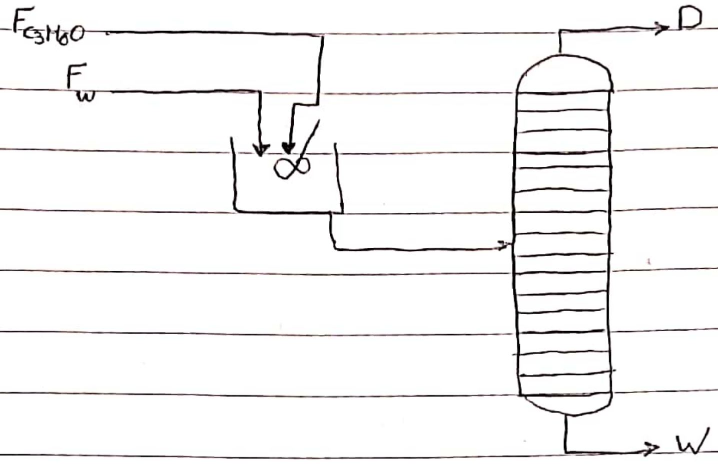
Subject: [Industrial Principle's Hysys Project] Date: / /

Unit:



rxn: $C_3H_6O + H_2O \rightarrow C_3H_8O_2$

$r = k C_{H_2O} \cdot C_{C_3H_6O}$

$F_{C_3H_6O}$: 2754 kg/hr, sat. liq., 1 atm

F_w : B kg/hr, 45 °C, 1 atm

goal. 0.995 $C_3H_8O_2$

Problem 01. "Find k and E_a"

2 PFR sets were used; SS 1" with Sch. 40, 4 m long, (H_2O C_3H_6O) (0.5 − 0.5) mass weight, $T_1 = 50$ °C, $T_2 = 60$ °C | $x_1 = 0.05$, $x_2 = 0.06$

P = 1 atm, u = 2 m/s, $k = k_0 \cdot \exp(-\frac{E_a}{RT})$

Nominal pipe size = 1 in (outside diameter = 1.315 in), Schedule no. = 40, wall thickness = 0.133 in

inside diameter = 1.049 in, cross-sectional area of metal = 0.494 in², inside sectional area = 0.006 ft²

circumference = 0.344 ft of length (outside) = 0.275 ft of length (inside), capacity at 1 ft/s = 1345 lb/hr water

pipe weigh = 1.68 lb/ft

Basis: 1000 gr of the mixture feed

→ 500 gr H_2O , $\frac{1 \text{ mol}}{18.015 \text{ g}}$ = 27.755 mol H_2O

→ 500 gr C_3H_6O , $\frac{1 \text{ mol}}{58.080 \text{ g}}$ = 8.609 mol C_3H_6O → Limiting component

stoichiometry table:

(case I.)
↓
$x_A = 0.05$

Comp.	N_0 (mol)	$x_A N_{A_0}$	N	W
A (C_3H_6O)	~~27.75~~ 8.609	−0.43045	8.179	475.036
B (H_2O)	27.755	−0.43045	27.325	492.260
C ($C_3H_8O_2$)	0	+0.43045	0.43	32.721 → 32.704

$\sum W_i = 1000$ (constraint)

$$\ln \frac{C_B \cdot C_{A_0}}{C_{B_0} \cdot C_A} = (C_{B_0} - C_{A_0}) kt$$

(case II.)

$x_A = 0.06$

	N_0	$x_A N_{A_0}$	N	W
A	8.609	−0.516	8.093	470.091
B	27.755	−0.516	27.239	490.712
C	0	+0.516	0.516	39.266 → 39.247

s.a.m

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$$\ln \frac{C_B \cdot C_{A_0}}{C_{A_0} \cdot C_{B_0}} = (C_{B_0} - C_{A_0}) k t \Rightarrow \ln \frac{N_B \cdot N_{A_0}}{N_A \cdot N_{B_0}} = \frac{(N_{B_0} - N_{A_0})}{V} k t$$

For case I & II $\Longrightarrow$ $t_1 = t_2$, $V_1 = V_2$

$$\left[\frac{\ln\left(\frac{N_B \cdot N_{A_0}}{N_A \cdot N_{B_0}}\right)}{(N_{B_0} - N_{A_0}) k} \right]_{case\ I} = \left[\frac{\ln\left(\frac{N_B \cdot N_{A_0}}{N_A \cdot N_{B_0}}\right)}{(N_{B_0} - N_{A_0}) k} \right]_{case\ II} \quad (I)$$

$k = k_0 \cdot \exp\left(\frac{-E_a}{RT}\right)$ $\Longrightarrow$

$$\left[\frac{\ln\left(\frac{N_B \cdot N_{A_0}}{N_A \cdot N_{B_0}}\right)}{(N_{B_0} - N_{A_0}) \cdot k_0 \cdot \exp\left(\frac{-E_a}{RT}\right)} \right]_{case\ I} = \left[\frac{\ln\left(\frac{N_B \cdot N_{A_0}}{N_A \cdot N_{B_0}}\right)}{(N_{B_0} - N_{A_0}) \cdot k_0 \cdot \exp\left(-\frac{E_a}{RT}\right)} \right]_{case\ II} \quad (II)$$

substitution $\Longrightarrow$

$$\frac{\ln\left(\frac{27.325 \times 8.609}{8.179 \times 27.755}\right)}{(27.755 - 8.609) k_0 \cdot \exp\left(\frac{-E_a}{82.06 \times 10^{-6} \frac{m^3 atm}{mol \cdot k} \times 323.15}\right)} = \frac{\ln\left(\frac{27.239 \times 8.609}{8.093 \times 27.755}\right)}{(27.755 - 8.609) k_0 \cdot \exp\left(\frac{-E_a}{82 \times 10^{-6} \times 333.15}\right)}$$

$$\Longrightarrow 0.0356 \times \exp\left(\frac{E_a}{0.0265}\right) = 0.0430 \times \exp\left(\frac{E_a}{0.0273}\right) \Longrightarrow 1.208 = \exp\left(\frac{E_a}{0.0265} - \frac{E_a}{0.0273}\right)$$

$$\overset{\ln}{\Longrightarrow} 0.189 = \frac{0.0008 E_a}{7.2345 \times 10^{-4}} \Longrightarrow E_a = 0.1709 \frac{m^3 atm}{mol} \times \frac{101392 \frac{J}{m^3}}{1\ atm} = 17329.42 \ J/mol$$

$$V = \frac{\pi d_{in}^2 L}{4} = \frac{\pi}{4} \left(1.049^{in} \times \frac{0.0254^m}{1^{in}}\right)^2 \times 9^m = 0.00223\ m^3$$

$$u = 2^{m/s} \Longrightarrow u = \frac{L}{t} \Longrightarrow t = \frac{L}{u} = \frac{9^m}{2^{m/s}} = 2^s$$

$$(I) \Longrightarrow \left[\frac{\ln\left(\frac{N_B \cdot N_{A_0}}{N_A \cdot N_{B_0}}\right)}{(N_{B_0} - N_{A_0}) k_0 \cdot \exp\left(\frac{-E_a}{RT}\right)} \right]_{case\ I} = \frac{t}{V} \Longrightarrow \frac{0.0356 \times \exp\left(\frac{0.1709}{0.0265}\right)}{19.146\ k_0 \times} = \frac{2^s \times \frac{1\,hr}{3600^s}}{0.00223}$$

$$\Longrightarrow \frac{1.1753}{k_0} = 0.2491 \Longrightarrow k_0 = 4.7182 \ \frac{m^3}{mol \cdot hr}$$

$A = 1.7e13$

$E_a = 3.29e9$ btu/lbmol

s.a.m

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Problem 02. what is the mass flow rate of water, B ?

Basis = 1 hr

$C_3H_6O = 2759 \, \frac{kg}{} \times \frac{1 \, kmol}{58.08 \, kg} = 47.417$ kmol C_3H_6O

$H_2O = B \, \frac{kg}{} \times \frac{1 \, kmol}{18.015 \, kg} = \frac{B}{18.015}$ kmol H_2O

for C_3H_6O to be the limiting component, there should be: $\frac{B}{18.015} \geq 47.417 \Rightarrow B > 854.217$ kg

Problem 03. Compute Equilibrium constant of the reaction. $C_3H_6O + H_2O \longrightarrow C_3H_8O_2$

(A, B, C)

- Due to the given rate of reaction, $(-r_A = kC_AC_B)$

there is no reverse path for reaction to take place. Thus: $K_{eq.} = \frac{k_f}{k_b} = \infty$