11.3 Dynamic analysis and time response

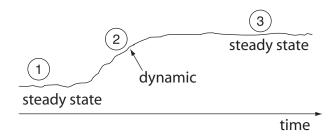


Figure 11.4: Dynamic response in output y to step change in input u

We want to understand what happens when we get an imbalance from the steadystate, such that the system's states change with time. For this purpose, let us consider the following incident (see Figure 11.4):

- 1. The system is initially "at rest" (steady state).
- 2. A change in one of the system's independent variables ("input" u) occurs, for example, a change in external conditions or a parameter change, such that we get an imbalance and the system's dependent variables (states and "outputs" y) change with time.
- 3. After a while (actually when $t \to \infty$), the system will eventually approach a new equilibrium state, where it is again "at rest" (new steady state).

Some examples are

- If we, on a winter's day, turn on more heat in a room, the temperature will start rising. The change is largest in the beginning, and "eventually" the temperature will approach a new steady state value (where again the system is at rest).
- If we push the accelerator ("gas") pedal of a car, then the car's speed will increase. The change is largest in the beginning, and "eventually" the speed will reach a new steady-state value (where again there is a balance between the forward force from the engine and the resistance force from the air).
- In a chemical reactor we have a continuous supply of reactant. If we increase ("disturb") the concentration of the reactant, the product concentration will also increase. The change is largest in the beginning, and "eventually" the product concentration will approach a new steady state value.

In all these cases, we go from one steady state to another, and a steady-state model is sufficient to calculate the initial and final states. However, we need a dynamic model to say something about the dynamic response and to quantify what we mean by "eventually." By the term **response**, we mean the time response for the dependent variable (output) y when we change the independent variable (input) y. In the three cases mentioned above we have

- Room: u = Q (heating), y = T
- Car: u = w (fuel flow), y = v (speed)
- Reactor: u = cin, y = cout

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Four important responses are (see Figure 11.5):

Step response. This is the response in the dependent variable y to a *step change* (persistent change) in the independent variable u. Mathematically, the change in u is

$$u(t) = \left\{ \begin{array}{ll} u_0 & t \le t_0 \\ u_\infty = u_0 + \Delta u & t > t_0 \end{array} \right\}$$

where Δu is the magnitude of the step. A step response was considered in the three cases above.

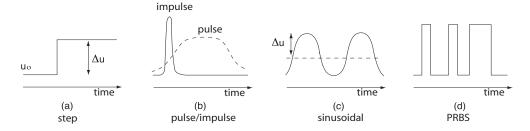


Figure 11.5: Time signals for input u(t)

Impulse response. A **pulse** is a temporary change of the independent variable u, and if the duration is very short (negligible) compared to the system's dynamics, we have an **impulse**. The impulse response is the resulting response in y. For a process engineer, an example of an impulse is to "throw a bucket" of something into a tank. For a chemist or a medical doctor, an injection with a needle gives an impulse.

For a flow system, the so-called **residence time distribution (RTD)** is actually the concentration impulse response of a non-reacting component.

Frequency response (sinusoidal input). This is the resulting response in y to a persistent sinusoidal variation in the independent variable u,

$$u(t) = u_0 + \Delta u \cdot \sin(\omega t)$$

For small changes, we can assume that the system is linear, and the output signal is also sinusoidal with the same frequency ω :

$$y(t) = y_0 + \Delta y \cdot \sin(\omega t + \phi)$$

The frequency response is characterized by two parameters: The gain $\Delta y/\Delta u$, and the phase shift, ϕ . Both depend on the frequency ω [rad/s], and by varying the frequency ω , we get information on how the system reacts to quick (ω large) and slow (ω small) input variations. Frequency analysis is an important tool in control engineering.

PRBS response. This is the response in y when the independent variable u changes at "random" times between two given values (PRBS = pseudo-random binary sequence). This may give a good "dynamic distribution" and is sometimes an

effective method for obtaining experimental data that can be used for estimating (="identify" in control engineering) parameters in an empirical dynamic model for the relationship between u and y.

The step response is very popular in process engineering because it is simple to perform, understand and analyze. In the following, we study the step response in more detail.

11.3.1 Step response and time constant

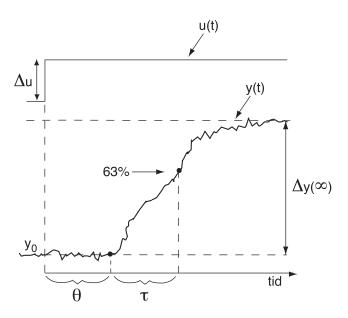


Figure 11.6: Experimental step response

We consider a system that is initially "at rest," that is, at steady state with dy/dt = 0. A step-change then occurs in the independent variable u, which takes the system away from its initial steady state. We assume that the system is stable such that it eventually approaches a new steady state. The resulting **step response** in y(t) is often characterized by the following three parameters (see Figure 11.6):

(Steady state) Gain $k = \frac{\Delta y(\infty)}{\Delta u}$.

(Effective) Delay θ – the time it takes before y "takes off" in the "right" direction. Thus, $\Delta y(\theta) \approx 0$.

Time constant τ – additional time it takes to reach 63% of the total change in y (that is, $\Delta y(\tau + \theta) = 0.63 \Delta y(\infty)$).

Here

- $\Delta u = u(\infty) u(t_0)$ magnitude of step change in u
- t_0 time when step change in u occurs (often $t_0 = 0$ is chosen)

- $\Delta y(t) = y(t) y(t_0)$ the resulting change in y
- $y(t_0) = y_0$ initial (given) steady state
- $y(\infty)$ final (new) steady state

The value of $\Delta y(\infty) = y(\infty) - y(t_0)$, and thereby of the steady state gain k, can be determined from a steady state model, if one is available.

The cause of the delay (time delay) θ may be a transport delay (for example a pipe) or a delay in a measurement, but in most cases it represents the contribution from many separate dynamic terms that, altogether, give a response that resembles a delay (hence the term "effective" delay).

The time constant τ characterizes the system's dominant "inertia" against changes. It is defined as the additional time (after the time delay) it takes the variable to reach 63% (more precisely, a fraction $1-e^{-1}=1-0.3679\approx 0.63$, see below) of its total change. Why do we not let the time constant be the time it takes to reach all (100%) of its change? Because it generally take an infinitely long time for the system to reach exactly its final state, so this would not give a meaningful value.

The values of the parameters k, τ and θ are independent of the size of the step (independent of the value of Δu), provided the step Δu is sufficiently small such that we remain in the "linear region." On page 301, we show how we can derive a linear model.

11.3.2 Step response for first-order system

The basis for the definition of τ given above is the simplest case with one linear differential equation (first-order system). Here, we study this system in more detail. A first-order system can be written in the following standard form

$$\tau \frac{dy}{dt} = -y + ku, \quad y(t_0) = y_0$$
 (11.21)

where

- u is the independent variable (input)
- y is the dependent variable (output)
- \bullet τ is the time constant
- k is the gain

We now assume that

- 1. The system is "at rest" at time t_0 with dy/dt = 0, that is, for $t \le t_0$ we have $u = u_0$ and $y_0 = ku_0$.
- 2. The independent variable u changes from u_0 to a constant value $u = u_0 + \Delta u$ at time t_0 .

As proven below, the solution ("step response") can then be written as

$$y(t) = y_0 + \left(1 - e^{-t/\tau}\right) k\Delta u$$
(11.22)

or

$$\underbrace{\Delta y(t)}_{y(t)-y_0)} = \underbrace{\Delta y(\infty)}_{y(\infty)-y_0} \left(1 - e^{-t/\tau}\right)$$
(11.23)

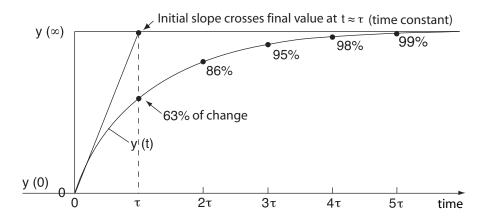


Figure 11.7: Step response for first-order system

(you should try to remember this one). k is the steady state gain, and when $t \to \infty$ we have $e^{-t/\tau} \to 0$ and the system approaches a new steady state where $\Delta y(\infty) = k\Delta u$. Notet that the exponential term $1 - e^{-t/\tau}$ describes how fast the system approaches its new steady state, and as a function of the non-dimensional time t/τ we have:

t/ au	$1 - e^{-t/\tau}$	Value	Comment
~	$1 - e^0 =$	_	
-	$1 - e^{-0.1} =$		
0.5	$1 - e^{-0.5} =$	0.393	
			63% of change is reached after time $t = \tau$
	$1 - e^{-2} =$		
3	$1 - e^{-3} =$	0.950	
4	$1 - e^{-4} =$	0.982	98% of change is reached after time $t = 4\tau$
5	$1 - e^{-5} =$	0.993	
∞	$1 - e^{-\infty} =$	1	

The time response is plotted in Figure 11.7. We note that at time $t = \tau$ (the time constant), we have reached 63% of the total change, and after four time constants, we have reached 98% of the change (and we have for all practical purposes arrived at the new steady state). Note also from Figure 11.7 that the initial slope of the response (at time t = 0) goes through to the point $(\tau, y(\infty))$. This can be shown mathematically from (11.23):

$$\frac{dy}{dt} = (y(\infty) - y_0) \frac{1}{\tau} e^{-t/\tau} \quad \Rightarrow \quad \left(\frac{dy}{dt}\right)_{t=0} = \frac{y(\infty) - y_0}{\tau} \tag{11.24}$$

This means that the response y(t) would reach the final value $y(\infty)$ at time τ if it continued unaltered (in a straight line) with its initial slope.

Comments.

1. As seen from the proof below, (11.23) applies also to cases where the system is not initially at rest. This is not the case for (11.22).

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2. For cases where τ is negative, the system is unstable, and we get that y(t) goes to infinity when t goes to infinity.

3. From (11.24) and $\Delta y(\infty) = k\Delta u$, we derive that

$$\frac{1}{\Delta u} \left(\frac{dy}{dt} \right)_{t=0} = \frac{k}{\tau} \tag{11.25}$$

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This means that the initial slope k' of the "normalized" response $\Delta y(t)/\Delta u$ is equal to the ratio k/τ , i.e., $k' \triangleq k/\tau$.

Proof: Step response for a first-order system

Consider a first-order system in standard form, (11.21),

$$\tau \frac{dy}{dt} = -y + ku; \quad y(0) = y_0$$
 (11.26)

where both τ and ku are constant. There are many ways of solving the linear differential equation (11.26). We can for example use separation of variables and derive

$$\frac{dy}{y - ku} = -\frac{dt}{\tau}$$

Integration gives

$$\int_{y_0}^y \frac{dy}{y - ku} = \int_0^t -\frac{dt}{\tau} \quad \Rightarrow \quad \ln \frac{y - ku}{y_0 - ku} = -\frac{t}{\tau}$$

and we get the general solution

$$y(t) = ku + e^{-t/\tau}(y_0 - ku)$$

We subtract y_0 from both sides and get

$$y(t) - y_0 = \left(1 - e^{-t/\tau}\right)(ku - y_0) \tag{11.27}$$

Since $e^{-t/\tau} \to 0$ as $t \to \infty$, we have that $y(\infty) = ku$, and by introducing deviation variables

$$\Delta y(t) \stackrel{\triangle}{=} y(t) - y(0) \tag{11.28}$$

we find that (11.27) can be written in the following general form

$$\Delta y(t) = \Delta y(\infty) \left(1 - e^{-t/\tau} \right) \tag{11.29}$$

We have so far <u>not</u> assumed that the system is "at rest" at $t = t_0$, but let us do this now. We then have at $t = t_0$ that dy/dt = 0, which gives

$$y_0 = ku_0$$

and (11.27) gives for a system that is initially at rest:

$$\underbrace{\Delta y(t)}_{y(t)-y_0} = \left(1 - e^{-t/\tau}\right) k \underbrace{\Delta u}_{u-u_0}$$
(11.30)

Example 11.4 Concentration response in continuous stirred tank

We consider the concentration response for component A in a continuous stirred tank without chemical reaction (see Figure 11.8). We assume constant liquid density ρ and constant volume V. The system is assumed to be at rest at t=0. We want to find the step response for t>0 given the following data

$$V = 5m^3; \quad q = 1m^3/h$$

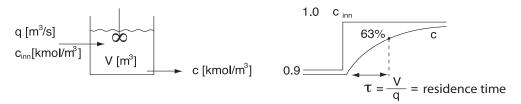


Figure 11.8: Continuous stirred tank without reaction

$$c_{A, \rm in} = \left\{ \begin{array}{ll} c_0 = 0.9 \ kmol/m^3 & t \leq 0 \\ c_{\infty} = 1.0 \ kmol/m^3 & t > 0 \end{array} \right\}$$

Solution. With constant density and constant volume, the mass balance gives that the volumetric inlet and outlet flow rates are equal, $q_{\rm in} = q_{\rm out} = q$. We further assume perfect mixing in the tank such that $c_{A,{\rm out}} = c_A$. The component balance for A in the tank is then $[mol\ A/s]$

$$\frac{d}{dt}(c_A V) = q c_{A, \text{in}} - q c_A \tag{11.31}$$

With constant volume V this gives

$$\frac{V}{q}\frac{dc_A}{dt} = -c_A + c_{A,\text{in}} \tag{11.32}$$

This is in standard form (11.21) with

$$u = c_{A,in}; \quad y = c_A$$

and

$$k=1;$$

$$\boxed{\tau=rac{V}{q}} \quad rac{[m^3]}{[m^3/s]}=[s]$$

Here, V/q [s] is the residence time for mass in the tank, that is, the time constant in this case equals the residence time. From (11.22), the solution of (11.32) (the step response) is given by

$$c_A(t) = c_0 + \left(1 - e^{-t/\tau}\right) \Delta c_{A,\text{in}}$$
 (11.33)

where $\Delta c_{A,\text{in}} = c_{\infty} - c_0 = 0.1 \text{ kmol/m}^3$. At time t = 0, we then have that $c_A(0) = c_0 = 0.9 \text{ kmol/m}^3$, and concentration rises such that it is, at time $t = \tau = 5 \text{ h}$ (the residence time), $c_A = 0.9 + (1 - e^{-1}) \cdot 0.1 = 0.963 \text{ kmol/m}^3$, and at time $t = \infty$, $c_A(\infty) = 0.9 + 0.1 = 1 \text{ kmol/m}^3$ (as expected).

11.3.3 Additional examples of step responses for first-order systems

Here, we consider some relatively simple examples with only one differential equation which give first-order step responses (Figure 11.7).

Example 11.5 Temperature dynamics in continuous stirred tank. Consider the continuous process in Figure 11.9 where a liquid stream of 1 kg/s (constant) flows through a mixing tank with constant volume 1.2 m^3 . The density of the liquid is 1000 kg/ m^3 (constant) and the heat capacity is 4 kJ/kg K. Perfect mixing in the tank is assumed.

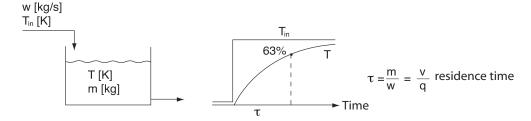


Figure 11.9: Temperature dynamics in continuous stirred tank without reaction

The process is initially operated at steady state such that the inlet temperature $T_{\rm in}$ is 50° C and the outlet temperature $T_{\rm out} = T$ is 50° C (so we assume no heat loss). Suddenly, the temperature of the inflow is changed to 60° C (step change). The outlet temperature will also "eventually" reach 60° C. The question is: What is the time constant, that is, how long does it take before the temperature in the tank (and outlet stream) has increased by $0.63\cdot10 = 6.3^{\circ}$ C to 56.3° C?

Solution. Since the mass in the tank is constant, the mass balance gives $w_{\text{out}} = w_{\text{in}} = w = 1 \text{ kg/s}$. The energy balance (11.12) for the tank is (liquid)

$$\frac{dH}{dt} = H_{\rm in} - H_{\rm out} \quad [J/s]$$

With the assumption of constant heat capacity c_p , this gives

$$mc_p \frac{dT}{dt} = wc_p(T_{\rm in} - T)$$

or equivalently

$$\frac{m}{w}\frac{dT}{dt} = -T + 1 \cdot T_{\rm in}$$

With y=T and $u=T_{\rm in}$ we see that this is in standard form (11.21) with

$$\tau = \frac{m}{w} = \frac{\rho V}{w} = \frac{1000 \cdot 1.2}{1} = 1200 \ s; \quad k = 1$$

In other words, it will take $\tau = 1200~s = 20$ min (the residence time m/w) before the outlet stream's temperature reaches 56.3 °C (and it will take an infinitely long time before it reaches 60 °C).

Note that the time constant also for this example equals the residence time. This is true for changes in both concentration and temperature for a continuous stirred tank without reaction or heating.

Example 11.6 Temperature dynamics in continuous stirred tank with heat exchange.

Consider the same example as above, where the inlet temperature is changed from 50 °C (initial steady state) to 60 °C, but we have heating (see Figure 11.10) such that the temperature in the tank is 70 °C (initial steady state). We consider the response and determine the time constant for the following two cases:

- 1. An electric heater is used such that the supplied heat Q is independent of the temperature T in the tank.
- 2. We have a heat exchanger with condensing stream on the hot side. The supplied heat is $Q = UA(T_h T)$ where T_h (hot side temperature) is constant at 110 °C.

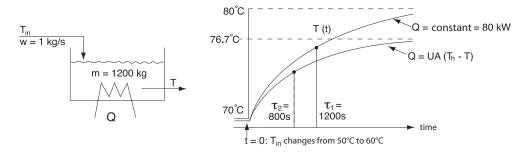


Figure 11.10: Continuous stirred tank with heating

Solution. The energy balance (11.12) becomes [J/s]

$$mc_p \frac{dT}{dt} = wc_p(T_{\rm in} - T) + Q$$

At the initial steady state (dT/dt = 0), we have (before the change in $T_{\rm in}$)

$$Q = -wc_p(T_{\rm in} - T) = -1 \text{ kg/s} \cdot 4000 \text{ J/kg } K \cdot (50 - 70)K = 80000\text{J/s} = 80 \text{ kW}$$

- 1. For the case when Q is independent of T, transformation to the standard form (11.21) gives that the time constant is $\tau = m/w = 1200$ s (residence time), and that the gain from $T_{\rm in}$ to T is k=1, that is, the steady-state temperature rise in the tank is 10 °C, that is, it will eventually rise to 80 °C.
- 2. For the case where Q depends on T, the energy balance becomes

$$mc_p \frac{dT}{dt} = wc_p(T_{\rm in} - T) + UA(T_h - T)$$
(11.34)

and transformation to the standard form (11.21) gives

$$\tau = \frac{mc_p}{wc_p + UA}; \quad k = \frac{wc_p}{wc_p + UA}$$

The time constant τ and the gain k are both smaller than in case 1. The reason is that the heat exchanger counteracts some of the temperature change ("negative feedback"). For numerical calculations, we need to know the value of UA. We have $UA = Q/(T_h - T)$, and from the initial steady state data, we find $UA = 80 \cdot 10^3/(110 - 70) = 2000$ W/K. The time constant and the gain are then

$$\tau = \frac{mc_p}{wc_p + UA} = \frac{1200 \cdot 4000}{1 \cdot 4000 + 2000} = 800 \ s; \quad k = \frac{4000}{4000 + 2000} = 0.67$$

that is, the temperature in the tank only increases by 6.7 °C to 76.7 °C – while in case 1 with an electric heater it increased by 10 °C.

Although k and τ are different, we note that $k' = k/\tau = 1/1200$ is the same in both cases, and since from (11.25) $\lim_{t\to 0} \Delta T'(t) = (k/\tau) \cdot \Delta T_{\rm in}$, this means that the initial responses are the same (see also Figure 11.10). This is reasonable also from physical considerations, since the "counteracting" negative feedback effect from the heat exchanger only comes in after the tank temperature T starts increasing which leads to a reduction in $Q = UA(T_h - T)$.

Example 11.7 Dynamics of cooking plate. Let us consider a cooking plate with mass m=1 kg and specific heat capacity $c_p=0.5$ kJ/kg K. The cooking plate is heated by electric power and the supplied heat is $Q_1=2000$ W. The heat loss from the cooking plate is $UA(T-T_o)$ where T is the cooking plate's temperature, $T_o=290$ K is the temperature of the surroundings, $A=0.04m^2$ and U is the overall heat transfer coefficient. If we leave the plate unattended, then we find that $T\to 1000$ K when $t\to\infty$. What is the time constant for the cooking plate (defined as the time it takes to obtain 63% of the final temperature change)?

Solution. This is a closed system without mass flows and shaft work, and since the cooking plate is solid, we can neglect energy related to pressure-volume changes. The energy balance (11.12) around the cooking plate (the system) gives

$$\frac{dH}{dt} = Q$$

Here, there are two contributions to the supplied heat Q, from electric power and from heat loss, that is,

$$Q = Q_1 - UA(T - T_o)$$

The enthalpy of the cooking plate is a function of temperature, that is, $dH/dt = mc_p dT/dt$. The energy balance becomes

$$mc_p \frac{dT}{dt} = Q_1 - UA(T - T_o) \tag{11.35}$$

In order to determine the overall heat transfer coefficient U, we use the steady state temperature $T^* = 1000$ K. At steady state, the energy balance is $0 = Q_1 - UA(T^* - T_o)$ and we find

$$U = \frac{Q_1}{A(T^* - T_o)} = \frac{2000}{0.04(1000 - 290)} = 70.4 \quad [W/m^2 \ K]$$

We assume that the overall heat transfer coefficient U is constant during the heating. The dynamic energy balance (11.35) is then a linear first-order differential equation which can be written in standard form

$$\tau \frac{dT}{dt} = -T + ku \tag{11.36}$$

where

$$\tau = \frac{mc_p}{UA} = 177.5 \ s$$

and

$$ku = \underbrace{\frac{1}{UA}}_{k_1} \underbrace{Q_1}_{u_1} + \underbrace{1}_{k_2} \cdot \underbrace{T_0}_{u_2}$$

In other words, we find that it takes time $t = \tau = 177.5$ s (about 3 min) to obtain 63% of the final change of the cooking plate's temperature.

Example 11.8 Response of thermocouple sensor in coffee cup. Temperature is often measured with a thermocouple sensor based on the fact that electric properties are affected by temperature. We have a thermocouple and a coffee cup and perform the following experiments:

- 1. Initially, we hold the thermocouple sensor in the air (such that it measures the air temperature).
- 2. We put the thermocouple into the coffee (and keep it there for some time so that the thermocouple's temperature is almost the same as the coffee's temperature).
- 3. We remove it from the coffee (the temperature will decrease and eventually approach the temperature of air actually, it may temporarily be lower than the air temperature because of the heat required for evaporation of remaining coffee drops).

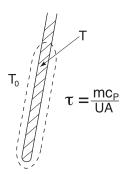


Figure 11.11: Thermocouple

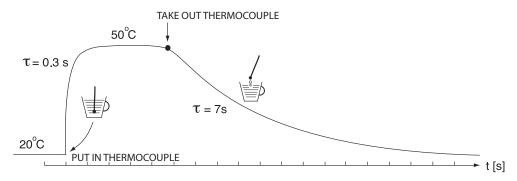


Figure 11.12: Coffee cup experiment

Task 1. What happens? Sketch the expected temperature response.

Solution: The result of an actual experiment performed by the author is shown in Figure 11.12. We see that the response is similar to a standard first-order response. However, it is striking that the response is much quicker when we put the sensor into the coffee (time constant about 0.3 s) than when we remove it (time constant about 7s).

Task 2. Can you explain this? Formulate a dynamic model and find an analytical expression for the time constant.

Solution: Since we want to find the response in temperature, we need to formulate an energy balance, and since it is the thermocouple's temperature, the energy balance should be around the thermocouple. The general energy balance is given in (11.12). Since there are no streams, we have that $H_{\rm in}-H_{\rm out}=0$. There is also no shaft work ($W_s=0$), and the contribution from "pressure-volume changes" can be neglected. The energy balance (11.12) around the thermocouple is then simply

$$\frac{dH}{dt} = Q$$

Here, $dH/dt = mc_p dT/dt$ where m is the mass of the thermocouple and T its temperature. The supplied heat to the thermocouple from the surroundings is

$$Q = UA(T_o - T)$$

The energy balance then becomes

$$mc_p \frac{dT}{dt} = UA(T_o - T) \tag{11.37}$$

where

- T temperature of thermocouple [K]
- T_o temperature of surroundings (coffee or air) [K]
- m mass of thermocouple [kg]
- $c_p(T)$ specific heat capacity of thermocouple [J/kg K]
- A area of thermocouple $[m^2]$
- U heat transfer coefficient from surroundings to thermocouple $[W/m^2 \ K]$

(11.37) can be rewritten as

$$\frac{mc_p}{UA}\frac{dT}{dt} = T_o - T$$

With y = T and $u = T_o$ this is in standard form (11.21) with

$$\tau = \frac{mc_p}{UA}; \quad k = 1 \tag{11.38}$$

(note that we get the same expression for the time constant as for the cooking plate in Example 11.7). At steady state, dT/dt = 0, and we have as expected that $T = T_o$. Thus, following a step in the surrounding's temperature T_o , the thermocouple's temperature T should exponentially (with time constant τ) approach T_o , and this is indeed confirmed by the experiment.

Some comments on coffee cup experiment

- 1. The time constant is independent of the temperatures T and T_o (this is not immediately obvious for someone who does not know any process dynamics).
- 2. The time constant τ is constant if c_p and U are constant (this seems to be a reasonable assumption during each of the two experiments).
- 3. The time constant was observed to be 7s/0.3s = 23 times larger when the thermocouple was removed from the coffee. Since $\tau = \frac{mc_p}{UA}$ where mc_P/A is constant, this must be (provided our theory is correct) because U is about 23 times higher when the thermocouple is in the coffee than when it is in air. This seems reasonable because heat transfer is usually much better to liquid than to gas.
- 4. In general, we desire a fast measurement, that is, we want the time constant τ to be small for the sensor. This is obtained by reducing the thermocouple's heat capacity mc_p [J/K], and making a design such that UA [W/K] is large. In order to protect the thermocouple, it is often placed in a pocket, which is not favorable because it increases the mass m and also reduces U. We can reduce this effect by choosing a pocket material with a small heat capacity mc_p (but at the same time with a good conductivity) and designing the pocket such that the outer area A is as large as possible.

Final comment on comparison of coffee cup experiment with theory

Being good engineers, we are very eager to compare our experimental results with theoretical calculations. I used a cylindrical thermocouple, that is,

$$\frac{V}{A} = \frac{(\pi/4)D^2L}{\pi DL} = \frac{1}{4}D$$

where D = 1.6 mm, $\rho = 2700$ kg/m³ and $c_p = 800$ J/kg K (aluminium). We can from (11.38) calculate the overall heat transfer coefficient U (SI units):

$$U = \frac{V\rho c_p}{A\tau} = \frac{1}{4} \frac{D\rho c_p}{\tau} = \frac{864}{\tau} \quad \text{[using SI units]}$$

Here, I found experimentally $\tau = 0.3s$ (coffee, that is, water) and $\tau = 7s$ (air), which gives $U = 2880 \ W/m^2 \ K$ (water) and $U = 123 \ W/m^2 \ K$ (air). Immediately, the value 2880 $W/m^2 \ K$ seems very high, because it is similar to values we find in heat exchangers with forced convection, and here we have natural convection. Let us compare with theoretical values for natural convection to air and water. For natural convection, $^1 \ Nu = 0.5 (Gr \cdot Pr)^{0.25}$, where the non-dimensional groups Nu, Gr and Pr are defined as

$$Nu = \frac{hD}{k}; \quad Pr = \frac{c_p \mu}{k}; \quad Gr = \frac{g\beta \Delta T D^3}{(\mu/\rho)^2}$$

Inserting and rearranging gives

$$h = 0.5 \left(\frac{k^3 c_p \rho^2 g \beta}{\mu}\right)^{0.25} \cdot \left(\frac{\Delta T}{D}\right)^{0.25}$$

where k is the thermal conductivity, β the thermal expansion coefficient and μ the viscosity of the fluid. We use the following physical and transport data:

$$\begin{aligned} \mathbf{Air}: & k = 0.027 \frac{W}{K\ m}; c_p = 1000 \frac{J}{kg\ K}; \mu = 1.8 \cdot 10^{-5} \frac{kg}{m\ s}; \rho = 1.2 \frac{kg}{m^3}; \beta = \frac{1}{T} = 0.003 \frac{1}{K} \end{aligned}$$

$$\mathbf{Water}: & k = 0.7 \frac{W}{K\ m}; c_p = 4200 \frac{J}{kg\ K}; \mu = 10^{-3} \frac{kg}{m\ s}; \rho = 1000 \frac{kg}{m^3}; \beta = 0.001 \frac{1}{K} \end{aligned}$$

We then find for natural convection (SI units)

Air:
$$h = 1.31 \cdot \left(\frac{\Delta T}{D}\right)^{0.25}$$

Water:
$$h = 173 \cdot \left(\frac{\Delta T}{D}\right)^{0.25}$$

Note from this that with natural convection, the heat transfer coefficient h to water is more than 100 times higher than to air. If we use $D=10^{-3}$ m and $\Delta T=10$ K (mean temperature difference between coffee and air; the exact value is not that important since it is raised to the power 0.25) we get $\left(\frac{\Delta T}{D}\right)^{0.25}=10$ (SI units) and if we assume $U\approx h$ (that is, we assume that the heat conduction inside the thermocouple is very fast), we estimate theoretically that U=13.1 W/m²K (air) and U=1730 W/m²K (water). We see that the theoretical U-value for water (1730 W/m² K) is quite close to the experimental (2880 W/m² K), while the theoretical U-value for air (13.1 W/m² K) is much lower than the experimental (123 W/m² K) estimated from the experiment. The reason for this is probably remaining water droplets on the thermocouple which evaporate and improve the heat transfer for the case when we remove the thermocouple from the coffee.

Example 11.9 Mass balance for filling a bathtub without plug. Here, we consider the dynamics for the volume (level) in a bathtub with no plug, see Figure 11.13. The model can also describe the dynamics of the outflow for a tank or the change in the water level in a lake following a rainfall. We consider a rectangular bathtub with liquid volume V = Ah where $A [m^2]$ is the base of the tub and h [m] is the liquid height. We assume that the density ρ is constant.

The control volume (boundary) for the system is the whole bathtub, and the inventory of mass is $m = \rho V$ [kg]. Mass is a conserved quantity, and from (11.3) we get that

$$\frac{dm}{dt} = w_{\rm in} - w_{\rm out} \quad [kg/s] \tag{11.39}$$

¹ For more details on this, and in general on modeling and balance equations, see: R.B. Bird, W.E. Stewart and E.N. Lightfoot, *Transport Phenomena*, Wiley, 1960.

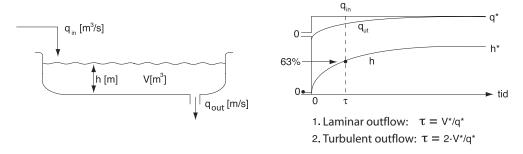


Figure 11.13: Bathtub without plug

and with the assumption of constant density we get the "volume balance"

$$\frac{dV}{dt} = q_{\rm in} - q_{\rm out} \quad [m^3/s] \tag{11.40}$$

This equation describes the volume change in a bathtub while it is filled or emptied. With a plug, we have $q_{out} = 0$, and the process is a "pure integrator," that is, there is no natural feedback that counteracts the increase in V. However, here we consider the case with no plug, and there is a "natural negative feedback," because q_{out} is a function of amount of water in the bathtub, that is, q_{out} increases when the liquid height h increases. We have from the static momentum balance (= mechanical energy balance):²

1. Laminar flow exit: $q_{\text{out}} = k_l h$ 2. Turbulent flow exit: $q_{\text{out}} = k_t \sqrt{h}$

The flow pattern is probably turbulent, but for simplicity let us assume laminar flow.

1. Laminar outflow. Inserting V = Ah into the "volume balance" gives

$$\frac{d(Ah)}{dt} = A\frac{dh}{dt} = q_{\rm in} - k_l h \quad [m^3/s]$$
(11.41)

This is a first-order differential equation in h(t) that can be rearranged into the standard form (11.21),

$$\tau \frac{dh}{dt} = -h + k \cdot q_{\rm in}$$

Thus, we have $\tau = A/k_l$ and $k = 1/k_l$ and the solution is

$$h(t) = \frac{1}{k_l} \left(1 - e^{-\frac{k_l t}{A}} \right) q_{\text{in}}$$
 (11.42)

We find that h(t) increases with time, most sharply at first, but then the increased level (h) results in a larger outflow, and we eventually reach (for $t \to \infty$) at a balance point (steady state) where $q_{\text{out}}^* = q_{\text{in}}$ and h no longer increases. The steady-state value, h^* , $t = \infty$ is from (11.42)

$$h^* = h(\infty) = \frac{q_{\rm in}}{k_l} \tag{11.43}$$

The outlet stream of the bathtub is driven by the pressure difference ρgh over the hole where the water exits. At steady state this pressure difference equals the friction pressure drop, i.e., $\Delta p_f = \rho gh$. From fluid mechanics (see page 243) we have $\Delta p_f \sim q$ for laminar flow and $\Delta p_f \sim q^2$ for turbulent flow, and it follows that $q \sim h$ (laminar) and $q \sim \sqrt{h}$ (turbulent).

- We can alternatively derive (11.43) from the steady state mass balance, $q_{\rm in} = q_{\rm out} \ [m^3/s]$. Here, $q_{\rm out} = k_l h$ and (11.43) follows.
- The time constant is $\tau = A/k_l$. Here, the steady-state flow rate is $q^* = k_l h^* (= q_{\text{out}}^* = q_{\text{in}}^*)$, that is, $k_l = q^*/h^*$, and it follows that

$$\tau = \frac{A}{k_l} = \frac{Ah^*}{q^*} = \frac{V^*}{q^*}$$

which equals the residence time of the bathtub. However, so that you won't think that the time constant always equals the residence time, please note that for turbulent outflow the time constant is twice the residence time; this is shown on page 302.

The following example illustrates that the dynamics of gas systems are usually very fast. This is primarily because of a short residence time, but it is usually further amplified by small relative pressure differences.

Example 11.10 Gas dynamics. A large gas tank is used to dampen flow rate and pressure variations. Derive the dynamic equations and determine the time constant for the pressure dynamics. We assume for simplicity that the inlet and outlet flow rates of the tank are given by $F_{\rm in} = c_1(p_{\rm in} - p)$ [mol/s] and $F_{\rm out} = c_2(p - p_{\rm out})$ [mol/s] where the "valve constants" c_1 and c_2 are assumed to be equal $(c_1 = c_2 = c)$.

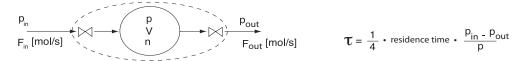


Figure 11.14: Gas dynamics

Solution. The mass balance is

$$\frac{dn}{dt} = F_{\rm in} - F_{\rm out} \quad [\text{mol/s}]$$

We assume constant volume V and ideal gas,

$$n = \frac{pV}{RT}$$

The mass balance then gives:

$$\frac{V}{RT}\frac{dp}{dt} = c(p_{\rm in} - p) - c(p - p_{\rm out})$$

This equation can be used to compute p as a function of $p_{\rm in}$, $p_{\rm out}$ and time. Rearranged into standard form (11.21), we see that the time constant is

$$\tau = \frac{V}{2cRT} = \frac{n}{2cp} \tag{11.44}$$

From the steady-state mass balance we get $p^* = (p_{in}^* + p_{out}^*)/2$, so at steady state

$$F^* = F_{\text{in}}^* = F_{\text{out}}^* = c \cdot \frac{p_{\text{in}}^* - p_{\text{out}}^*}{2}$$

Substituting the resulting value for c into (11.44) gives

$$\tau = \frac{n^*}{2cp^*} = \frac{1}{4} \cdot \frac{n^*}{F^*} \cdot \frac{p_{\text{in}}^* - p_{\text{out}}^*}{p^*}$$
 (11.45)

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that is, the time constant is 1/4 of the residence time, n/F, multiplied by the relative pressure difference, $(p_{\rm in}-p_{\rm out})/p$. For gas systems, both these terms are usually small, which explains why the pressure dynamics are usually very fast.

For example, with $p_{in}^* = 10.1$ bar, $p^* = 10$ bar and $p_{out}^* = 9.9$ bar we get

$$\tau = \frac{1}{4} \cdot \frac{n^*}{F^*} \cdot \frac{10.1 - 9.9}{10} = \frac{1}{4} \cdot \frac{1}{50} \cdot \frac{n^*}{F^*}$$

that is, the time constant for the pressure dynamics in the tank is only 1/200 of the (already small) residence time.

Example 11.11 First-order reaction in batch reactor (or in beaker)

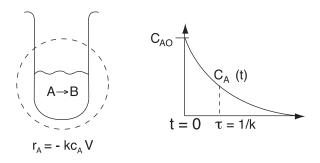


Figure 11.15: Reaction in beaker

Consider a beaker where component A reacts according to the first-order irreversible reaction $A \to B$. Derive the equation that describes the concentrations dynamics when temperature is assumed constant.

Solution. There are no inlet and outlet streams, so the component balance for the beaker is

$$\frac{d(c_A V)}{dt} = r_A V \quad [\text{mol A/s}] \tag{11.46}$$

where r_A is the reaction rate for "generation" of component A, which for a first-order reaction is $r_A = -kc_A$ [mol A/m^3 , s], where k [s^{-1}] is constant since the temperature is constant. If we, in addition, neglect changes in the volume, we get

$$\frac{dc_A}{dt} = -kc_A \tag{11.47}$$

which gives a first-order response $c_A(t) = c_A(0)e^{-t/\tau}$ with time constant $\tau = 1/k$ (note that k here is the reaction rate constant and not the gain). We note that $c_A \to 0$ when $t \to \infty$, that is, the final steady state has complete conversion of A.

Comment. This is a batch process, so the system is not initially at steady state. However, this is not a requirement, and (11.47) can be solved when we know the initial concentration $c_A(0)$ at the start of the experiment.

Exercise 11.2* Evaporator. Take another look at the evaporator in Example 11.2 (page 280). What is the time constant for the temperature response?

Exercise 11.3 First-order reaction in CSTR. Consider a continuous stirred tank reactor (CSTR) where component A decomposes in a first-order irreversible reaction $A \to B$ with reaction rate $r = (-r_A) = kc_A V$ [mol A/s]. (Note that k here is the reaction rate

constant and not the process gain). The feed concentration is $c_{A,F}$. Derive the equation that describes the concentration dynamics when temperature is assumed constant. Find the time constant and gain for the response.

11.3.4 Time response for more complex systems

In the previous section, we considered in detail the step response for systems with only one differential equation which can be written in "standard" form $\tau dy(t)/dt = -y(t) + k \ u(t)$. This gave rise to a first-order response. Although many systems can be written (or approximated) by a first-order response, it must be emphasized that the responses are generally far more complex.

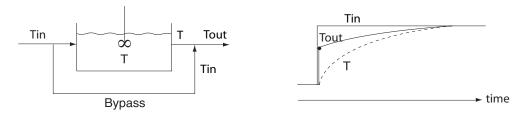


Figure 11.16: Temperature response for stirred tank with bypass

• Even for systems with only one linear differential equation, the response can be different from that described above, either because the system is non-linear or because the response has a "direct term," that is, the equation can be written in the form

$$\tau dx(t)/dt = -x(t) + ku(t); \quad y(t) = c \cdot x(t) + d \cdot u(t)$$

where the $d \neq 0$ gives a "direct term" from u to y (see for example Figure 11.16 which shows the response of a stirred tank with bypass).

- If we have two first-order systems in series, for example two stirred tanks, the total response will be second-order, and if we have n first-order systems in a series, the total response is nth-order. The response for such higher-order systems will usually have a "flatter" initial response (see Figure 11.22, page 309), and is often approximated as an effective time delay.
- We will also have a higher-order response if the model consists of several coupled differential equations, for example, an adiabatic reactor with coupled material and energy balance (see Figure 11.24, page 312).

The analytic expression for the time response of higher-order system is usually rather complicated, and often there is no analytical solution. However, by linearizing the system, as discussed in the next section (Section 11.4), it is possible to use effective mathematical tools for analyzing the system, for example, by computing the system's "poles" (=eigenvalues = -1/time constant) and "zeros." The most important tool for analyzing more complex systems is nevertheless "dynamic simulation," that is, numerical solution of the equations. This is discussed in Section 11.5.

11.6 Process control

Automatic **feedback control** is widely used in the process industry, and the instrumentation and control system typically represents 30% of the investments in a plant. For each process variable y that one wants to control one needs

- a measurement of the process variable (y),
- an independent manipulated variable u (usually a valve) that influences y.

We use the following notation

- CV = controlled variable (y, "output")
- MV = manipulated variable (u, "input", independent variable)
- DV = disturbance variable (d, independent variable that we cannot influence)

The MV should have a "direct" and large effect on the CV (with fast dynamics and a small delay or inverse response). The idea of control is to adjust the MV (u) such that the CV (y) is kept close to its desired setpoint y_s , in spite of disturbances d, that is, we want a small control error,

$$e(t) = y(t) - y_s$$

We use **negative feedback**, where the sign of the control action is opposite the sign of the process. This implies that the MV (u) is adjusted such that it counteracts changes in the CV (y). A well-known feedback controller from daily life is the on/off controller used in thermostats, where the heat is the MV and temperature is the CV. The on/off controller is simple, but it gives large MV changes (between max and min), and fluctuations in the CV (temperature) are unavoidable. This is undesirable, so in the process industry one normally uses the proportional-integral-derivative (PID) controller with algorithm

$$u(t) = u_0 - K_c \left(e(t) + \frac{1}{\tau_I} \int_0^t e(t)dt + \tau_D \frac{de(t)}{dt} \right)$$
 (11.54)

We see that the MV-change away from its nominal value $(u - u_0)$ is a weighted sum of the present value of the error e (the P-term), the integral of the error e (the I-term) and the derivative of the error e (the D-term). The PID controller has three adjustable parameters:

- Gain K_c
- Integral time τ_I [s]
- Derivative time τ_D [s]

The proportional term is usually the most important, and a large value of K_c results in a faster initial response. The integral action causes the MV to change until the error e(t) is zero, that is, we get no steady state off-set. A small value of the integral time τ_I [s] results in the controller returning faster to steady state. For this reason, the integral time is often called the "reset time." The derivative term can give faster responses for some processes, but it often gives "nervous control" with large sensitivity to measurement noise. For this reason, a PI controller (with $\tau_D = 0$) is most common.

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There are also other variants of the PID controller, for example, the cascade form, but the differences are usually small for practical purposes. One should, however, note that the vendors use different names and definitions for the three PID parameters. For example, some vendors use the integral gain $K_I = K_c/\tau_I$ and the derivative gain $K_D = K_c\tau_D$. Others use the "proportional band" $100/K_c$, and "reset rate" $1/\tau_I$.

The main problem with negative feedback is that we can get instability if we overreact (if K_c is too large or τ_I is too small) such that we get variations that grow over time.

On-line tuning. Finding good control parameters ("tunings") is not as simple as one may believe. A common (and serious) mistake is to use the wrong sign for K_c , which usually causes the system to drift to an operating point with a fully open or fully closed valve. Tuning is often performed "on-line" using trial-and-error. One usually starts with a controller with a low gain (K_c) and with no integral action $(\tau_I = \infty)$. K_c is then gradually increased until either (a) the control performance to disturbances and set-point changes is acceptable, (b) the MV change is too large or (c) the system starts oscillating. If the system starts oscillating, then K_c is reduced by approximately a factor 2 or more. Next, one gradually reduces the integral time τ_I until (a) the settling time (back to the set-point) is acceptable or (b) the system starts oscillating. If the system oscillates, then τ_I is increased by a factor of approximately 2 or more compared to the value that gave oscillations. If the response is too slow then one may try introducing derivative time τ_D , which can be increased until (a) the MV changes become too nervous or (b) the system starts oscillating. If the system starts oscillating, then τ_D is reduced with approximately a factor 2 or more compared to the value that gave oscillations.

Model-based tuning for fast response. Alternatively, model-based tuning is used. The response (without control) from the MV (u) to the CV (y) is recorded and then approximated as a first-order response with a delay, that is, one obtains the model parameters k, τ and θ (see page 286). The following SIMC⁴ PI-tunings are recommended

$$K_c = \frac{1}{k} \frac{\tau}{\tau_c + \theta}; \quad \tau_I = \min\{\tau, \ 4(\tau_c + \theta)\}$$
 (11.55)

Here, the "closed-loop" response time τ_c [s] is the only tuning parameter. A smaller τ_c gives a faster response for the CV, but one may get oscillations and the MV-changes are larger. In order to avoid oscillations and have good robustness (with a good margin to instability), it is recommended to choose τ_c larger than the effective delay, that is, $\tau_c \geq \theta$.

If the response is dominant second order, meaning that the response is well approximated by a second-order response with $\tau_2 > \theta$, then a substantial improvement can sometimes be obtained by adding derivative action, provided there is not too much measurement noise. The response is then approximated by a second-order model with parameters k, τ, τ_2 and θ . For a PID controller on cascade form, K_c and τ_I are then as given in (11.55) (but note that the parameter values will change because θ is smaller when we use a second-order model) and the derivative time is

$$\tau_D = \tau_2 \tag{11.56}$$

⁴ S. Skogestad, "Simple analytic rules for model reduction and PID controller tuning," J. Process Control, Vol. 13 (2003), 291–309.

Note that this is for a so-called cascade PID-form. To get the corresponding PID-parameters for the "ideal" PID form in (11.54), compute the factor $\alpha = 1 + \tau_D/\tau_I$, and multiply K_c and τ_I by α , and divide τ_D by α .

Conservative tuning for smooth response. The tuning procedure outlined above is often time consuming, and as a starting point the following minimum ("conservative") gain can be used⁵

$$|K_{c,\min}| = \frac{|u_0|}{|y_{\max}|}$$
 (11.57)

where $|u_0|$ is the MV change required to counteract the largest expected disturbance and $|y_{\text{max}}|$ is the largest accepted CV deviation. In industry, the variables have often already been scaled such that $|u_0| \approx |y_{\text{max}}|$ (for example equal to 1) and we get $|K_{\text{c,min}}| \approx 1$. Indeed, this is a common factory setting for the gain. In addition, it is crucial that the sign of K_c is chosen correctly – remember that the control is supposed to counteract and not intensify changes in the CV. As a conservative starting point for the integral time, $\tau_I = \tau$ can be chosen, where τ is the dominant time constant for the effect of the MV on the CV.

Example 11.19 Control of exothermic CSTR. This is a continuation of Example 11.16 (page 311). We want to keep the reactor temperature y = T approximately constant at $y_s = 444K$. We assume that the reactor temperature can be measured and that we can affect y = T by changing the coolant temperature $u = T_c$. The objective is to design a feedback PI-controller with y = T as the controlled variable (CV) and $u = T_c$ as the manipulated variable (MV). We consider, as before, an increase in the feed rate of 20% (from 0.10 to $0.12 \text{ m}^3/\text{min}$) – this is the "disturbance" to the process. Without control, we have found that the reactor temperature T will eventually drop to 441.9 K, but with PI control the MV will counteract the disturbance such that CV = T returns to its desired value (setpoint) of 444 K; see Figure 11.28.

To tune the controller, we obtained first, without control, the response from the cooling temperature (MV, u) to the reactor temperature (CV, y). This response (not shown in Figure 11.28) can be closely approximated as a first-order response (without time delay θ) with gain $k = \Delta y(\infty)/\Delta u \approx 0.5$ and time constant $\tau \approx 7$ min. For example, this is obtained by simulating a small step in T_c (for example, by changing T_c from 430 to Tc=431 and setting q=0.1 in the MATLAB code on page 312), but it can also be found analytically by linearizing the model. We chose the closed-loop response time to be $\tau_c = 3$ min (a lower value gives a faster response, but with larger changes in the MVT_c). From (11.55), this gives the PI-settings

$$K_c = \frac{1}{0.5} \frac{7}{3+0} = 4.7, \quad \tau_I = \min\{7, 12\} = 7 \text{ min}$$

The response with control is shown in Figure 11.28. We see that the temperature y=T returns to its setpoint $T_s=444$ K after about 9 minutes (about three times τ_c). The simulation was performed by adding the following lines after point II in the MATLAB code on page 312:

```
% PI-CONTROLLER: u = u0 - Kc*e - (Kc/taui)*eint, where deint/dt = e
% Note: (1) The integrated error eint is introduced as an extra state: eint = y(4)
% (2) The process ''output" (CV) yreg is in this case the reactor temperature T
% (3) The process ''input" (MV) u is in this case the cooling temperature Tc
yreg = T; yregs= 444; e=yreg-yregs; u0 = 430; eint=y(4); Kc=4.7; taui=7;
u = u0 - Kc*e - (Kc/taui)*eint;
Tc = u;
```

⁵ S. Skogestad, "Tuning for smooth PID control with acceptable disturbance rejection," Ind. Eng. Chem. Res., Vol. 45, 7817-7822 (2006).

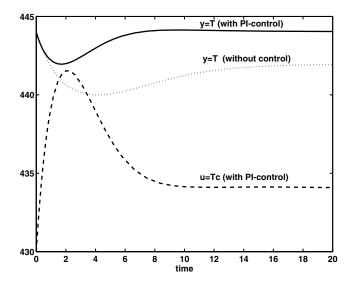


Figure 11.28: Exothermic CSTR with and without control: Temperature response after a 20% increase in feed flow rate

and by changing the last line to: DYDT=[f1; f2; f3; e];. The modified code is saved in the file cstrTpi.m and can be run by entering:

 $[\mathtt{T}, \mathtt{Y}] = \mathtt{ode15s}(\mathtt{@cstrTpi}, [\mathtt{0}\ \mathtt{50}], [\mathtt{2274}\ \mathtt{7726}\ \mathtt{444.0}\ \mathtt{0}]);.$

11.7 Summary

Typically, the following steps are involved for the derivation and analysis of a dynamic model:

- 1. Formulate the relevant dynamic balance equations. The main problem is often: Which balance? Which control volume?
- 2. Use steady state data (obtained at the nominal operating point) to determine any missing parameters in the dynamic model equations.
- 3. Linearize and analyze the model.
- 4. Find the dynamic response by solving the dynamic equations ("dynamic simulation").
- 5. The model can, also, be used to design the control system, for example, to tune a PID controller.