

$$\begin{cases} k_1 = 3 \text{ } \mu\text{mol} \cdot \text{min} \\ k_{2,f} = 0.1 \text{ } \mu\text{min}^{-1} \quad k_{2,r} = 0.05 \text{ } \mu\text{min}^{-1} \end{cases}$$

$$V_0 = 10 \text{ L}$$

$$C_{A_0} = C_{B_0} = C_{C_0} = C_{D_0} = 0$$

$$C_A = 0.2 \text{ mol/L} \quad C_D = 0.4 \text{ mol/L}$$

$$T_A = [0; 1; 50] \text{ } \mu\text{min}$$

$$T_B = [10; 1; 50] \text{ } \mu\text{min}$$

$$T = 300 \text{ } \mu\text{min}$$

$$\dot{V}_a = 1 \text{ L/min}$$

$$\dot{V}_b = 0.6 \text{ L/min}$$

$$r_A = r_B = -k_1 C_A C_B$$

$$r_C = k_{2,f} C_C - k_{2,r} C_D - k_{2,f} C_C$$

$$r_D = k_{2,f} C_C$$

$$A = I - O + G - C$$

$$\frac{d}{dt} \int_V C_j dV = Q_0 C_{j_0} - Q C_j + \int_V R_j dV$$

$$R_j = \sum_i V_{ij} \cdot r_i$$

$$V_{C(t)} = V_0 + t \cdot \dot{V}_0 = \dot{V}_a(t) + \dot{V}_b(t)$$

$$C_A \frac{dV}{dt} + V \frac{dC_A}{dt} = -k_1 C_A C_B V + C_A \dot{V}_a$$

$$C_D$$

$$\frac{dC_A V}{dt} = -k_{2,f} C_A C_D \cdot V +$$

$$r = k_1 C_A C_B$$

$$V \frac{dC_A}{dt} = \dot{V}_a (1 - H(t-50)) - k_{2,f} C_A C_D \cdot V$$

$$V \frac{dC_D}{dt} = \dot{V}_b (1 -$$

$$V \frac{dC_C}{dt} = k_{2,f} C_A C_D \cdot V + k_{2,r} C_D \cdot V - k_{2,f} C_C V$$

$$1 \{1 - H(t-50)\} + 0.6 \{H(t-10) - H(t-50)\}$$

(e)

$$V_{C(t)} = V_0 + \dot{V}_{C(t)} \cdot t$$

$$\dot{V}_{C(t)} = \dot{V}_a + \dot{V}_b$$

$$= 1 \cdot [1 - H(t-50)] + 0.6 [H(t-10) - H(t-50)]$$

$$\begin{cases} t < 10 \rightarrow \dot{V} = 1 + 0.6(0-0) \\ \quad \quad \quad = 1 \\ 10 < t < 50 \rightarrow \dot{V} = 1 + 0.6 \\ \quad \quad \quad = 1.6 \\ t > 50 \rightarrow \dot{V} = 0 \end{cases}$$

$$C_{A(i+1)} = C_{A(i)} + dt \left(\frac{\dot{V}_a}{V} - k_1 C_{A(i)} C_{B(i)} \right)$$

$$C_{B(i+1)} = C_{B(i)} + dt \left(\frac{\dot{V}_b}{V} - k_1 C_{A(i)} C_{B(i)} \right)$$

$$C_{C(i+1)} = C_{C(i)} + dt (k_{2,f} C_{A(i)} C_{B(i)} - k_{2,r} C_{C(i)} + k_{2,r} C_{D(i)})$$

$$C_{D(i+1)} = C_{D(i)} + dt (k_{2,f} C_{C(i)} - k_{2,r} C_{D(i)})$$

(c) What is the steady-state volume in the tank?

(d) What is the steady-state concentration of D?

(e) How long does the reaction need to proceed for the concentration of D to reach 90% of its steady-state value?

$$c) \quad V = 10 \text{ L}$$

(d)

$$\text{Steady-state conc of D} = 0.140932 \text{ mol/L}$$

$$\text{Time consumed to reach 90\% cd} = 0.1268388 \text{ mol/L}$$

$$t_{\text{times}} = 116 \text{ s}$$

Problem 2. (Dorfman 1.38) In this problem, you are going to look into the error due to the addition of small numbers and the subtraction of very similar numbers. You should start with the large number $x = 10^{10}$. We want to look at the different ways to add 1 to this number and then subtract x from the result. If the calculation is perfect, the final result should be 1. If there are round-off errors or chopping errors, you will not get 1.

Define a small number ϵ . In this problem, you will consider the values $\epsilon = 0.1, 0.01, \dots, 10^{-10}$. Your program should perform the following calculation for each value of ϵ ,

$$R = \left(x + \sum_{j=1}^{\epsilon^{-1}} \epsilon \right) - x$$

where R is the final result of the calculation. To compute the term in brackets, compute the value of $x + \epsilon$, then add ϵ to that answer to get the value of $x + 2\epsilon$, add ϵ to that answer to get $x + 3\epsilon$, and so on so that computing the term in brackets involves the addition of very different sized numbers. In other words, do not compute the summation then add it to x . You should not store the value of every step in the calculation- for $\epsilon = 10^{-10}$ this would be a huge memory cost and your program would take a very long time to run. This entire program should execute in less than a minute on a reasonable computer if you write it well. Your program should make a semilog plot of the value of R as a function of ϵ .

$$\left. \begin{array}{l} R = x \\ R = x + \sum_{j=1}^{\epsilon^{-1}} \epsilon \\ R = R - x \end{array} \right\}$$

$$x = 10^{10} \quad R = \left(x + \sum_{j=1}^{\epsilon^{-1}} \epsilon \right) - x$$

$$\epsilon = (10)^{-n} \quad R = (x + \text{sum}) - x$$

$$n = 1:10 \Rightarrow 10$$

$$R = 1$$

$$\epsilon = \epsilon \Rightarrow$$

$$x = 10^{10}$$

$$i = 1:10$$

$$\epsilon_0 = 1$$

$$\epsilon_1 = \epsilon_0 / 10$$

$$R = x$$

$$\text{for } j = 1 : \epsilon^{-1}$$

$$R = R + \epsilon$$

$$T_2 =$$

Problem 3. (Shelfman 3.25) This problem involves the analysis of a cross-current heat exchanger. The design requires the counter-current heat exchanger to have a heat transfer rate of $Q = 0.8 \text{ MW}$, where Q is the heat transferred between streams. A is the area of the exchanger, and the log mean temperature is defined as

$$\Delta T_{lm} = \frac{(T_2 - T_1) - (T_2' - T_1')}{\ln\left(\frac{T_2 - T_1}{T_2' - T_1'}\right)}$$

where T_1 is the inlet temperature of the inner stream, T_2 is the outlet temperature of the inner stream, T_1' is the inlet temperature of the outer stream, and T_2' is the outlet temperature of the outer stream. The first law of thermodynamics requires that

$$\dot{Q} = \dot{m}_i c_p (T_2 - T_1) = \dot{m}_o c_p (T_2' - T_1')$$

where \dot{m}_i is the mass flow rate of the inner stream, \dot{m}_o is the mass flow rate of the outer stream, and we have chosen to set $T_2 > T_1$, so that Q is positive. A similar energy balance applies to the outer stream.

a) We will begin by reviewing the analysis of a cross-current heat exchanger. The inner fluid has a flow rate of 3 kg/s and a heat capacity of $2.3 \frac{\text{kJ}}{\text{kg} \cdot \text{C}}$ and the outer fluid has a flow rate of 5 kg/s and a heat capacity of $4 \frac{\text{kJ}}{\text{kg} \cdot \text{C}}$. The heat exchanger cools the inner fluid from 100°C to 15°C , and the outer fluid enters at 50°C . The overall heat transfer coefficient is $1 \frac{\text{MW}}{\text{m}^2 \cdot \text{C}}$. Determine the outlet temperature of the cooling fluid and the area of the heat exchanger. Use of MathLab is not required for this page.

b) We now want to figure out the outlet temperature of the inner fluid if we change the flow rate of the cooling fluid. Write a MATLAB program that uses the function method to compute this quantity. Test your program using the same parameters as part (a).

c) Repeat part (b) instead writing a MATLAB program that implements Newton's method and an initial guess of 100°C (which makes no sense physically) and demonstrate quadratic convergence. Include all relevant calculations in your review (e.g., the nonlinear equation and its derivative) and include a plot of the data demonstrating quadratic convergence.

d) Use your Newton's method algorithm from part (c) to compute the outlet temperature of the inner fluid as a function of the cooling fluid flow rate for exponentially spaced flow rates (logspace) from 10^{-2} to 10^2 kg/s . Your program should automatically generate a contour plot of data demonstrating quadratic convergence.

$$Q = UA \Delta T_{lm}$$

$$\Delta T_{lm} = \frac{(T_2' - T_2) - (T_1' - T_1)}{\ln\left(\frac{T_2' - T_2}{T_1' - T_1}\right)}$$

$$= \frac{(T_2' - T_2) - (T_1' - T_1)}{\ln\left(\frac{T_2' - T_2}{T_1' - T_1}\right)}$$

$$Q = \dot{m}_i c_p (T_2 - T_1)$$

$$U = 1 \frac{\text{MW}}{\text{m}^2 \cdot \text{C}}$$

Inner: $T_1 > T_2$

$$\dot{m}_i = 3 \text{ kg/s}$$

$$C_{p,i} = 2.3 \text{ kJ/kg} \cdot \text{C}$$

Outer: $T_1' > T_2'$

$$\dot{m}_o = 5 \text{ kg/s}$$

$$C_{p,o} = 4 \text{ kJ/kg} \cdot \text{C}$$

$$T_1 - T_2 = (100 - 50^\circ\text{C}) = 50^\circ\text{C}$$

$$\Delta T_i = 50^\circ\text{C}$$

$$T_2' = 15^\circ\text{C}$$

$$T_1 = 17.25^\circ\text{C}$$

2nd $T_1' = ?$ & $A = ?$

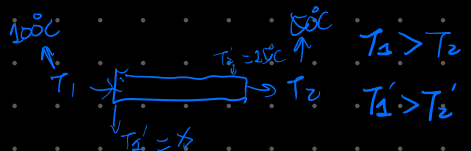
$$\dot{m}_i C_{p,i} \Delta T_i = \dot{m}_o C_{p,o} \Delta T_o$$

$$T_1' = \frac{\dot{m}_i C_{p,i} \Delta T_i}{\dot{m}_o C_{p,o}} + T_2'$$

$$= \frac{3 \times 2.3 \times 50}{5 \times 4} + 15$$

$$= 32.25^\circ\text{C}$$

$$\Delta T_o = T_1' - T_2' = 32.25 - 15 = 17.25$$



$$\Delta T_{lm} = \frac{(15 - 50) - (32.25 - 100)}{\ln\left(\frac{15 - 50}{32.25 - 100}\right)} = -49.59^\circ\text{C}$$

$$A = \frac{Q}{U \Delta T_{lm}}$$

$$= \frac{3 \times 2.3 \times 50}{1 \times (-49.59^\circ\text{C})} = 6.96 \text{ m}^2$$

$$cb) T_2 = 100^\circ\text{C}$$

$$T_2' = 15^\circ\text{C}$$

$$\dot{m}_i = 3 \text{ kg/s}$$

$$A = 7.134 \text{ m}^2$$

$$U = 1 \frac{\text{MW}}{\text{m}^2 \cdot \text{C}}$$

$$\dot{m}_o = \text{change}$$

$$T_2 = ?$$

$$T_2' = ?$$

$$m = ?$$

$$T_1' = \frac{\dot{m}_i C_{p,i} (T_1 - T_2)}{\dot{m}_o C_{p,o}} + T_2'$$

$$Q = \dot{m}_i C_{p,i} (T_2 - T_1) = UA \Delta T_{lm}$$

$$\Rightarrow \dot{m}_i C_{p,i} \Delta T + UA \Delta T_{lm} = 0$$

$$\frac{\dot{m}_i C_{p,i} \Delta T}{UA} + \Delta T_{lm} = 0$$

$$\dot{m}_i \cdot C_{p,i} \cdot (T_2' - T_2) - U \cdot A \cdot \frac{(T_2' - T_2) - (T_1' - T_1)}{\ln\left(\frac{T_2' - T_2}{T_1' - T_1}\right)} = 0$$

$$\dot{m}_i \cdot C_{p,i} (T_2 - T_2) - \dot{m}_o \cdot C_{p,o} (T_2' - T_2) = 0$$

$$\textcircled{1} \dot{m}_i C_{p,i} (T_1 - T_1) - \dot{m}_o C_{p,o} (T_2' - \left(\frac{\dot{m}_i C_{p,i} (T_2 - T_1)}{\dot{m}_o C_{p,o}} + T_2'\right)) = 0 \quad \checkmark$$

$$\textcircled{2} \dot{m}_i C_{p,i} \cdot (T_2' - \left(\frac{\dot{m}_i C_{p,i} (T_1 - T_2)}{\dot{m}_o C_{p,o}} + T_2'\right)) + UA \cdot \left(\frac{(T_2' - T_2) - (T_1' - T_1)}{\ln\left(\frac{T_2' - T_2}{T_1' - T_1}\right)}\right) = 0$$

(c)

$$T_1' = \frac{\dot{m}_1 C_p (T_1 - T_2)}{\dot{m} C_p} + T_2'$$

$$= \frac{6.9(100 - T_2)}{4m} + 15$$

$$f(x) = 6.9(T_2 - 100) - 6.957 \cdot \frac{(15 - T_2) - \left(\frac{6.9(100 - T_2)}{4m} + 15 \right) - 100}{\ln \left(\frac{15 - T_2}{\left(\frac{6.9(100 - T_2)}{4m} + 15 \right) - 100} \right)}$$

$$f'(x) = 6.9 - \frac{6.957(m - 1.725)(T - 100)(m - 2.50393 \times 10^{-18}T - 1.725)}{m(T - 15)(m + 0.0202941T - 2.02941) \cdot \left(\log \left(\frac{m(0.0117647T - 0.176471)}{m + 0.0202941T - 2.02941} \right) \right)^2} + \frac{6.957m - 12.0008}{m \cdot \log \left(\frac{m(0.0117647T - 0.176471)}{m + 0.0202941T - 2.02941} \right)}$$

(c) $T_2 = 1000^\circ\text{C}$

$T_1 = 100^\circ\text{C}$

$T_2' = 15^\circ\text{C}$

$$f(x) = f(x^{(k)}) + f'(x^{(k)})(x - x^{(k)}) + \dots$$

$$0 \approx f(x^{(k)}) + f'(x^{(k)})(x - x^{(k)})$$

$$x = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

$$\Rightarrow x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$