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

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

Energy in system → total

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

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

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

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

Assume total pressure is nonchanging →

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

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

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. $\frac{dN_i}{dt} = -\nu_i\, r_A V + \underbrace{q_{i_{in}} - q_{out}}$

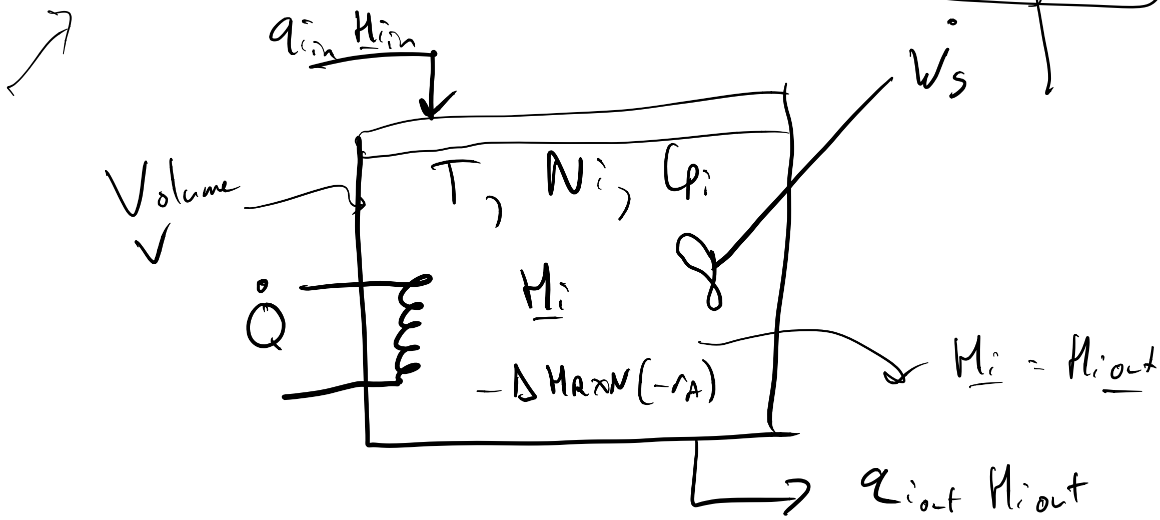
ν_i: stocchiometric coeffishant

r_A: RxN rate A

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

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

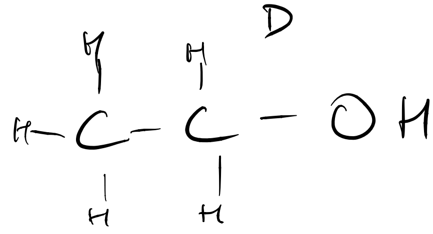
$$\boxed{\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum q_{io}(\underline{H}_i - \underline{H}_{in}) + (-\Delta H_{Rxn})(-r_A V)}{\sum N_i \underline{C}_{p_i}}}$$



In Class Problem

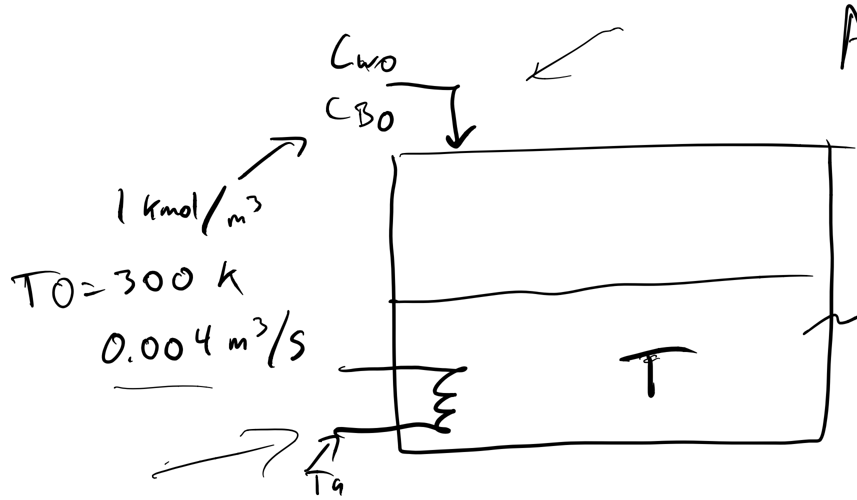
$$\underset{A}{C_2H_5(CH_3COO)_{aq}} + \underset{B}{Na(OH)_{aq}} \rightleftharpoons$$

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



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

Apocolypse Now problem



initial T in system.

$V = 0.2\ m^3$
contains H_2O + ethyl acetate.

initial concentrations $\left\{ \begin{array}{l} C_{Ai} = 5\ kmol/m^3 \\ C_{Wi} = 30.7\ kmol/m^3 \end{array} \right.$

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

inlet rates lead to dilution

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

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

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

$C_D = C_c \Leftarrow$ 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

$-r_A = kC_AC_B - k_-C_CC_D \rightarrow K_C = k/k_-$

$$-r_A = k\left(C_AC_B - \frac{C_CC_D}{K_C}\right)$$

is also a f(T)

Stoichiometry

$-r_A = -r_B = r_C = r_D$

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

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

$$k = 0.39175 \exp\left[5472.7\left(\frac{1}{273} - \frac{1}{T}\right)\right]$$

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

exothermic RXN

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

$C_{PA} = 170.7 \text{ J/mol·K}$

$C_{PB} = C_{PC} = C_{PD} = C_{PW} = C_P = 75.24 \text{ J/mol K}$

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

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

Recall from earlier:

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

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

heat exchanger temperature

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

$$\frac{dC_A}{dt} = r_A - (v0 * C_a)/V$$

$$\frac{dC_B}{dt} = rB + (v0 * (Cb0 - Cb)/V)$$

$$\frac{dC_C}{dt} = r_c - ((C_c * v0))/V$$

$$\frac{dT}{dt} = [UA * (Ta - T) - Fb0 * cp * (1+55) * (T - T0) + rA * V * dh]/NCp$$

$$\frac{dN_w}{dt} = v0 * Cw0$$

$vO = 0.004$

$CbO = 1$

$UA = 3000$

$Ta = 290$

$cp = 75240$

$TO = 300$

$dh = -7.9076 \cdot 10^7$

$CwO = 55$

$k = 0.39175 * exp(5472.7 * ((1/273) - \frac{1}{T}))$

$Cd = Cc$

$Vi = 0.2$

$Kc = 10^\wedge(3885.44/T)$

$cp_a = 170700$

$V = V_i + vO * t$

$F_{b0} = C_{b0} * v0$

$r_a = -k * ((C_a * C_b) - ((C_c * C_d)/K_c))$

$N_a = V * C_a$

$N_b = V * C_b$

$N_c = V * C_c$

$r_b = r_a$

$r_c = -r_a$

$N_d = V * C_d$

$rate = -r_a$

$NC_p = c_p * (N_b + N_c + N_d + N_w)$
$+ c_{pa} * N_a$

Solve from $t = 0$ to $t = 360$

initial conditions

$C_{a0} = 5$ $\quad N_{W0} = 6.14$

$C_{b0} = 0$ $\quad T0 = 300$

$C_{c0} = 0$