Fischer-Tropsch Database Calculations

Conversions: CO, H_2, and Syngas

$$f = \frac{n_{in} - n_{out}}{n_{in}} \cdot 100$$

n: (mols per hour)
f: Conversion (%)

Efficiency:

$$e = \frac{n_{CO\_in} - \left(n_{CO\_out} + n_{CO_2\_out}\right)}{n_{CO\_in} - n_{CO\_out}} \cdot 100$$

n: (mols per hour)
e: Efficiency (%)

Weight Hourly Space Velocity:

$$S_v = \frac{Q_{in} \cdot 100}{M}$$

S_v: Weight hourly space velocity WHSV (slph per g metal)
Q_{in}: Feed gas flow rate (slph)
M: Catalysts active metal (g)

Contraction:

$$C = \frac{Q_{in} - Q_{out}}{Q_{in}} \cdot 100$$

Q_{in}: Gas feed flow rate (slph)
Q_{out}: Gas out flow rate (slph)
C: Gas contraction (%)

Syngas ratio (H_2:CO):

$$s_r = \frac{n_{H_2\_in}}{n_{CO\_in}}$$

n: (mols per hour)
s_r: Syngas ratio

Rates (CO, H_2):

$$r = \frac{n_{in} \cdot f}{M}$$

n: (mols per hour)
M: Catalysts active metal (g)
f: Fractional conversion
r: Rate (mols / hr / g metal)

Rate CO_2:

$$r = \frac{n}{M}$$

n: CO_2 produced (mols per hour)
M: Catalysts active metal (g)
r: Rate (mols / hr / g metal)

Rate H_2O:

$$r = \frac{n_{gas} + n_{liquid}}{M}$$

n_{gas}: H_2O in gas phase (mols per hour)
n_{liquid}: H_2O in liquid phase, assumes water phase is pure water (mols per hour)
M: Catalysts active metal (g)
r: Rate (mols / hr / g metal)

Rate Syngas:

$$r_{syngas} = r_{H_2} + r_{CO}$$

r_{syngas}: Syngas rate (mols / hr / g metal)
r_{CO}: CO rate (mols / hr / g metal)
r_{H2}: H_2 rate (mols / hr / g metal)

Rate FT:

$$r_{FT} = r_{CO} - r_{CO_2}$$

r_{FT}: FT rate (mols / hr / g metal)
r_{CO}: CO rate (mols / hr / g metal)
r_{CO2}: CO_2 rate (mols / hr / g metal)

Rate Hydrocarbon:

$$r_{Hydrocarbon} = r_{FT} \cdot 14.329$$

$r_{Hydrocarbon}$: Hydrocarbon rate (mols / hr / g metal)
r_{FT}: FT rate (mols / hr / g metal)

H_2/CO Usage:

$$u = \frac{r_{H_2}}{r_{CO}}$$

r_{H2}: H_2 rate (mols / hr / g metal)
r_{CO}: CO rate (mols / hr / g metal)
u: H_2/CO usage

Selectivity CH_4:

$$s_{CH_4} = \frac{r_{CH_4}}{r_{FT}} \cdot 100$$

r_{CH4}: CH_4 rate (mols / hr / g metal)
r_{FT}: FT rate (mols / hr / g metal)
S_{CH4}: CH_4 selectivity

Selectivity CO_2:

$$S_{CO_2} = \frac{n_{CO_2\_out}}{n_{CO\_in} - n_{CO\_out}} \cdot 100$$

n: (mols / hr)
S_{CO2}: CO_2 selectivity