



11

Process dynamics

In a dynamic system, the values of the variables change with time, and in this chapter we quantify the well-known fact that “things take time.” We also consider dynamic modeling, dynamic responses (analysis), dynamic simulation (numerical calculation) and process control.

11.1 Introduction

Some reasons for considering a system’s dynamics and obtaining dynamic models are:

1. To describe the time behavior of a batch process.
2. To describe the transient response of a continuous process (e.g., dynamic change from one steady state to another).
3. To understand the dynamics of the process (analysis), for example, as expressed by the time constant.
4. To develop a “training simulator” for operator training.
5. For “what occurs if” studies, for example, as a tool in a HAZOP analysis (“what happens if this valve is closed?”).
6. For optimization and control (control structure, tuning of controllers, model-based control).

Note that when it comes to dynamics, there is no difference between a model for a batch process a continuous process.

The dynamic models we consider in this chapter are given in the form of differential equations,

$$\frac{dy}{dt} = f(y, u) \quad (11.1)$$

where u is the independent variable and y the dependent variable, as seen from a cause-and-effect relationship. With a dynamic model, it is possible, given the system’s initial state ($y(t_0) = y_0$) and given the value of all of the independent variables ($u(t)$ for $t > t_0$), to compute (“simulate”) the value of the dependent variables as a function of time ($y(t)$ for $t > t_0$).

Up to now, we have studied steady-state behavior, where time t was not a variable. The steady-state model $f(y, u) = 0$ gives the relationship between the variables u and y for the special case when $dy/dt = 0$ (“the system is at rest”).

The basis for a dynamic model can be

1. Fundamental: From balance equations + physics/chemistry; see the next section
2. Empirical (regression-based): From experimental data (measurements)

Often we use a combination, where the parameters of a fundamental model are obtained from experimental measurement data.

Comment on notation. The dot notation (\dot{X}) is used other places in this book to indicate rate variables (e.g., \dot{m} [kg/s] denotes the mass flow rate). However, in other fields and books, particularly in control engineering, the dot notation indicates time derivative (that is $\dot{m} \equiv dm/dt$). Since we work, in this chapter, with both time derivatives and rates, we here choose to avoid the dot notation altogether. The following special symbols are instead used for rates (amount of stream per unit of time):

- Molar flow rate: $F \equiv \dot{n}$ [mol/s]
- Mass flow rate: $w \equiv \dot{m}$ [kg/s]
- Volumetric flow rate: $q \equiv \dot{V}$ [m³/s]

11.2 Modeling: Dynamic balances

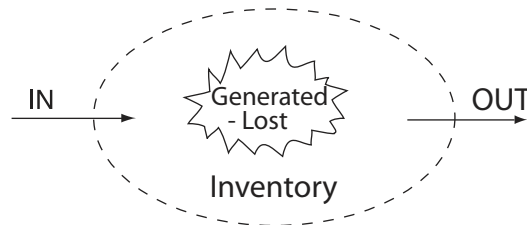


Figure 11.1: The balance principle

Here, we show how dynamic models can be derived from the balance equations for total mass, energy and component mass (mole). This gives, at the same time, an overview and a review of the material presented in previous chapters. Consider a system with a well-defined boundary (“control volume”), see Figure 11.1. The starting point for a fundamental model is the balance equations (see Chapter 2).

$$\underbrace{\text{Change Inventory}}_{\text{accumulated in the system}} = \underbrace{\text{In} - \text{Out}}_{\text{through the system's boundary}} + \underbrace{\text{Generated} - \text{Loss}}_{\text{internally in the system}}$$

In this chapter, the terms “change,” “in,” “out,” “generated” and “loss” are always per unit of time. Mathematically, the general balance equation *per unit of time* is (see (2.8) on page 42):

$$\boxed{\frac{dB}{dt} = B_{\text{in}} - B_{\text{out}} + B_{\text{generated}} - B_{\text{loss}}} \quad \left[\frac{\text{kg}}{\text{s}}, \frac{\text{mol}}{\text{s}}, \frac{\text{J}}{\text{s}}, \dots \right] \quad (11.2)$$

Here B is the inventory of the quantity that we are considering (inside the system’s boundary), $\frac{dB}{dt}$ is the change in the inventory per unit of time, $B_{\text{in}} - B_{\text{out}}$ is net

supplied through the system's boundary (with mass flows or through the wall) and $B_{\text{generated}} - B_{\text{loss}}$ is net supplied internally in the system. For conserved quantities (*mass* and *energy*), we have $B_{\text{generated}} = 0$ and $B_{\text{loss}} = 0$. *Component mass (mol)* is not conserved, so we have to include a term for "net generated in chemical reactions," which represents the sum of "generated" and "lost." Similarly, *momentum* (mechanical energy) is not conserved and we have to include a friction term.

In principle, the balance equations are easy to formulate, but we need to decide:

1. Which control volume (where do we draw the boundary for the quantity we are balancing)?
2. Which balance (which quantity are we considering, for example, mass or energy)?

The answer to the last question is typically:

- Interested in mass, volume or pressure: *mass balance*
- Interested in concentration: *component balance*
- Interested in temperature: *energy balance*
- Interested in the interaction between flow and pressure: *Mechanical energy balance* (= *momentum balance* = Bernoulli = Newton's second law) (in some of the examples below, we use the static momentum balance where the term for acceleration is neglected).

11.2.1 Dynamic total mass balance

The total mass balance per unit of time is

$$\boxed{\frac{dm}{dt} = w_{\text{in}} - w_{\text{out}}} \quad [\text{kg/s}] \quad (11.3)$$

where m [kg] is the system's mass ("inventory of mass inside the control volume"), dm/dt [kg/s] is the change in mass inventory per unit of time and $w_{\text{in}} - w_{\text{out}}$ [kg/s] are the mass flow rates for for the entering and exiting streams (bulk flow). By introducing the density, we get

$$\frac{d(\rho V)}{dt} = \rho_{\text{in}} q_{\text{in}} - \rho_{\text{out}} q_{\text{out}} \quad [\text{kg/s}]$$

where V [m³] is the system's volume, q_{in} [m³/s] and q_{out} [m³/s] are the volumetric flow rates and ρ , ρ_{in} and ρ_{out} [kg/m³] are the (average) densities.

For liquid-phase systems, it can often be assumed that the density ρ is constant (that is, $\rho = \rho_{\text{in}} = \rho_{\text{out}} = \text{constant}$), and the mass balance becomes a "volume balance"

$$\text{Constant density: } \frac{dV}{dt} = q_{\text{in}} - q_{\text{out}} \quad [\text{m}^3/\text{s}] \quad (11.4)$$

Quotation marks are here used to show that volume is generally *not* a conserved quantity. In practice, it is often the liquid level (or height h [m]) that is of interest. The relationship between volume and level is $V = Ah$ for a tank with constant cross section area A [m²], and more generally $V = \int A(h)dh$ when A varies with height. We then get

$$\frac{dV}{dt} = A \frac{dh}{dt} + h \frac{\partial A}{\partial h} \frac{dh}{dt}$$

where the last term is zero for a constant cross section area A (since $\partial A/\partial h = 0$).

Note that the total number of moles in the system is generally not a conserved quantity, that is, the total mole balance is

$$\frac{dn}{dt} = F_{\text{in}} - F_{\text{out}} + G \quad [\text{mol/s}] \quad (11.5)$$

where G [mol/s] is the net generated number of moles in chemical reactions.

11.2.2 Dynamic component balance

The dynamic **component balance** can, for an arbitrary component A, be written

$$\boxed{\frac{dn_A}{dt} = F_{A,\text{in}} - F_{A,\text{out}} + G_A} \quad [\text{mol A/s}] \quad (11.6)$$

(we normally use mole basis, but the component balance can also be written on weight basis [kg A/s]). Here, n_A [mol A] is the inventory (amount) of component A inside the system's boundary, $F_{A,\text{in}} - F_{A,\text{out}}$ [mol A/s] are the molar flow rates of A in the streams (bulk flow) and G_A [mol A/s] is net generated in the chemical reactions. This can, from (3.7), be calculated from

$$G_A = \sum_j \nu_{A,j} \xi_j \quad [\text{mol A/s}]$$

where $\nu_{A,j}$ is the stoichiometric coefficient for component A in reaction j , and ξ_j [mol/s] is the extent of reaction for reaction j . Instead of the extent of reaction, one can alternatively use the reaction rate, and from (10.7), write

$$G_A = \int_0^V \underbrace{\sum_j \nu_{A,j} r_j}_{r_A} dV \quad [\text{mol A/s}] \quad (11.7)$$

where r_j [mol/ m³ s] is the reaction rate for reaction j . Note that we in the dynamic case usually do *not* restrict ourselves to independent reactions because this makes it more difficult to introduce the reaction rate. The reaction rate is a function of concentration and composition, and generally varies with the position in the reactor (and therefore the integral in (11.7)).

For example, for a first-order reaction $A \rightarrow B$, we can have that

$$r = k(T)c_A \quad [\text{mol A/s m}^3]$$

Here, we have $r_A = -r$, where the sign is negative because A is consumed in the reaction and the stoichiometric coefficient is $\nu_A = -1$. We often assume that the temperature dependency of the reaction rate constant k follows Arrhenius' equation

$$k(T) = Ae^{-E/RT}$$

where A is a constant and E [J/mol] is the activation energy. We also introduce

$$\bar{c}_A = n_A/V; \quad c_{A,\text{in}} = F_{A,\text{in}}/q_{\text{in}}; \quad c_{A,\text{out}} = F_{A,\text{out}}/q_{\text{out}}$$

where \bar{c}_A [mol/m³] is the average concentration of A in the reactor. Similarly, the average reaction rate is defined $\bar{r}_A = (\int r_A dV)/V$. Then $G_A = \bar{r}_A V$ and the component balance can be written

$$\boxed{\frac{d(\bar{c}_A V)}{dt} = c_{A,\text{in}} q_{\text{in}} - c_{A,\text{out}} q_{\text{out}} + \bar{r}_A V} \quad [\text{mol A/s}] \quad (11.8)$$

Here we have used concentration c , but we may alternatively use mole fraction or weight fraction.

Example 11.1 Ideal continuous stirred tank reactor (CSTR). Here we have perfect mixing and we do not need to use average values, that is, $\bar{c}_A = c_A$ and $\bar{r}_A = r_A$. Furthermore, we have that $c_{A,\text{out}} = c_A$ and the component balance (11.8) is

$$\frac{d(c_A V)}{dt} = c_{A,\text{in}} q_{\text{in}} - c_A q_{\text{out}} + r_A V \quad (11.9)$$

If we, in addition, assume constant density ρ , we can introduce the “volume balance” (11.4) such that the left side of (11.9) is

$$\frac{d(c_A V)}{dt} = c_A \frac{dV}{dt} + V \frac{dc_A}{dt} = c_A (q_{\text{in}} - q_{\text{out}}) + V \frac{dc_A}{dt}$$

The “out term” in (11.9) then drops out and the component balance for a CSTR becomes

$$\boxed{V \frac{dc_A}{dt} = (c_{A,\text{in}} - c_A) q_{\text{in}} + r_A V} \quad [\text{mol A/s}] \quad (11.10)$$

Note that, with the assumption of constant density, this equation applies even if the reactor volume V varies.

With a little practice, the balance (11.10) may be set up directly: “The concentration change in a CSTR is driven by the inflow having a different composition plus the contribution for chemical reaction.” However, it is generally recommended to start from equation (11.6).

11.2.3 Dynamic energy balance

The general energy balance (4.10) over a time period Δt with $\Delta U = U_f - U_0$ gives, as $\Delta t \rightarrow 0$, the dynamic energy balance:

$$\boxed{\frac{dU}{dt} = H_{\text{in}} - H_{\text{out}} + Q + W_s - p_{\text{ex}} \frac{dV}{dt}} \quad [\text{J/s}] \quad (11.11)$$

Here, U [J] is the internal energy for the system (inside the control volume), while $H_{\text{in}} - H_{\text{out}}$ is the sum of internal energy in the streams plus the flow work that the streams perform on the system as they are “pushed” in or out of the system. The term $-p_{\text{ex}} \frac{dV}{dt}$ is the work supplied to the system when its volume changes; it is negligible for most systems. Q [J/s] is supplied heat (through the system’s wall), while W_s [J/s] is supplied useful mechanical work (usually shaft work, for example, from a compressor, pump or turbine). Note that there is no term of the kind “heat generated in chemical

reaction” because the heat of reaction is indirectly included in the internal energy, and thus in the terms dU/dt , H_{in} , and H_{out} .

“Complete” general energy balance. Note that I, as before, have been a bit lazy when writing the energy balance in the “general” form in (11.11). When necessary, terms for kinetic and potential energy must be added to U and H , and other work terms such as electrochemical work W_{el} must be included. Thus, as stated in the “energy balance reading rule” on page 4.4:

- Shaft work W_s [J/s] really means $W_s + W_{\text{el}} + \text{other work forms}$.
- Internal energy U of the system [J] really means $E = U + E_K + E_P + \text{other energy forms}$. Here E_K is kinetic energy and E_P is potential energy of the system.
- Enthalpy H of the in- and outstreams [J/s] really means $H + E_K + E_P + \text{other energy forms}$. For a stream, $E_K = w\alpha v^2/2$ and $E_P = wgz$, see page 125, where w [kg/s] is the flow rate.

Energy balance in enthalpy

We usually prefer to work with enthalpy, and introducing $U = H - pV$ in (11.11), gives

$$\boxed{\frac{dH}{dt} = H_{\text{in}} - H_{\text{out}} + Q + W_s - \underbrace{(p_{\text{ex}} - p) \frac{dV}{dt} + V \frac{dp}{dt}}_{\text{pressure-volume changes}}} \quad [\text{J/s}] \quad (11.12)$$

Here, $H = mh$ [J] is the enthalpy of the system (inside the control volume), where m [kg] is system mass and h [J/kg] is its specific enthalpy.

Comments:

1. The term “pressure-volume changes” in (11.12) and (11.13) is often negligible.
 - The term is exactly zero (also for gases) for cases with constant pressure and volume.
 - The term is exactly zero (also for gases) for cases where the pressure is constant and equal to the surrounding’s pressure ($p = p_{\text{ex}} = \text{constant}$).
 - Even with varying pressure, the term is approximately zero for liquids and solids, because the volume V is relatively small for such systems.

However, the term “pressure-volume changes” can be considerable for gases with varying pressure, for example, for a gas pipeline.

2. We have $\frac{dH}{dt} = m \frac{dh}{dt} + h \frac{dm}{dt}$ and by introducing the mass balance (11.3), the energy balance on “mass flow basis” becomes

$$m \frac{dh}{dt} = w_{\text{in}}(h_{\text{in}} - h) - w_{\text{out}}(h_{\text{out}} - h) + Q + W_s - \underbrace{(p_{\text{ex}} - p) \frac{dV}{dt} + V \frac{dp}{dt}}_{\text{pressure-volume changes}} \quad [\text{J/s}] \quad (11.13)$$

3. All enthalpies must refer to a common reference state. If we use, for example, the elements at 298 K and 1 bar as the reference, the enthalpy H (or h) is the sum of (1) chemical formation energy, (2) “latent” phase transition energy (if the phase differs from the standard state), (3) thermal energy (“sensitive heat c_p ”), (4) mixing energy and (5) pressure-correction energy; see page 364.
4. Enthalpy $H(T, p, f, n_j)$ [J/kg] is generally a function of temperature T , pressure p , phase distribution f (where f is fraction of light phase) and composition (n_j). The time derivative

of the enthalpy in (11.12) can then be written

$$\frac{dH}{dt} = \underbrace{\frac{\partial H}{\partial T}}_{C_p} \frac{dT}{dt} + \frac{\partial H}{\partial p} \frac{dp}{dt} + \underbrace{\frac{\partial H}{\partial f}}_{\Delta_{\text{trs}} H} \frac{df}{dt} + \sum_j \frac{\partial H}{\partial n_j} \frac{dn_j}{dt} \quad (11.14)$$

This expression may be useful in some cases, but for numerical calculations it is generally recommended to work directly with H (or U) as the internal variable (“state”) rather than T ; see page 316 on solving the resulting differential-algebraic equations (DAE).

11.2.4 Energy balance in temperature

Here, we want to derive a differential equation in temperature, $dT/dt = \dots$. This gives insight and is useful for some calculations. The expressions for dT/dt presented below depend on the following assumptions:

- The enthalpy’s dependency of pressure is neglected, which is reasonable in most cases.
- The phase distribution in the system and in each stream does not change, which is reasonable in most cases.
- The enthalpy’s dependency of composition is neglected, which is reasonable in many cases, for example, if each stream’s composition is constant (actually, this assumption is not made for the case with chemical reaction in case III).

This means that the three last terms in (11.14) drop out, and the specific enthalpies in (11.13) are only a function of temperature, that is,

$$h(T) = h(T_{\text{ref}}) + \int_{T_{\text{ref}}}^T c_p(T) dT \quad (11.15)$$

Here $h(T_{\text{ref}})$ is constant, because the composition and phase distribution is constant. When we put everything into the energy balance (11.13), the contribution from the reference-terms ($h(T_{\text{ref}})$, $h_{\text{in}}(T_{\text{ref}})$, $h_{\text{out}}(T_{\text{ref}})$) will appear as terms for heat of phase change (e.g., heat of vaporization) or heat of reaction. Let us next consider three cases.

I. No reaction and no phase transition

For the case with *no reaction and no phase transition*, the reference-terms drop out and (11.13) becomes

$$m c_p(T) \frac{dT}{dt} = w_{\text{in}} \int_T^{T_{\text{in}}} c_p(T) dT - w_{\text{out}} \int_T^{T_{\text{out}}} c_p(T) dT + Q + W_s \underbrace{-(p_{\text{ex}} - p) \frac{dV}{dt} + V \frac{dp}{dt}}_{\text{pressure-volume changes}}$$

If we, in addition, assume that the *heat capacity is constant* (independent of temperature), the energy balance becomes

$$m c_p \frac{dT}{dt} = w_{\text{in}} c_p (T_{\text{in}} - T) - w_{\text{out}} c_p (T_{\text{out}} - T) + Q + W_s \underbrace{-(p_{\text{ex}} - p) \frac{dV}{dt} + V \frac{dp}{dt}}_{\text{pressure-volume changes}} \quad (11.16)$$

This is further simplified for an ideal stirred tank (CSTR), where we have $T_{\text{out}} = T$.

II. With phase transition

Let us consider a somewhat more complex case with phase transition, where we cannot use (11.16), because the reference terms $h(T_{\text{ref}})$ do not drop out of the energy balance.

Example 11.2 Phase transition: Energy balance for evaporator.

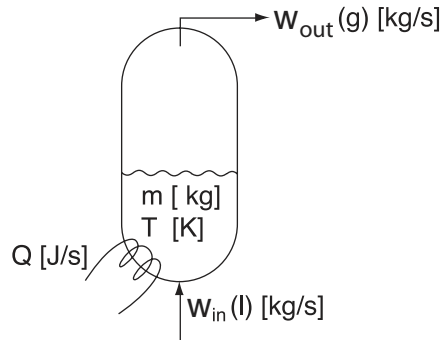


Figure 11.2: Evaporator for water

We consider an evaporator for water as shown in Figure 11.2. We neglect the mass of gas compared to the mass of liquid in the system (inside the evaporator). The mass balance is

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

Since we assume only liquid in the tank, we can neglect the terms with “pressure-volume changes” (even when the pressure varies). We also have no shaft work ($W_s = 0$). The energy balance (11.13) then becomes

$$m \frac{dh}{dt} = w_{\text{in}}(h_{\text{in}} - h) - w_{\text{out}}(h_{\text{out}} - h) + Q \quad [\text{J/s}]$$

The enthalpy h [J/kg] of the liquid in the tank is only a function of temperature (because the remaining terms in (11.14) can be neglected or are zero). Thus, we have $dh/dt = c_{pL}dT/dt$, where we use c_{pL} [J/K kg] with subscript L to indicate that it is a liquid.

The inflow and the mass in the evaporator have the same composition and phase (liquid). We then have

$$h_{\text{in}}(T_{\text{in}}) - h(T) = \int_T^{T_{\text{in}}} c_{pL}(T) dT \quad [\text{J/kg}]$$

We assume perfect mixing such that $T = T_{\text{out}}$. Since the outlet stream is in gas phase, we then get

$$h_{\text{out}}(T) - h(T) = \Delta_{\text{vap}}h(T) \quad [\text{J/kg}]$$

where $\Delta_{\text{vap}}h(T)$ is the heat of vaporization for water at T (which takes into account the change in reference due to the phase transition). The energy balance (11.13) for the evaporator then becomes

$$\boxed{m c_{pL}(T) \frac{dT}{dt} = w_{\text{in}} \int_T^{T_{\text{in}}} c_{pL}(T) dT - w_{\text{out}} \Delta_{\text{vap}}h(T) + Q} \quad [\text{J/s}] \quad (11.17)$$

Note that (11.17) also applies when the mass m in the tank varies with time, because the mass balance $\frac{dm}{dt} = w_{\text{in}} - w_{\text{out}}$ was used when deriving (11.13).

Comments.

1. The heat of vaporization is often given at a temperature T_{ref} (for example, at the normal boiling point at 1 atm). The heat of vaporization at T can then be found by adding the following subprocesses: (1) Cooling the liquid from T to T_{ref} , (2) evaporation at T_{ref} , and (3) heating the gas from T_{ref} to T . We then get

$$\Delta_{\text{vap}}h(T) = \Delta_{\text{vap}}h(T_{\text{ref}}) + \int_{T_{\text{ref}}}^T (c_{pV} - c_{pL})dT$$

where $\Delta_{\text{vap}}h(T_{\text{ref}})$ is the heat of vaporization at temperature T_{ref} , and c_{pV} is the heat capacity of the steam.

2. Temperature and pressure are related by the equilibrium vapor pressure: $p = p^{\text{sat}}(T)$ (see page 180).

With a little practice, it is possible to formulate energy balances of this kind directly: We imagine “standing in the tank” (the system) and use the temperature and phase here as the reference. Then we consider what can be the source of changes in the system’s temperature. In the example with the evaporator, (11.17) can be derived as follows:

“The temperature change in the tank (left side) is driven by the inflow having a different temperature than the tank (first term right side), and by enthalpy being removed by evaporation (second term) and by heat being supplied (third term).”

The term for the outlet stream drops out since it has the same temperature as the tank. More generally, it is recommended to start from the basic equations.

Exercise 11.1 Derive the energy balance for a flash tank with inventory n [mol], feed F [mol/s], vapor product D [mol/s] and liquid product B [mol/s] (make a flow sheet). Show that it becomes

$$nC_{pL} \frac{dT}{dt} = FC_{pL}(T_F - T) + D \cdot \Delta_{\text{vap}}H(T)$$

What are the units for the quantities in the equation? Which assumptions have been made when deriving this?

III. With chemical reaction

For cases with chemical reaction, it is usually most convenient to use a molar basis. We return to (11.12) and introduce $H(T, p, n_j) = \sum_j n_j \bar{H}_{m,j}(T, p)$. Here, $\bar{H}_{m,j}$ [J/mol] is the “partial molar enthalpy” for component j in the mixture. For cases with negligible heat (enthalpy) of mixing, we have that $\bar{H}_{m,j} = H_{m,j}$, where $H_{m,j}$ is the molar enthalpy of pure component j in its actual phase. With this as a starting point, let us derive the general energy balance in terms of temperature (dT/dt) for a continuous stirred tank reactor (CSTR).

Example 11.3 Energy balance with temperature for CSTR. We consider an ideal continuous stirred tank reactor (CSTR) where a chemical reaction takes place (Figure 11.3). Let us, as an example, consider the reaction $2A \rightarrow B$, but the derivation below is general and applies to any reaction. The reaction rate is $r(T, c_A)$ [mol/s m³], and if we take into consideration the stoichiometry, the component balances are:

$$\frac{dn_A}{dt} = F_{A,\text{in}} - F_{A,\text{out}} + \underbrace{\nu_A r V}_{G_A} \quad [\text{mol A/s}]$$

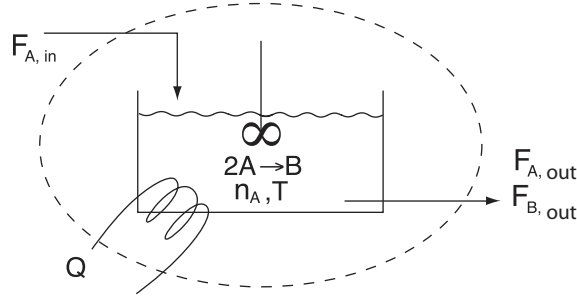


Figure 11.3: Continuous stirred tank reactor (CSTR) with heating

$$\frac{dn_B}{dt} = F_{B,in} - F_{B,out} + \underbrace{\nu_B r V}_{G_B} \quad [\text{mol B/s}]$$

where the stoichiometric coefficients in our example are $\nu_A = -2$ and $\nu_B = 1$. We assume no shaft work and neglect the “pressure-volume contribution.” The energy balance is then

$$\frac{dH}{dt} = H_{in} - H_{out} + Q \quad [\text{J/s}] \quad (11.18)$$

If we neglect the enthalpy of mixing, the enthalpy can be written

$$H(T, p, n_A, n_B) = n_A H_{m,A}(T, p) + n_B H_{m,B}(T, p) \quad [\text{J}]$$

where $H_{m,j}(T, p)$ [J/mol] is the molar enthalpy for component j . Here, we choose the elements in their standard states at 298.15 K and $p^\ominus = 1$ bar as the reference. If we neglect the pressure’s influence on the enthalpy, we then have

$$H_{m,j}(T, p) = H_j^\ominus(T) + \Delta H_{\text{trs}} \quad [\text{J/mol}]$$

where $H_j^\ominus(T) = \Delta_f H_j^\ominus(T)$ [J/mol] is the standard enthalpy of formation for generating component i in its standard state at T and 1 bar from the elements at 298 K and 1 bar, and ΔH_{trs} is the enthalpy change for the change in reference from the standard state to actual state (phase). If we assume that there is no phase change, we can then write

$$\begin{aligned} H &= n_A H_A^\ominus(T) + n_B H_B^\ominus(T) \quad [\text{J}] \\ H_{in} &= F_{A,in} H_A^\ominus(T_{in}) + F_{B,in} H_B^\ominus(T_{in}) \quad [\text{J/s}] \\ H_{out} &= F_{A,out} H_A^\ominus(T_{out}) + F_{B,out} H_B^\ominus(T_{out}) \quad [\text{J/s}] \end{aligned}$$

Inserting into the energy balance (11.18) gives

$$\begin{aligned} & n_A \overbrace{\frac{dH_A^\ominus(T)}{dT}}^{C_{p,m,A}(T)} \frac{dT}{dt} + n_B \overbrace{\frac{dH_B^\ominus(T)}{dT}}^{C_{p,m,B}(T)} \frac{dT}{dt} + H_A^\ominus(T) \frac{dn_A}{dT} + H_B^\ominus(T) \frac{dn_B}{dT} \\ &= F_{A,in} H_A^\ominus(T_{in}) + F_{B,in} H_B^\ominus(T_{in}) - F_{A,out} H_A^\ominus(T_{out}) - F_{B,out} H_B^\ominus(T_{out}) + Q \end{aligned}$$

We assume perfect mixing such that $T = T_{out}$. By inserting the expressions for dn_A/dt and dn_B/dt from the mass balance, and rearranging the terms (a bit of a work is needed here...), we finally derive the energy balance in “temperature form”:

$$\boxed{n C_{p,m} \frac{dT}{dt} = F_{in} \int_T^{T_{in}} C_{p,m,in}(T) dT + (-\Delta_r H^\ominus(T)) r V + Q} \quad (11.19)$$

(For cases with many reactions, the term $(-\Delta_r H^\ominus(T)) rV$ is replaced by $\sum_j (-\Delta_r H_j^\ominus(T)) r_j V$. For our reaction $2A \rightarrow B$, we have

$$\Delta_r H^\ominus(T) = \sum_j \nu_j H_j^\ominus = H_B^\ominus - 2H_A^\ominus \quad [\text{J/K mol}] \quad (11.20)$$

Furthermore,

$$n = n_A + n_B \quad [\text{mol}]$$

$$F_{\text{in}} = F_{A,\text{in}} + F_{B,\text{in}} \quad [\text{mol/s}]$$

and the molar heat capacities for the reactor (system) and feed are

$$C_{p,m} = \frac{n_A}{n} C_{p,m,A}(T) + \frac{n_B}{n} C_{p,m,B}(T) \quad [\text{J/K mol}]$$

$$C_{p,m,\text{in}}(T) = \frac{F_{A,\text{in}}}{F_{\text{in}}} C_{p,m,A}(T) + \frac{F_{B,\text{in}}}{F_{\text{in}}} C_{p,m,B}(T) \quad [\text{J/K mol}]$$

Let us summarize the assumptions that have been made when deriving (11.19):

1. All streams have the same phase.
2. Perfect mixing such that $T = T_{\text{out}}$.
3. Heat of mixing is neglected.
4. The pressure's influence on the enthalpy is neglected.

Note that (11.19) applies to the case with varying composition in the reactor and a varying amount of n ("holdup") in the reactor. For a more detailed example with dynamic simulation, see page 311.

With a little experience, it is again possible to directly formulate the energy balance (11.19) in temperature form for a continuous stirred tank reactor:

"The temperature change in the reactor (left side) is driven by the difference between the feed and reactor temperatures (first term left side), by the heat of reaction (second term) and by the supplied heat (third term)."

Comments.

1. We note that the "heat of reaction" appears as a separate term when we choose to write the energy balance in the "temperature form" in (11.19).
2. The energy balance in temperature form (11.19) gives interesting insights and is useful in many situations. However, it is usually simpler for numerical calculations (dynamic simulation) to stay with the original form (11.11) or (11.12) with U or H as the state (differential) variables. See page 316 for solving the resulting DAE equations.

11.2.5 Steady-state balances

The dynamic balances derived above are all in the form $dy/dt = f(y, u)$. We usually assume that the system is initially "at rest" (steady-state) with $dy/dt = 0$. The steady-state (nominal) values for u and y are here indicated by using superscript *, and we have that $f(y^*, u^*) = 0$.

11.3 Dynamic analysis and time response

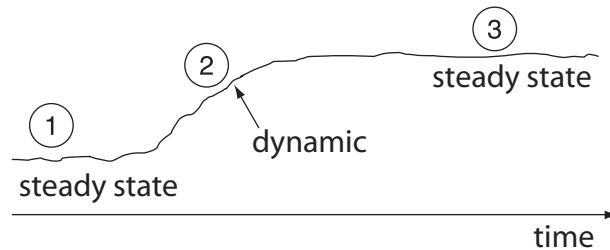


Figure 11.4: Dynamic response in output y to step change in input u

We want to understand what happens when we get an imbalance from the steady-state, 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 $t \rightarrow \infty$), 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) u . In the three cases mentioned above we have

- Room: $u = Q$ (heating), $y = T$
- Car: $u = w$ (fuel flow), $y = v$ (speed)
- Reactor: $u = c_{in}$, $y = c_{out}$

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

$$u(t) = \begin{cases} u_0 & t \leq t_0 \\ u_\infty = u_0 + \Delta u & t > t_0 \end{cases}$$

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

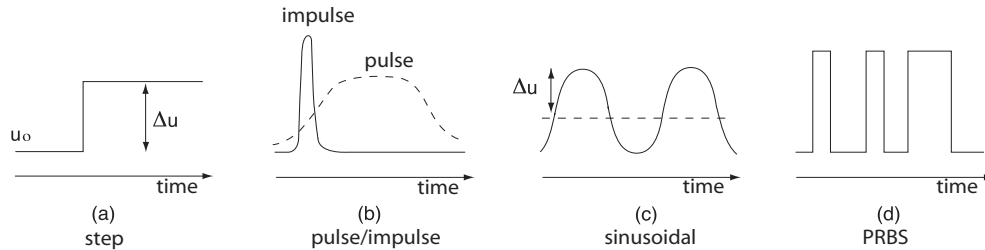


Figure 11.5: Time signals for input $u(t)$

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

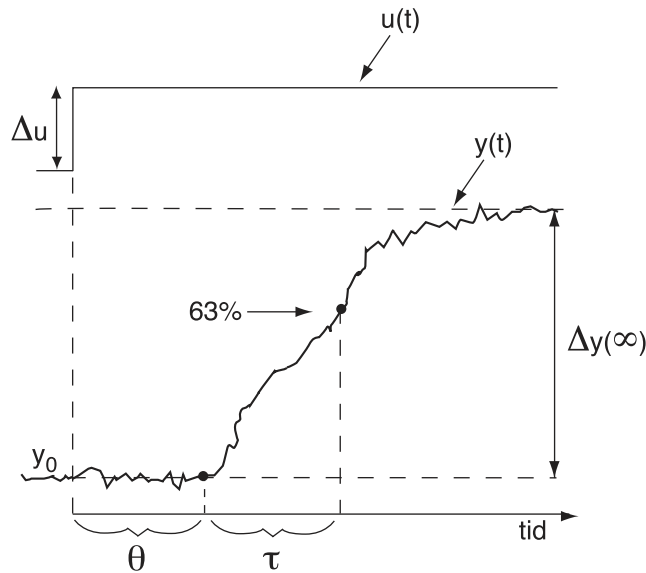


Figure 11.6: Experimental step response

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

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

where

- u is the independent variable (input)
- y is the dependent variable (output)
- 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 $t \leq t_0$ 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

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

or

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

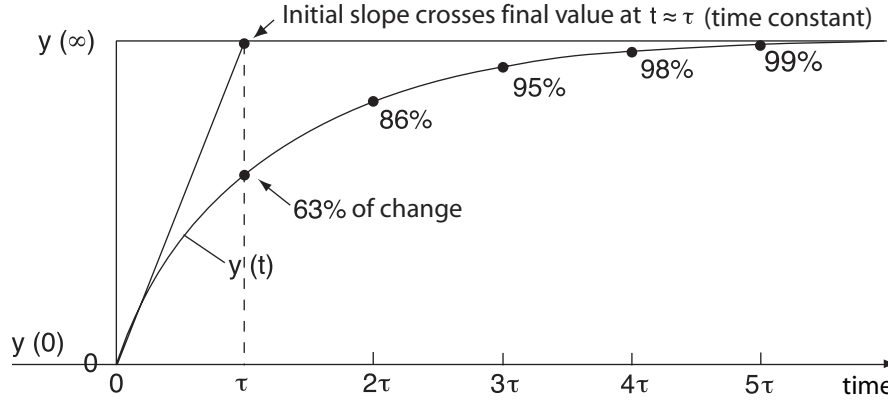


Figure 11.7: Step response for first-order system

(you should try to remember this one). k is the steady state gain, and when $t \rightarrow \infty$ we have $e^{-t/\tau} \rightarrow 0$ and the system approaches a new steady state where $\Delta y(\infty) = k\Delta u$. Note 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/τ	$1 - e^{-t/\tau}$	Value	Comment
0	$1 - e^0 =$	0	
0.1	$1 - e^{-0.1} =$	0.095	
0.5	$1 - e^{-0.5} =$	0.393	
1	$1 - e^{-1} =$	0.632	63% of change is reached after time $t = \tau$
2	$1 - e^{-2} =$	0.865	
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):

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

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).

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

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

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),

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

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

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

and we get the general solution

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

We subtract y_0 from both sides and get

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

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

$$\Delta y(t) \triangleq y(t) - y_0 \quad (11.28)$$

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

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

We have so far not 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:

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

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

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

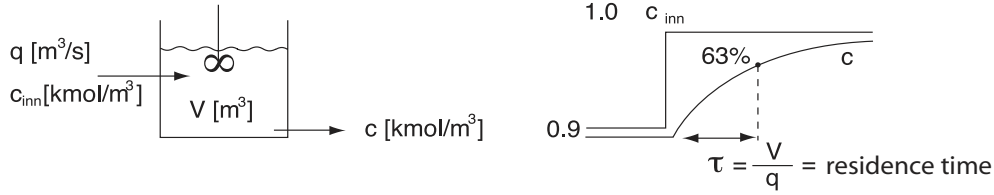


Figure 11.8: Continuous stirred tank without reaction

$$c_{A,\text{in}} = \begin{cases} c_0 = 0.9 \text{ kmol/m}^3 & t \leq 0 \\ c_\infty = 1.0 \text{ kmol/m}^3 & t > 0 \end{cases}$$

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

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

With constant volume V this gives

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

This is in standard form (11.21) with

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

and

$$k = 1; \quad \tau = \frac{V}{q} \quad \frac{[m^3]}{[m^3/s]} = [s]$$

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

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

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.

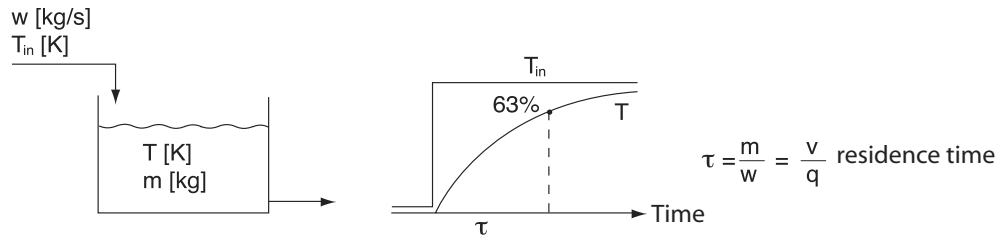


Figure 11.9: Temperature dynamics in continuous stirred tank without reaction

The process is initially operated at steady state such that the inlet temperature T_{in} is $50^\circ C$ and the outlet temperature $T_{out} = T$ is $50^\circ C$ (so we assume no heat loss). Suddenly, the temperature of the inflow is changed to $60^\circ C$ (step change). The outlet temperature will also “eventually” reach $60^\circ C$. **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 $0.63 \cdot 10 = 6.3^\circ C$ to $56.3^\circ C$?

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

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

With the assumption of constant heat capacity c_p , this gives

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

or equivalently

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

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

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

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

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 $50^\circ C$ (initial steady state) to $60^\circ C$, but we have heating (see Figure 11.10) such that the temperature in the tank is $70^\circ C$ (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 $110^\circ C$.

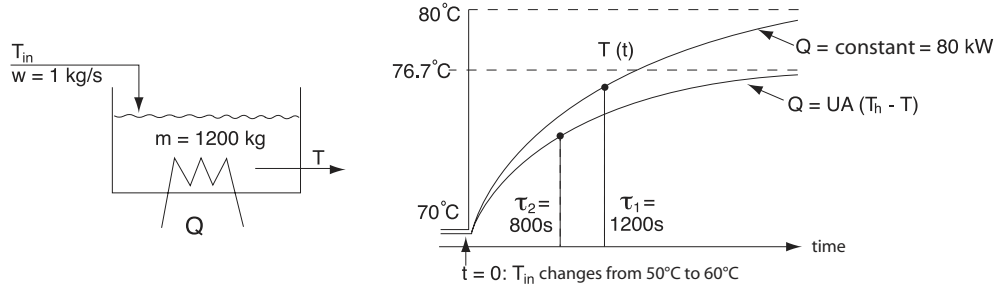


Figure 11.10: Continuous stirred tank with heating

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

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

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

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

1. For the case when Q is independent of T , transformation to the standard form (11.21) gives that the time constant is $\tau = m/w = 1200 \text{ s}$ (residence time), and that the gain from T_{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

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

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 $UA = 80 \cdot 10^3 / (110 - 70) = 2000 \text{ W/K}$. The time constant and the gain are then

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

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) $\lim_{t \rightarrow 0} \Delta T'(t) = (k/\tau) \cdot \Delta T_{in}$, 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, $A = 0.04$ m² and U is the overall heat transfer coefficient. If we leave the plate unattended, then we find that $T \rightarrow 1000$ K when $t \rightarrow \infty$. 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

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

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

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

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

$$\tau \frac{dT}{dt} = -T + ku \quad (11.36)$$

where

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

and

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

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).

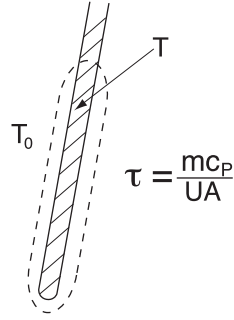


Figure 11.11: Thermocouple

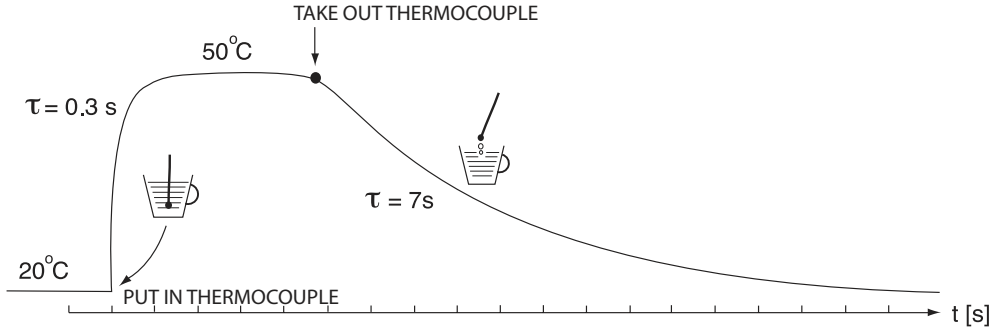


Figure 11.12: Coffee cup experiment

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 $H_{in} - H_{out} = 0$. 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

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

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 [m²]
- U – heat transfer coefficient from surroundings to thermocouple [W/m² 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

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

(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 $U = 2880 \text{ W/m}^2 \text{ K}$ (water) and $U = 123 \text{ W/m}^2 \text{ K}$ (air). Immediately, the value $2880 \text{ W/m}^2 \text{ K}$ 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:

$$\begin{aligned} \text{Air :} \quad & k = 0.027 \frac{\text{W}}{\text{K m}}; c_p = 1000 \frac{\text{J}}{\text{kg K}}; \mu = 1.8 \cdot 10^{-5} \frac{\text{kg}}{\text{m s}}; \rho = 1.2 \frac{\text{kg}}{\text{m}^3}; \beta = \frac{1}{T} = 0.003 \frac{1}{\text{K}} \\ \text{Water :} \quad & k = 0.7 \frac{\text{W}}{\text{K m}}; c_p = 4200 \frac{\text{J}}{\text{kg K}}; \mu = 10^{-3} \frac{\text{kg}}{\text{m s}}; \rho = 1000 \frac{\text{kg}}{\text{m}^3}; \beta = 0.001 \frac{1}{\text{K}} \end{aligned}$$

We then find for natural convection (SI units)

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

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

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 $D = 10^{-3} \text{ m}$ and $\Delta T = 10 \text{ K}$ (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 $U = 13.1 \text{ W/m}^2 \text{ K}$ (air) and $U = 1730 \text{ W/m}^2 \text{ K}$ (water). We see that the theoretical U -value for water ($1730 \text{ W/m}^2 \text{ K}$) is quite close to the experimental ($2880 \text{ W/m}^2 \text{ K}$), while the theoretical U -value for air ($13.1 \text{ W/m}^2 \text{ K}$) is much lower than the experimental ($123 \text{ W/m}^2 \text{ K}$) 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 $A [\text{m}^2]$ is the base of the tub and $h [\text{m}]$ 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

$$\frac{dm}{dt} = w_{\text{in}} - w_{\text{out}} \quad [\text{kg/s}] \quad (11.39)$$

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.

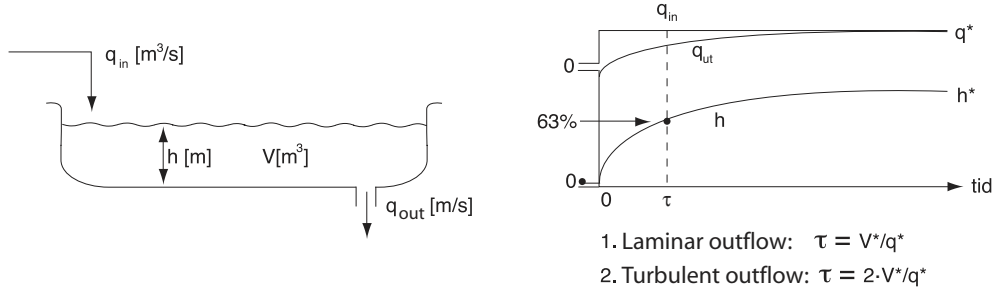


Figure 11.13: Bathtub without plug

and with the assumption of constant density we get the “volume balance”

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

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

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

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

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

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

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

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

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 $t \rightarrow \infty$) at a balance point (steady state) where $q_{out}^* = q_{in}$ and h no longer increases. The steady-state value, h^* , $t = \infty$ is from (11.42)

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

² 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, $q_{\text{in}} = q_{\text{out}}$ [m^3/s]. Here, $q_{\text{out}} = k_l h$ 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 $F_{\text{in}} = c_1(p_{\text{in}} - p)$ [mol/s] and $F_{\text{out}} = c_2(p - p_{\text{out}})$ [mol/s] where the "valve constants" c_1 and c_2 are assumed to be equal ($c_1 = c_2 = c$).

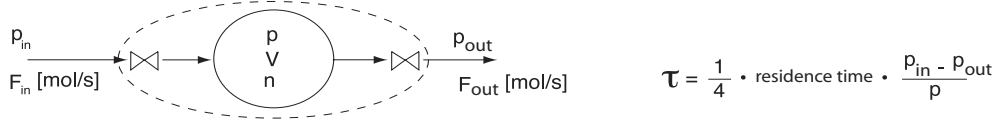


Figure 11.14: Gas dynamics

Solution. The mass balance is

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

We assume constant volume V and ideal gas,

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

The mass balance then gives:

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

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

$$\tau = \frac{V}{2cRT} = \frac{n}{2cp} \quad (11.44)$$

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

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

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

For example, with $p_{\text{in}}^* = 10.1$ bar, $p^* = 10$ bar and $p_{\text{out}}^* = 9.9$ 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)

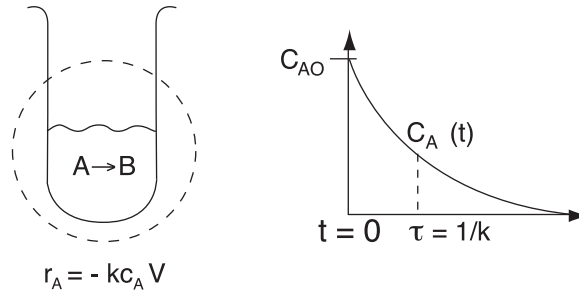


Figure 11.15: Reaction in beaker

Consider a beaker where component A reacts according to the first-order irreversible reaction $A \rightarrow B$. 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

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

where r_A is the reaction rate for “generation” of component A , which for a first-order reaction is $r_A = -k c_A$ [mol A/m³, s], where k [s⁻¹] is constant since the temperature is constant. If we, in addition, neglect changes in the volume, we get

$$\frac{dc_A}{dt} = -k c_A \quad (11.47)$$

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 $c_A \rightarrow 0$ when $t \rightarrow \infty$, 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 $A \rightarrow B$ with reaction rate $r = (-r_A) = k c_A V$ [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.

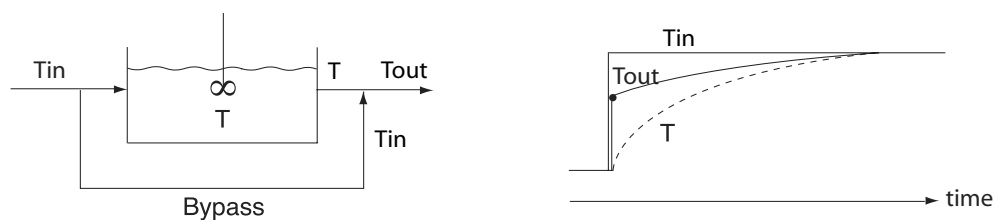


Figure 11.16: Temperature response for stirred tank with *bypass*

- 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 n th-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 = $-1/\text{time constant}$) 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.

Exercise 11.4 (a) Derive the model for the stirred tank with bypass shown in Figure 11.16 and (b) find an analytical expression for the time response.

11.4 Linearization

Consider a dynamic model

$$\frac{dy}{dt} = f(y, u) \quad (11.48)$$

This model is **linear** if the function $f(y, u)$ is linear, which means that if we double the change in u (or in y) then the change in f is doubled. In general our models are nonlinear, but we are often interested in studying the response of small changes in u , and we can then use a linearized model. The most important use of linearized models is in control engineering, where the objective of the control is indeed to keep y close to its desired value (that is, Δy is indeed small) such that the assumption of linear model often holds well.

Let y^* and u^* denote the values of y and u at the operating point $*$ (or along the nominal trajectory $y^*(t)$) where we linearize the model. This is often a steady-state point but does not need to be. A first-order **Taylor-series expansion** (“tangent approximation”) of the function $f(y, u)$, where we neglect the second-order (with $\Delta u^2, \Delta y^2, \Delta u \Delta y$) and higher-order terms, gives a linearized approximation

$$f(y, u) \approx \underbrace{f(y^*, u^*)}_{f^*} + \underbrace{\left(\frac{\partial f}{\partial u}\right)^* \Delta u + \left(\frac{\partial f}{\partial y}\right)^* \Delta y}_{\Delta f} \quad (11.49)$$

where $\Delta u = u - u^*$ and $\Delta y = y - y^*$ represent the deviations from the nominal operating point. The approximation is exact for small values of Δu and Δy . Further, we have that

$$\frac{d\Delta y}{dt} = \frac{d(y - y^*)}{dt} = \frac{dy}{dt} - \underbrace{\frac{dy^*}{dt}}_{f^*}$$

For the non-linear model (11.48) we have then derived a **linearized model in deviation variables**,

$$\frac{d\Delta y}{dt} = \Delta f = \underbrace{\left(\frac{\partial f}{\partial y}\right)^*}_{a} \Delta y + \underbrace{\left(\frac{\partial f}{\partial u}\right)^*}_{b} \Delta u \quad (11.50)$$

where the coefficients a and b denote the local derivatives with respect to y and u , respectively. Comparing this with the standard form for first-order systems in (11.21),

$$\tau \frac{d\Delta y}{dt} = -\Delta y + k\Delta u$$

we find

$$\tau = -\frac{1}{a}; \quad k = \frac{b}{a}$$

Thus, linearized models can be used to determine the time constant τ .

Example 11.12 Linearized model for turbulent outflow of tank. This is a continuation of Example 11.9 (page 296) where we considered laminar outflow of a bathtub. For case 2 with turbulent outflow, $q_{\text{out}} = k_t \sqrt{h}$, the “volume balance” (11.41) for filling the bathtub becomes

$$A \frac{dh}{dt} = q_{\text{in}} - k_t \sqrt{h} = f(h, q_{\text{in}}) \quad [m^3/s] \quad (11.51)$$

Here, the function f is non-linear in h . Linearizing f and introducing deviation variables gives, see (11.50),

$$A \frac{d\Delta h}{dt} = \Delta f = \Delta q_{\text{in}} - k_t \frac{1}{2\sqrt{h^*}} \Delta h$$

Comparison with the standard form with $y = \Delta h$ and $u = \Delta q_{\text{in}}$ gives $\tau = 2\sqrt{h^*} A/k_t$, where from (11.51), $k_t = q^*/\sqrt{h^*}$ and q^* is the steady state flow. Further rearrangement of the expression for the time constant gives

$$\tau = 2 \frac{\sqrt{h^*} A}{k_t} = 2 \frac{h^* A}{q^*} = 2 \cdot \frac{V^*}{q^*}$$

That is, the time constant is two times the residence time (while it was equal to the residence time with laminar outflow). In other words, we can, by comparing the experimental time constant with the residence time, predict whether the outflow is laminar or turbulent. Also note that the steady state gain $k = \Delta h(\infty)/\Delta q_{\text{in}} = 2h^*/q^*$ for turbulent flow is twice that of laminar flow.

Comment. Note that the initial response for $h(t)$ (expressed by the slope $k' = k/\tau$) is the same for both cases, $k' = k/\tau = 1/A$. This is reasonable since the outlet flow (where the difference between turbulent and laminar flow lies) is only affected after the level starts changing.

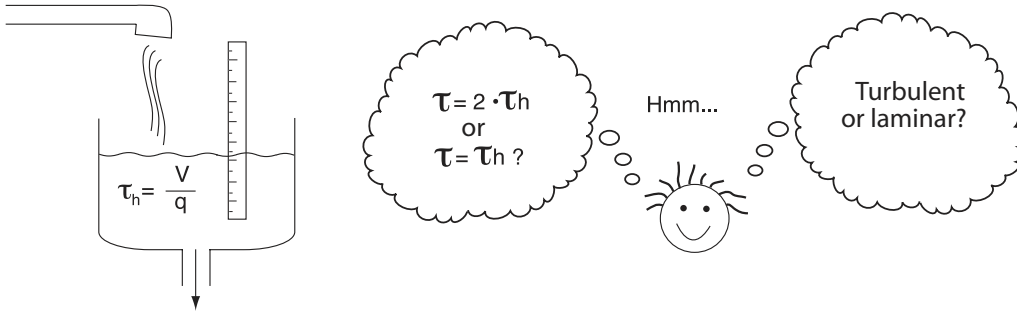


Figure 11.17: Student anxious to check the outflow from a sink

Exercise 11.5 Experiment at home. You should check whether the outflow from your sink is laminar or turbulent by comparing the time constant τ of the dynamic response in sink level with the residence (holdup) time $\tau_h = V/q$:

1. With the plug out, adjust the inflow such that the level is at a steady state where the sink is a little more than half full.
2. Reduce the inflow and record the level response (use a ruler and read off the level at regular intervals). From this experiment estimate the time constant τ (when 63% of the steady-state change is reached). This assumes that the area A is reasonably constant in the region between the two steady-state levels.

3. Temporarily lead the water somewhere else (but keep the same flow), for example, into a bucket, such that the sink is emptied. Put in the plug and let again the water flow into the sink. Measure the time it takes to fill the tank to its previous level. This is the residence time $\tau_h = V/q$.
4. If $\tau \approx \tau_h$, the outflow is laminar, and if $\tau \approx 2\tau_h$, it is turbulent. (Note that it is possible, but not very likely, that you get a transition from turbulent to laminar flow when q is reduced).
5. Another way of checking whether the flow is laminar or turbulent is to find the residence time τ_h for two different steady state levels (see point 3); if the flow is laminar, then $\tau_h = A/k_l$ is independent (!) of the level h , but if the flow is turbulent, then $\tau_h = \sqrt{h}A/k_t$ increases with the square root of the level.

Multivariable and higher-order systems. We have above assumed that we have a scalar model with one input variable u and one output variable y . It is, however, easy to generalize the linearization to the multi-dimensional case where the coefficients (derivatives) $A = \partial f/\partial y$ and $B = \partial f/\partial u$ become matrices. The model in deviation variables is then

$$\frac{d\Delta y}{dt} = A\Delta y + B\Delta u$$

Δu : vector of independent variables (inputs or disturbances)

Δy : vector of dependent state variables (often denoted x)

(Note that we, for simplicity, have not introduced separate symbols for vectors, but we could for clarity have written \underline{u} and \underline{y}).

The concept of time constant is less clear in the multivariable case, but we can instead compute the eigenvalues λ_i of the matrix A :

- We find that the “time constants” $\tau_i = -1/\lambda_i(A)$ appear in the linearized time response which contains the term e^{-t/τ_i} . For the scalar case with only one equation ($A = a = \text{scalar}$), the eigenvalue of A equals a , and we find $\tau = -1/a$.
- The system is (locally) stable if and only if all eigenvalues of A have a negative real part (i.e., the eigenvalues are in the left-half complex plane).

11.5 Dynamic simulation with examples

By the expression “dynamic simulation,” we mean “numerical solution (integration) of the system’s differential equations as a function of time.”

We consider a dynamic system described by the differential equations

$$\frac{dy}{dt} = f(y, u)$$

where

1. The initial state $y(t_0) = y_0$ is known (we need one for every differential equation).
2. The independent variables $u(t)$ are known for $t > t_0$.

Using “dynamic simulation,” we compute numerically $y(t)$ for $t > t_0$ by integrating the above equation,

$$y(t) = y_0 + \int_{t_0}^t f(y(\tau), u(\tau)) d\tau$$

(strictly speaking, this should be $y(t) = y_0 + \int_{t_0}^t f(y(\tau), u(\tau)) d\tau$ but we are a bit sloppy to simplify the notation).

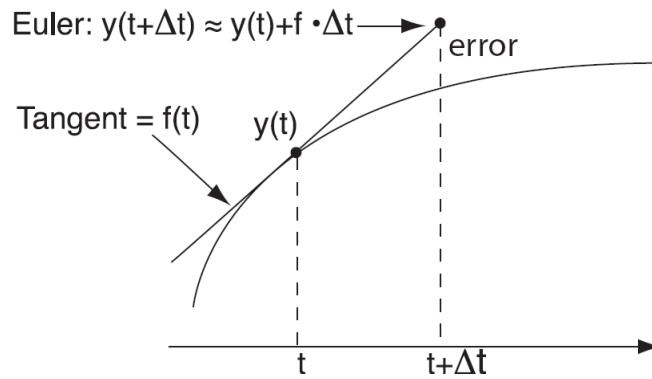


Figure 11.18: Euler integration

The simplest method is **Euler integration**, see Figure 11.18, where we assume that the derivative $f(y, u)$ is piecewise constant over a time interval Δt . If we are at time t , then the value of y at time $t + \Delta t$ is

$$y(t + \Delta t) = y(t) + \int_t^{t+\Delta t} f(y, u) dt \approx y(t) + f(y, u) \Delta t$$

where $f(y, u)$ is the local derivative (tangent) at time t . We repeat this at time $t + \Delta t$ and so on, as explained next.

Algorithm for Euler integration:

1. Start at $t = t_0$ with a known initial state y_0 .
2. Compute the derivative $f = f(y(t), u(t))$ at time t .
3. Euler approximation: Assume the derivative f is constant over the period Δt and compute $y(t + \Delta t) \approx y(t) + f \cdot \Delta t$.
4. Stop if $t \geq t_{\text{final}}$; otherwise set $t := t + \Delta t$ and $y(t) := y(t + \Delta t)$ and go to step 2.

The algorithm is best understood by considering an example.³

Example 11.13 Euler integration: Concentration response for tank.

Consider the continuous stirred tank in Figure 11.19 with the following given data:

- $V = 5 \text{ m}^3 = \text{constant}$
- $q = 1 \text{ m}^3/\text{min}$ (assumed constant)

³The unit for time (t) is minutes [min] in almost all examples in this chapter.

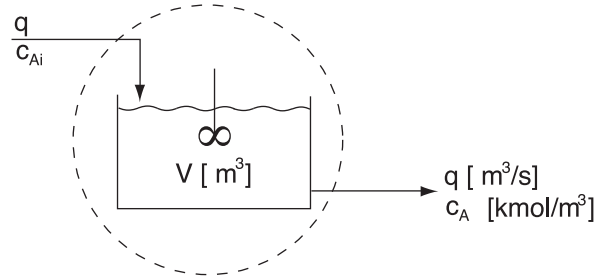


Figure 11.19: Stirred tank without reaction

- Step change in $c_{Ai} = \begin{cases} 0.9 \text{ kmol/m}^3, & t \leq 0 \\ 1.0 \text{ kmol/m}^3, & t > 0 \end{cases}$
- Ideal mixing and constant density is assumed.

The component balance $d(c_A V)/dt = qc_{Ai} - qc_A$ [kmol A/s] is rearranged to:

$$\frac{dc_A}{dt} = \frac{q}{V}(c_{Ai} - c_A) = f(c_A)$$

For $t \leq 0$, we assume the system is at steady state and the component balance gives $c_A = c_{Ai} = 0.9 \text{ kmol/m}^3$ (the initial value for c_A). The exact solution of the differential equation for $t \geq 0$ is from (11.22)

$$c_A(t) = 0.9 + 0.1 \cdot (1 - e^{-t/5})$$

where the time constant is $\tau = V/q = 5 \text{ min}$ (residence time).

Let us compare this with Euler integration using $\Delta t = 0.1 \text{ min}$, which is a relatively small step compared to the time constant of 5 min. The steps of the algorithm are:

1. At $t = t_0 = 0$ set $c_A(t) = 0.9$.
2. With $c_{Ai} = 1$ (constant), we have for $t \geq 0$:

$$f(c_A) = \frac{q}{V}(c_{Ai} - c_A) = 0.2(1 - c_A)$$

3. Euler approximation: Value of c_A at time $t + \Delta t$ is:

$$c_A(t + \Delta t) \approx c_A(t) + f(c_A) \cdot \Delta t = c_A + 0.2(1 - c_A) \cdot 0.1 = 0.98c_A(t) + 0.02$$

4. Set the value for $c_A(t + \Delta t)$ to $c_A(t)$ and go to step 2.

We then get:

t	$c_A(t)$	$f(c_A) = 0.2(1 - c_A)$	$f \cdot \Delta t$	Euler $c_A(t + \Delta t) \approx c_A(t) + f \cdot \Delta t$	Exact $c_A(t + \Delta t)$
0^+	0.9	0.02	0.002	0.902	0.90198
0.1	0.902	0.0196	0.00196	0.90396	0.90392
0.2	0.90396	0.0192	0.00192	0.90588	0.90582
0.3	0.90588	0.0188	0.00188	0.90776	0.90768
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
5.0	0.9636	0.0073	0.00073	0.9643	0.9628
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
20.0	0.9982	0.0004	0.00004	0.9982	0.9982

We see, as expected, that Euler integration gives a numerical error; see also Figure 11.20. This error can be reduced by reducing the step length Δt , but this increases the computational effort and if it becomes too small it may conflict with the accuracy of the computer. On the other hand, if Δt gets too large, the Euler integration may go unstable.

There are many possible improvements to Euler integration

- Higher-order method: Include more terms in the Taylor-series expansion for y (Euler assumes $y \approx y_0 + f\Delta t$).
- Introduce step length control (adjusting Δt during integration).
- Use an implicit solution that avoids the possible instability, for example, implicit Euler:

$$y(t + \Delta t) \approx y(t) + f(y(t + \Delta t), u(t + \Delta t)) \cdot \Delta t$$

which has to be solved with respect to $y(t + \Delta t)$.

Examples of MATLAB routines which include improvements of this kind are `ode45` and `ode15s` (the latter is recommended for most problems).

Euler integration with MATLAB

We continue Example 11.13. First, we write the following MATLAB routine to compute the derivative $dc_A/dt = f(c_A)$ (and save it in the file `conctank.m`):

```
function DYDT=f(t,y)
% This is file conctank.m
% Concentration response of tank with no reaction
% inlet: Time t and state vector y
% OUTPUT: derivatives DYDT
%
% Usage with odeeuler: [T,Y]=odeeuler(@conctank,[0 10],0.9,0.1)
% Usage with ode15s: [T,Y]= ode15s(@conctank,[0 10],0.9)
% Plot results:      plot(T,Y)
%
% I. Data (parameters and independent variables)
V=5;      % tank volume
q=1;      % volumetric flow rate
tau=V/q; % residence time
cai=1;    % inlet concentration for t>0
% II. Extract present value of states
ca=y;    % tank concentration
% III. Evaluate derivatives of states
f=(cai - ca)/tau;
DYDT=f;
```

We note that the routine that calculates the derivative (in this case `conctank.m`) generally contains the following parts:

- I. Data** (given values for parameters and independent variables u).
- II. Extract variables from the state vector y** (in this example there is only one state so the “vector” y has only one element). It is recommended that the variables be given physical names in order to enhance the readability of the code, for example `ca=y`.
- III. Evaluate the derivative**, that is, compute function f (which is returned to the MATLAB integration routine).

In addition, we need a program that computes the numerical solution (“performs the integration”). Below is a simple program for **Euler integration** which is saved in the file `odeeuler.m`:

```
function [tout,yout]=odeeuler(odefile,tspan,y0,H)
% This is the function odeeuler.m
% Simple integration routine written by SiS in 1998
% Usage:      [T,Y]=odeeuler(@F,TSPAN,Y0,H)
% for example: [T,Y]=odeeuler(@conctank,[0 10],0.9,0.1)
%
%   T - solution time vector.
%   Y - solution state (output) vector.
%   F - filename with diff.eqns. (see also help ode15s).
%   TSPAN = [initial_time final_time]
%   Y0 - initial state vector
%   H - integration step size
%
t0=tspan(1); tfinal=tspan(2);
% Initialize
tout=t0; yout=y0; neq=length(y0); t=t0; y=y0;
% Integrate
while t < tfinal,
    t=t+H;
    f=feval(odefile,t,y);
    for i=1:neq,
        y(i)=y(i)+H*f(i);
    end
    tout=[tout;t]; yout=[yout; y];
end
```

We can now use MATLAB to compute the concentration response using Euler integration:

```
>> [T,Y]=odeeuler(@conctank,[0 1],0.9,0.1)
```

```
T =
    0
    0.1000
    0.2000
    0.3000
    0.4000
    0.5000
    0.6000
    0.7000
    0.8000
    0.9000
    1.0000
    1.1000
```

```
Y =
    0.9000
    0.9020
    0.9040
    0.9059
    0.9078
    0.9096
    0.9114
    0.9132
    0.9149
    0.9166
    0.9183
    0.9199
```

```

>> [T,Y]=odeeuler(@conctank,[0 20],0.9,0.1); % semicolon avoids output to the screen
% The result is compared with the more exact solution with ode15s:
>> [T1,Y1]=ode15s(@conctank,[0 20],0.9);
>> plot(T,Y,T1,Y1,'--') % see plot in Figure

```

Figure 11.20 compares the results of the Euler integration with a more accurate and effective integration method (ode15s in MATLAB). The difference is small in this case.

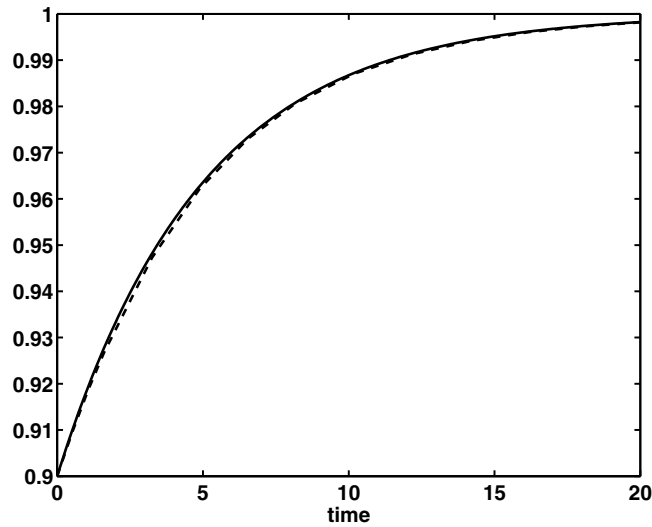


Figure 11.20: Concentration response with `odeeuler` (solid) and `ode15s` (dashed) for a tank.

Example 11.14 Three tanks in series. *This is an extension of Example 11.13, where we had a feed of $1 \text{ m}^3/\text{min}$ to a large tank of $V_1 = 5 \text{ m}^3$. We add two smaller tanks with volume $V_2 = V_3 = 1.5 \text{ m}^3$ (Figure 11.21).*

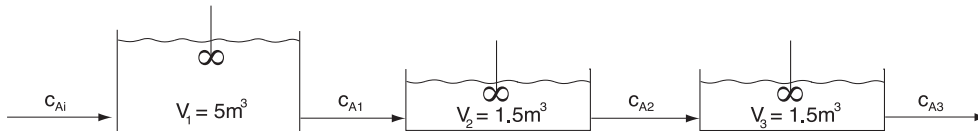


Figure 11.21: Three tanks in a series

The component balance for the “old” tank (tank 1) gives

$$\frac{dc_A}{dt} = \frac{q}{V_1} (c_{Ai} - c_{A1}) = f_1(c_{A1}, c_{Ai})$$

The component balances for the new tanks 2 and 3 give

$$\frac{dc_{A2}}{dt} = \frac{q}{V_2} (c_{A1} - c_{A2}) = f_2(c_{A1}, c_{A2})$$

$$\frac{dc_{A3}}{dt} = \frac{q}{V_3} (c_{A2} - c_{A3}) = f_3(c_{A2}, c_{A3})$$

For $t \leq 0$, steady-state conditions are assumed and the component balances give $c_{A1} = c_{A2} = c_{A3} = c_{Ai} = 0.9 \text{ kmol/m}^3$ (which is the initial value for the three states). The dynamic

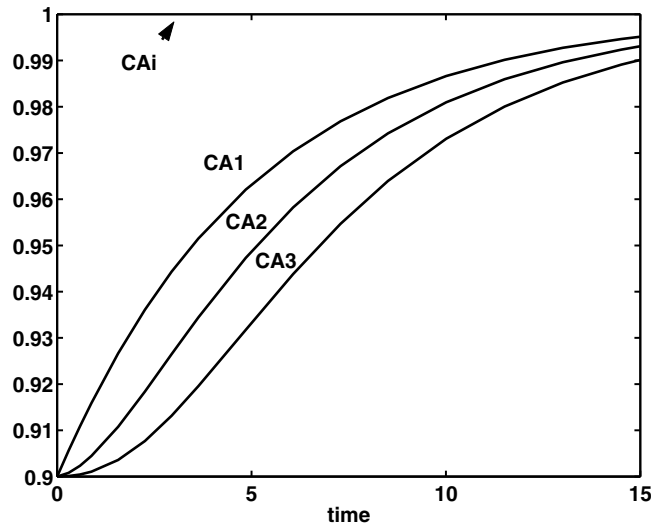


Figure 11.22: Concentration response for three tanks in series

response is shown in Figure 11.22. Note the typical second-order response for c_{A2} , which starts “flat,” that is, the first derivative is initially zero. For c_{A3} , the initial response is even “flatter” since the second derivative is also initially zero.

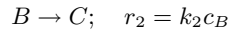
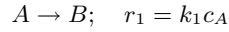
Here, we used the following routine to compute the derivatives (saved in file `conctank3.m`):

```
function DYDT=f(t,y)
% This is file conctank3.m
% INPUT: Time t and state vector y
% OUTPUT: derivatives DYDT
% Usage with ode15s: [T,Y]= ode15s(@conctank3,[0 15],[0.9 0.9 0.9])
%
% I. Data (parameters and independent variables)
V1=5;      % volume tank 1
V2=1.5;    % volume tank 2
V3=1.5;    % volume tank 3
q=1;      % volumetric flow rate
tau1=V1/q; tau2=V2/q; tau3=V3/q; % residence time
cai=1;    % inlet concentration for t>0
% II. Extract present value of states
ca1=y(1); % concentration big tank 1
ca2=y(2); % concentration small tank 2
ca3=y(3); % concentration small tank 3
% III. Evaluate derivatives of states
f1=(cai - ca1)/tau1;
```

```
f2= (ca1 - ca2)/tau2;
f3= (ca2 - ca3)/tau3;
DYDT=[f1; f2; f3];
```

Example 11.15 Isothermal continuous stirred tank reactor (CSTR).

In an isothermal continuous stirred tank reactor (CSTR) with constant volume V , two reactions take place



Data: $c_{AF} = 10 \text{ kmol/m}^3$ (feed concentration), $c_{BF} = 0 \text{ kmol/m}^3$, $c_{CF} = 0 \text{ kmol/m}^3$, $V = 0.9 \text{ m}^3$, $q = 0.1 \text{ m}^3/\text{min}$, $k_1 = 1 \text{ min}^{-1}$, $k_2 = 1 \text{ min}^{-1}$.

Task: Plot the responses of c_A and c_B to a step increase in q of 20%.

Solution. Component balances for A , B and C give

$$\frac{d}{dt}(c_A V) = q c_{AF} - q c_A - k_1 c_A V$$

$$\frac{d}{dt}(c_B V) = 0 - q c_B + k_1 c_A V - k_2 c_B V$$

$$\frac{d}{dt}(c_C V) = 0 - q c_C + k_2 c_B V$$

The steady-state concentrations are found by setting the time derivatives to 0. We find

$$c_A^* = \frac{q c_{AF}}{q + k_1 V} = 1 \text{ kmol/m}^3$$

$$c_B^* = \frac{k_1 V}{q + k_2 V} c_A^* = 0.9 \text{ kmol/m}^3$$

$$c_C^* = \frac{k_2 V}{q} c_B^* = 8.1 \text{ kmol/m}^3$$

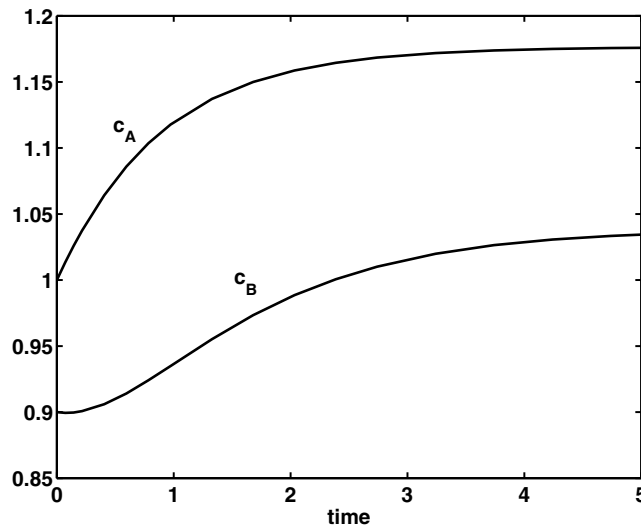


Figure 11.23: Concentration response for isothermal CSTR after a step increase in flowrate

The resulting time response is shown in Figure 11.23. We observe, as expected, a typical “first-order” response for c_A with time constant $V/(q + k_1V) = (0.9/(0.12 + 1 \cdot 0.9)) \text{ min} = 0.88 \text{ min}$. The response for c_B is however not a typical second-order response – we have a so-called inverse response where c_B initially drops (it is not so easy to see) and then reverses and ends up with a steady state increase from 0.90 to 1.034 kmol/m^3 . The reason is that an increase in the feed rate initially lowers c_B because of the dilution effect. However, in the long run the lower residence time results in less B being consumed in the reaction $B \rightarrow C$.

Here, we used the following MATLAB routine in order to compute the derivative of the three concentrations (state variables):

```
function DYDT=f(t,y)
% This is file cstr3.m
% INPUT: Time t and state vector y
% OUTPUT: derivatives DYDT
% Usage with ode15s: [T,Y]= ode15s(@cstr3,[0 5],[1.0 0.9 8.1])
%
% I. Data (parameters and independent variables)
cAF=10; cBF=0; cCf=0; % inlet concentrations
V = 0.9; % reactor volume (constant)
q = 0.1*1.2; % 20% increase in q
k1 = 1; k2 = 1; % rate constants
% II. Extract present value of states
cA=y(1);
cB=y(2);
cC=y(3);
% III. Evaluate derivatives of states
f1= (q*cAF - q*cA - k1*cA*V) /V;
f2= (q*cBF - q*cB + k1*cA*V - k2*cB*V) /V;
f3= (q*cCf - q*cC + k2*cB*V) /V;
DYDT=[f1; f2; f3];
```

Let us now take a look at some more complicated examples where the temperature varies and we also need to use the energy balance.

Example 11.16 Exothermic CSTR with cooling.

In a continuous stirred tank reactor (CSTR) with constant volume V and cooling, we have the exothermic reversible reaction $A \rightleftharpoons B$. The component balances for A and B give

$$V \frac{dc_A}{dt} = q c_{AF} - q c_A - r V \quad [\text{mol A/min}]$$

$$V \frac{dc_B}{dt} = q c_{BF} - q c_B + r V \quad [\text{mol B/min}]$$

where the reaction rate is $r = k_1 c_A - k_2 c_B$ [$\text{mol/m}^3 \text{ min}$]. The energy balance (11.19) gives

$$\rho V c_p \frac{dT}{dt} = \rho q c_p (T_F - T) + r V (-\Delta_r H^\ominus(T)) + Q \quad [\text{J/min}]$$

where the “supplied” heat by cooling is $Q = UA(T_c - T)$. The reactor feed $c_{AF} = 10 \text{ kmol/m}^3$, $c_{BF} = 0$ and $T_F = 300\text{K}$, and the cooling temperature is $T_c = 430\text{K}$. We assume that the heat capacity and heat of reaction $\Delta_r H^\ominus$ are independent of temperature.

The remaining data are as given in the MATLAB file `cstrT.m` (see below). By using a long simulation time (10000 min) in MATLAB, the steady state values in the reactor are numerically determined to be

$$c_A^* = 2.274 \text{ kmol/m}^3; c_B^* = 7.726 \text{ kmol/m}^3; T^* = 444.0 \text{ K}$$

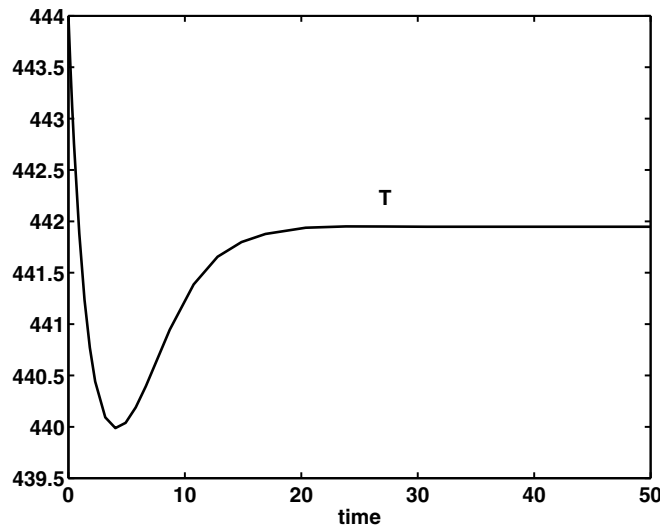


Figure 11.24: Temperature response for exothermic CSTR to a 20% feedrate increase

Increasing the feed rate q by 20% (from 0.10 to 0.12 m³/min) (by editing the file `cstrT.m`; try yourself!) gives a drop in the steady-state temperature from 444.0 K to 441.9 K. The dynamic response is shown in Figure 11.24, and we note that we have a rather strange response. The temperature first drops (because we supply more cold feed), but then it rises because more reactant is converted and the reaction is exothermic. This is not an inverse response because the response does not cross its original value.

If we increase the feed rate q by 50% (to 0.15 m³/min; try yourself!), we find that the temperature drop is so large that the reaction “extinguishes” (that is, the reactor becomes unstable), and the temperature drops all the way down to 348.7 K, which is much lower than the “cooling” temperature (try yourself!).

Further simulations. (1) With a very large (infinite) reactor volume, we approach chemical equilibrium and the steady-state reactor temperature is 453.4 K (independent of q , but you may need to run for a very long time). (2) Removing the cooling gives an equilibrium temperature of 461.0 K (“adiabatic temperature rise”). (3) If the cooling is removed at normal conditions the reactor temperature is 453.5 K (rather than 444.0 K). (Try this and other changes yourself! It is easy with the MATLAB program; and if you think it is too much work to write it yourself then you can get it from the author’s home page).

```
function DYDT=f(t,y)
% This is file cstrT.m
% INPUT: Time t and state vector y

% OUTPUT: derivatives DYDT
% Usage with ode15s: [T,Y]= ode15s(@cstrT,[0 50],[2274 7726 444.0])
% Plot: plot(T,Y(:,3))

% All in SI units except time which is in minutes.
% I. Data (parameters and independent variables)
cAF=10000; % feed concentration of A [mol/m3]
cBF=0; % feed concentration of B [mol/m3]
TF=300; % feed temperature [K]
V = 0.9; % reactor volume [m3]
```



```

q = 0.10;           % volumetric flow rate [m3/min] (CAN CHANGE, e.g., to 0.12)
dhr= -80e3;        % Heat of reaction [J/mol]
cp= 4.e3;          % specific heat capacity [J/kg K]
rho = 1000;        % mean density [kg/m3]
U = 1000*60;       % overall heat transfer coefficient [J/min,m2,K]
A = 5;             % heat transfer area [m2]
Tc = 430;          % cooling temperature [K]
k1_400 = 0.1;      % rx1: rate constant at 400K [1/min]
k2_400 = 0.001;    % rx2: rate constant at 400K [1/min]
E1 = 60e3;         % rx1: activation energy [J/mol]
E2 = E1 - dhr;     % rx2: activation energy [J/mol]
R = 8.31;          % gas constant [J/K mol]
% II. Extract present value of states
cA=y(1);
cB=y(2);
T=y(3);
% IIIa. Intermediate calculations
k1 = k1_400 * exp(-(E1/R) * (1/T - 1/400));
k2 = k2_400 * exp(-(E2/R) * (1/T - 1/400));
r = k1*cA - k2*cB;
Q = U*A*(Tc-T);
% IIIb. Evaluate derivatives of states
Vdcadt = q*cAF - q*cA - r*V;           % [mol A/min]
Vdcbdt = q*cBF - q*cB + r*V;         % [mol B/min]
mcpdTdt = rho*q*cp*(TF-T) + r*V*(-dhr) + Q; % [J/min]

f1 = Vdcadt/V;
f2 = Vdcbdt/V;
f3 = mcpdTdt / (rho*cp*V);

DYDT=[f1; f2; f3];

```

In the above example, we assumed that the heat capacities and the heat of reaction were independent of temperature. For the more general cases, it is recommended that the energy balance is written in its original form with U (or H) as a state, and that T is found numerically from the implicit algebraic equation $U = U_0(T, p, n_i)$, as described for the flash tank in Example 11.18.

Exercise 11.6 Second-order reaction in CSTR Consider a continuous stirred tank reactor (CSTR) where component A decomposes in a second-order irreversible reaction $2A \rightarrow B$ with reaction rate $r = r_B = kc_A^2V$ [kmol/s]. The following steady state data are given: $V^* = 30 \text{ m}^3$ (constant), $q^* = 0.5 \text{ m}^3/\text{s}$, $c_{AF}^* = 4 \text{ kmol}/\text{m}^3$, $c_{BF}^* = 0 \text{ kmol}/\text{m}^3$ (feed), $c_B^* = 1 \text{ kmol}/\text{m}^3$ (product and tank).

- Derive the equations that describe the concentration dynamics when the temperature and volume are assumed constant.
- Use the steady state data to determine c_A^* and the reaction rate constant k .
- Linearize the model and determine an expression for the time constant for the concentration response for component A in the nominal working point.
- Sketch the expected response $c_A(t)$ (in product/tank) when we at $t = 0$ throw in some catalyst such that k is doubled. (For calculations by hand you can for example use Euler integration of the balance for component A with $\Delta t = 5 \text{ s}$). What is the new steady state value of c_A ? What is the time constant?

Distillation examples

Example 11.17 Dynamics of distillation column (Figure 11.25). In a distillation column, the components are separated based on their difference in volatility, and multiple

stages and countercurrent flow are used to enhance this. Here, we look at a very simple distillation column with only three equilibrium stages (a reboiler, a feed stage, and a stage above the feed) plus a total condenser. We separate a binary mixture with a constant relative volatility of 4.78. The MATLAB file `dist.m` given below should be self-explainable. In order to find the steady state column profile, we simulate for a very long time. We then find the following mole fractions of the lightest component on the four stages (including the total condenser):

```
xss =
0.0998    0.3160    0.6536    0.9002
```

That is, we have about 10 mol% light component in the bottom product and about 90 mol% in the top product. The subsequent response to a step in the feed rate F by 20%, with constant reflux (L) and boilup (V), is shown in Figure 11.25. We note that the responses are close to first-order, in spite of the fact that we have four coupled differential equations.

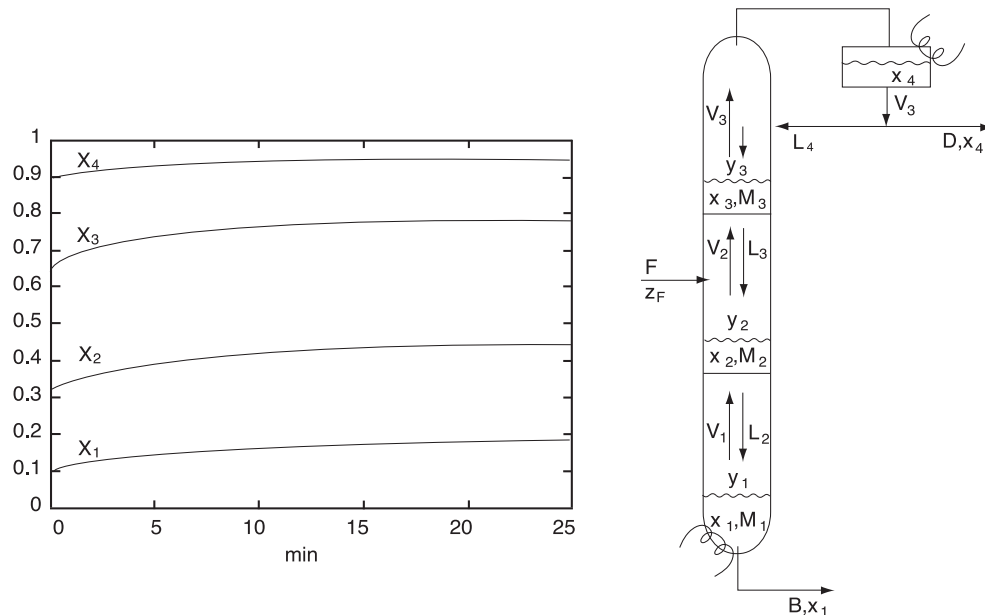


Figure 11.25: Concentration response for distillation column

```
function DXDT = f(t,x)
% This is the file dist.m
% Distillation column with reboiler (stage 1), a feed stage (stage 2),
% ... a stage above this (stage 3) and a total condenser (stage 4)
% Assumptions; Binary mixture with constant alpha and constant molar flows
% Molar holdup on all stages is 1 kmol (M=1)
% States x : vector of liquid mole fractions of light component on the stages
% Usage:
% x0 = [0.5, 0.5, 0.5, 0.5]; % initial states (not steady-state)
% [T,X] = ode15s(@dist,[0 1000],x0) % First simulate to t=1000 (steady-state)
% xss = X(length(X),:) % Save the steady-state mole fractions
% [T,X] = ode15s(@dist,[0 20],xss) % Run new simulation (e.g change F=1.2)

% I. Data (parameters and independent variables)
```

```

% Assume constant relative volatility
alfa = 4.78;

% Feed rate [kmol/min] and feed composition (may change this)
F=1.0; zF=0.5;

% Flows in the column [kmol/min] (feed liquid; constant molar flows)
V=3.55; V1=V; V2=V; V3=V;
L=3.05; L4=L; L3=L; L2=L+F;
% Assume constant condenser and reboiler holdup (perfect level control):
D=V3-L4; B=L2-V1;

% II. Extract present value of states
% ..... Not needed here since x is the state which is already a good name

% IIIa. Intermediate calculations
% Vapor-liquid equilibrium (constant relative volatility)
y(1) = alfa*x(1)/(1+(alfa-1)*x(1));
y(2) = alfa*x(2)/(1+(alfa-1)*x(2));
y(3) = alfa*x(3)/(1+(alfa-1)*x(3));
y(4)=x(4); % total condenser

% IIIb. Evaluate derivatives of states
% Component balances (assume constant stage holdups M1=M2=M3=M4=1 [kmol])
DXDT(1) = L2*x(2)-V1*y(1)-B*x(1);
DXDT(2) = L3*x(3)+V1*y(1)-L2*x(2)-V2*y(2)+F*zF;
DXDT(3) = L4*x(4)+V2*y(2)-L3*x(3)-V3*y(3);
DXDT(4) = V3*y(3)-L4*x(4)-D*x(4);

% Change vector DXDT to a column vector (MATLAB requires this..).
DXDT=DXDT';

```

The above routine does not make use of MATLAB's vector calculation features. However, below is given an excerpt from a more general routine which uses vectors. Note that we use element-by-element operators `*`, `./` to multiply and divide vectors. This code also allows for variable stage holdup $M(i)$, which is important if the model is to be used for control purposes. It is simple to change the number of stages NT in the column.

```

% From code for general distillation column dynamics
% Vapor-liquid equilibria
i=1:NT-1; y(i)=alpha*x(i)./(1+(alpha-1)*x(i));

% Need algebraic for computing L(i) (e.g., Francis weir)
% and V(i) (e.g., constant molar flows or "valve" equation)
% ..... but these are not given here.

% Column mass balances
i=2:NT-1;
dMdt(i) = L(i+1) - L(i) + V(i-1) - V(i);
dMxdt(i)= L(i+1).*x(i+1) - L(i).*x(i) + V(i-1).*y(i-1) - V(i).*y(i);

% Correction for feed at the feed stage
% The feed is assumed to be mixed into the feed stage
dMdt(NF) = dMdt(NF) + F;
dMxdt(NF)= dMxdt(NF) + F*zF;

% Reboiler (assumed to be an equilibrium stage)
dMdt(1) = L(2) - V(1) - B;
dMxdt(1)= L(2)*x(2) - V(1)*y(1) - B*x(1);

```

```

% Total condenser (no equilibrium stage)
dMdt(NT) = V(NT-1) - LT - D;
dMxdt(NT) = V(NT-1)*y(NT-1) - LT*x(NT) - D*x(NT);

% Compute the derivative for the mole fractions from d(Mx) = x dM + M dx
i=1:NT;
dxdt(i) = (dMxdt(i) - x(i).*dMdt(i) )./M(i);

% Output
DYDT=[dxdt';dMdt'];

```

Systems with algebraic equations (DAE system)

In the above examples, all the model equations were differential equations. Actually, we had some algebraic expressions, e.g., the reaction rate constant as function of temperature, but these were explicit in the (dynamic) state variables y_1 , i.e., $y_2 = f(y_1, u)$, such that they could easily be evaluated (using IIIa. **Intermediate calculations** in the MATLAB code).

However, more generally, one will in addition to the differential equations

$$\frac{dy_1}{dt} = f_1(y_1, y_2, u) \quad (11.52)$$

also have “implicit” algebraic equations of the form

$$0 = f_2(y_1, y_2, u) \quad (11.53)$$

where y_2 are the extra algebraic variables. Three approaches of dealing with systems with both differential and algebraic equations (DAE systems) are:

1. **Eliminate the algebraic variables** y_2 by substituting relationships for them into the differential equations (which is actually what we do with the “intermediate calculations” in the above examples). This approach does not generally work for all the equations, but it should be used to some extent to reduce the number of variables. However, you should avoid that things get too complicated, because otherwise the code becomes difficult to read and you will make errors.
2. **Use a separate “equation solver” for the algebraic equations** $f_2 = 0$, which is “inside” an ordinary differential equation (ODE) solver (integrator). This approach is common, but may be inefficient in terms of computing time.
3. **Use a DAE-solver that solves the differential and algebraic equation simultaneously.** The equation set is then written in the form

$$M \frac{dy}{dt} = f(y, u)$$

where the “*mass matrix*” M is a square matrix that tells the solver which equations are algebraic. Usually, M is a diagonal matrix with 1’s on the diagonal for differential equations and 0’s for algebraic equations. This is a general approach and complicated “fixes” are avoided.

To illustrate the three approaches, consider a **dynamic flash**. We derive differential equations (and dynamic states) from the dynamic balances for component mass and

energy. The energy balance has internal energy U (or enthalpy H) as the “natural” differential variable (dynamic state):

$$dU/dt = Fh_F(T, \dots) - Gh_G(T, \dots) - Lh_L(T, \dots)$$

where, as indicated, the enthalpies h_F , h_G and h_L are (explicit) functions of temperature T . In addition, we have the algebraic equations, which mostly are associated with the vapor-liquid equilibrium (VLE). Again, these algebraic equations do not depend explicitly on U , but rather on temperature T , etc. As discussed above, there are three approaches to overcome this:

1. In simple cases, we can **eliminate** U as a state variable by substituting its dependency on T and other variables into dU/dt , and rewrite the energy balance with T as a state ($dT/dt = \dots$). This approach was used in all the previous examples, but generally it will not work, or at least be very cumbersome, see (11.14). For the flash example, it will not work because U depends on the phase distribution f and we lack an expression for df/dt in (11.14).
2. In general, with internal energy U and the component holdups as state variables, we can solve an “**UV-flash**” to compute the temperature, pressure and phase distribution. Here, we make use of the fact that the total volume V of the flash tank is fixed. The UV flash must be performed as a **separate “intermediate” calculation**, which requires a separate solver, in addition to the solver for the differential equations (integrator). This approach may require a long computation time because of the nested loops.
3. The recommended approach, used in the example below, is to use a **DAE solver** (`ode15s` in our case) to solve the flash equations and the differential equations **simultaneously**. However, also here we should use “intermediate calculations” (elimination; approach 1) to reduce the number of algebraic equations, for example, for computing physical properties. For each remaining algebraic equation, we need an associated (algebraic) state variable, which should be chosen such that algebraic equations in the “intermediate calculations” depend explicitly on the state variables. In many cases, we need the temperature T in the “intermediate calculations,” so it is recommended to choose T as a (algebraic) state variables. In summary, it is recommended to include both U and T in the state vector, by using the following DAE set

$$\begin{aligned} \frac{dU}{dt} &= f_1(T, n_i, \dots) \\ 0 &= \underbrace{U - U_0(T, n_i, \dots)}_{f_2} \end{aligned}$$

This corresponds to including U in the differential variables y_1 and T in the algebraic variables y_2 in (11.52)-(11.53).

We next consider an example with a flash tank where we use the simultaneous DAE approach.

Example 11.18 Adiabatic flash. *We have an adiabatic flash tank with feed stream F [mol/s], vapor product G [mol/s] and liquid product L [mol/s]. The feed consists of methanol*

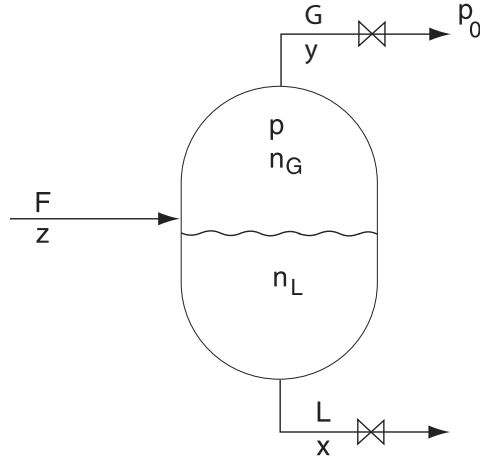


Figure 11.26: Adiabatic flash tank

(1) and ethanol (2). The mole fractions of the light component in the three streams are denoted z (feed), y (vapor) and x (liquid), respectively. The feed is assumed to be liquid and the pressure p_0 downstream the tank (which must be lower than the bubble point pressure of the feed to get flashing) is assumed given; see Figure 11.26. The vapor/liquid equilibrium (VLE) is assumed to be ideal and follow Raoult's law.

For a system with N_c components, we can generally set up N_c mass balances (we choose to use 1 total mass balance, and $N_c - 1$ component balances) and 1 energy balance (11.11);

$$\begin{aligned} \frac{dn}{dt} &= F - G - L \\ \frac{dn_i}{dt} &= Fz_i - Gy_i - Lx_i \quad (i = 1, \dots, N_c - 1) \\ \frac{dU}{dt} &= Fh_F - Gh_G - Lh_L \end{aligned}$$

Here n [mol] is the total holdup in the tank (in both phases), n_i [mol i] is the holdup of component i in the tank (in both phases) and U [J] is the internal energy in the tank. We have assumed, in the energy balance, that the volume of the tank V_{tot} is constant, such that $p_{\text{ex}} \frac{dV_{\text{tot}}}{dt} = 0$. This gives $N_c + 1$ differential equations, corresponding to $N_c + 1$ dynamic state variables (n, n_i, U). However, in addition we generally have a large number of algebraic equations, which may require us to add algebraic state variables, at least if the algebraic equations are implicit.

First, we have the following algebraic relationships for mass and energy holdups

$$\begin{aligned} n &= n_G + n_L \\ n_i &= n_G y_i + n_L x_i \quad (i = 1, \dots, N_c - 1) \\ U &= n_G h_G + n_L h_L - pV_{\text{tot}} \end{aligned}$$

where n_G and n_L is the amount of gas and liquid (the phase distribution) in the tank. Furthermore, we have algebraic expressions for $h_G(T, p, x_i)$ and $h_V(T, p, y_i)$ [J/mol], for G (e.g., valve equation $G = k_g(p - p_0)$), for L (e.g., level control equation $L = k_L(V - V_0)$), for the VLE (from which we can compute p and y_i from T and x_i), for the gas holdup n_G (e.g., ideal gas law), etc. For details, see the MATLAB code below, which should be self-explainable.

It is possible to set up all of these equations as one large equation set (and solve with a DAE solver), but this gives many algebraic variables. In practice, we want to reduce the number of algebraic equations (and the corresponding number of state variables) by inserting any explicit algebraic relationships into the differential equations, as we did earlier using “intermediate computations.” There are many ways of doing this, and it will depend on which variables we select as the algebraic state variables.

For the present flash example, we select T and V_L (liquid volume) as the algebraic state variables, in addition to the three dynamic state variables n , n_1 and U . With this choice, all the algebraic equations are explicit in the state variables, except for two algebraic equations for n and U (which are implicit in V_L and T). For details see the MATLAB file `flash.m` below. Note that the mass matrix M has 0’s on the last two diagonal entries, to signal that the last two equations are algebraic rather than differential.

The steady-state solution is, as before, found by simulating the dynamic response for a long time (unfortunately, it is not allowed in MATLAB to set the mass matrix $M = 0$, which in principle should have been OK). We find at steady state

$$n = 100.4\text{e}3 \text{ mol}, \quad n_1 = 48.1\text{e}3 \text{ mol}, \quad U = 5.02\text{e}8 \text{ J}, \quad T = 344.5 \text{ K}, \quad V_L = 5.02 \text{ m}^3$$

We start from this steady-state when performing further simulations. The liquid feed rate is $0.1 \text{ m}^3/\text{s}$ (2012 mol/s), so the residence time in the flash tank is about 50 s . The dynamic response in the flash tank temperature T to a step increase in the feed temperature T_f from 400K to 440 K is shown in Figure 11.27. This corresponds to an increase in feed enthalpy. Note that the feed is liquid, and the feed pressure (20 bar) is above the bubble point. There is a fast initial temperature increase from 344.5 K to about 345.1 K , related to a fast pressure increase (from $p = 1.03 \text{ bar}$ to 1.05 bar), followed by a slow temperature increase towards 345.3 K at the new steady state, related to the composition change in the liquid phase (from $x_1 = 0.479$ to 0.467 at the new steady state). The increase in vapor flow is from $G = 302 \text{ mol/min}$ to 533 mol/s at the new steady state. The MATLAB file used for this simulation is given below.

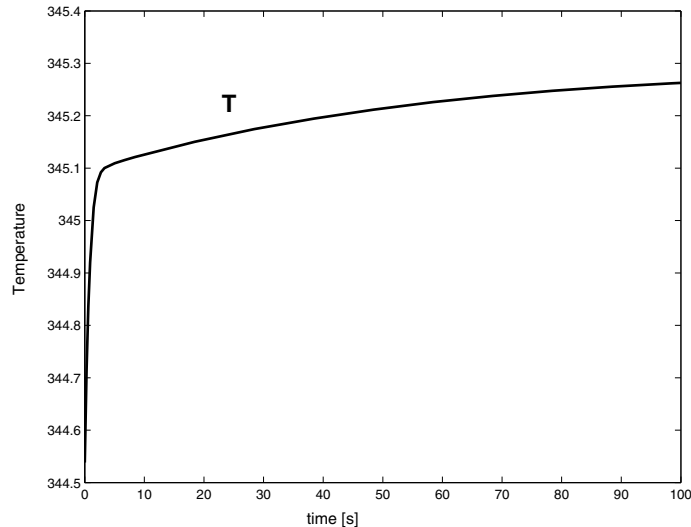


Figure 11.27: Adiabatic flash: temperature response after step in the feed enthalpy

```

function F=f(t,y)
% This is file flash.m
% INPUT: Time t and state vector y
% OUTPUT: Right hand side of DAE set: M dy/dt = f(y)
% States n=y(1); n1=y(2); U=y(3); T=y(4); VL=y(5);
% Usage with ode15s:
%   options = odeset('mass',diag([1 1 0 0]));
%   y0 = [100.4e3 48.1e3 5.02e8 344.5 50.17]
%   [t,y]= ode15s(@flash,[0 100],y0,options)
% Plot temperature:   plot(t,y(:,4))

% All in SI units
% I. Data (parameters and independent variables)
% Data for: 1-methanol, 2-ethanol
A1=8.08097; B1=1582.271; C1=239.726; % Antoine psat1 [mmHg] w/ T [C] (T-range: 15C - 84C)
A2=8.11220; B2=1592.864; C2=226.184; % Antoine psat2 [mmHg] w/ T [C] (T-range: 20C - 93C)
cpl1=80; cpl2=131; cpv1=44; cpv2=65; % heat capacity [J/K mol]
T0=298.15; hvap01=38000; hvap02=43000; % heat of vap. at T0 [J/mol]
Vl1= 40.7e-6; Vl2=58.7e-6; % liquid molar volumes [m3/mol]
R=8.13; % J/mol K

% Feed data
q=0.1; % m3/s
z1=0.5; % mol1/mol
Tf=1.1*400; % K (increase from 400K to 440K)
p0=1e5; % N/m2 (=1 bar downstream pressure)
Vf = z1*Vl1 + (1-z1)*Vl2; % m3/mol (molar volume feed)
F = q/Vf; % mol/s (feed rate)

% Total tank volume
Vtot = 10; % m3

% Valve constant and controller gain
kg=0.1; kl=100e3; % note that the P-controller gain kl is large

% II. Extract present value of states
n=y(1); % total holdup in tank (both phases) [mol]
n1=y(2); % component 1 holdup in tank (both phases) [mol1]
U=y(3); % total internal energy (both phases) [J]
T=y(4); % temperature (same in both phases) [K]
VL=y(5); % liquid volume [m3]

% IIIa. Intermediate calculations
% VLE
x1 = n1/n;
p1s=10.^(A1-B1/(T-273.15+C1))/750e-5; % psat1 from Antoine [N/m2]
p2s=10.^(A2-B2/(T-273.15+C2))/750e-5; % psat2 from Antoine [N/m2]
p1 = x1*p1s; % partial pressure component 1 [N/m2]
p2 = (1-x1)*p2s; % partial pressure component 2 [N/m2]
p = p1+p2; % pressure = sum of partial pressures [N/m2]
y1 = p1/p; % vapor fraction component 1 [mol1/mol]
Vm = x1*Vl1 + (1-x1)*Vl2; % molar volume (liquid phase) [m3/mol]

% Phase distribution
VG = Vtot - VL; % gas volume [m3]
nL = VL / Vm; % liquid holdup [mol]
nG = p*VG / (R*T); % gas holdup (ideal gas law) [mol]

% Enthalpies [J/mol] (Ref.state: pure liquid at T0)
hF = [z1*cpl1 + (1-z1)*cpl2] * (Tf-T0);
hL = [x1*cpl1 + (1-x1)*cpl2] * (T -T0);
hG = [y1*cpv1 + (1-y1)*cpv2] * (T -T0) + y1*hvap01 + (1-y1)*hvap02;

```



```

% Vapor and liquid flow
G = kg*(p-p0);           % simple valve equation for outflow of gas      [mol/s]
VLs = Vtot/2;           % Setpoint level (volume): keep 50% liquid in tank [m3]
L = kl*(VL-VLs);       % Level controller with proportional gain kl    [mol/s]

% IIIb. Evaluate right hand side of DAE-set: M dy/dt = f(y)
f1 = F - G - L;         % =dn/dt Dynamic: Overall mass balance
f2 = F*z1 - G*y1 - L*x1; % =dn1/dt Dynamic: Component 1 mass balance
f3 = F*hF - G*hG - L*hL; % =dU/dt Dynamic: Energy balance
f4 = U + p*Vtot - hL*nL - hG*nG; % = 0 Algebraic: Internal energy U
f5 = n - nG - nL;      % = 0 Algebraic: Total holdup n
F = [f1; f2; f3; f4; f5];

```

Finding the steady-state. Above, the steady state was found by simulating the dynamic response for a long time. Alternatively, one may find the steady-state directly, for example, using the function `fmincon` in MATLAB:

```
yss = fmincon('1',y0,[],[],[],[],[],[],@flashss)
```

where the file `flashss.m` is identical to `flash.m` (above) except that the first line is changed to function `[c,ceq]=f(y)` and the following line is added at the end: `c=[]; ceq=F;`.

Remark 1 Removing or adding algebraic state variables. In the MATLAB code given above, we have two algebraic state variables (T and V_L), but actually we can get rid of V_L as a state variable if we do a little work. This follows because the holdup equations are simple, so we can combine them (including $n = n_G + n_L$ which MATLAB solved using `f5` in the code above), and derive an explicit expression for V_L as a function of n , p , V_{tot} and V_m (try yourself, it is easy!). In the MATLAB code above, we then replace the line `VG = Vtot - VL` by the following two lines of “intermediate calculations”:

```

VG = (Vtot-n*Vm)/(1 - (p*Vm)/(R*T));
VL = Vtot - VG;

```

We now have only 4 state variables, so we delete the algebraic equation `f5 = n - nG - nL` at the end. Of course, we also need to change the mass matrix and the call to `ode15s`. The final result is of course the same as before.

The main problem when we reduce the number of state variables is that the equations get a bit more messy and it is easy to make mistakes. For this reason, we often choose to *add* “unnecessary” state variables in the problem. This also makes plotting the results easier, as MATLAB stores all the state variables. For example, if we want to plot pressure, then we can simply add a “dummy” state variable (`pdummy=y(6);`) together with a “dummy” algebraic equation (`f6= p - pdummy;`).

Remark 2 Fixing pressure and index problem. In the model of the flash tank given in the MATLAB code above, we let the pressure vary dynamically, but from the very quick initial rise in temperature in Figure 11.27 it follows that the pressure dynamics are very fast. In such cases it might be tempting to say that the pressure is fixed by introducing the algebraic equation $p = p_0$ (`f6 = p-p0;`) and an additional state variable G (and omitting the valve equation for G). This is in principle OK, but it turns out that the integration routine `ode15s` is unable to solve this – we get an error message: “This DAE appears to be of index greater than 1.” An “index problem” is often an indication of a non-physical assumption (in this case, it is not physically possible to keep the pressure p constant), and the problem can often be avoided by rewriting the equations, and/or avoiding non-physical assumptions.

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

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

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.

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 over-react (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

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

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

$$\tau_D = \tau_2 \quad (11.56)$$

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

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

where $|u_0|$ is the MV change required to counteract the largest expected disturbance and $|y_{\max}|$ is the largest accepted CV deviation. In industry, the variables have often already been scaled such that $|u_0| \approx |y_{\max}|$ (for example equal to 1) and we get $|K_{c,\min}| \approx 1$. 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 $y_s = 444\text{K}$. 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 m^3/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 $T_c=431$ 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 $MV T_c$). 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).

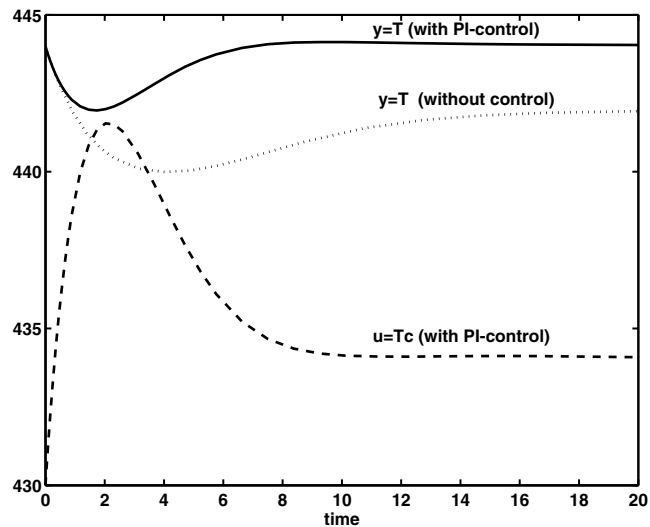


Figure 11.28: Exothermic CSTR with and without control: Temperature response after a 20% increase in feed flow rate

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:

```
[T,Y]=ode15s(@cstrTpi,[0 50],[2274 7726 444.0 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.

