Fischer-Tropsch

There are several Fischer-Tropsch reactors in operation: multi-tubular fixed bed (trickle flow), fluidized bed / risers and slurry columns. For this workshop we will consider the low temperature (< 260 °C) slurry reactor. We will approach the problem in the simplest way possible while still capturing the essentials.

For simplicity we will only consider the main reaction:

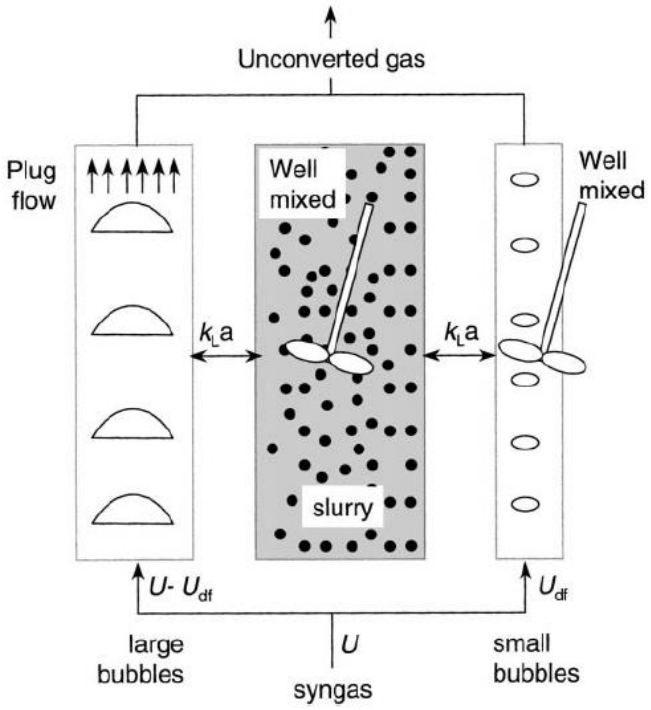
Reaction 1: $CO + 2H_2 \rightarrow CH_2 + H_2O$ $\qquad \Delta H_r = -76 \times 10^3 \ \frac{J}{mol\ H_2}$

The reaction rate is given by:

$$-R_{CO} = K_r C_{CO}^l = 1.5 \times 10^{-4} C_{CO}^l \qquad \frac{mol\ CO}{kg_{cat} s}$$

C_{CO}^l is the CO concentration in the liquid phase. K_r is determined at 515 K.

For the modelling we use the model proposed by Krishna, which includes the liquid phase, small bubbles and large bubbles. The large bubbles move in plug flow, while the liquid and the small bubbles are close to a CSTR. The latter we will model using the axial dispersion model.



The dense phase consists of the liquid phase plus the catalyst plus the small bubbles.

The following correlations can be used:

Rise (linear) velocity of the small bubbles:

$$V_{SB} = 0.095 \times (1 + \frac{0.8\epsilon_p}{0.095})$$

In which ϵ_p is the hold-up of catalyst in the dense phase in m^3 catalyst / m^3 dense phase. The dense phase is the liquid plus catalyst plus the small bubbles.

The hold-up of small bubbles is given by (m^3 small bubble / m^3 volume dense phase):

$$\epsilon_{SB} = 0.6072 \times (1 - \frac{0.7\varepsilon_p}{0.27})$$

We can now calculate the superficial velocity of the small bubbles (U_{SB}):

$$U_{SB} = V_{SB}\varepsilon_{SB}$$

By means of the over balance we now also know the superficial velocity of the large bubbles (U_{LB}):

$$U_{LB} = U_g - U_{SB}$$

In this equation U_g is the overall superficial velocity (m^3 gas / s divided by the total flow area of the column). We will use U_g as a design variable which we can vary.

The hold-up of large bubbles is given by (m^3 large bubble / m^3 total volume (small bubbles + large bubble + liquid+catalyst)) :

$$\epsilon_{LB} = 0.7 \times U_{LB}^{0.58}$$

In which U_{LB} is the superficial velocity of the large bubbles.

The total gas hold-up is now given by:

$$\varepsilon_g = \varepsilon_{LB} + \varepsilon_{SB}(1 - \varepsilon_{LB})$$

For $k_l a$ the following relations hold:

$$kla_{LB} = 2.25\epsilon_{LB}, \;\; kla_{SB} = 4.5\epsilon_{SB}$$

The equations that we need to solve are:

Mol balance CO (C_{LB}) in large bubbles:

$$-U_{LB}\frac{dC_{LB}}{dx} - kla_{LB}\left(\frac{C_{LB}}{m_{co}} - C_L\right) = 0$$

C_L is the CO concentration in the liquid

Mol balance CO (CS_B) in small bubbles:

$$-U_{SB}\frac{dC_{SB}}{dx} + D_{SB}\frac{d^2C_{SB}}{dx^2} - kla_{SB}\left(\frac{C_{SB}}{m_{co}} - C_L\right) = 0$$

Mol balance CO (C_L) in the liquid

$$-U_L\frac{dC_L}{dx} + D_L\frac{d^2C_L}{dx^2} + kla_{SB}\left(\frac{C_{SB}}{m_{co}} - C_L\right) + kla_{LB}\left(\frac{C_{LB}}{m_{co}} - C_L\right) - (1-\varepsilon_{LB})\varepsilon_p\rho_c K_r C_L = 0$$

Of course we will solve this with BVP4C in matlab.

The boundary conditions are:
At the inlet (x = 0):

$$C_{LB} = C_{in}, \qquad D_{SB}\frac{dC_{SB}}{dx} - U_{SB}(C_{CB} - C_{in}) = 0, \qquad D_L\frac{dC_L}{dx} - U_L\left(C_L - \frac{C_{in}}{m_{co}}\right) = 0$$

C_{in} is the inlet concentration of CO in the gas phase.

At X =L → the gradients of C_{SB} and C_L are zero

Assignment:

Design a slurry reactor system for the production of 6000 ton / day CH_2. T = 515 K, P = 30 bar.
You may use a constant gas velocity and work with an isothermal model. Do calculate how many vertically placed cooling tubes of 2 inch are required (cooling medium = 500K). Investigate numerically the effects of mixing in the liquid phase.
For the modelling you may get inspired by the bubble column model of last week.

Restrictions:
Maximal reactor diameter = 8 m
Maximal reactor height = 30 m
Maximal catalyst hold-up, ϵ_p = 0.3
Maximal superficial gas velocity = 0.4 m/s

Other parameters:
You can use a superficial liquid velocity of 0.01 m/s
Catalyst density = 2000 kg/m^3 catalyst
No restriction to mass transfer in the gas phase
The equilibrium distribution for CO is 2.5 (C^g/C^l) [mind the definition]
Information on dispersion coefficients: see slides on bubble & slurry reactors
I varied the D_L between 0.01 and 1000 m^2/s. According to the (co)relations it lies between 1 and 10.
For the heat transfer coefficient I have taken 750 W/m^2/K

Information on heat transfer coefficients: see slides on bubble & slurry reactors

Simulations:

Let's do some first calculations. I took the max diameter of 8 meters, the max gas velocity and a catalyst hold-up of 0.25. I varied the height of the reactor. D_L = 1 m^2/s, D_{SB} = 10 m^2/s

Height	**CO conversion**	**Productivity mol CO / m^3 /s**	**Productivity ton CH_2 / day**	**# of cooling tubes (% of flow area)**
10	0.32	3	1827	8118 (46)
15	0.42	2.67	2413	7151 (40)
20	0.50	2.37	2874	6398 (36)
25	0.57	2.15	3262	5800 (32)
30	0.62	1.96	3584	5310 (30)

Area / volume of cooling tubes needs to be taken into account in model (not done yet).

We need, for sure, two of these large reactors.

Look at the amount of cooling capacity: for the reactor of 30 meters in height this 450 MW!

Effect of the liquid dispersion coefficient: same parameters as above, height = 30 meters.

Liquid dispersion m^2/s	CO conversion	Productivity mol CO / m^3 /s	Productivity ton CH_2 / day	# of cooling tubes (% of flow area)
0.01	0.63	1.98	3600	
0.1	0.63	1.97	3600	
1	0.63	1.97	3590	
10	0.62	1.93	3522	
100	0.59	1.85	3370	
1000	0.58	1.81	3309	

Small effect of liquid dispersion!

Effect of gas velocity