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L-21 9/11/2012

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Tubular Reactors heated/Cooled From Wall.

$$v C_p \frac{dT}{dV} = \sum_{i=1}^{p} r_i (-\Delta H_i^*) + q - W_s$$

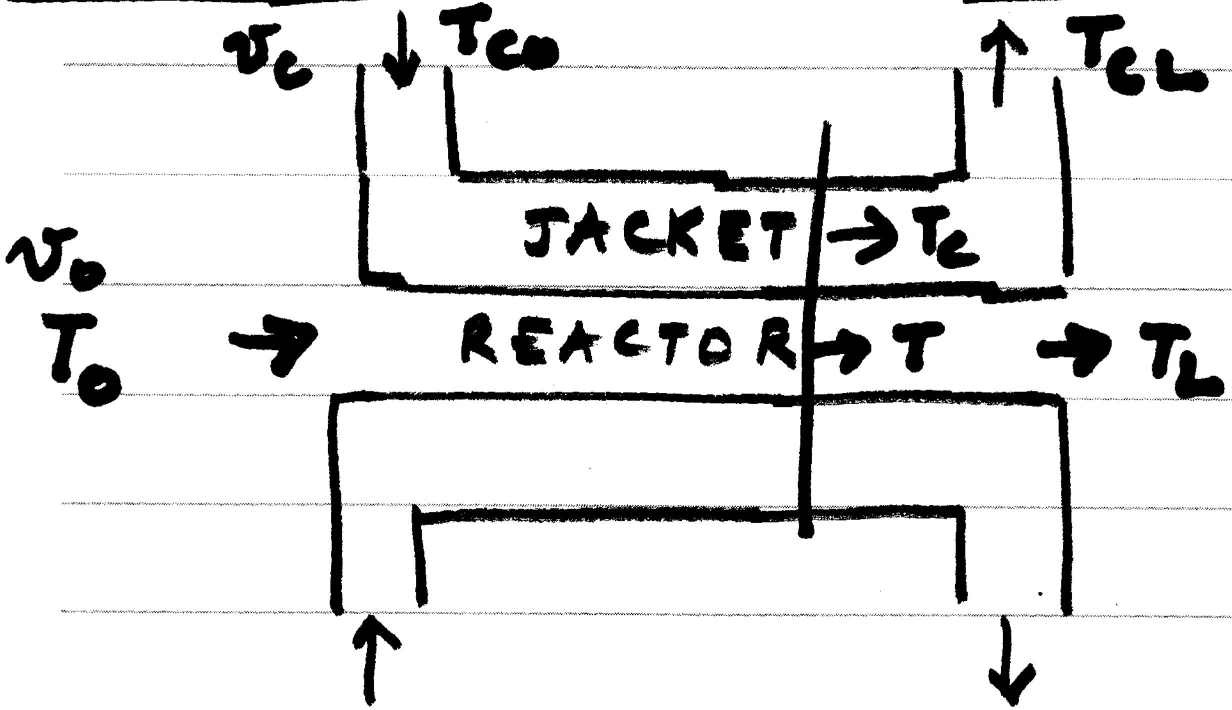
$$= \sum r_i (-\Delta H_i^*) + \frac{4h}{D}(T_c - T).$$

Friday 9 Nov 12

T_c

T

Tubular Reactor heated or Cooled from Wall



cocurrent

No phase change

$$\frac{dx_j}{dV} = f_j(x_1 \ldots x_r, T) \quad (r \text{ equations}) - (1)$$

$$v C_p \frac{dT}{dV} = \sum_{i=1}^{p} (-\Delta H_i^*)\, r_i(x_1, x_2 \ldots x_r, T) + \frac{4h}{D}(T_c - T) \quad \ldots (2)$$

Overall balance (no phase change)

$$v_0 C_p (T_0 - T_R) + v_c C_{pc} (T_{c0} - T_R) + \sum_{i=1}^{r} F_{A0} X_i (-\Delta H_i^*) = v_0 C_p (T - T_R) + v_c C_{pc} (T_c - T_R) \quad -(3)$$

where $F_{A0} X_i$ is the mol/s of 'i' independent reaction and so $\sum_{i=1}^{r} F_{A0} X_i (-\Delta H_i^*)$ is the heat absorbed or released per unit time

~~Substituting~~ From (3)

$$T_c = T_{c0} + \frac{v_0 C_p (T_0 - T) + \sum_{i=1}^{r} F_{A0} X_i (-\Delta H_i^*)}{v_c C_{pc}} \quad -(4)$$

So the differential eqn governing are

$$\frac{dX_j}{dV} = f_j(X_1, X_2 \ldots X_r, T)$$

$$\nu C_p \frac{dT}{dV} = \frac{4h}{D}(T_c - T) + \sum_{i=1}^{p} (-\Delta H_i^*) r_i (X_1, X_2 \ldots X_r, T)$$

$$T_c = T_{c0} + \nu_0 C_p (T_0 - T) + \sum_{i=1}^{r} F_{A0} X_i (-\Delta H_i^*)$$

$\nu_c C_{pc}$

$X_1 \ldots X_r = 0$ @ $V = 0$

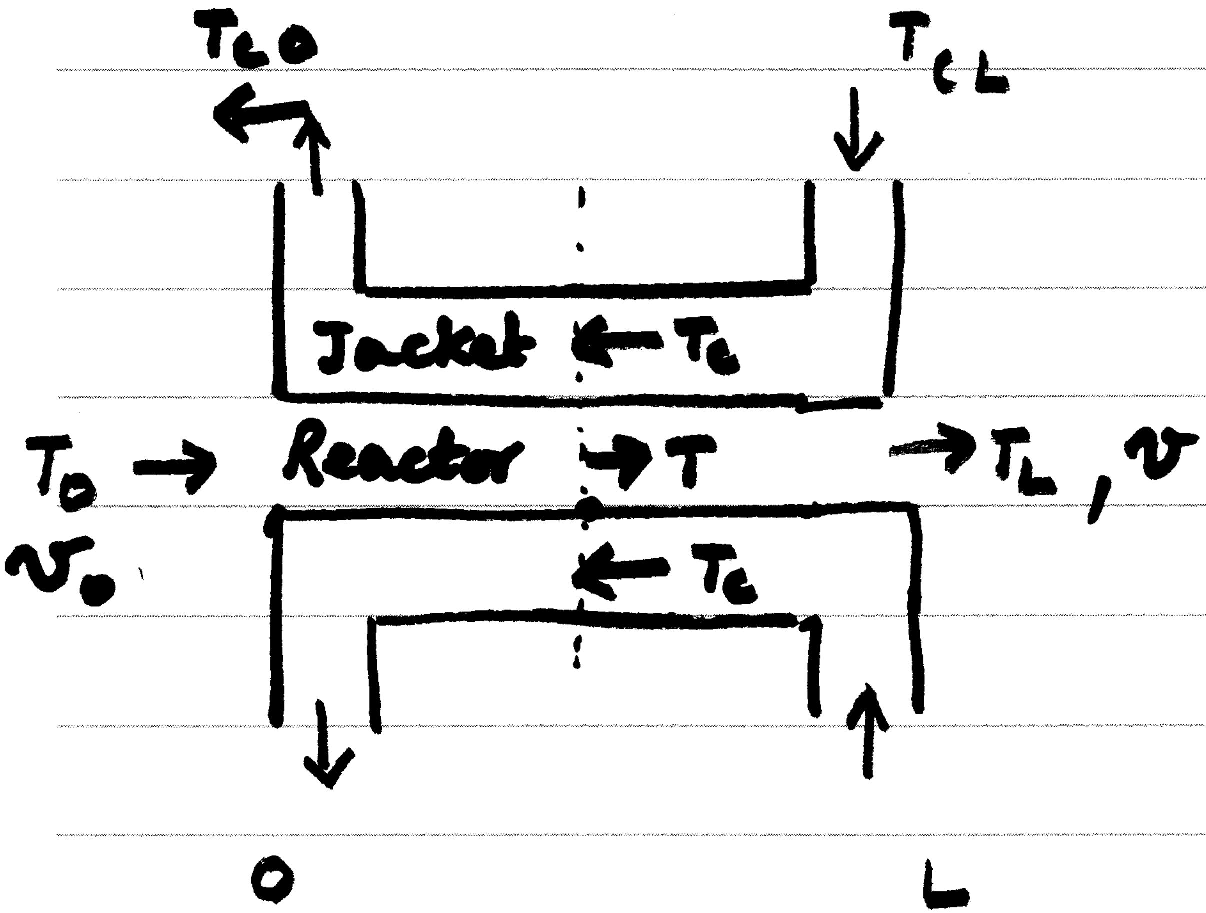
$T = T_0$ @ $V = 0$

$T_c = T_{c0}$ @ $V = 0$

So Equations can be integrated by a forward Marching Routine

Tubular Reactors heated / cooled from Wall

Countercurrent Flow



$$v C_p \frac{dT}{dV} = \sum_{i=1}^{p \text{ rxns}} r_i (-\Delta H_i^*) + \frac{4h}{D}(T_c - T) \quad - (1)$$

$$\frac{dx_j}{dV} = f_j(x_1 \cdots x_r, T) \quad \text{.. r equations} \quad \text{.. (2)}$$

overall balance between '0' & any position

$$v_0 C_p (T_0 - T_R) + v_c C_{pc} (T_c - T_R) + \sum_{i=1}^{r} F_{A0} x_j (-\Delta H_j^*)$$

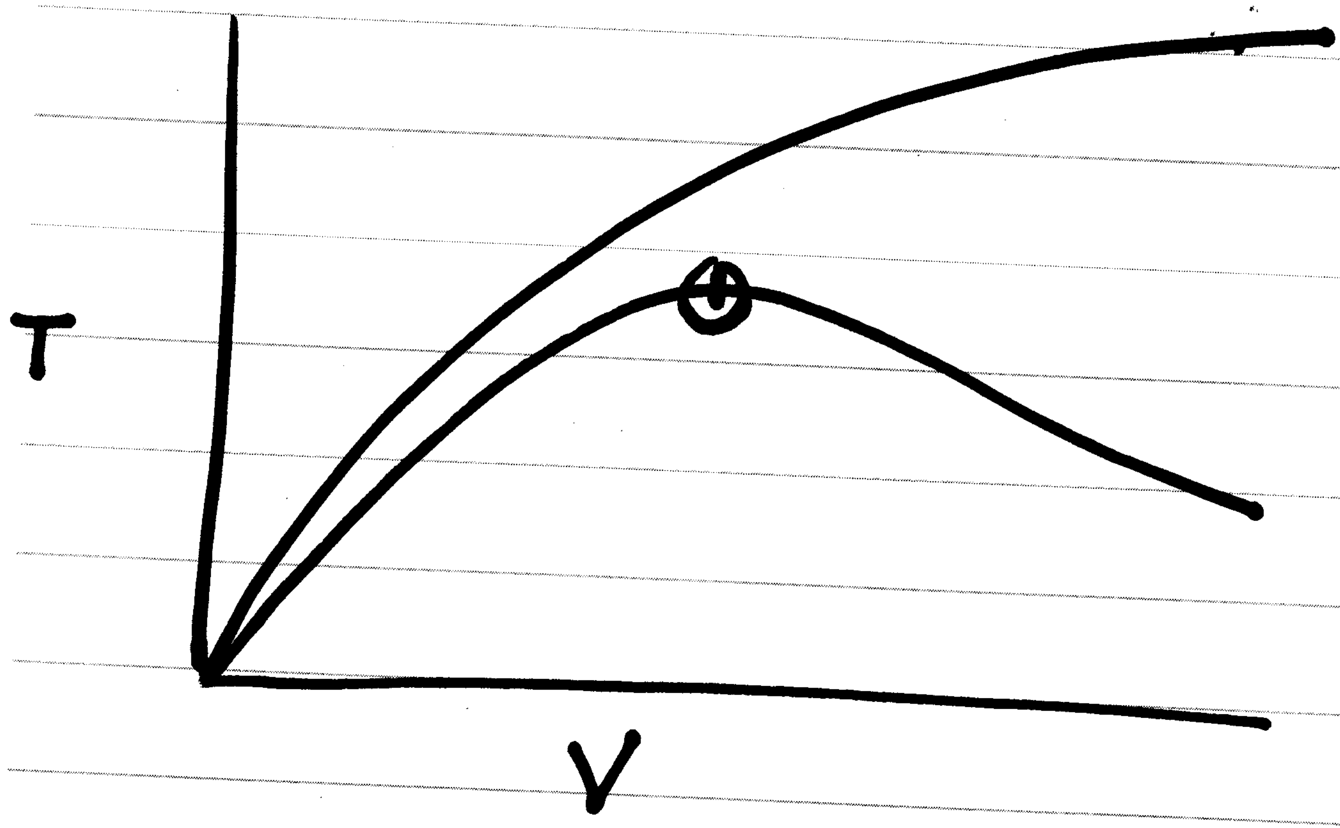
$$= v_c C_{pc} (T_{c0} - T_R) + v C_p (T - T_R) \quad - (3)$$

$$T_c = \frac{T_{c0} + v C_p (T - T_0) - \sum_{i=1}^{r\ (\text{ind rxns})} F_{A0} X_j (-\Delta H_j^*)}{v_c C_{pc}} \quad \ldots (4)$$

overall balance between 0 + L

$$v C_p (T_0 - T_R) + v_c C_{pc} (T_{cL} - T_R) + \sum_{i=1}^{r} F_{A0} X_j(L) (-\Delta H_j^*)$$

$$= v C_p (T_L - T_R) + v_c C_{pc} (\underline{T_{c0}} - T_R) \quad \ldots (5)$$



exo.

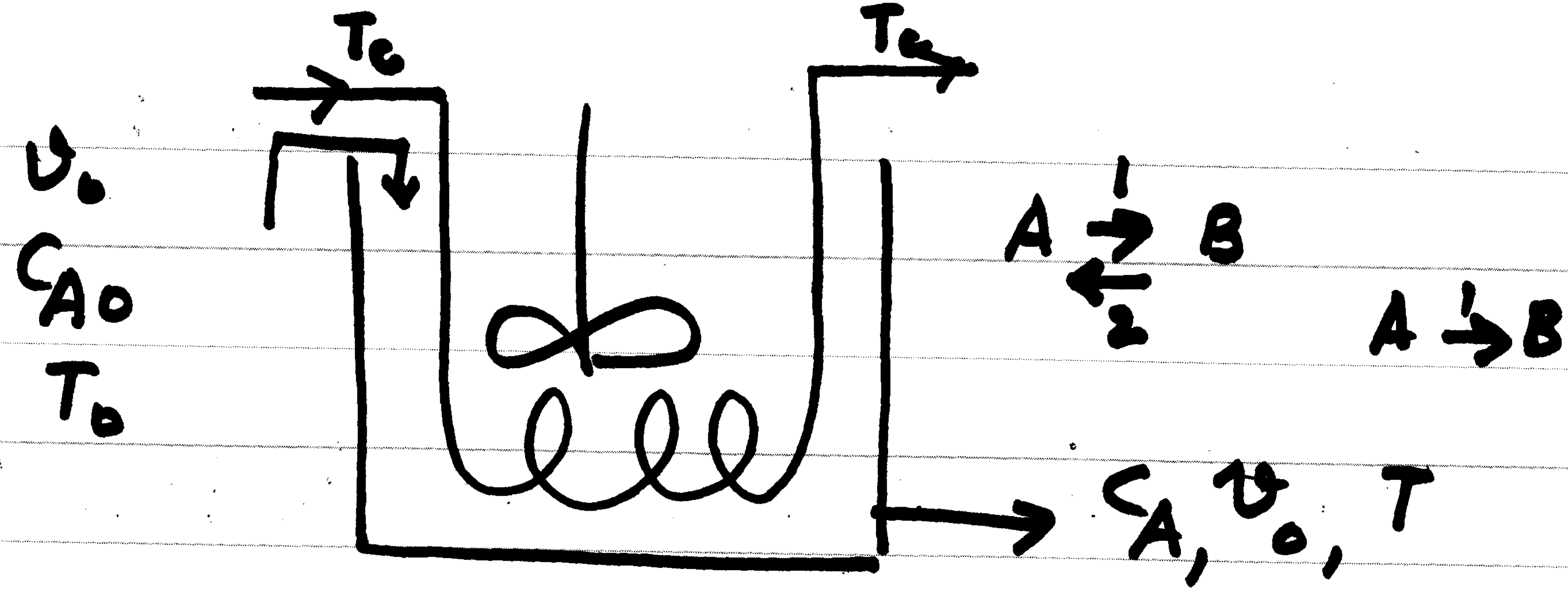
SOLUTION PROCEDURE

1) Assume T_{co}
2) Replace T_c in Eqn (1) from Eqn (4)

3) Now Eqn (1) and (2) RHS is fully specified since T_c at $z=0$, x_j (at $z=0$, T at $z=0$ are all specified. So Eqn (1) and (2) can be integrated by forward march Runge Kutta. The integration gives T, T_c, x_j (for all r eqns). for all $z = 0$ to L.
4) Using T (at $z=L$) check if Eqn (5) is satisfied. Else repeat with new value of T_{co} till Eqn (5) is

Advanced Reaction Engineering

Transient Behavior of Exothermic Reactions in CSTR



$$F_{A0} - F_A + r_A V = \frac{d}{dt} N_A \qquad -(1)$$

Let us define a variable $x = \dfrac{C_{A0} - C_A}{C_{A0}}$

Note x has meaning of Conversion only at Steady State. Under Unsteady State its just a variable

$$\cancel{v_0} C_{A0} - \cancel{v} C_A - r_1 \left(\frac{V}{v_0}\right) = \left(\frac{V}{v_0}\right) \frac{dC_A}{dt}$$

$A \rightarrow B$

Not $r_A = (-1)\, r_1$; V = Constant assumed

$v = v_0$ assumed so that;

$$-\tau \frac{dx}{dt} = x - \frac{r_1 \tau}{C_{A0}}$$

$$\tau \frac{dx}{dt} = -x + \frac{r_1 \tau}{C_{A0}} \qquad (1)$$

where $\tau = V/v_0$

Energy Balance

A → B

$$V\hat{C}_p \frac{dT}{dt} = v_0 \bar{C}_p (T_0 - T) + r_1 V(-\Delta H_1^*) + Q - \cancel{W_s}$$

$$\frac{V\hat{C}_p}{v_0 \bar{C}_p}\frac{dT}{dt} = (T_0 - T) + \frac{r_1 V(-\Delta H_1^*)}{v_0 \bar{C}_p} + \frac{Q}{v_0 \bar{C}_p}.$$

$$(\tau)\frac{dT}{dt} = (T_0 - T) + r_1 \tau J_1 + \left(\frac{hA}{v_0 \bar{C}_p}\right)(T_c - T) \qquad -(2)$$

$$J_1 = (-\Delta H_1^*)/\tilde{C}_p \qquad \frac{hA}{v_0 C_p} = \beta.$$

$$\tau \frac{dT}{dt} = (T_0 - T) + \lambda_1 \tau J_1 + \beta (T_c - T).$$

where $\beta = \frac{hA}{v_0 C_p} : \frac{(\text{kcal}/\text{m}^2 \cdot {}^\circ\text{C}/\text{hr})\,\text{m}^2}{(\text{m}^3/\text{hr})(\text{kcal}/\text{m}^3 \cdot {}^\circ\text{C})}$ = dimensionless

$$\tau \frac{dT}{dt} = \left[(1+\beta)(T_c^* - T)\right] + (\lambda_1 \tau J_1). \quad \cdots (3)$$

where $T_c^*(1+\beta) = T_0 + \beta T_c$ — (3 a)

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$$\tau \frac{dx}{dt} = -x + \frac{r_1 \tau}{c_{x0}}$$

$$\tau \frac{dT}{dt} = (1+\beta)(T_c^{*} - T) + r_1 \tau J_1$$

At steady state

$$\tau \frac{dT_s}{dt} = 0 = \underbrace{(1+\beta)(T_c^* - T_s)}_{-U_{rs}} + \underbrace{r_{1s} J_1 \tau}_{U_{gs}} \quad \text{- (5)}$$

$$\tau \frac{dX_s}{dt} = 0 = -X_s + \frac{r_{1s}\tau}{c_{A0}} \quad \text{-- (4)}$$

Let $U_{gs} = r_{1s} \tau J_1$ and

$U_{rs} = (1+\beta)(T_s - T_c^*)$ so that

steady state is represented by $U_{gs} = U_{rs}$

Example

$$r_{1S} = k_{1S} C_{AS} = k_{1S} C_{A0} (1 - x_S)$$

From (4)

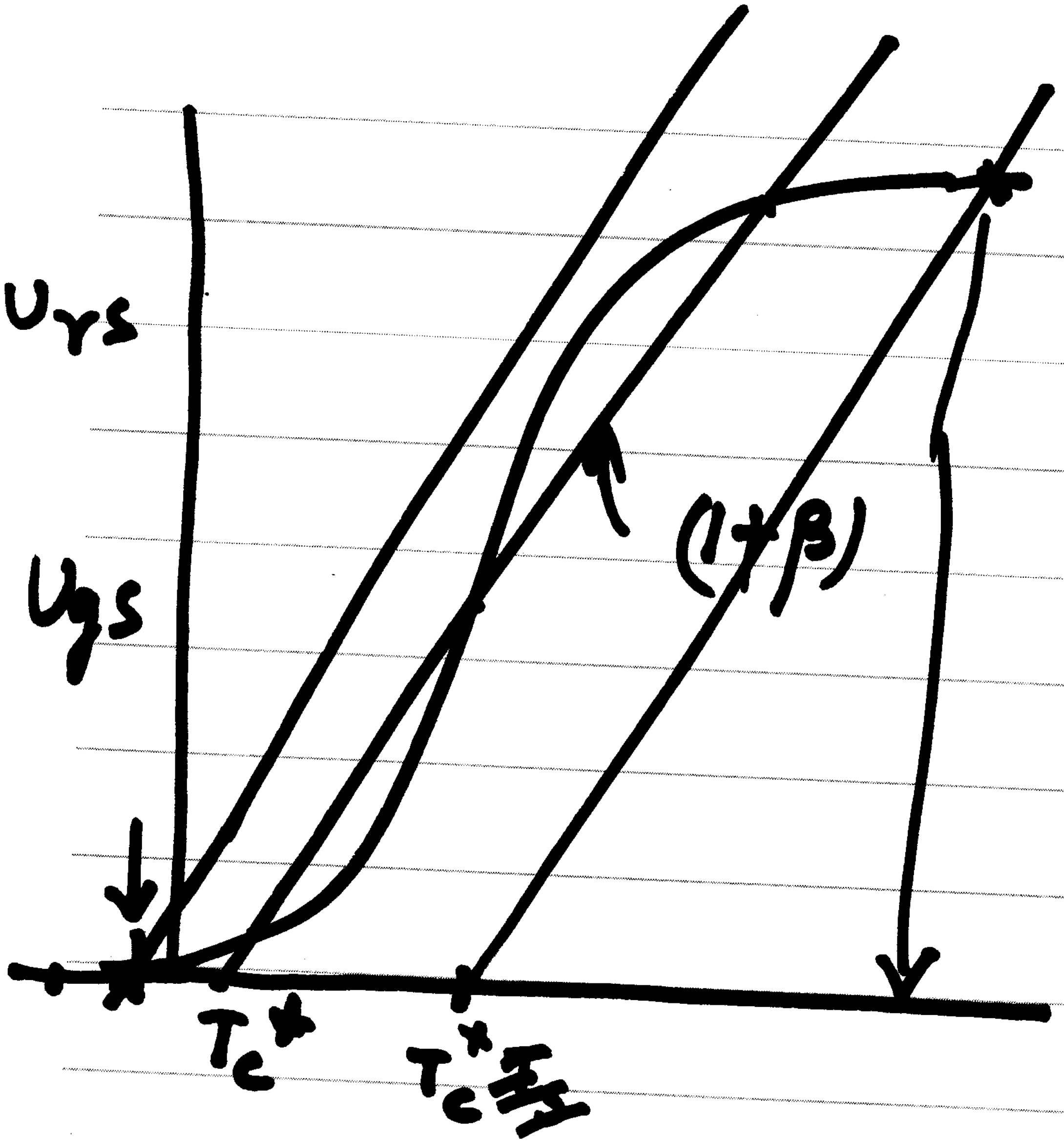
$$x_S = k_{1S} C_{A0} (1 - x_S) \tau / C_{A0}$$

$$x_S = k_{1S} \tau (1 - x_S)$$

$$x_S = \frac{k_{1S} \tau}{(1 + k_{1S} \tau)} = k_{1S}(T) \tau / (1 + k_{1S}(T) \tau)$$

$$U_{gS} = r_{1S} \tau J_1 = k_{1S} C_{A0} (1 - x_S) \tau J_1$$

$$= (k_{1S} \tau) C_{A0} J_1 / (1 + k_{1S} \tau) = \underline{C_{A0} x_S J_1}$$



$$U_{gs} = \frac{k_{1s}\tau}{1+k_{1s}\tau} c_{A0} J_1$$

$$U_{rs} = (1+\beta)(T_s - T_c^*)$$

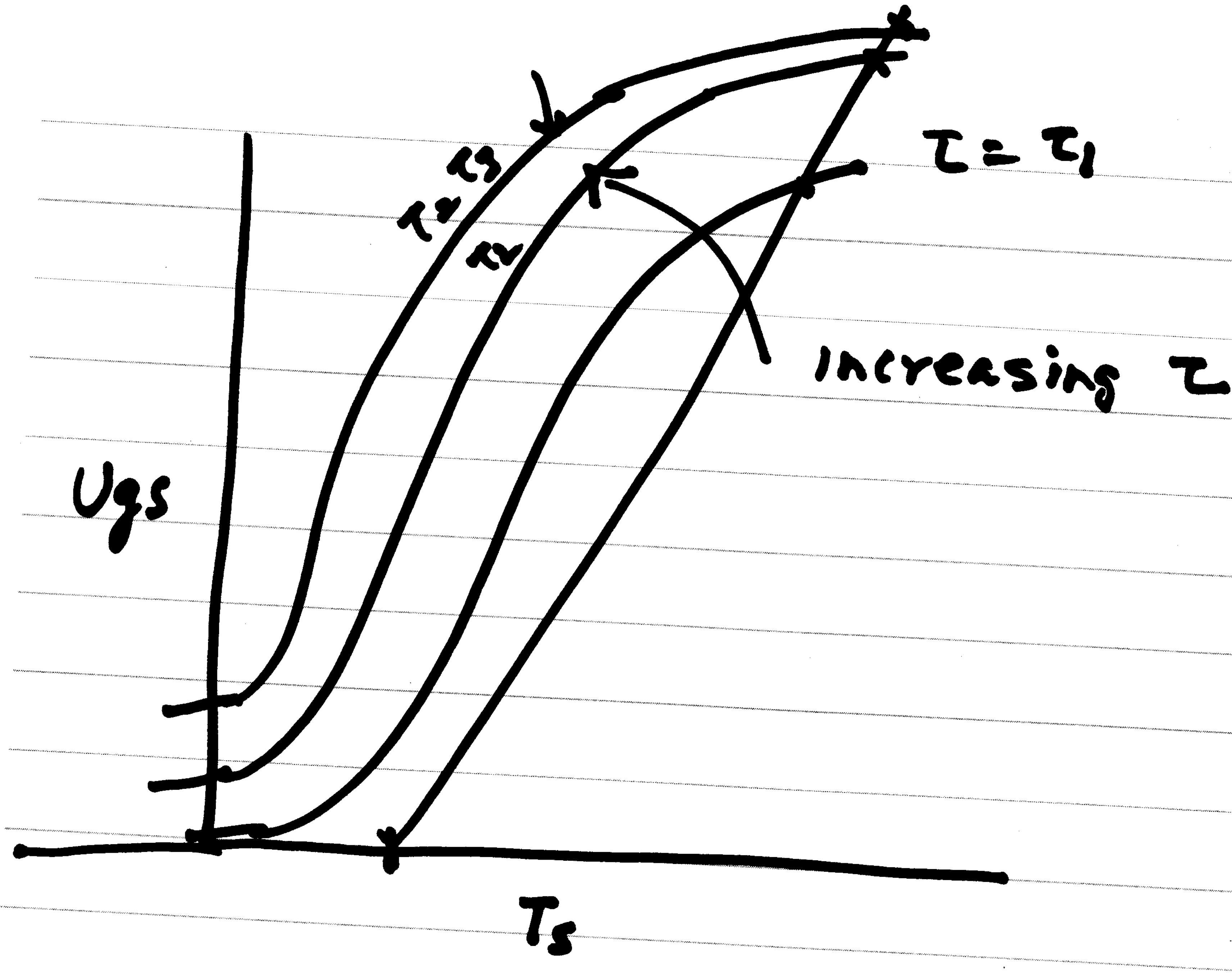
$$U_{gs} = U_{rs}$$

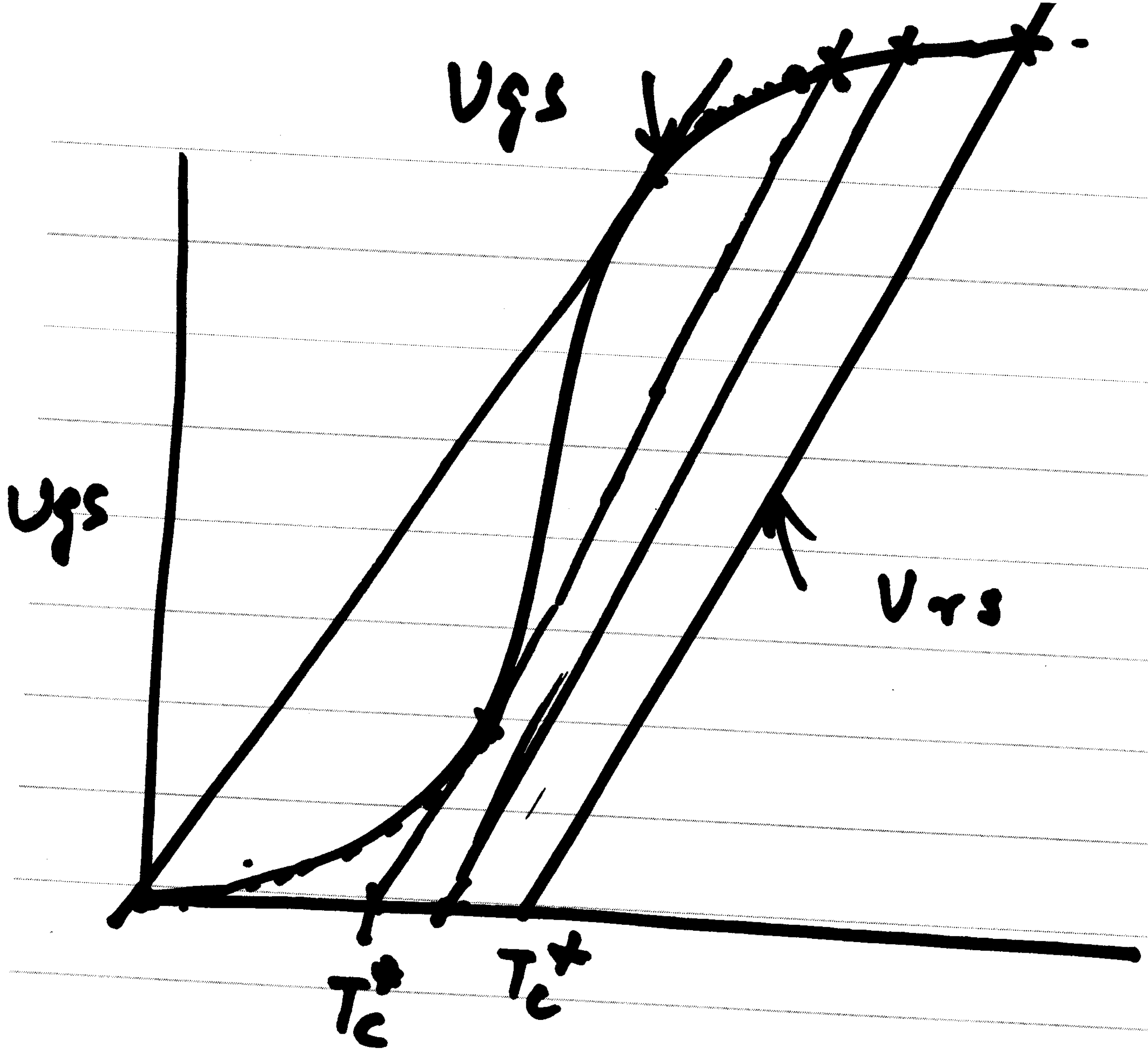
Exothermic Stirred Tank.

1 SS. (Lower

1 SS (upper).

3 SS ( )


τ = τ1
Increasing τ
Ugs
Ts



4

Stability of Steady States.

$$\tau \frac{dx}{dt} = -x + \frac{r_1 \tau}{C_{A0}} \qquad (1)$$

$$\tau \frac{dT}{dt} = (1+\beta)(T_c^* - T) + r_1 \tau J_1 \qquad (2)$$

SS

$$\tau \frac{dx_s}{dt} = 0 = -x_s + r_{1s} \tau / C_{A0}. \qquad (3)$$

$$\tau \frac{dT_s}{dt} = 0 = (1+\beta)(T_c^* - T_s) + r_{1s} \tau J_1 \qquad (4)$$

$$\tau \frac{d}{dt}(X - X_s) = -(X - X_s) + (r_1 - r_{1s})\frac{\tau}{C_{A0}} \quad (5)$$

$$\tau \frac{d}{dt}(T - T_s) = -(1+\beta)(T - T_s) + (r_1 - r_{1s})\tau J_1 \quad -(6)$$