Equilibrium conversion & interstage cooling

In a reversible reaction, X_e represents the highest conversion. One cannot exceed this value. So if I ask you to maximise conversion, how do you do this?

Remember Haber-Bosch?

* interstage cooling !

Consider a simple example:

$$A + B \rightleftharpoons 2C \qquad \text{(gas phase)}$$

Start with the stoichiometry table:

Species	Initial	Change	Final
A	N_{A0}	$-N_{A0}X_e$	$N_{A0}(1-X_e)$
B	$N_{B0}=\Theta_B N_{A0}$	$-N_{A0}X_e$	$N_{A0}(\Theta_B-X_e)$
C	0	$2N_{A0}X_e$	$2N_{A0}X_e$
Total	$N_{A0}(1+\Theta_B)$		$N_{A0}(1+\Theta_B)$

Note: $\Delta = 0 \quad \therefore \quad \varepsilon = 0$

$\therefore$ Volume changes will only occur due to temperature changes

$$\therefore \quad v = v_0 (1 + \varepsilon X_e) \left(\frac{P_0 T}{P T_0} \right)$$

$$\therefore \quad v = \frac{v_0 P_0 T}{P T_0}$$

Assume no pressure drop

* If there is, we have to use the Ergun equation that relates:

$\Rightarrow$ (P_0/P) to the weight of the bed traversed,

& $P/P_0 = y$, $\frac{dy}{dW}$ = long expression

$$\therefore \quad v = \frac{v_0 T}{T_0}$$

Now, K_e = equilibrium constant = $\frac{C_C^2}{C_A \cdot C_B}$

$$\therefore \ K_e = \frac{\left(\frac{N_C}{v}\right)^2}{\frac{N_A}{v} \cdot \frac{N_B}{v}} = \frac{N_C^{\,2}}{N_A \cdot N_B}$$

$$\therefore \ K_e = \frac{4 N_{A0}^{\,2} X_e^{\,2}}{N_{A0}^{\,2} (\theta_B - X_e)(1 - X_e)}$$

$$\therefore \ K_e = \frac{4 X_e^{\,2}}{(\theta_B - X_e)(1 - X_e)}$$

$$\therefore \ K_e = \frac{4 X_e^{\,2}}{\theta_B - \theta_B X_e - X_e + X_e^{\,2}}$$

$$\therefore \ K_e \left[X_e^{\,2} - X_e(1 + \theta_B) + \theta_B \right] = 4 X_e^{\,2}$$

$$\therefore \ K_e X_e^{\,2} - (1 + \theta_B) K_e X_e + \theta_B K_e - 4 X_e^{\,2} = 0$$

$$\therefore \ (K_e - 4) X_e^{\,2} - (1 + \theta_B) K_e X_e + \theta_B K_e = 0$$

$$\therefore \ X_e = \frac{(1 + \theta_B) K_e \pm \sqrt{(1+\theta_B)^2 K_e^{\,2} - 4 \theta_B K_e (K_e - 4)}}{2(K_e - 4)}$$

$$\therefore \ X_e = \frac{(1 + \theta_B) K_e \pm \sqrt{K_e^{\,2}(1 + 2\theta_B + \theta_B^{\,2}) - 4\theta_B K_e^{\,2} + 16\theta_B K_e}}{2(K_e - 4)}$$

$$\therefore X_e = \frac{(1+\Theta_B)K_e \pm \sqrt{K_e^2 + 2\Theta_B K_e^2 + \Theta_B^2 K_e^2 - 4\Theta_B K_e^2 + 16\Theta_B K_e}}{2(K_e - 4)}$$

$$\boxed{\therefore X_e = \frac{(1+\Theta_B)K_e \pm \sqrt{K_e^2 - 2\Theta_B K_e^2 + \Theta_B^2 K_e^2 + 16\Theta_B K_e}}{2(K_e - 4)}}$$

→ ①

(from eqb., i.e. MB)

Energy balance:

Adiabatic:

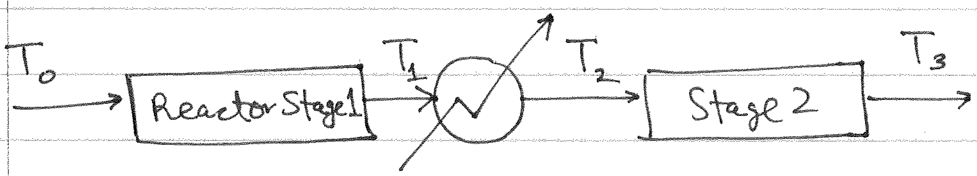
$$-F_{A0}\sum \Theta_i C_{pi}(T - T_{i0}) - F_{A0} X_A\left[\Delta H_{rxn}^{\circ}(T_R) + \Delta C_{p\,rxn}(T - T_R)\right] = 0$$

Non-adiabatic:

$$\frac{dT}{dV} = \frac{r_A \Delta H_{rxn} - Ua(T - T_c)}{F_{A0}\left[\left(\sum \Theta_i C_{pi}\right) + \Delta C_{p\,rxn} X_e\right]}$$

$$\frac{dT_c}{dV} = \frac{Ua(T - T_c)}{\dot{m}_c C_{p\,cool}}$$

Let's ponder about this :



How do we operate the reactors?

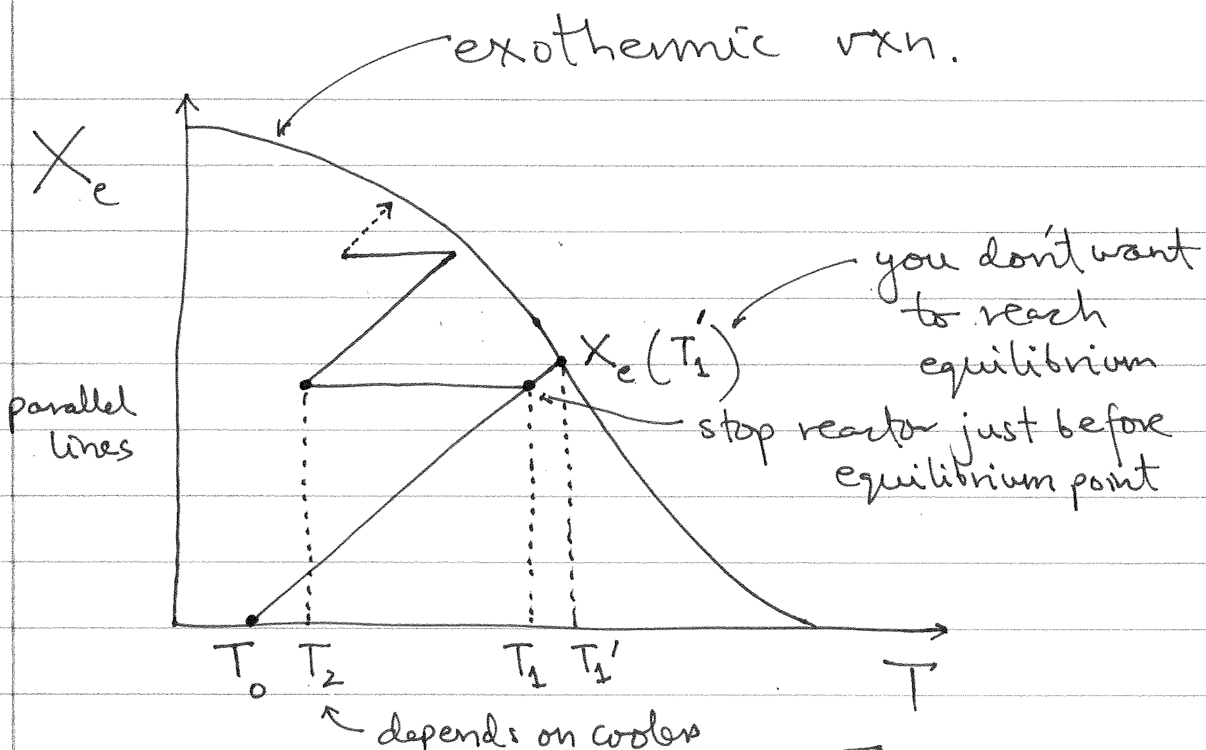
How does one operate the coolers?

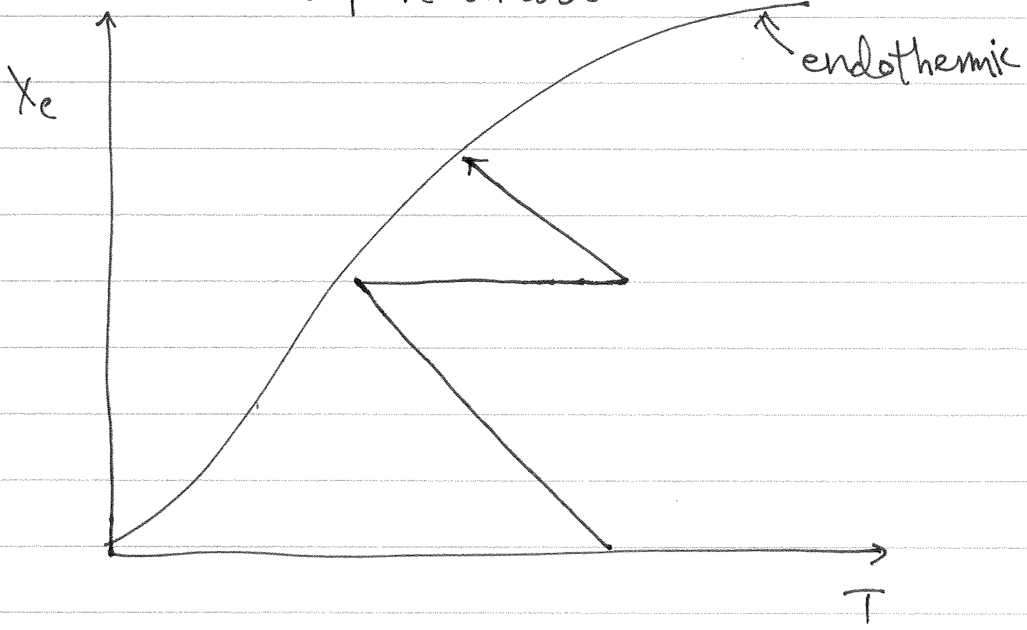
↳ flash cooling = you want this to be instantaneous so that equilibrium X_e is not changed

Adiabatic preferred since it allows stoppage of reactor before Xe is reached.

$$\therefore X^{EB} = \frac{\sum \Theta_i C_{p_i} (T - T_{i0})}{-\Delta H^{\circ}_{rxn}(T_R) - \Delta C_{p_{rxn}} (T - T_R)}$$

straight line

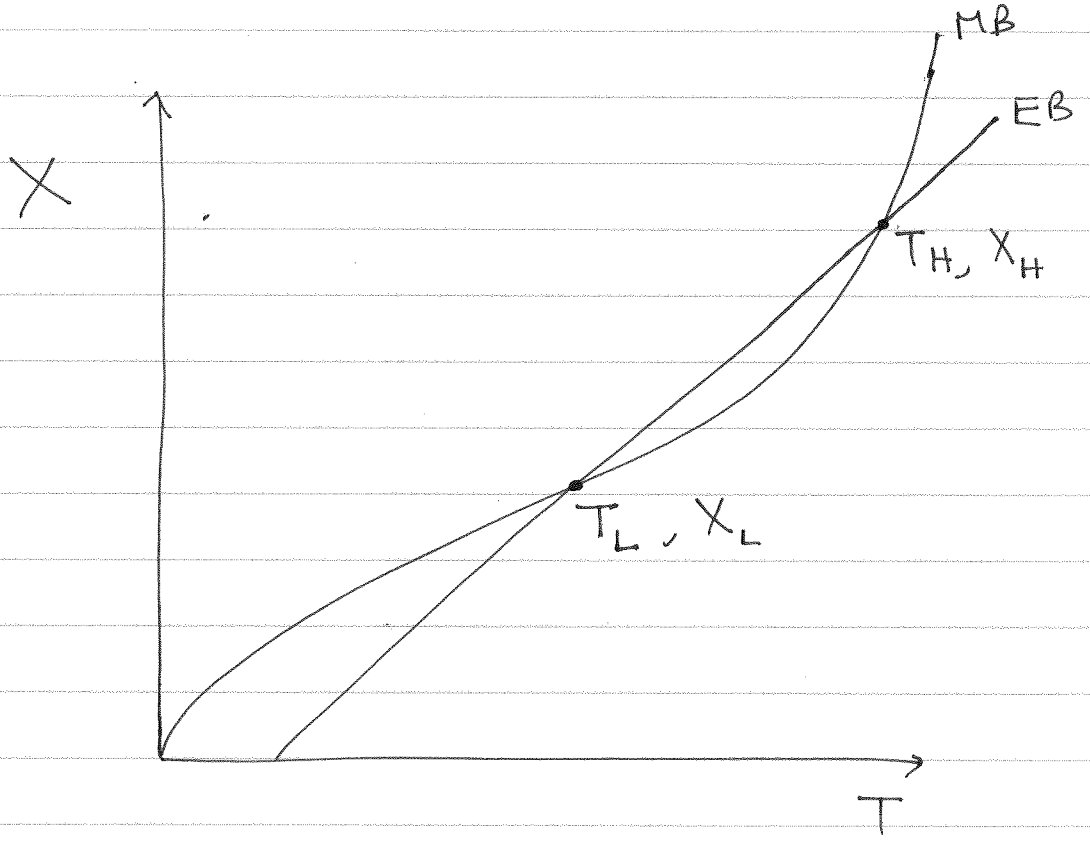




* One is able to exceed nominal X_e through use of interstage flash cooling!

Metastability & accidents

Consider a CSTR:-



- There are multiple operating points. {you can get this for PFRs ~~too~~ but very common for CSTR}

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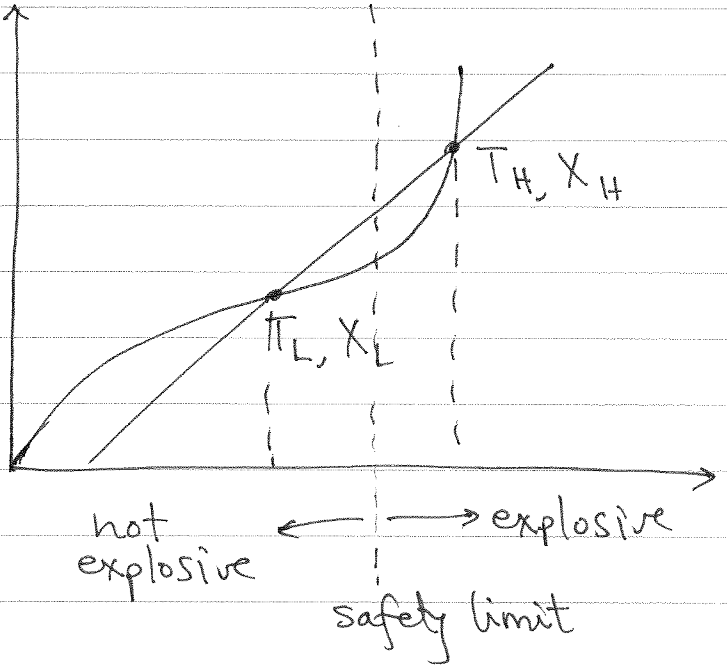
- This is called case of multiple steady states
- when this happens, control goes out the window!

Consider a case:



* This is a common cause of accidents in the industry.

* PFRs have better control ≡ you can simply manipulate volume/residence time

* CSTRs are trickier!