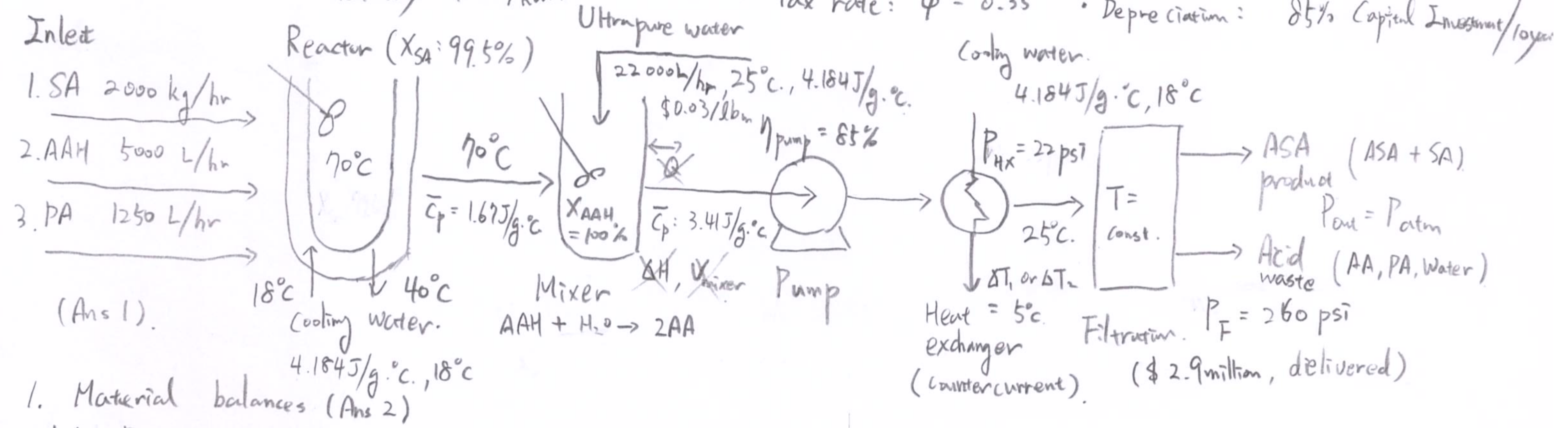
Aspirin production

- Chemical reaction

salicylic acid + acetic anhydride + phosphoric acid
(SA, \$1.33/lbm) (AAH, \$0.49/lbm) (PA, \$0.34/lbm)

⟶ acetylsalicylic acid + acetic acid + phosphoric acid
$k_r = 0.5 s^{-1}$
$\Delta H_r = -85600 J/mol$
(ASA, \$3.97/lbm) (AA, \$0.013/lbm) (PA, \$0.34/lbm)

- Cost information (cooling water : \$0.03/1000 gal ; electricity : \$0.05/kW.hr)
- Operating cost : 1.55 (feed + cooling water + electricity)
- Tax rate : $\phi = 0.35$
- Depreciation : 85% Capital Investment/10year



1. Material balances (Ans 2)

1.1. Reactor

Stoichiometry

SA: $\dot{n}_{SA,in} = \dot{n}_{SA,out} + r_{c,SA}$

AAH: $\dot{n}_{AAH,in} = \dot{n}_{AAH,out} + r_{c,AAH}$ $\quad r_{c,AAH}/r_{c,SA} = 1, \quad r_{c,AAH} = 14.41\ kgmol/hr$

PA: $\dot{n}_{PA,in} = \dot{n}_{PA,out}$

ASA: $r_{f,ASA} = \dot{n}_{ASA,out}$ $\quad r_{f,SAS}/r_{c,SA} = 1, \quad r_{f,SAS} = 14.41\ kgmol/hr$

AA: $r_{f,AA} = \dot{n}_{AA,out}$ $\quad r_{f,AA}/r_{c,SA} = 1, \quad r_{f,AA} = 14.41\ kgmol/hr$

$$r_{c,SA} = 0.995 \cdot \dot{n}_{SA,in} = 0.995 \frac{\dot{m}_{SA,in}}{MW_{SA}} = 0.995 \cdot \frac{2000\ kg/hr}{138.1\ kg/kgmol} = 14.41\ kgmol/hr$$

$$\dot{n}_{SA,out} = \dot{n}_{SA,in} - r_{c,SA} = \frac{2000\ kg/hr}{138.1\ kg/kgmol} - 14.41\ kgmol/hr = 0.07\ kgmol/hr \quad (9.67\ kg/hr)$$

$$\dot{n}_{AAH,out} = \dot{n}_{AAH,in} - r_{c,AAH} = \frac{\rho_{AAH} \cdot \dot{V}_{AAH,in}}{MW_{AAH}} - r_{c,AAH} = \frac{1.08\ g/cm^3 \cdot 5000\ L/hr}{102.1\ kg/kgmol} - 14.41\ kgmol/hr = 38.48\ kgmol/hr \quad (3928.81\ kg/hr)$$

$$\dot{n}_{PA,out} = \dot{n}_{PA,in} = \frac{\rho_{PA} \dot{V}_{PA}}{MW_{PA}} = \frac{1.68\ g/cm^3 \cdot 1250\ L/hr}{98\ kg/kgmol} = 21.43\ kgmol/hr \quad (2100.14\ kg/hr)$$

$\dot{n}_{ASA,out} = r_{f,ASA} = 14.41\ kgmol/hr\ (2596.68\ kg/hr)$, $\dot{n}_{AA,out} = r_{f,AA} = 14.41\ kgmol/hr\ (866.04\ kg/hr)$

$$\therefore \dot{m}_{reactor,out} = 9.67 + 3928.81 + 2100.14 + 2596.68 + 866.04 = 9501.34\ kg/hr$$

SA AAH PA ASA AA

1.2 Mixer

Stoichiometry

AAH : $\dot{n}_{AAH,in} = \dot{n}_{AAH,out} + r_{c,AAH}$

Water : $\dot{n}_{w,in} = \dot{n}_{w,out} + r_{c,w}$

AA : $\dot{n}_{AA,in} + r_{f,AA} = \dot{n}_{AA,out}$

$r_{c,w}/r_{c,AAH} = 1$, $r_{c,w} = 38.48$ kgmol/hr

$r_{f,AA}/r_{c,AAH} = 2$, $r_{f,AA} = 76.96$ kgmol/hr

$$r_{c,AAH} = 1.0 \times \dot{n}_{AAH,in} = 38.48 \text{ kgmol/hr}$$

$$\dot{n}_{w,out} = \dot{n}_{w,in} - r_{c,w} = \frac{\rho_w \dot{V}_{w,in}}{MW_w} - r_{c,w} = \frac{1 \text{ g/cm}^3 \cdot 22000 \text{ L/hr}}{18 \text{ kg/kgmol}} - 38.48 \text{ kgmol/hr} = 1183.74 \text{ kgmol/hr}$$

(21307.32 kg/hr)

$$\dot{n}_{AA,out} = \dot{n}_{AA,in} + r_{f,AA} = 14.41 + 76.96 = 91.37 \text{ kgmol/hr } (5491.34 \text{ kg/hr})$$

$$\dot{m}_{mixer,out} = \dot{m}_{reactor,out} + \dot{m}_{w,in} = 9501.34 + 22000 = 31501.34 \text{ kg/hr}$$

1.3 Filtration

ASA product : (ASA : 14.41 kgmol/hr
SA : 0.07 kgmol/hr

Acid waste : (AA : 91.37 kgmol/hr
PA : 21.43 kgmol/hr
Water : 1183.74 kgmol/hr.

2. Equipment sizing.

2.1. Reactor

$$r_{c,SA} = k_r \cdot C_{SA,out} \cdot V_r = k_r \cdot \frac{\dot{n}_{SA,out}}{\dot{V}_{out}} \cdot V_r = k_r \cdot \dot{n}_{SA,out} \frac{\rho_{out}}{\dot{m}_{out}} \cdot V_r$$

$$\therefore V_r = \frac{r_{c,SA} \cdot \dot{m}_{out}}{k_r \cdot \dot{n}_{SA,out} \cdot \rho_{out}} = \frac{14.41 \text{ kgmol/hr} \cdot 9501.34 \text{ kg/hr}}{0.5 \text{ s}^{-1} \cdot 0.07 \text{ kgmol/hr} \cdot 1.2 \text{ g/cm}^3} = 905.5 \text{ L} = 239.2 \text{ gal} \quad (\text{Ans } 5,9)$$

고려서에서 주어지지 않음.

2.2 Pumps.

$$\frac{P_2 - P_1}{\rho} + \frac{1}{2}(\alpha_2 V_{avg,2}^2 - \alpha_1 V_{avg,1}^2) + g(z_2 - z_1) = W_s - W_f$$

same diameter   same level

$$W_s = \frac{P_2 - P_1}{\rho} = \frac{20 \text{ psi} + 260 \text{ psi}}{1.2 \text{ g/cm}^3} \cdot \left(\frac{1 \text{ g/cm}^3}{62.43 \text{ lb}_m/\text{ft}^3}\right) \cdot \left(\frac{\text{lb}_f/\text{in}^2}{1 \text{ psi}}\right) \cdot \left(\frac{144 \text{ in}^2}{\text{ft}^2}\right) \left(\frac{1 \text{ hp}}{550 \text{ ft lb}_m/\text{s}}\right) = 0.986 \frac{\text{hp}}{\text{lb}_m/\text{s}}$$

고려서에서 주어지지 않음.

$$W = \dot{m}_{mixer,out} \cdot W_s = 31501.34 \text{ kg/hr} \cdot 0.986 \frac{\text{hp}}{\text{lb}_m/\text{s}} \cdot \frac{1 \text{ hr}}{3600 \text{ s}} \cdot \frac{2.205 \text{ lb}_m}{1 \text{ kg}} = 19.02 \text{ hp}$$

$$\therefore \text{Power to operating pump} = \frac{\text{Power delived to the fluid}}{\text{efficiency}} = \frac{19.02 \text{ hp}}{0.85} = 22.38 \text{ hp} \quad (\text{Ans } 6,9)$$

3. Energy balance (Ans 3)

3.1. Reactor

$$\dot{Q}_{reaction} = \Delta \hat{H}_{reaction} \cdot r_{c,SA} = -85800\ J/gmol \cdot 14.41\ kgmol/hr = -1.24 \times 10^{9}\ J/hr$$

$$\dot{Q}_{cooling\ water} = \dot{m}_{cooling\ water} \cdot \overline{C}_{p,w} \cdot (T_{out} - T_{in}) = 1.24 \times 10^{9}\ J/hr \quad (\text{Ans } 9)$$

$$\dot{m}_{cooling\ water} = \frac{\dot{Q}_{cooling\ water}}{\overline{C}_{p,w}(T_{out} - T_{in})} = \frac{1.24 \times 10^{9}\ J/hr}{4.184\ J/g\cdot°C \cdot (40°C - 18°C)} = 1.35 \times 10^{7}\ g/hr \quad (3550\ gal/hr)$$

(Ans 4,9)

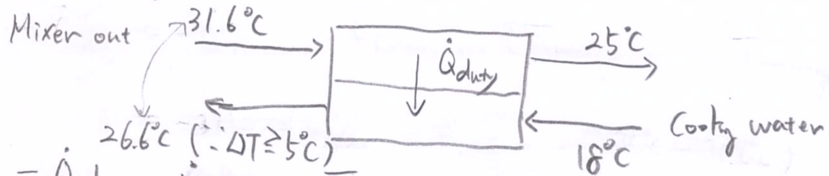
3.2. Mixer

$$\dot{Q}_{reactor\ out} = -\dot{Q}_{ultrapure,\ water}$$

$$\dot{m}_{reactor\ out} \cdot \overline{C}_{p,reactor\ out}(T_f - T_{reactor\ out}) = -\dot{m}_{ultrapure\ water} \cdot \overline{C}_{p,w}(T_f - T_{ultrapure\ water})$$

$$T_f = \frac{9501.34\ kg/hr \cdot 1.67\ J/g\cdot°C \cdot 70°C + 22000\ kg/hr \cdot 4.184\ J/g\cdot°C \cdot 25°C}{9501.34\ kg/hr \cdot 1.67\ J/g\cdot°C + 22000\ kg/hr \cdot 4.184\ J/g\cdot°C} = 31.6°C$$

3.3. Heat exchanger



Hot: $-\dot{Q}_{duty} = \dot{m}_{mixer\ out} \cdot \overline{C}_{p,mixer\ out} \cdot (T_{exchanger\ out} - T_{exchanger\ in})$

$$= 31501.34\ kg/hr \cdot 3.41\ J/g\cdot°C \cdot (25°C - 31.6°C)$$

$$\therefore \dot{Q}_{duty} = 709000\ kJ/hr = 672000\ Btu/hr \quad (\text{Ans } 9)$$

Cold: $\dot{Q}_{duty} = \dot{m}_{cooling\ water} \cdot \overline{C}_{p,w} \cdot (T_{out} - T_{in}) = 709000\ kJ/hr$

$$\dot{m}_{cooling\ water} = \frac{709000\ kJ/hr}{4.184\ J/g\cdot°C \cdot (26.6 - 18°C)} = 19.7 \times 10^{6}\ g/hr \quad (5200\ gal/hr)\ (\text{Ans } 4,9)$$

$$\Delta T_1 = 5°C = 9°F, \quad \Delta T_2 = 7°C = 12.6°F \quad \therefore T_{log\ mean} = \frac{12.6 - 9}{\ln(12.6/9)} = 10.7°F$$

$$U_o = 50\ Btu/hr\cdot ft^2\cdot°F \quad (\text{from Table } 10.4)$$

$$\therefore A = \frac{\dot{Q}_{duty}}{U \cdot \Delta T_{log\ mean}} = \frac{672000\ Btu/hr}{50\ Btu/hr\cdot ft^2\cdot°F \cdot 10.7°F} = 1260\ ft^2 \quad (\text{Ans } 7,9)$$

4. Economics

4.1. Capital investment

· Equipment

Reactor : $\frac{M\&S}{814} \cdot 47.0\,(V/gal)^{0.61} = \frac{1469}{814} \cdot 47.0 \cdot (239.2\,gal)^{0.61} \doteqdot \$2400$

Heat exchanger : $\frac{1469}{814} \cdot 398 \cdot (1260\,ft^2)^{0.65} \doteqdot \$74400$

Pump : $\frac{1469}{814} \cdot 421 \cdot (139\,gal/min)^{0.46} \doteqdot \$7300$

$\dot{V} = 31501.34\,kg/hr \cdot \frac{1\,m^3}{1\,kg} \doteqdot 139\,gal/min.$

From mixer

$\rho \approx$ water.

Filtration (delivery included) : \$ 2900000

Total delivered cost = $(2400 + 74400 + 7300) \times 1.1 + 2900000 = \$2992500$

Capital investment : $6.0 \times \$2992500 = \$17955000$

Depreciation : $(0.85 \times \$17955000)/10 = \$1526200/yr$

4.2 Operating cost

· Feed

SA : $\$1.33/lb_m \cdot 2000\,kg/hr = \$51380000/yr$

AAH : $\$0.49/lb_m \cdot 5000\,L/hr \cdot \rho_{AAH} = \$51110000/yr$

PA : $\$0.34/lb_m \cdot 1250\,L/hr \cdot \rho_{PA} = \$13790000/yr$

· Ultrapure water : $\$0.03/lb_m \cdot 22000\,L/hr \cdot \rho_w = \$12750000/yr$

· Cooling water : $\$0.03/1000\,gal\,(3550\,gal/hr + 5200\,gal/hr) = \$2300/yr$

· Electricity : $\$0.05/kW\text{-}hr \cdot 22.4\,hp = \$7300/yr$

$\therefore$ operating cost = $1.55\,(\text{feed} + \text{water} + \text{electricity}) \doteqdot \$200000000/yr$

4.3 Sales

ASA(aspirin) : $\$3.97/lb_m \cdot 2600\,kg/hr = \$199910000/yr$

Acid waste (AA) : $\$0.013/lb_m \cdot 28900\,kg/hr = \$7260000/yr$ (31500 − 2600)

Total: $\$207170000/yr$

4.4 Gross profit = sales − operating cost − depreciation

$= \$207170000/yr - \$200000000/yr - \$1526200/yr$

$= \$5643800/yr$

4.5 NAPAT = $\$5643800/yr \cdot (1-0.35) = \$3668500/yr$

4.6 ROI : $\frac{NAPAT}{\text{Capital investment}} = \frac{\$3668500/yr}{\$17955000} = 20.4\,\%$ (Ans 10)

↳ (Ans 11).