Solutions for Tutorial 3 Modelling of Dynamic Systems

3.1 Mixer: Dynamic model of a CSTR is derived in textbook Example 3.1. From the model, we know that the outlet concentration of A, C_A , can be affected by manipulating the feed concentration, C_{A0} , because there is a causal relationship between these variables.

- a. The feed concentration, C_{A0} , results from mixing a stream of pure A with solvent, as shown in the diagram. The desired value of C_{A0} can be achieved by adding a right amount of A in the solvent stream. Determine the model that relates the flow rate of reactant A, F_A , and the feed concentration, C_{A0} , at constant solvent flow rate.
- b. Relate the gain and time constant(s) to parameters in the process.
- c. Describe a control valve that could be used to affect the flow of component A. Describe the a) valve body and b) method for changing its percent opening (actuator).



Figure 3.1

a. In this question, we are interested in the behavior at the mixing point, which is identified by the red circle in the figure above. We will apply the standard modelling approach to this question.

<u>Goal</u>: Determine the behavior of $C_{A0}(t)$

<u>System:</u> The liquid in the mixing point. (We assume that the mixing occurs essentially immediately at the point.)

Balance: Since we seek the behavior of a composition, we begin with a component balance.

(1)
$$MW_A(V_mC_{A0}|_{t+\Delta t} - V_mC_{A0}|_t) = MX_A\Delta t(F_SC_{AS} + F_AC_{AA} - (F_S + F_A)C_{A0}) + 0$$

Note that no reaction occurs at the mixing point. We cancel the molecular weight, divide by the delta time, and take the limit to yield

(2)
$$\frac{V_m}{(F_S + F_A)} \frac{dC_A}{dt} = \frac{F_S}{F_S + F_A} C_{AS} + \frac{F_A}{F_S + F_A} C_{AA} - C_{A0}$$

No reactant (A) appears in the solvent, and the volume of the mixing point is very small. Therefore, the model simplifies to the following algebraic form.

(3)
$$\frac{F_A}{F_S + F_A}C_{AA} = C_{A0}$$

Are we done? We can check degrees of freedom.

DOF =
$$1 - 1 = 0$$

C_{A0}
Therefore, the model is complete.
(F_S, F_A, and C_{AA} are known)

You developed models similar to equation (3) in your first course in Chemical Engineering, Material and Energy balances. (See Felder and Rousseau for a refresher.) We see that the dynamic modelling method yields a steady-state model when the time derivative is zero.

Note that if the flow of solvent is much larger than the flow of reactant, $F_S >> F_A$, then,

(4)
$$C_{A0} = \left(\frac{C_{AA}}{F_S}\right) F_A$$

If F_S and C_{AA} (concentration of pure reactant) are constant, the concentration of the mixed stream is <u>linearly dependent</u> on the flow of reactant.

b. For the result in equation (4),

Time constant = 0	(This is a steady-state process.)
$Gain = C_{AA}/F_{S}$	(The value will change as F_S is changed.)

- c. The control valve should have the following capabilities.
- 1. Introduce a restriction to flow.
- 2. Allow the restriction to be changed.
- 3. Have a method for automatic adjustment of the restriction, not requiring intervention by a human.
- 1&2 These are typically achieved by placing an adjustable element near a restriction through which the fluid must flow. As the element's position in changed, the area through which the fluid flows can be increased or decreased.
- 3 This requirement is typically achieved by connecting the adjustable element to a metal rod (stem). The position of the rod can be changed to achieve the required restriction. The power source for moving the rod is usually air pressure, because it is safe (no sparks) and reliable. A rough schematic of an automatic control valve is given in the following figure.



valve plug and seat

See a Valve You can see a picture of a typical control valve by clicking here. Many other valves are used, but this picture shows you the key features of a real, industrial control valve.

> Hint: To return to this current page after seeing the valve, click on the "previous view" arrow on the Adobe toolbar.

You can read more about valves at the McMaster WEB site.

3.2 Stirred tank mixer

- a. Determine the dynamic response of the tank temperature, T, to a step change in the inlet temperature, T_{0} , for the continuous stirred tank shown in the Figure 3.2 below.
- b. Sketch the dynamic behavior of T(t).
- c. Relate the gain and time constants to the process parameters.
- d. Select a temperature sensor that gives accuracy better than ± 1 K at a temperature of 200 K.



Figure 3.2

We note that this question is a simpler version of the stirred tank heat exchanger in textbook Example 3.7. Perhaps, this simple example will help us in understanding the heat exchanger example, which has no new principles, but more complex algebraic manipulations. Remember, we use heat exchangers often, so we need to understand their dynamic behavior.

a/c. The dynamic model is derived using the standard modelling steps.

<u>Goal:</u> The temperature in the stirred tank.

<u>System</u>: The liquid in the tank. See the figure above.

Balance: Since we seek the temperature, we begin with an energy balance.

Before writing the balance, we note that the kinetic and potential energies of the accumulation, in flow and out flow do not change. Also, the volume in the tank is essentially constant, because of the overflow design of the tank.

accumulation = in - out (no accumulation!)

(1)
$$(U|_{t+\Delta t} - U|_t) = \Delta t(H_{in} - H_{out})$$

We divide by delta time and take the limit.

(2)
$$\frac{dU}{dt} = (H_{in} - H_{out})$$

The following thermodynamic relationships are used to relate the system energy to the temperature.

 $dU/dt = V\rho C_v dT/dt$ $H = F\rho C_p (T-T_{ref})$ For this liquid system, $C_v \approx C_p$

Substituting gives the following.

(3)
$$V\rho \frac{dT}{dt} = F\rho(T_0 - T)$$

Are we done? Let's check the degrees of freedom.

$$DOF = 1 - 1 = 0$$
T
(V, and T₀ known)

This equation can be rearranged and subtracted from its initial steady state to give

(4)
$$\tau \frac{dT'}{dt} + T' = KT'_0$$
 with $\tau = V/F$ $K = 1$

Note that the time constant is V/F and the gain is 1.0. These are not always true! We must derive the models to determine the relationship between the process and the dynamics. See Example 3.7 for different results for the stirred tank heat exchanger.

The dynamic response for the first order equation differential equation to a step in inlet temperature can be derived in the same manner as in Examples 3.1, 3.2, etc. The result is the following expression.

(5)
$$T' = K\Delta T_0 (1 - e^{-t/\tau})$$

and $T = T_{initial} + K\Delta T_0 (1 - e^{-t/\tau})$



d. We base the temperature sensor selection on the information on advantages and disadvantages

of sensors. A table is available on the McMaster WEB site, and links are provided to more extensive sensor information. A version of such a table is given below.

Since a high accuracy is required for a temperature around 200 K, an RTD (a sensor based on the temperature sensitivity of electrical resistance) is recommended. Even this choice might not achieve the 1 K accuracy requirement.

sensor type	limits of application (°C)	accuracy ^(1,2)	dynamics, time constant (s)	advantages	disadvantages
4 1					
thermocouple type E (chromel-constantan)	-100 to 1000	$\pm 1.5 \text{ or } 0.5\%$	(3)	1. good reproducibility	1. minimum span, 40 °C
type J		(0 10 900 C)		2. white fullige	not exactly linear
(iron-constantan)	0 to 750	± 2.2 or 0.75%			 drift over time low emf corrupted by
type K					noise
(chromel-nickel)	0 to 1250	± 2.2 or 0.75%			
type T (copper-constantan)	-160 to 400	± 1.0 or 1.5% (-160 to 0 °C)			
RTD	-200 to 650	(0.15 +.02 T) °C	(3)	1. good accuracy	1. self heating
				2. small span possible	2. less physically
				3. linearity	rugged
Thermister	-40 to 150	0.10°C	(3)	1 good accuracy	1 highly nonlinear
Thermister	40 10 150	0.10 C	(3)	2. little drift	2. only small span
				2	3. less physically
					rugged
					4. drift
Bimetallic		± 2%		1. low cost	 local display
				2. physically rugged	
Filled system	-200 to 800	$\pm 1\%$	1-10	1. simple and low cost	1. not high temperatures
				2. no hazards	2. sensitive to external
					pressure

1. °C or % of span, whichever is larger

2. for RTDs, inaccuracy increases approximately linearly with temperature deviation from 0 °C

3. dynamics depend strongly on the sheath or thermowell (material, diameter and wall thickness), location of element in the sheath (e.g.,

bonded or air space), fluid type, and fluid velocity. Typical values are 2-5 seconds for high fluid velocities.

3.3 Isothermal CSTR: The model used to predict the concentration of the product, C_B , in an isothermal CSTR will be formulated in this exercise. The reaction occurring in the reactor is

$$A \rightarrow B$$
 $r_A = -kC_A$

Concentration of component A in the feed is C_{A0} , and there is no component B in the feed. The assumptions for this problem are



Figure 3.3

- a. Develop the differential equations that can be used to determine the dynamic response of the concentration of component B in the reactor, $C_B(t)$, for a given $C_{A0}(t)$.
- b. Relate the gain(s) and time constant(s) to the process parameters.
- b. After covering Chapter 4, solve for $C_B(t)$ in response to a step change in $C_{A0}(t)$, ΔC_{A0} .
- c. Sketch the shape of the dynamic behavior of $C_B(t)$.
- d. Could this system behave in an underdamped manner for different (physically possible) values for the parameters and assumptions?

In this question, we investigate the dynamic behavior of the product concentration for a single CSTR with a single reaction. We learned in textbook Example 3.2 that the concentration of the reactant behaves as a first-order system. Is this true for the product concentration?

a. We begin by performing the standard modelling steps.

Goal: Dynamic behavior of B in the reactor.

System: Liquid in the reactor.

Balance: Because we seek the composition, we begin with a component material balance.

Accumulation = in - out + generation

(1)
$$MW_B(VC_B |_{t+\Delta t} - VC_B |_t) = MW_B\Delta t(FC_{B0} - FC_B + VkC_A)$$

We can cancel the molecular weight, divide by delta time, and take the limit to obtain the following.

(2)
$$V \frac{dC_B}{dt} = FC_{B0} - FC_B + VkC_A$$

We can subtract the initial steady state and rearrange to obtain

(3)
$$\tau_{\rm B} \frac{dC'_{\rm B}}{dt} + C'_{\rm B} = K_{\rm B}C'_{\rm A}$$
 $\tau_{\rm A} = \frac{V}{F}$ $K_{\rm B} = \frac{Vk}{F}$

Are we done? Let's check the degrees of freedom.

DOF =
$$2 - 1 = 1 \neq 0$$
 No!
C_B and C_A

The first equation was a balance on B; we find that the variable C_A remains. We first see if we can evaluate this using a fundamental balance.

Goal: Concentration of A in the reactor. **System:** Liquid in the reactor. **Balance:** Component A

(4)
$$MW_A(VC_A|_{t+\Delta t} - VC_A|_t) = MW_A\Delta t(FC_{A0} - FC_A - VkC_A)$$

Following the same procedures, we obtain the following.

(5)
$$\tau_A \frac{dC'_A}{dt} + C'_A = K_B C'_{A0}$$
 $\tau_A = \frac{V}{F + Vk}$ $K_A = \frac{F}{F + Vk}$

Are we done? Let's check the degrees of freedom for equations (3) and (5).

DOF =
$$2 - 2 = 0$$
 Yes!
C_B and C_A

The model determining the effect of C_{A0} on C_B is given in equations (3) and (5).

b. The relationship between the gains and time constants and the process are given in equations (3) and (5).

c. We shall solve the equations for a step in feed concentration using Laplace transforms. First we take the Laplace transform of both equations; then we combine the resulting algebraic equations to eliminate the variable C_A .

(6)
$$\tau_{B}(sC'_{B}(s) - c'_{B}(t)|_{t=0}) + C'_{B}(s) = K_{B}C'_{A}(s)$$

(7)
$$\tau_{A}(sC'_{A}(s) - C'_{A}(t)|_{t=0}) + C'_{A}(s) = K_{A}C'_{A0}(s)$$

(8)
$$C'_{B}(s) = \frac{K_{A}K_{B}}{(\tau_{A}s+1)(\tau_{B}s+1)}C'_{A0}(s)$$

We substitute the input forcing function, $C'_{A0}(s) = \Delta C_{A0}/s$, and invert using entry 10 of Table 4.1 (with a=0) in the textbook.

(9)
$$C'_{B}(s) = \frac{K_{A}K_{B}}{(\tau_{A}s+1)(\tau_{B}s+1)} \frac{\Delta C'_{A0}}{s}$$

(10)
$$C'_{B}(t) = K_{A}K_{B}\Delta C_{A0}\left[1 + \frac{\tau_{A}}{\tau_{B} - \tau_{A}}e^{-t/\tau_{A}} - \frac{\tau_{B}}{\tau_{B} - \tau_{A}}e^{-t/\tau_{B}}\right]$$

c. The shape of the response of C_B using the numerical values from textbook Example 3.2 is given in the following figure. Note the overdamped, "S-shaped" curve.

This is much different from the response of C_A .

Compare the responses and explain the differences.

d. Because the roots of the denominator in the Laplace transform are real, this process can never behave as an underdamped system.



3.4 Inventory Level: Process plants have many tanks that store material. Generally, the goal is to smooth differences in flows among units, and no reaction occurs in these tanks. We will model a typical tank shown in Figure 2.4.

a. Liquid to a tank is being determined by another part of the plant; therefore, we have no influence over the flow rate. The flow from the tank is pumped using a centrifugal pump. The outlet flow rate depends upon the pump outlet pressure and the resistance to flow; it <u>does not</u> depend on the liquid level. We will use the valve to change the resistance to flow and achieve the desired flow rate. The tank is cylindrical, so that the liquid volume is the product of the level times the cross sectional area, which is constant.

Assume that the flows into and out of the tank are initially equal. Then, we decrease the flow out in a step by adjusting the valve.

i. Determine the behavior of the level as a function of time.



Figure 2.4

We need to formulate a model of the process to understand its dynamic behavior. Let's use our standard modelling procedure.

Goal: Determine the level as a function of time.

Variable: L(t)

System: Liquid in the tank.

Balance: We recognize that the level depends on the <u>total</u> amount of liquid in the tank. Therefore, we select a total material balance. Note that no generation term appears in the total material balance.

(accumulation) = in - out $(\rho AL)_{t+\Delta t} - (\rho AL)_t = \rho F_{in} \Delta t - \rho F_{out} \Delta t$

We cancel the density, divide by the delta time, and take the limit to yield

$$A\frac{dL}{dt} = F_{in} - F_{out}$$

The flow in and the flow are independent to the value of the level. In this problem, the flow in is constant and a step decrease is introduced into the flow out. As a result,

$$A\frac{dL}{dt} = F_{in} - F_{out} = \mathbf{constant} > 0$$

We know that if the derivative is constant, i.e., independent of time, the level will increase linearly with time. While the mathematician might say the level increases to infinity, we know that it will increase until it overflows. Thus, we have the following plot of the behavior.



Note that the level never reaches a steady-state value (between overflow and completely dry). This is very different behavior from the tank concentration that we have seen. Clearly, we must closely observe the levels and adjust a flow to maintain the levels in a desirable range. If you are in charge of the level – and you do not have feedback control – you better not take a coffee break!

The level is often referred to as an integrating process – Why? The level can be determined by solving the model by separation and integration, as shown in the following.

$$\int A \, dL = \int (F_{in} - F_{out}) dt$$
$$L = A \int (F_{in} - F_{out}) dt$$

Thus, the level integrates the difference between inlet and outlet flows.

ii. Compare this result to the textbook Example 3.6, the draining tank.



Key Issue	Example 3.6 Draining tank	This question Tank with outlet pump	
Level model	By overall material balance	By overall material balance	
Flow out	Depends on the level	Independent of the level	
		(or very nearly so)	
Level behavior	First order exponential for a step	Linear, unbounded response	
	change	to a step change	
Level stability	stable	unstable	

iii. Describe a sensor that could be used to measure the level in this vessel.

Naturally, we could tell you the answer to this question. But, you will benefit more from finding the answer. Click to access the instrumentation resources and review Section 2.4 and links to more detailed resources. <u>CLICK HERE</u>



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3.5 **Designing tank volume**: In this question you will determine the size of a storage vessel. Feed liquid is delivered to the plant site periodically, and the plant equipment is operated continuously. A tank is provided to store the feed liquid. The situation is sketched in Figure 3.5. Assume that the storage tank is initially empty and the feed delivery is given in Figure 2.5. Determine the minimum height of the tank that will prevent overflow between the times 0 to 100 hours.



Figure 3.5 Tank between the feed delivery and the processing units.

This problem shows how the dynamic behavior of a process unit can be important in the design of the process equipment.

Our approach to solving the problem involves determining the liquid volume over the complete time period from 0 to 100 hours. The maximum volume during the period can be used to evaluate the size of the tank; any tank smaller would experience an overflow.

The dynamic model for the tank was formulated in the previous solution, which we will apply in this solution. The behavior of the system is summarized in the following table and sketched in the figure.

Time (h)	F _{in}	F _{out} (m ³ /h)	$\frac{dV/dt = F_{in} - F_{out}}{(m^3/h)}$	V beginning of period (m ³)	V end of period (m ³)
0 - 20	30	12	18	0	360
20-40	0	12	-12	360	120
40-50	30	12	18	120	300
50-70	0	12	-12	300	60
70-80	30	12	18	60	240
80-100	30	12	-12	240	0

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We see in the table and figure that the maximum volume is 360 m^3 . Since the cross sectional area is 50 m^2 , the minimum height (or level) for the tank is calculated to be 7.2 m.

 $L = 360 \text{ m}^3 / 50 \text{ m}^2 = 7.2 \text{ m}$

We should note that this calculation results in the tank being completely full at t = 20 hours; there is <u>no margin for error</u>. We should look into the likely **variability** of the feed deliveries and the production rates before making a final decision on the correct volume.

3.6 Modelling procedure: Sketch a flowchart of the modelling method that we are using to formulate dynamic models.

We should develop this type of sketch so that we can <u>visualize the procedure</u> and clarify the sequence of steps. A flowchart is given on the following page. Did yours look similar?

