 flow; $F_{CO}(\frac{ml}{min})$ is CO flow; $X_{CO}(\%)$ is CO conversion.

Finally, the C_{5+} selectivity is calculated using equation (8):

$$S_{C_{5+}} = 1 - \left(S_{CH_4} + S_{C_2} + S_{C_3} + S_{C_4} + S_{CO_2}\right) \tag{8}$$

Where S_{C_2}, S_{C_3}, S_{C_4} are selectivities to C_2, C_3, C_4, respectively calculated using the same procedure described above.