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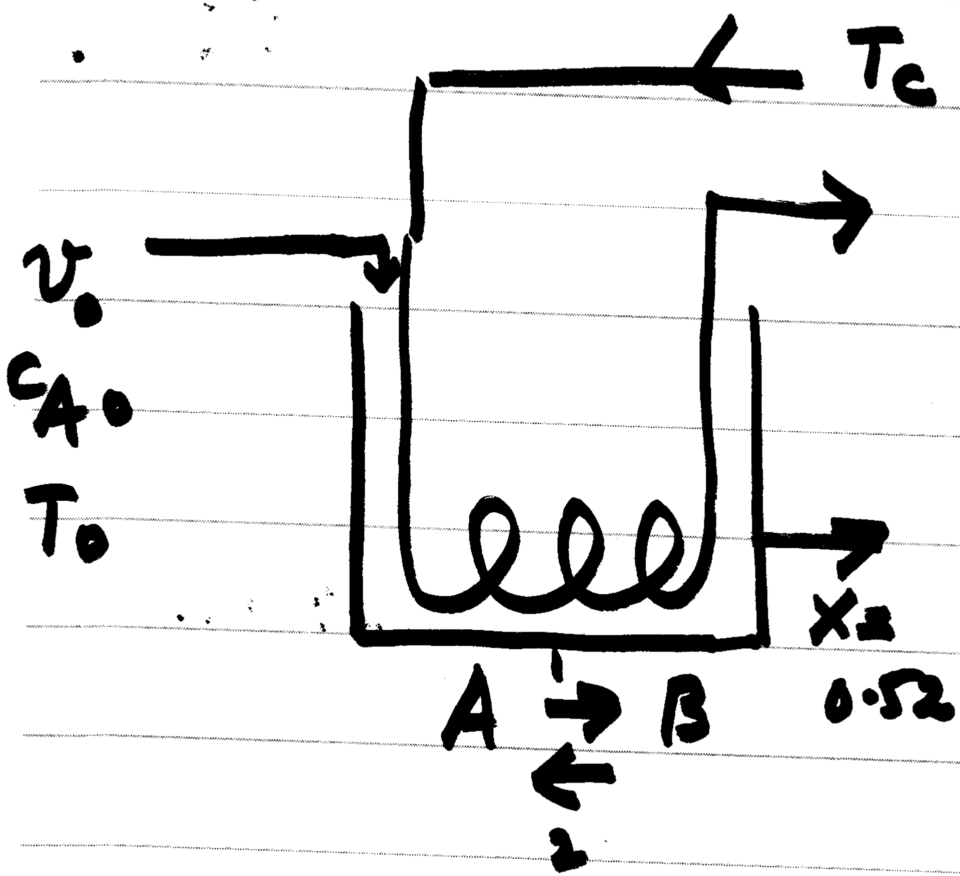
Lec. 28 22/11/2012

Advanced Reaction Engineering

Practice Problem (Energy Balance)

22 NOV 12
Thursday
1400-1500



$C_{A0} = 1.66 \text{ kmol}/m^3$

$T_0 = 21 \, C$

$v_0 = 0.6 \, m^3/hr$

$E_1 = 25000 \text{ kcal/kmol}$

$T_c = 10 \, C$

$h(\text{Coolant-Reactants}) = 1000 \dfrac{\text{kcal}}{m^2 \, hr \, C}$

$\Delta H_{(A \to B)} = -20{,}000 \text{ kcal/kmol.}$

T(K)	293	303	(315)	323
k_1	1.06	4.37	21.3	57.2
K_e	21.6	6.96	1.97	0.89

$$A \underset{2}{\overset{1}{\rightleftarrows}} B$$

(1) Derive locus of max rates

$$r_B = k_1 C_A - k_2 C_B$$

$$= k_1 C_{A0}(1-X) - k_2\left(\cancel{C_{B0}} + C_{A0} X\right)$$

$$\left(\frac{\partial r_B}{\partial T}\right)_X =$$

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$$r_B = k_1 C_{A0}(1-X) - k_2 C_{A0} X$$

$$\left(\frac{\partial r_B}{\partial T}\right)_X = \frac{k_1 E_1}{RT^2} C_{A0}(1-X) - \frac{k_2 E_2}{RT^2} C_{A0} X = 0$$

$$(1-X_m)\frac{k_1 E_1}{RT^2} C_{A0} = \frac{k_2 E_2}{RT^2} C_{A0} X_m$$

$$\left(\frac{X_m}{1-X_m}\right) = \frac{k_1}{k_2}\left(\frac{E_1}{E_2}\right) = K\left(\frac{E_1}{E_2}\right) \Rightarrow X_m = \frac{K\delta}{K\delta+1}$$

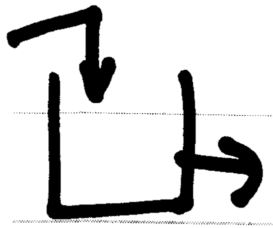
$\Rightarrow \delta$

$$r_B = k_1 C_{A0}(1-X) - k_2 C_{A0} X$$

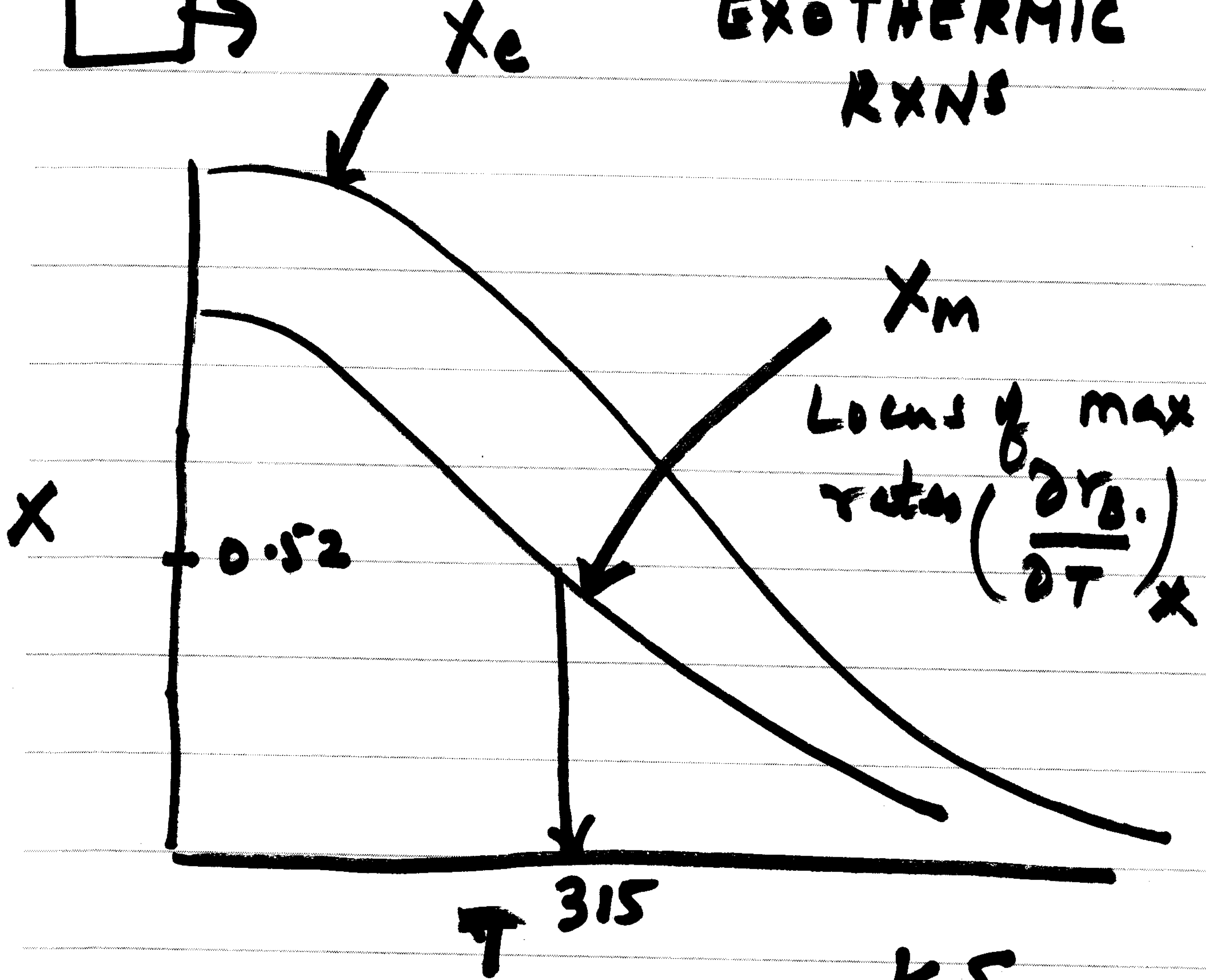
at equilibrium $r_B = 0$

$$k_1 C_{A0}(1-X_e) = k_2 C_{A0} X_e$$

$$\frac{X_e}{1-X_e} = \frac{k_1}{k_2} = K \Rightarrow \quad X_e = \frac{K}{K+1}$$



EXOTHERMIC RXNS

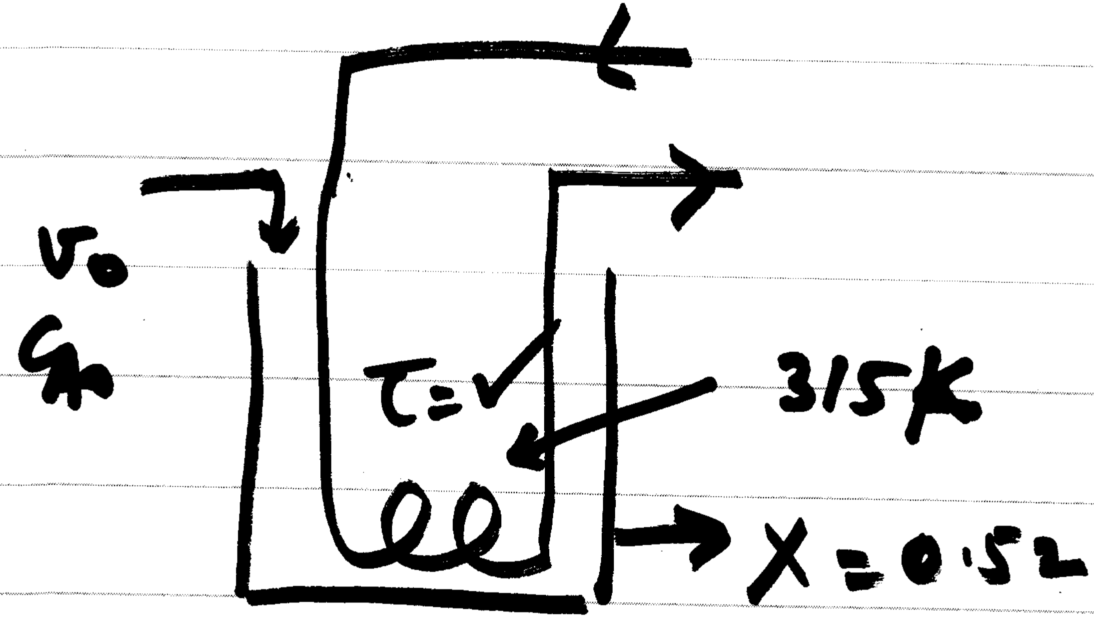


$$X_e = \frac{K}{K+1} = \frac{1}{\left(1 + 1/K\right)}$$

K decreases as T increases

$$X_m = \frac{K\delta}{1+K\delta} = \frac{1}{\left(1+\frac{1}{K\delta}\right)}$$

$$X_m = 0.52 = \frac{K\delta}{1+K\delta}$$

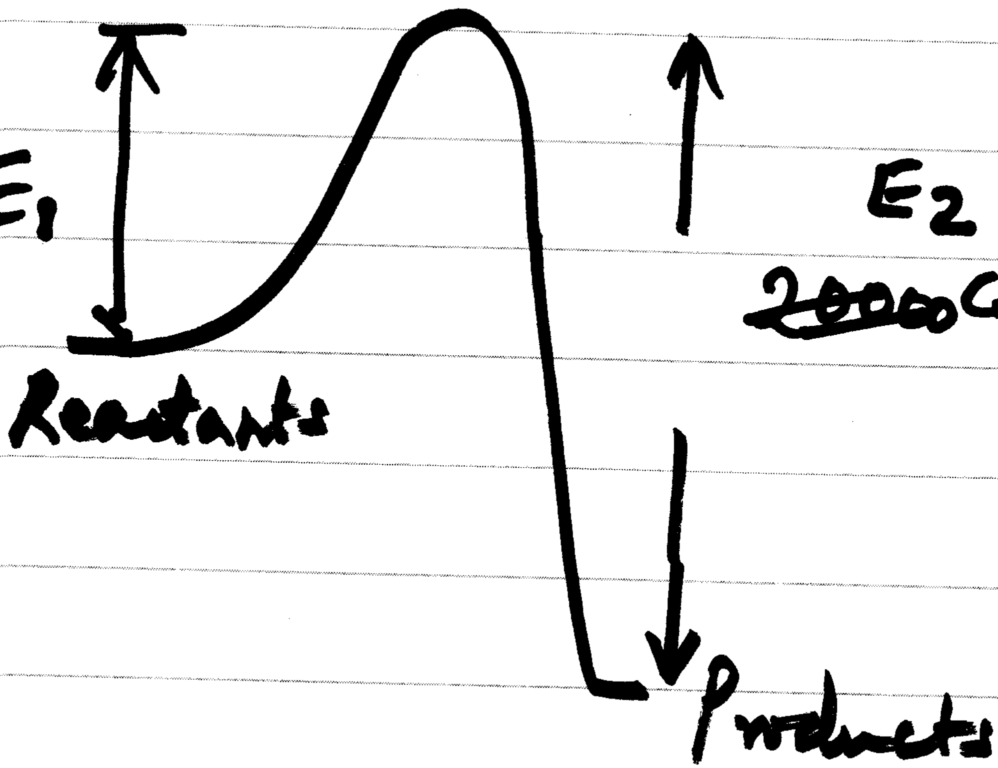


optimum conditions to achieve X = 0.52

$$\frac{X_m}{1-X_m} = \frac{1}{(1 + 1/k\tau)}$$

$$\frac{0.52}{1-0.52} = \frac{1}{(1 + 1/k\tau)}$$

$$\delta = \frac{E_1}{E_2} \; ; \; \frac{25000}{45000} = \frac{5}{9} = \underline{\underline{0.55}}.$$



$E_2 = 45000$

~~20000 cal/mol.~~

$-20{,}000 \frac{\text{cal}}{\text{mol.}}$

$$E_1 - E_2 = (\Delta H)$$

$$25000 - E_2 = -20000$$

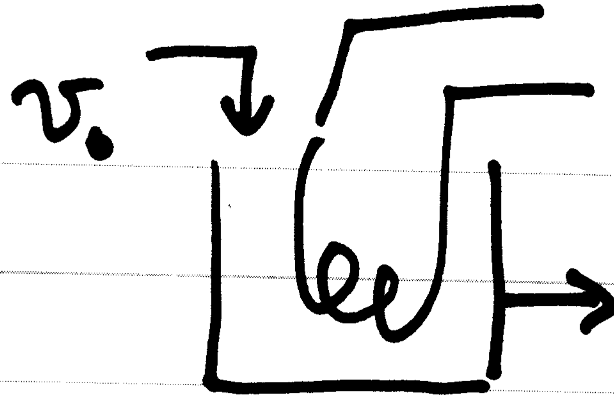
$$E_2 = 45000 \text{ cal/mol.}$$

$$\frac{0.52}{1-0.52} = K \cdot \frac{25000}{45000}$$

$$K = 1.97$$

So choose T of reactor so that $K = 1.97 \Rightarrow$

$$T = 315\ K$$



$x = 0.52$

$T = 315°$

$\tau = ?$

$Q = ?$

$C_A = C_{A0}(1-x)$

$C_B = \cancel{C_{B0}} + C_{A0}x$

Material Balance

$$F_{A0} - F_A + r_A V = \cancel{\text{Accumulation}}$$

$$F_{A0} - F_{A0}(1-x) - (k_1 C_A - k_2 C_B) V = 0$$

$$F_{A0}x - (k_1 C_{A0}(1-x) - k_2 C_{A0}x) V = 0$$

$$x - (1-x)k_1\tau + k_2\tau x = 0$$

Material Balance

$$X(1+k_1\tau+k_2\tau) = k_1\tau$$

$$X = \frac{k_1\tau}{1+k_1\tau+k_2\tau}$$

$k_1(315) = 2.34/hr$

$k_2(315) = 10.8/hr$

$k_1(315)$; $k_2(315\ K)$

$$0.52 = \frac{2.34\tau}{1+2.34\tau+10.8\tau} \Rightarrow \tau = \underline{\underline{0.11/hr}}$$

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$$V = v_0 \tau = (0.6)(0.1) = 0.06\ m^3$$

$$= \cancel{0.6}\ m^3/hr$$

$F_{A0} X$

Energy Balance for CSTR

$$\overset{0}{\cancel{V C_p \frac{dT}{dt}}} = v_0 C_p (T_0 - T) + (r_1 - r_2)(-\Delta H_1^{*}) V + Q - \cancel{W_s}$$

(SS)

$$0 = 0.6\ \frac{m^3}{hr} \cdot 1000 (40 - 42) + F_{A0} X (-\Delta H_1^{*}) + Q$$

$$+ (0.6)(166)(0.5)(2000) \times 0.52 + Q.$$

$$Q = -3158\ kcal/hr$$

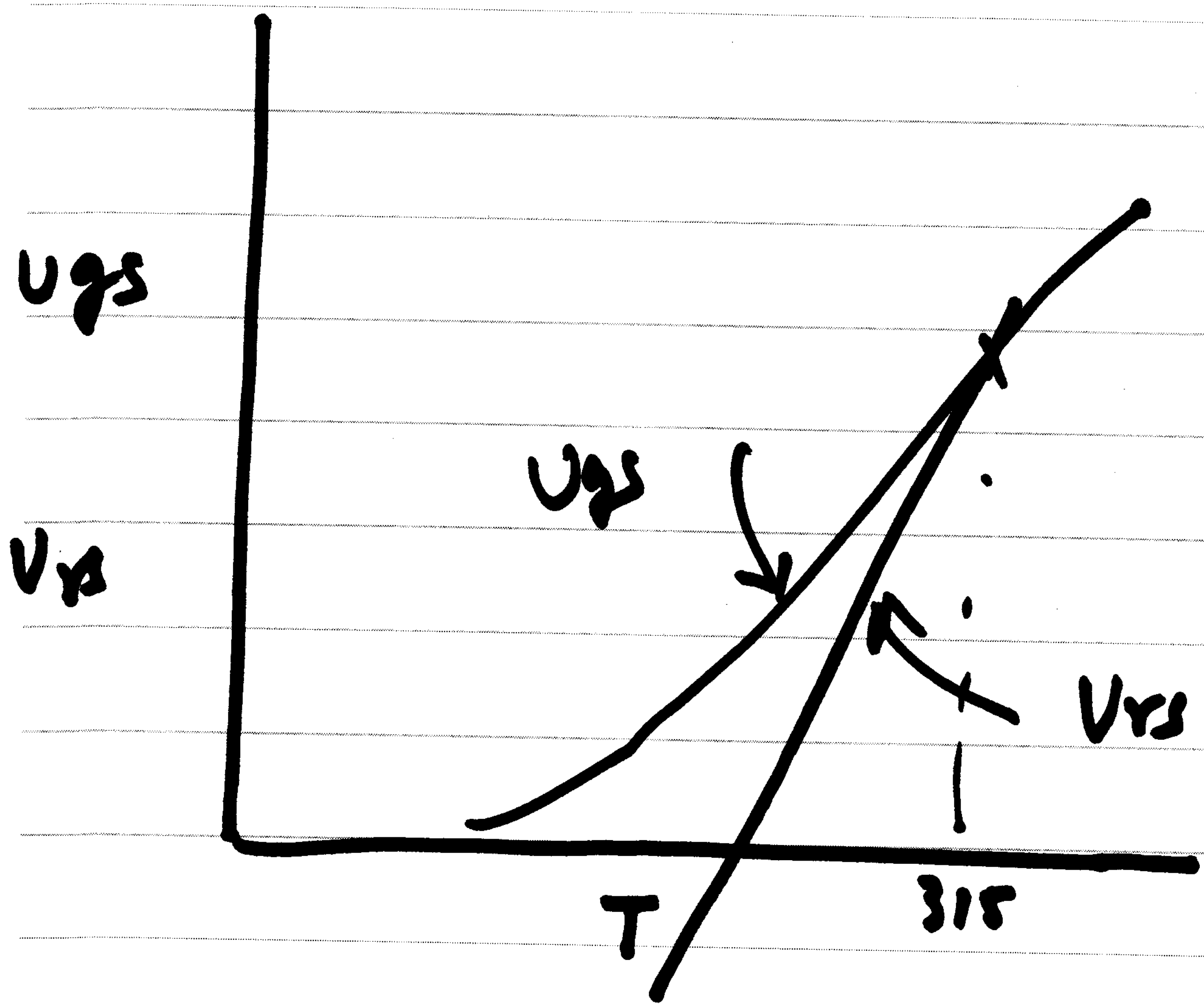
$Q = -3158$ Kcal/hr

$h A \Delta T = Q$

$$A = \frac{Q}{h \Delta T} = \frac{3158}{(1000)(42-10)} = 0.26 M^2$$

$(315K - 10c)$.

Steady State Stability



U_g = heat ~~removal~~ generation

U_r = heat removal

$$U_{gs} = (r_{1s} - r_{2s})\,\tau\,J_1$$

$$= (r_{1s} - r_{2s}) = C_n X_s / J$$

$$U_{gs} = C_n X_s J = \frac{C_n k_{1s} \tau J_1}{(1 + k_{1s}\tau + k_{2s}\tau)}$$

$$k_1 = k_{10}\, e^{-E_1/RT}$$

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

$$T_c^* = (T_0 + \beta \, T_c) / (1+\beta)$$

$$\beta = kH / v_0 C_p .$$

T	293	303	315	323
h_1				
h_2				
$h_1 \tau$				
$k_2 \tau$				
X_s				
$U_{gs} = C_{p0} X_s T_1$	3.32	7.9	12.2	267
$U_{rs} = (1+\beta)(T_s - T_c^*)$	-15.6	-1.29	15.9	41.6

$$L = 1 - \frac{\tau}{C_{A0}} \frac{\partial}{\partial x} (r_1 - r_2)_s$$

$$M = 1 + \beta \qquad \beta = hA/r_0 C_p$$

$$N = T_f \, \tau \left[\frac{\partial (r_1 - r_2)}{\partial T} \right]_s$$

$$L + M > N$$
$$LM > N$$

steady is stable if these two criteria are satisfied

$$r_1 - r_2 = k_1 C_{A0}(1-x) - k_2 C_{A0} x$$

$$\frac{\partial(r_1 - r_2)}{\partial x} = (-k_{1s} - k_{2s}) C_{A0} = -(k_{1s} + k_{2s}) C_{A0}$$

$$L = 1 + \frac{\tau}{C_{A0}}(k_{1s} + k_{2s}) C_{A0} = 1 + k_{1s}\tau + k_{2s}\tau$$

$$= 1 + (21.3)(0.11) + (10.08)\,0.11$$

$$= 4.45$$

$$M = 1 + \beta = 1 + \frac{hA}{v_0 C_p}.$$

$$= 1 + \frac{(1000)\,0.24}{(0.6)(1000)} = 0.43$$

$$J_1 = \frac{(-\Delta H)}{C_p}$$

$$N = J_1 \tau \left[\frac{\partial}{\partial T} (r_1 - r_2) \right]_s$$

$$N = J_1 \tau \left[\frac{k_{1s} E_1}{R T_s^2} C_{A0} (1-x) - \frac{k_2 E_2 C_{A0} x_s}{R T_s^2} \right]$$

$$= 0.03$$

$L = 4.45$

$M = 0.43$

$N = 0.03$

$L + M > N$

$LM > N$

Both the criteria are satisfied. Steady state is stable.