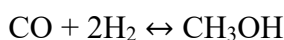


**Assignment 5**

(Submission deadline-18 Sept 2020, 5 PM)

1. Methanol is synthesized in a
- gas phase
- reaction



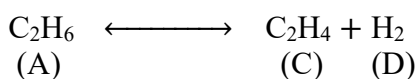
under constant pressure adiabatic PFR. The feed is as per the stoichiometric proportion at 300 K.

Standard Gibbs free energy of formation ( $g_{f,298K}^0$ ) and standard enthalpy of formation ( $h_{f,298K}^0$ ) of CO and CH<sub>3</sub>OH at 298 K are given in the table below.

Species	$g_{f,298K}^0$ kJ/mol	$h_{f,298K}^0$ kJ/mol
CO	-137.17	-110.53
CH <sub>3</sub> OH	-161.96	-200.66

Assuming that heat of reaction is independent of temperature, calculate equilibrium conversion of CO over a temperature range of 300 - 500 K (take an interval of 50 K), and show a rough sketch of the profile. [Note that concentration equilibrium constant ( $K_C$ ) and true equilibrium constant ( $K$ ) are related by  $K_C C_{A0}^2 = K$ , for the above reaction.]

2. Consider the gas phase pyrolysis of ethane



Thermodynamic data are given below. Heat capacity as a function of temperature for each species is given by:  $\frac{C_{P,i}}{R} = \alpha_i + \beta_i T + \gamma_i T^2$  (T in K)

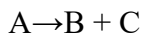
Species	$h_{f,298K}^0$ kJ/mol	$\alpha$	$\beta$	$\gamma$
C <sub>2</sub> H <sub>6</sub>	-84.68	1.131	$19.225 \times 10^{-3}$	$-5.561 \times 10^{-6}$
C <sub>2</sub> H <sub>4</sub>	52.26	1.424	$14.394 \times 10^{-3}$	$-4.392 \times 10^{-6}$
H <sub>2</sub>	-	3.249	$0.422 \times 10^{-3}$	0

Mean heat capacity is defined over a temperature range  $T_1$  to  $T_2$  as:

$$\bar{C}_P = \frac{1}{T_2 - T_1} \int_{T_1}^{T_2} C_P dT$$

Calculate  $\bar{C}_P$  over a temperature range of 298 K to 500 K for each species. Using the mean heat capacities, calculate heat of reaction for the above reaction over a temperature range of 298 K - 500K. Based on your result, can you suggest whether or not the heat of reaction can be considered to be independent of temperature over the range 298 - 500?

## 3. The elementary, irreversible gas-phase reaction



is carried out adiabatically in a PFR packed with a catalyst. Pure A enters the reactor at a volumetric flow rate of  $20 \text{ dm}^3/\text{s}$ , at a pressure of 10 atm, and a temperature of 450 K.

*Additional information:*

$$C_{P,A} = 40 \text{ J/mol.K}, C_{P,B} = 25 \text{ J/mol.K}, C_{P,C} = 15 \text{ J/mol.K}$$

$h_{f,A}^0 = -70 \text{ kJ/mol}$ ,  $h_{f,B}^0 = -50 \text{ kJ/mol}$ ,  $h_{f,C}^0 = -40 \text{ kJ/mol}$ . All heats of formation are referenced to 273 K.

$$k = 0.133 \exp \left[ \frac{E}{R} \left( \frac{1}{450} - \frac{1}{T} \right) \right] \frac{\text{dm}^3}{\text{kg-cat} \cdot \text{s}} \text{ with } E = 31.4 \text{ kJ/mol}$$

Plot the conversion and temperature down the plug-flow reactor until an 80% conversion (if possible) is reached. (The maximum catalyst weight that can be packed into the PFR is 50 kg.) Assume that pressure drop is negligible.