INDUSTRIAL ORGANIC CHEMISTRY – EXERCISE 2

Methanol synthesis: design of the multi-stage adiabatic reactor

Methanol synthesis is carried out in multi-stage adiabatic reactors with intermediate cooling in order to maintain a high reaction rate.

The main reaction involved in the methanol synthesis is:

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

Since CO_2 is fed to the reactor, the following reaction takes also place:

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

By assuming that the intermediate cooling is carried out by means of external heat exchangers, the temperature of the reacting mixture leaving the exchanger is equal to 240 °C. The maximum temperature in the catalytic bed has to be lower than 270 °C to avoid catalyst deactivation. The pressure drops along the reactors are negligible.

Based on the reported data:

a) write the mass and heat balance equations for the generic adiabatic bed adopting a pseudo-homogeneous model;
b) evaluate the volume of the reactor and the number of beds required to obtain a molar fraction of methanol in the outlet stream equal to 0.061

Input data:

1. <u>Physycal-chemical properties</u>

$$\rho_{\text{catalyst}} = 1.98\text{g}/(\text{cm}\text{\^{}}3\ )$$
$$\varepsilon = 0.4\ (\text{void fraction of the catalyst bed})$$
$$\langle \text{Cp}_{\text{mix}} \rangle = 4.081\text{kJ/kg}$$
$$\Delta \text{H}_{\text{R1}} \approx -23460\text{cal/mol}$$
$$\Delta \text{H}_{\text{R2}} \approx 9510\ \text{cal/mol}$$

2. Operating conditions

Absolute pressure: 51 bar
Feeding temperature: 513 K

	Q (kmol/h)	y_i
CO	2008.6	13.39%
CO_2	1495.0	9.97%
H_2	9500.2	63.33%
CH_4	1996.2	13.31%
CH_3OH	0.0	0.00%
H_2O	0.0	0.00%
tot	15000	100.00%

3. Kinetic equations

KINETIC EQUATION [mol/g_{cat}/min]	Reaction constants
$R_1 = \dfrac{f_{CO} f_{H_2}^2 - \dfrac{f_{CH_3OH}}{K_{eq,1}}}{\left(C_1 + C_2 f_{CO} + C_3 f_{CO_2} + C_4 f_{H_2}\right)^2}$	$C_1 = \exp\left[3.49 + 4883\left(\frac{1}{T} - \frac{1}{506}\right)\right]$ $C_2 = \exp\left[2.53 - 39060\left(\frac{1}{T} - \frac{1}{506}\right)\right]$ $C_3 = \exp\left[3.70 + 15948\left(\frac{1}{T} - \frac{1}{506}\right)\right]$ $C_4 = \exp\left[1.54 + 8229\left(\frac{1}{T} - \frac{1}{506}\right)\right]$
$R_2 = \dfrac{f_{CO2} f_{H2} - \dfrac{f_{CO} f_{H2O}}{K_{eq,2}}}{C_5}$	$C_5 = \exp\left[5.18 + 938\left(\frac{1}{T} - \frac{1}{506}\right)\right]$
f = fugacity, atm (P.L. Villa, P. Forzatti, G. Buzzi-Ferraris, G. Garone, I. Pasquon, I&EC Process Design & Development 24 (1985) 12)	

To evaluate the equilibrium constants, the $\Delta G°$ of reaction are reported:

$\Delta G_1^0 = -22.858 + 0.05602 \cdot T$ (K) kcal/mol
$\Delta G_2^0 = 9.418 - 0.00907 \cdot T$ (K) kcal/mol

The fugacity are evaluate accordingly to what reported in Exercise 1