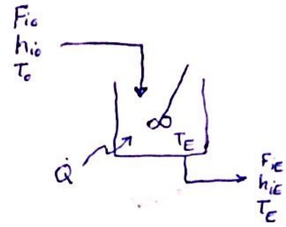
① Non-Isothermal CSTRs



- EBE
  - → Let us start with the general energy balance.
  - . h_i's are specific enthalpy on a molar basis $\frac{dE_{sys}}{dt} = \dot{Q} + \sum_i F_{io}h_{io} - \sum_i F_{iE}h_{iE}$ ①
  - → We can re-write eq.1 on a mass basis. let:

$$\dot{m}_o h'_o = \sum_i F_{io}h_{io} \quad ② \qquad , \qquad \dot{m}_E h'_E = \sum_i F_{iE}h_{iE} \quad ③$$

  - . note now h'_o and h'_E are specific enthalpy of feed and product streams, respectively, on a mass basis.
  - → because of conservation of mass: $\dot{m}_o = \dot{m}_E = \dot{m}$ ④
  - → Furthermore, for SS ops. we have: $dE_{sys}/dt = 0$ ⑤
  - → substituting for eqs.2 to5 in eq.1, we obtain: $\longrightarrow 0 = \dot{Q} + \dot{m}(h'_o - h'_E)$ ⑥
  - → or rearranging: $\underbrace{\dot{Q}}_{J/s} = \underbrace{\dot{m}}_{kg/s}\underbrace{(h'_E - h'_i)}_{J/kg}$ ⑦

- Again
  - → we consider thermal and chemical contribution to h' and re-write eq.7 as:

$$\dot{Q} = \dot{m}\left[(h'_{E,thermal} + h'_{E,chemical}) - (h'_{o,thermal} - h'_{o,chemical})\right] \quad ⑧$$

  - → Thermal term: $h'_{E,thermal} = \int_{T_R}^{T_E} C'_{PE}\,dT \quad , \quad h'_{o,thermal} = \int_{T_R}^{T_o} C'_{Po}\,dT$, where T_R is some reference T.
  - → chemical term: $\underbrace{\dot{m}}_{kg/s}\underbrace{h'_{E,chemical}}_{J/kg} = \underbrace{(\Delta H_{RA})}_{J/mol}\underbrace{(-r_{AE})}_{mol/m^3.s}\underbrace{V_R}_{m^3} \quad , \quad \dot{m}h'_{o,chemical} = 0$
    - ↳ since no rxn has taken place at the inlet of reactor.
  - → Let us now ~~consider~~ choose T_o, the inlet T, as our reference T, T_R. i.e.: $T_R = T_o$
  - → hence eq.8 can be written as: $\dot{Q} = \dot{m}\int_{T_o}^{T_E} C'_{PE}\,dT + (\Delta H_{R,A})_{T_o}(-r_{AE})V_R$ ⑨
  - → Recall the comp. balance eq.: $\boxed{-r_{AE} = \frac{F_{Ao}X_{AE}}{V}}$ ⑩
  - → the heat flow to the reactor, $\dot{Q}$, can be expressed as: $\dot{Q} = U_oA(T_a - T_E)$
  - → hence, eq.9 becomes: $\Longrightarrow \boxed{U_oA(T - T_E) = \dot{m}\int_{T_o}^{T_E} C'_{PE}\,dT + (\Delta H_{R,A})_{T_o}(-r_{AE})V_R}$ ⑪
  - → eqs. 10 and 11 are a system of 2 eqs. with 2 unknowns (X_{AE}, T_E).

- Ex. 1
  - → "Non-Isothermal CSTR"
  - → gas phase rxn: $A + 2B \longrightarrow C$, $-r_A = kC_AC_B$, $k = 2.7\times10^6 \times e^{\frac{-12185}{T}}$ $(m^3/mol.s)$, $U_o = 10\ J/m^2.s.k$, $A = 10\ m^2$, $T_a = 600\ K$
  - → ideal gas, constant P, $F_{A_o} = 3\ mol/s$, $V = 0.4\ m^3$, inlet $T = 600\ K$, $C_{A_o} = 10\ mol/m^3$, $C_{B_o} = 20\ mol/m^3$, $C_{C_o} = 0$
  - → $\Delta H^o_{R,298} = -20\ kJ/mol$, $C_{P_A} = 27.7 + 0.003T\ J/mol.k$, $C_{P_B} = 25.1 + 0.0015T$, $C_{P_C} = 8.7 + 0.13T$
  - → Find the fractional conversion of A, X_{AE}, and exit T, T_E.

- Solution of ex.1 "MBE"
  - → for a CSTR: $-r_{AE} = \frac{F_{Ao}X_{AE}}{V} = kC_{AE}C_{BE}$
  - → construct the stoichiometric table:

comp.	@reactor inlet	@reactor outlet	in terms of X_{AE}
A	F_{Ao}	F_{AE}	$F_{A_o}(1 - X_{AE})$
B	$F_{B_o} = 2F_{A_o}$	$F_{B_o} - 2(F_{A_o} - F_{AE}) = 2F_{AE}$	$2F_{A_o}(1 - X_{AE})$
C	0	F_{CE}	$F_{A_o}X_{AE}$
			$F_{tE} = F_{A_o}(3 - 2X_{AE})$

  - → constant P: $P_o = P_E \Rightarrow C_{T_o}RT_o = C_{TE}RT_E$

$$\Rightarrow C_{TE} = C_{T_o}\left(\frac{T_o}{T_E}\right)$$

  - → $C_{AE} = \frac{F_{AE}}{F_{tE}}C_{TE} \Longrightarrow C_{AE} = \frac{1 - X_{AE}}{3 - 2X_{AE}}C_{T_o}\left(\frac{T_o}{T_E}\right)$, similarly: $C_{BE} = \frac{2(1 - X_{AE})}{3 - 2X_{AE}}C_{T_o}\left(\frac{T_o}{T_E}\right)$
  - → hence, the MBE becomes:

$$V = \frac{F_{A_o}X_{AE}}{2.7\times10^6\, e^{\frac{-12185}{T_E}} \times \frac{2(1 - X_{AE})^2}{(3 - 2X_{AE})^2}C^2_{T_o}\left(\frac{T_o}{T_E}\right)^2} \quad Ⓘ$$

  - → Note that there are 2 unknowns, T_E and X_{AE}, in the above eq. → thus, we need one more eq.

- Solution of ex.1 "EBE"

→ default eq.: $\dot{Q} = \dot{m}\int_{T_0}^{T_E} c'_{p_E}\,dT + (\Delta H_{R,A}|_{T_0})(-r_{AE})V$

$\Longrightarrow U_oA(T_a - T_E) = \sum_i \left(F_{iE}\int_{T_0}^{T_E} c_{p_i}dT\right) + (\Delta H_{R,A}|_{T_0})(-r_{AE})V$

→ $(-r_{AE})V = F_{A_0}X_{AE} \Longrightarrow U_oA(T_a - T_E) = \sum_i \left(F_{iE}\int_{T_0}^{T_E} c_{p_i}dT\right) + (\Delta H_{R,A}|_{T_0})F_{A_0}X_{AE}$

→ sigma term: $\sum_i \left(F_{iE}\int_{T_0}^{T_E} c_{p_i}dT\right) = F_{A_0}(1-X_{AE})\left[\alpha_A(T_E - T_0) + \frac{\beta_A}{2}(T_E^2 - T_0^2)\right]$

$+2F_{A_0}(1-X_{AE})\left[\alpha_B(T_E-T_0) + \frac{\beta_B}{2}(T_E^2 - T_0^2)\right] + F_{A_0}X_{AE}\left[\alpha_C(T_E - T_0) + \frac{\beta_C}{2}(T_E^2 - T_0^2)\right]$

→ $\Delta H_{R,A}|_{T_0} = \Delta H^{\circ}_{R,298} + \int_{298}^{T_0}(\Delta c_{p_i})dT$, where $\Delta c_{p_i} = \Delta\alpha + \Delta\beta . T$, where $\Delta\alpha = \sum_i \nu_i\alpha_i$, $\Delta\beta = \sum_i \nu_i\beta_i$

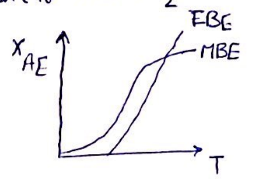
$= \Delta H^{\circ}_{R,298} + \Delta\alpha(T_0 - 298) + \frac{\Delta\beta}{2}(T_0^2 - 298^2)$

→ substituting: $U_oA(T_a - T_E) = F_{A_0}(T_E - T_0)\left[(1-X_{AE})\alpha_A + 2(1-X_{AE})\alpha_B + X_{AE}\alpha_C\right]$

$+ \frac{F_{A_0}(T_E^2 - T_0^2)}{2}\left[(1-X_{AE})\beta_A + 2(1-X_{AE})\beta_B + X_{AE}\beta_C\right]$

$+ F_{A_0}X_{AE}\left[\Delta H^{\circ}_{R,298} + \Delta\alpha(T_0 - 298) + \frac{\Delta\beta}{2}(T_0^2 - 298^2)\right]$

→ solving results: $X_{AE} = 0.796$, $T_E = 752.05^k$



② Multiple Steady States for CSTRs

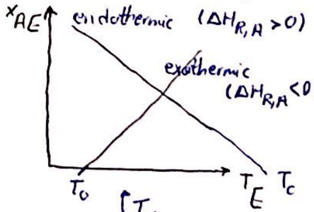
- Let us consider a simple case
  - → Liquid phase rxn, $C_{AE} = C_{A_0}(1 - X_{AE})$
  - → First order kinetics, $-r_{AE} = k_1 C_{AE}$
  - → $\Delta H_{R,A}$ constant, not a function of T
  - → $c'_{p_E} = \bar{c}_p$ " " " " " T
  - → $\dot{Q} = U_oA(T_a - T_E)$
  - → Arrhenius expression: $k_1 = A_1 e^{-E/RT}$

- MBE → $-r_{AE} = \frac{F_{A_0}X_{AE}}{V_R} \Longrightarrow k_1C_{AE} = A_1e^{-E/RT}.\cancel{C_{A_0}}(1 - X_{AE}) = \frac{F_{A_0}X_{AE}}{V_R} = \frac{\cancel{C_{A_0}}\nu_0}{V_R}X_{AE} = \frac{\cancel{C_{A_0}}}{\tau}X_{AE}$

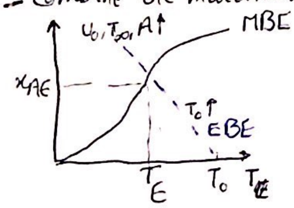
rearranging $\Longrightarrow$ $X_{AE} = \dfrac{A_1e^{-E/RT_E}}{\frac{1}{\tau} + A_1e^{-E/RT_E}}$

- EBE → $U_oA(T_a - T_E) = \dot{m}\bar{c}_p(T_E - T_0) + (\Delta H_{R,A})(-r_{AE})V_R = \dot{m}\bar{c}_p(T_E - T_0) + (\Delta H_{R,A})\frac{F_{A_0}X_{AE}}{\cancel{V_R}}\cancel{V_R}$

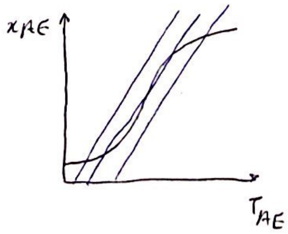
→ rearranging: $\Longrightarrow \frac{U_oA\,T_a + \dot{m}\bar{c}_pT_0}{(\Delta H_{R,A})F_{A_0}} - \frac{U_oA + \dot{m}\bar{c}_p}{(\Delta H_{R,A})F_{A_0}}T_E = X_{AE}$



-- combine the material and EBE:

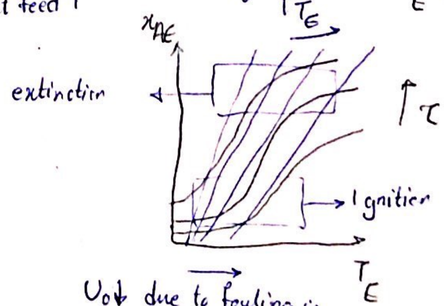


(Endothermic rxns)

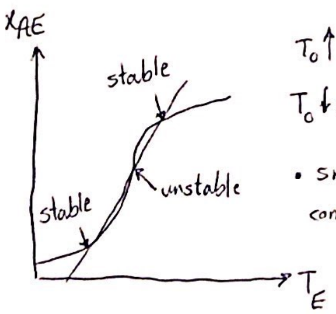


$T_a \triangleq$ ambient or jacket T

$T_0 \triangleq$ inlet feed T



$U_o\downarrow$ due to fouling in heat exchangers



$T_0\uparrow \equiv$ move up the MBE curve

$T_0\downarrow \equiv$ " down in " "

- small change in operating conditions can shift ss position.