Chapter 9

Professional Reference Shelf

R9.3. Linearized Stability of a CSTR

In this section we are going to develop a method to estimate the multiple steady states.† Begin with an unsteady mole balance for liquid phase reactions in a CSTR

$$\tau \frac{dC_A}{dt} = C_{A0} - C_A - (-r_A)\tau \tag{R9.3-1}$$

At steady state equation (R9.3-23) becomes

$$0 = C_{A0} - C_{AS} - (-r_{AS})\tau \tag{R9.3-2}$$

Substracting Equation (R9.3-23) and (R9.3-24)

$$\boxed{\tau \frac{dC_A}{dt} = -(C_A - C_{AS}) - \left[(-r_A) - (-r_{AS})\right]\tau} \tag{R9.3-3}$$

The unsteady energy balance is

$$\frac{dT}{dt} = \frac{F_{A0}\left[G(T) - R(T)\right]}{\sum N_i C_{P_i}} \tag{R9.3-4}$$

We are going to make the following approximation

$$\sum N_i C_{P_i} = N_A C_{P_A} + N_B C_{P_B} = N_{A0} C_{P_S} = V C_{A0} C_{P_S} \tag{R9.3-5}$$

Substituting Equation (R9.3-5) into Equation (R9.3-4) and considering the G(T) (Term 1) and R(T) (Term 2) separately

$$\text{Term 1:} \frac{F_{A0}G(T)}{VC_{A0}C_{P_S}} = \frac{F_{A0}(-r_A V/F_{A0})(-\Delta H_{Rx})}{VC_{A0}C_{P_S}} = -r_A \underbrace{\left(\frac{-\Delta H_{Rx}}{C_{A0}C_{P_S}}\right)}_{J} \tag{R9.3-6}$$

$$= -r_A J$$

$$\text{Term 2:} \frac{F_{A0}R(T)}{VC_{A0}C_{P_S}} = \frac{v_0 C_{A0}\left[C_{P_S}(1+\kappa)(T - T_C)\right]}{VC_{A0}C_{P_S}} = \frac{(1+\kappa)(T - T_C)}{\tau} \tag{R9.3-7}$$

Substituting Equations (R9.3-7) and (R9.3-8) into Equation (R9.3-4) we obtain

$$\tau \frac{dT}{dt} = -r_A J\tau - (1+\kappa)(T - T_C) \tag{R9.3-8}$$

At steady state

$$0 = -r_A J\tau - (1+\kappa)(T_S - T_C) \tag{R9.3-9}$$

Adding Equations (R9.3-30) and (R9.3-31)

$$\boxed{\tau \frac{dT}{dt} = J\tau\left[\left(-r_A\right) - \left(-r_{AS}\right)\right] - \left(1+\kappa\right)\left(T - T_S\right)} \qquad \text{(R9.3-10)}$$

Expanding $-r_A$ in a Taylor series about the steady state conditions C_{AS} and T_S

$$-r_A = -r_{AS} + \left(C_A - C_{AS}\right)\left.\frac{\partial\left(-r_A\right)}{\partial C_A}\right|_S + \left(T - T_S\right)\left.\frac{\partial\left(-r_A\right)}{\partial T}\right)_S \qquad \text{(R9.3-11)}$$

$$\frac{\partial\left(-r_A\right)}{\partial T} = Ae^{-E/RT} C_A \frac{E}{RT^2} = -r_A \frac{E}{RT^2}$$

Substituting and rearranging

$$\left[\left(-r_A\right) - \left(-r_S\right)\right] = k_S\left(C_A - C_{AS}\right) + \left(T - T_S\right)\frac{E}{RT_S^2}\left(-r_{AS}\right) \qquad \text{(R9.3-12)}$$

Substituting Equation (R9.3-12) into Equation (R9.3-3)

$$\boxed{\tau \frac{dC_A}{dt} = -\left(C_A - C_{AS}\right) - \tau k_S\left(C_A - C_{AS}\right) - \frac{E}{RT_S^2}\left(-r_{AS}\right)\left(T - T_S\right)} \qquad \text{(R9.3-13)}$$

Let

$$\Theta = t/\tau$$

$$x = C_A - C_{AS}$$

$$y = T - T_S$$

$$\frac{dx}{d\Theta} = -\underbrace{\left(1 + \tau k_S\right)}_{A} X - \underbrace{\frac{JE\tau\left(-r_{AS}\right)}{RT_S^2}}_{B} \frac{y}{J}$$

Let

$$A = 1 + \tau k_S$$

$$B = \frac{\tau JE\left(-r_{AS}\right)}{RT_S^2}$$

$$C = \left(1 + \kappa\right)$$

The linearized version of the mole balance is

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†This development follows that of R. Aris, *Elementary Chemical Reacitons Analysis,* Englewood Cliffs NJ: Prentice Hall, 1969.

$$\boxed{\frac{dx}{d\Theta} = -Ax - B\frac{y}{J}} \qquad \text{(R9.3-14)}$$

Substituting Equation (R9.3-12) into Equation (R9.3-10)

$$\tau\frac{dT}{dt} = \tau J\left[k_S\left(C_A - C_{AS}\right) + \frac{E\left(-r_{AS}\right)}{RT_S^2}\left(T - T_S\right)\right] - \left(1+\kappa\right)\left(T - T_S\right) \qquad \text{(R9.3-15)}$$

The linearized energy balance and mole balances are

$$\frac{dy}{d\Theta} = J\tau k_S x + By - Cy$$

$$\frac{dy}{d\Theta} = J\left(A-1\right)x + \left(B-C\right)y$$

The two coupled equation to be solved are

$$\boxed{\frac{dx}{d\Theta} = -Ax - \frac{By}{J}} \qquad \text{(R9.3-16)}$$

$$\boxed{\frac{dy}{d\Theta} = -J\left(1-A\right)x + \left(B-C\right)y} \qquad \text{(R9.3-17)}$$

In matrix notation

$$\boxed{\begin{matrix}\frac{dx}{d\Theta} \\ \frac{dy}{d\Theta}\end{matrix}} = \begin{bmatrix} -A & -\frac{B}{J} \\ -J\left(1-A\right) & \left(B-C\right)\end{bmatrix}\left[x, y\right] \qquad \text{(R9.3-18)}$$

$$= [\mathbf{M}]\ \left[x, y\right]$$

The solution is

$$x = K_1 e^{\lambda_1\Theta} + K_2 e^{\lambda_2\Theta} \qquad \text{(R9.3-19)}$$

$$y = K_3 e^{\lambda_1\Theta} + K_4 e^{\lambda_2\Theta} \qquad \text{(R9.3-20)}$$

Where the roots are found from the matrix **M**

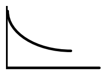
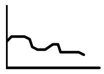
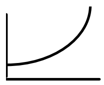
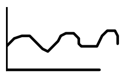
$$\lambda_1, \lambda_2 = \frac{\mathrm{Tr}\left(\mathbf{M}\right) \pm \sqrt{\mathrm{Tr}^2\left(\mathbf{M}\right) - 4\mathrm{Det}\left(\mathbf{M}\right)}}{2} \qquad \text{(R9.3-21)}$$

$$\boxed{\mathrm{Tr}\left(\mathbf{M}\right) = -A + B - C = B - \left(A + C\right)} \qquad \text{(R9.3-22)}$$

$$\mathrm{Det}\left(\mathbf{M}\right) = AC - B \qquad \text{(R9.3-23)}$$

The terms that the solution will take from a small perturbation from steady state are given in Table 1

TABLE R9.3-1 EIGEN VALUES OF COUPLED ODES

Tr < 0	Det > 0	Stable		
			$\left(\mathrm{Tr}^2(\mathbf{M}) - 4\mathrm{Det}(\mathbf{M})\right) > 0$	
			$\left(\mathrm{Tr}^2(\mathbf{M}) - 4\mathrm{Det}(\mathbf{M})\right) < 0$	
Tr > 0	Det > 0	Unstable		
			$\left[\mathrm{Tr}^2(\mathbf{M}) - 4\mathrm{Det}(\mathbf{M})\right] > 0$	
			$\left[\mathrm{Tr}^2(\mathbf{M}) - 4\mathrm{Det}(\mathbf{M})\right] < 0$	
$\mathrm{Tr}(\mathbf{M}) = 0$	$\mathrm{Det}\ (\mathbf{M}) > 0$	Pure Oscillation		

Example PRS.ER9.3-1 Linearized Stability

Let revisit Example 8-4. Let Examine the intersection of the two curves in Figure E8-8.2

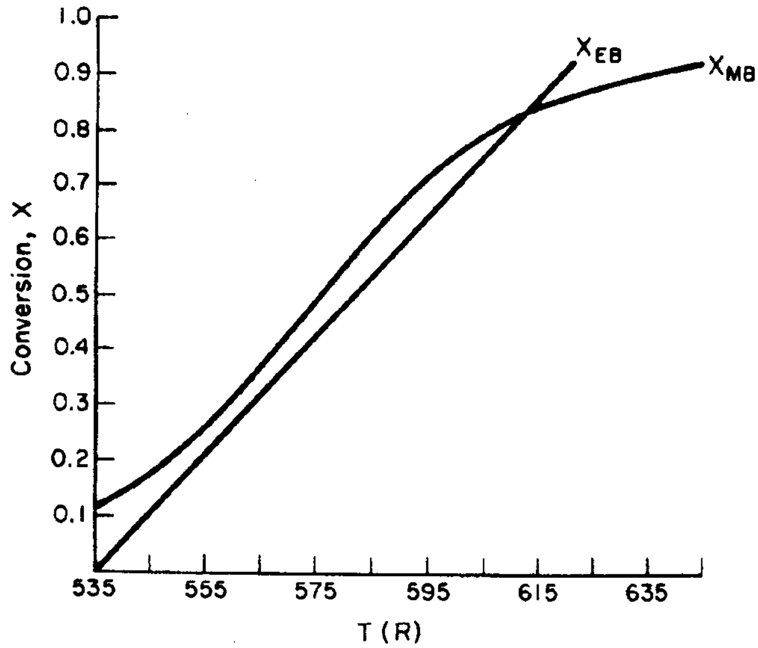


Figure E8-8.2

Determine the roots of Equation (R9.3-43) at the intersection of X_{EB} and X_{MB} and determine A the intersection we have

$$T_S = 613°R,\ \ X_S = 0.85,\ \ C_{AS} = 0.02 \qquad \text{(ER9.3-1.1)}$$

First let's calculate A

$$A = 1 + \tau k_S$$

$$\tau = 13\ \ h$$

From the problem statement in Example 8-4

$$k = 16.96 \times 10^{12} \exp[-32,400/RT] \qquad \text{(ER9.3-1.2)}$$

$$\text{At}\ \ T = 613°R$$

$$k_S = 47.5\ \ h^{-1}$$

$$A = 6.17$$

Next, let's calculate B

$$B = \tau J\left(\frac{E}{RT_S^2}\right)(-r_{AS}) \qquad \text{(ER9.3-1.3)}$$

to calculate B we need J.

$$J = \frac{(-\Delta H_{Rx})}{C_{A0}\sum\Theta_i C_{P_i}} = \frac{+36,400\,BTU/lbmol}{\left(0.13\dfrac{lbmol}{ft^3}\right)\left(\dfrac{403BTU}{lbmol°R}\right)} = 694.2\ ft^3/lbmol \qquad \text{(ER9.3-1.4)}$$

$$-r_{AS} = k_s C_{AS} = (47.5)(0.02) = \frac{0.94\,lbmol}{h\ \ ft^3} \qquad \text{(ER9.3-1.5)}$$

$$B = \tau J\left(\frac{E}{RT_S^2}\right)(-r_{AS}) \qquad \text{(ER9.3-1.3)}$$

$$B = (0.13)(694.2)(0.94)\frac{32,400}{(1.987)(613)^2}$$

$$B = 3.6$$

Next calculate C

$$C = (1 + \kappa) = 1 \qquad \text{(ER9.3-1.6)}$$

Now we can find the roots λ_1 and λ_2

$$\mathrm{Tr}(\mathbf{M}) = \mathrm{B} - (\mathrm{A} + \mathrm{C}) = 3.6 - (6.17 + 1) = 3.58 \quad \text{(ER9.3-1.7)}$$

$$\mathrm{Det}(\mathbf{M}) = (\mathrm{A})(\mathrm{C}) - \mathrm{B} = (6.17)(1) - 3.6 \quad \text{(ER9.3-1.8)}$$

$$= 2.7$$

$$\left[\mathrm{Tr}^2(\mathbf{M}) - 4\mathrm{Det}(\mathbf{M})\right] = \left[(3.58)^2 - 4(2.7)\right] = [12.8 - 10.8] = 2$$

$$\lambda_1,\ \lambda_2 = \frac{\mathrm{Tr}(\mathbf{M}) \pm \sqrt{\mathrm{Tr}^2(\mathbf{M}) - 4\mathrm{Det}(\mathbf{M})}}{2} = \frac{-3.58\sqrt{2}}{2} = -1.79 \pm 0.7$$

The system is stable with no oscillations.