

1. The elementary gas-phase reaction



is carried out isothermally in a flow reactor with no pressure drop. The specific reaction rate at 50°C is 10^{-4} min^{-1} and the activation energy is 85 kJ/mol . Pure A enters the reactor at 10 atm and 127°C and a molar flow rate of 2.5 mol/min . Calculate the reactor volume and space time to achieve 90% conversion in:

- (a) a CSTR (5 pts)
- (b) a PFR (5 pts)
- (c) If this reaction is to be carried out at 10 atm and 127°C in a batch mode with 90% conversion, what reactor size and cost would be required to process $(2.5 \text{ mol/min} \times 60 \text{ min/h} \times 24 \text{ h/day})$ 3600 mol of A per day? (5 pts)
- (d) Assume that the reaction is reversible with $K_C = 0.025 \text{ mol}^2/\text{dm}^6$ and calculate the equilibrium conversion and then redo (a) and (b) to achieve a conversion that is 90% of the equilibrium conversion. (10 pts)

2. (25 pts) 交通警語“喝酒後不開車”，主要是因喝酒之後血液中的酒精來不及分解，造成酒精濃度增高，進而影響神經控制能力，容易導致交通事故。因此為了避免危險事故，世界各國對於駕駛員血液中酒精濃度有一定嚴格的標準，符合標準才允許開車上路，例如美國標準為 1g of ethanol per liter of body fluid，瑞典為 0.5 g/L，台灣為 0.25 g/L。

各位化工人未來難免有應酬多少要喝酒，可否利用 kinetics 與以下生理 model 來評估自己酒後何時可再開車。從生理學知道，酒精首先被腸胃吸收至血液中，此反應為一級反應，其反應常數為 10 h^{-1} ；之後，酒精被血中酵素分解，此反應為零級反應，其反應速率為 $0.192 \text{ g/h} \cdot \text{L of body fluid}$ 。若某化學工程師於應酬時連續喝了兩杯高粱酒（假設每杯高粱約含 40 g 酒精），請問此人 (a) 在美國；(b) 在瑞典；(c) 在台灣 必須要休息多久才能上路？請畫出時間對血液中酒精濃度(C_B)作圖。

(Hint: Volume of body fluid = 40 L; 將此設為連續反應 $A \xrightarrow{\text{吸收}} B \xrightarrow{\text{分解}} C$

且 $t=0$ ，血液中酒精濃度 $C_B=0$)

3. (a) The Clausius-Clapeyron equation, $\ln P^o = c - (\Delta h/RT)$, is usually used to correlate the solid-vapor and liquid-vapor equilibrium cases (P^o and Δh are denoted as the vapor pressure and the latent heat). For example, the vapor pressure of solid and liquid hydrogen cyanides expressed in mmHg are given by

$$\text{Solid (from 243 to 258 K): } \log P^o = 9.33902 - (1864.8/T)$$

$$\text{Liquid (from 265 to 300 K): } \log P^o = 7.74460 - (1453.06/T)$$

Please calculate (1) the heat of sublimation; (2) the heat of vaporization; (3) the heat of fusion; (4) the triple point; and (5) the normal boiling point. ($R = 1.9872$ cal/g-mole = 8.3143 Joules/g-mole K = 82.06 atm-cm³/g-mole K) (20 分)

- (b) Please show the Clausius-Clapeyron equation: $\ln P^o = c - (\Delta h/RT)$ and describe the assumptions. (Hint: Start from the differentials of chemical potentials for each phase in terms of T and P) (15 分)

4. Based on the Gibbs-Duhem equation and the definition of excess Gibbs free energy,

$$G^E, \text{ please show } x_1 \frac{d \ln(y_1 P)}{dx_1} + x_2 \frac{d \ln(y_2 P)}{dx_1} = 0 \text{ under a constant temperature and}$$

pressure, if the vapor phase of this binary system is an ideal gas. (15 分)