$$\dot{Q} - \dot{W}_s + \sum_{i=1}^{n} q_i H_i|_{in} - \sum_{i=1}^{n} q_i H_i|_{out} =$$

$$\frac{\partial \hat{E}_{sys}}{\partial t}$$

Energy in system → total

include U, ~~KE~~, ~~PE~~

$$\hat{E}_{sys} = \sum_{i=1}^{n} \underbrace{N_i}\,\underbrace{E_i} = \sum_{i=1}^{n} N_i U_i$$

$$= \sum_{i=1}^{n} N_i (H_i - PV_i)$$

$$\boxed{\begin{aligned} &\dot{Q} - \dot{W}_s + \sum_{i=1}^{n} q_i \underline{H}_i|_{in} - \sum_{i=1}^{N} q_i \underline{H}_i|_{out} = \\ &\left[\sum_{i=1}^{n} N_i \frac{\partial \underline{H}_i}{\partial t} + \sum_{i=1}^{n} \underline{H}_i \frac{\partial N_i}{\partial t} - \frac{\partial \left(P \sum_{i=1}^{n} N_i V_i\right)}{\partial t}\right] \end{aligned}}$$

Assume total pressure is nonchanging →

Assume our vessels are static or slowly changing in time → neglect all PV contributions.

$$\dot{Q} - \dot{W}_s + \sum q_i \underline{H}_{i\,in} - \sum q_i \underline{H}_{i\,out} = \sum N_i \frac{d\underline{H}_i}{dt} + \sum$$

$$\sum \underline{H}_i \frac{dN_i}{dt}$$

Enthalpy relates to T

$$\frac{d}{dt}\left[\underline{H}_i = \underline{H}_i^{o}(T_R) + \int_{T_R}^{T} \underline{C}_{p_i}\, dT\right]$$

$$\boxed{\frac{d\underline{H}_i}{dt} = \underline{C}_{p_i} \frac{dT}{dt}}$$

$$\dot{Q} - \dot{W}_s + \sum q_i \underline{H}_i\Big|_{in} - \sum q_i H_i\Big|_{out} =$$

$$\sum N_i C_{p_i} \frac{dT}{dt} + \sum \underline{H}_i \frac{dN_i}{dt}$$

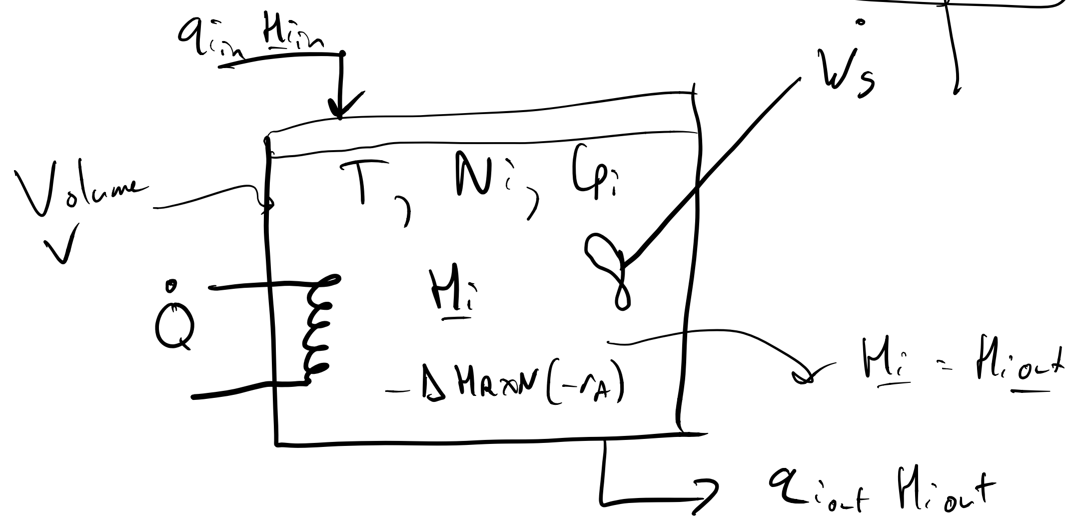
From mess balance:

e.g. $$\frac{dN_i}{dt} = -\underset{\substack{\uparrow \\ \text{stocchiometric} \\ \text{coeffishant}}}{\nu_i}\ \underset{\substack{\uparrow \\ \text{RXN rate A}}}{r_A}\, V + \underbrace{q_{i_{in}} - q_{out}}$$

$$\dot{Q} - \dot{W}_s + \underbrace{\sum q_{i_0}}_{\text{inlet}} \underline{H}_i\big|_{in} - \sum q_i \underline{H}_{i\,out} = \sum N_i C_{p_i} \frac{dT}{dt} +$$

$$\sum \nu_i \underline{H}_i (-r_A)(V) + \underbrace{\sum q_{i_{in}}}_{\text{outlet}} H_{i\,out} - \sum q_{i_{out}} H_{i\,out}.$$

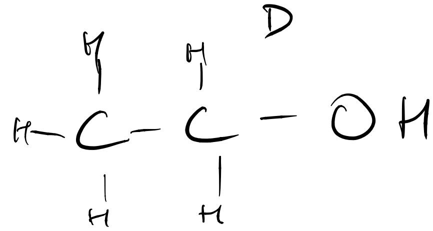
$$\boxed{\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum q_{io}(\underline{H}_i - \underline{H}_{in}) + (-\Delta H_{Rxn})(-r_A V)}{\sum N_i \underline{C}_{p_i}}}$$



In Class Problem

$$\underset{A}{C_2H_5(CH_3COO)_{aq}} + \underset{B}{Na(OH)_{aq}} \rightleftharpoons$$

$$\rightarrow \underset{C}{Na(CH_3COO)_{aq}} + \underset{D}{(C_2H_5OH)_{(aq)}}$$

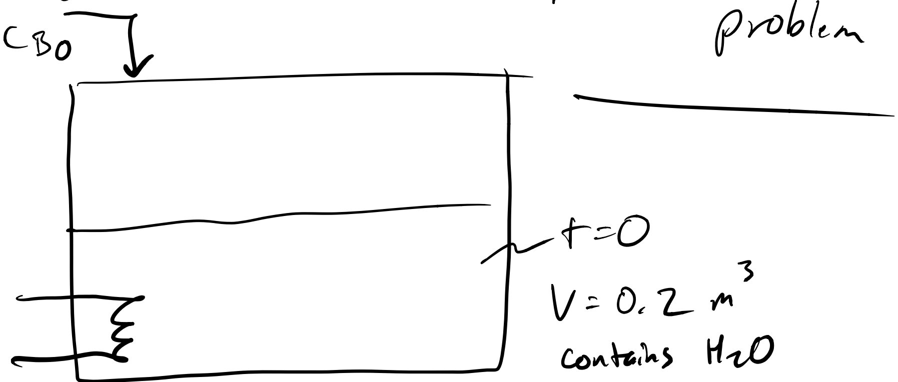


Stoichiometry $\quad -1 \quad -1 \quad 1 \quad 1$

Apocolypse now problem

C_{w0}
C_{B0}

1 kmol/m^3
300 K
0.004 m^3/s



t=0
V = 0.2 m^3
contains H_2O + ethyl acetate.

initial concentrations $\begin{cases} C_{Ai} = 5 \text{ kmol}/m^3 \\ C_{wi} = 30.7 \text{ kmol}/m^3 \end{cases}$

RXN is exothermic

Goal: keep below 315 K

Recall heat exchanger problem:
transfer coefficient of 3000 J/(s K)
T in exchanger ~ 290 K

Question: is exchanger sufficient?
How do you know? →
Plot, T, C_A, C_B, C_C as f(t)

Mole balance equations

$$\frac{dC_A}{dt} = r_A - \frac{q_0 C_A}{V}$$

inlet rates lead to dilution

$$\frac{dC_B}{dt} = r_B + q_0 \frac{(C_{B0} - C_B)}{V}$$

$$\frac{\partial C_c}{\partial t} = r_c - \frac{q_0 C_c}{V}$$

$C_D = C_c \Leftarrow$ stoichiometric equivalent to C_c

$$\frac{dN_w}{dt} = C_{wi0} \cdot q_0$$

Initial $N_{wi} = V_i \cdot C_{wi} =$

$(0.2)(30.7) = 6.14$ kmol

$-r_A = k C_A C_B - k_- C_C C_D \longrightarrow K_C = k/k_-$

$$-r_A = k\left(C_A C_B - \frac{C_C C_D}{K_C}\right)$$

is also a $f(T)$

Stoichiometry

$$-r_A = -r_B = r_C = r_D$$

$-1 \quad -1 \quad 1 \quad 1$

$$\boxed{V = V_0 + q_0 \cdot t}$$

$$k = 0.39175 \exp\left[54722.7\left(\frac{1}{273} - \frac{1}{T}\right)\right]$$

$$K_C = 10^{3885.44/T}$$

exothermic RXN

$\Delta H_{RX} = -79{,}076 \text{ kJ/kmol}$

$C_{PA} = 170.7 \ J/mol \cdot K$

$C_{PB} = C_{PC} = C_{PD} = C_{Pw} = C_p = 75.29 \ J/mol\,K$

Feed $C_{W0} = 55 \ kmol/m^3$

$C_{B0} = 1.0 \ kmol/m^3$

Recall from earlier:

$$\boxed{\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum q_i C_{pi}(T - T_{i0}) + [-\Delta H_{Rx}(T)](-r_A V)}{\sum N_i C_{pi}}}$$

$$\dot{Q} = 3000(T_a - T)$$

T_a: heat exchanger temperature

T: temp in system

water ratio of inlet

in your system

inlet temp.

$$\frac{dT}{dt} = \frac{\dot{Q} - q_0 C_p (1 + 55)(T - T_0) + r_A V \Delta H_{Rx}}{C_p(N_B + N_C + N_D + N_W) + C_{PA} \cdot N_A}$$

recall $N_i = V \cdot C_i$ $\quad V(t)$

Open your previous alcohol codes

Start inputting constants,

Change your ODE's

5 ODEs total

$$\frac{dC_A}{dt} =$$

$$\frac{dC_B}{dt} =$$

$$\frac{dC_C}{dt} =$$

$$\frac{dT}{dt} =$$

$$\frac{dN_w}{dt} =$$