

# Chapter 1

## Dynamic Modelling of Chemical Processes

### 1.1 References

Many textbooks and research books are available. When a precise reference is given for a textbook which describes a given topic particularly well, the present author has tried not to forget his colleagues and mentions them at the end of the concerned chapter. When general textbooks can be recommended for different points, they are mentioned at the end of this first chapter to avoid too much repetition. It is impossible to cite all textbooks and the fact that some are not cited does not mean that they are of lower value. Of course, research papers are referenced in the concerned chapter.

### 1.2 Applications of Process Control

A chemical plant represents a complex arrangement of different units (reactors; separation units such as distillation, absorption, extraction, chromatography and filtration; heat exchangers; pumps; compressors; tanks; ...). These units must be either maintained close to their steady states for continuous operation or follow optimal trajectories for batch operation.

The engineers in charge of a plant must ensure quantitative and qualitative product specifications and economic performance while meeting health, safety and environmental regulations.

The task of a control system is to ensure the stability of the process, to minimize the influence of disturbances and perturbations and to optimize the overall performance. These objectives are achieved by maintaining some variables (temperature, pressure, concentration, position, speed, quality, ...) close to their desired values or using set points which can be fixed or time-dependent.

When a chemical engineer designs a process control system, he or she must first study the process and determine its characteristics. The process variables

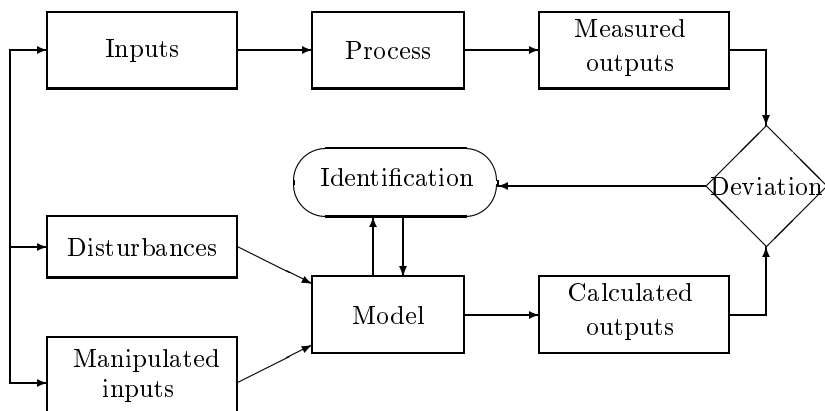
are classified as inputs, outputs, and states.

Subsequently, a process model with varying degrees of complexity (according to the ultimate use of the model) is derived. For an existing process, a black box model (where coefficients have no physical meaning) may be developed by system identification techniques, often with little effort. On the other hand, a physical model based on first principles involves a great deal of engineering effort.

The developed model is in general verified in an off-line manner and independently of the control scheme. Then, the model is used together with the chosen control scheme to check the process response to set point and disturbances variations.

The control scheme can be a simple proportional controller as well as a much more sophisticated algorithm, e.g. if nonlinear control based on a physical model of the process is utilized.

The outputs of the simulation model used for control can be compared to those of the real process or to those from an accurate model. System identification (Fig. 1.1) allows the engineer to estimate the parameters of the model or to evaluate the performances of the control law.

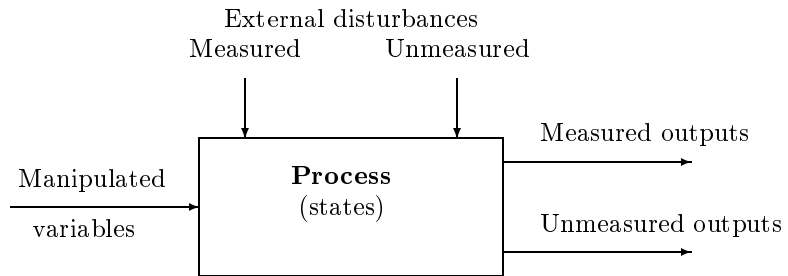


**Figure 1.1:** Design of a process model for control

## 1.3 Process Description from the Control Engineer's Viewpoint

The control engineer considers the process to be controlled as a dynamic system having inputs, outputs and internal variables called the state variables. His/her classification is different from the process engineer's point of view. Indeed, for a process engineer, inputs are essentially physical streams (such as a feed pipe) delivering material and energy to the process, possibly information such as electrical signals, and outputs are similarly physical streams, withdrawing

materials (the effluent stream to the downstream processing unit) and energy from the process.



**Figure 1.2:** Input-output block diagram representation of a process

From the control engineer's point of view, variables associated with a process (flow rate, concentration, temperature, pressure, quality, ...) are generally considered as signals transferring information. These variables are divided into two groups (Fig. 1.2):

- Inputs which represent the influence of environment on the process: these variables affect the process and thus modify its behaviour.
- Outputs which represent the process influence on environment: these variables represent the link with the outside. They should be maintained close to their set points.

Input and output variables are linked by state variables (see state representation) which are internal to the process and help to describe the evolution of the process with time. Any modification of the inputs affects dynamically the process states, which in turn influence algebraically the process outputs.

Input variables are divided into:

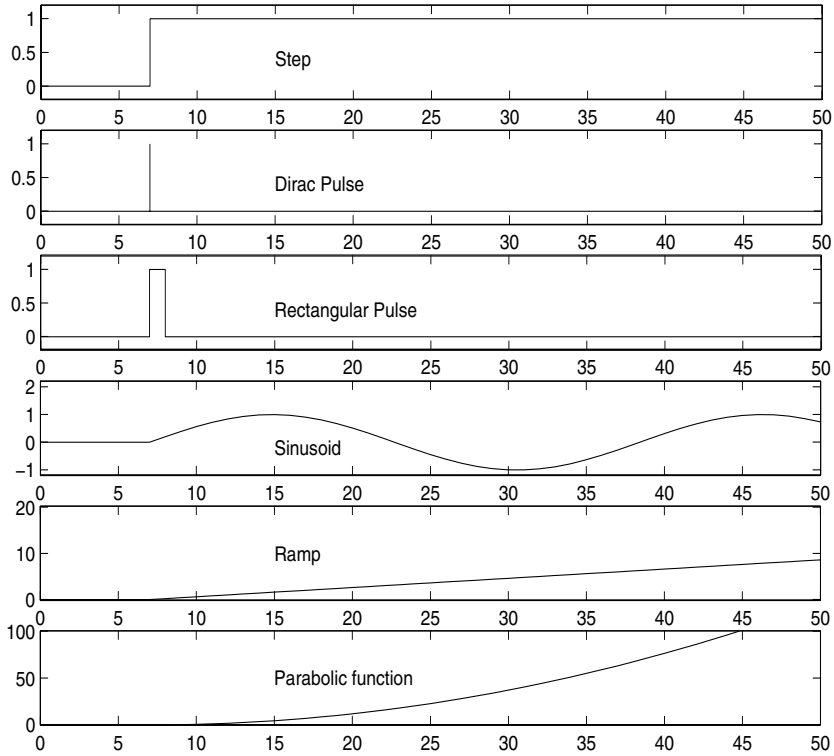
- Control variables or manipulated variables which can be adjusted freely by the operator or by regulatory means. For example, the position of a valve stem determines the flow rate through the valve. In this case, the input or manipulated variable will be the valve stem position or the flow rate in the pipe which is directly related to the valve position.
- Disturbances include all other inputs which are not set by the operator or a controller. For example, in the case of temperature control in a building, outside climate temperature and humidity changes are considered as disturbances which affect the controlled variable that is the inner temperature.

Output variables are divided into:

- Measured variables, whose values are known using direct on-line measurement by a sensor.
- Unmeasured variables, which may be estimated or inferred using an indirect or secondary measurement. This estimation of unmeasured variables by means of a model and other measurements constitutes a soft sensor (Chap. 18).

Figure 1.2 represents an input-output block diagram of a process.

A system is called single variable or single-input single-output (SISO) if it has only one input and one output. It is called multivariable or multi-input multi-output (MIMO) if it has several inputs and several outputs. In general, the number of inputs is larger than the number of outputs.



**Figure 1.3:** Different types of inputs starting at time  $t = 7$  after steady state

In order to study the behaviour of a process, the process inputs are generally varied by some simple and standard functions and the response of the process is monitored in each case. Apart from the disturbances, which can take any form, the standard input functions  $f$  (Fig. 1.3) are:

- A step function: a unit step function is defined as  $f = 1$  if  $t > 0$ ,  $f = 0$  if  $t \leq 0$ . Its response is called a step response.
- An impulse function: a unit impulse function is defined as:  $f = \delta$  (theoretical Dirac). Its response is called an impulse response.
- A sinusoidal function:  $f = a \cos(\omega t + \phi)$ . Its response is referred to as a frequency response.
- A ramp:  $f = kt$ . This determines the behaviour of the process output to an input with constant rate of change (constant velocity).
- A parabolic function:  $f = kt^2$ . This is used whenever the response to a

constant acceleration is desired.

The inputs to a controlled physical system can be further classified as disturbances (loads) (for regulatory control) or set point variations (for set point tracking or servo-control).

## 1.4 Model Classification

Models can be classified with respect to different user-specified criteria. In the steady-state models, the time derivatives of the state variables are set to zero ( $d/dt = 0$ ). In the dynamic models which describe the transient behaviour of the process, the process variables are time-dependent ( $f(t, x, u)$ ). In process control applications, the models must be dynamic in order to represent the process variations with respect to time.

Dynamic models can be of two kinds: deterministic, in which it is assumed that all the variables are perfectly known at a given instant of time, or probabilistic (stochastic) models, which make use of probability distributions to account for the variations and uncertainties associated with the process and its variables.

Dynamic models can be continuous when the function  $f(t, x, u)$  describing the process is continuous or discrete with respect to time (variables are only known at regular time intervals).

A model can be developed using merely the process input-output data series without physical knowledge of the process. This type of model is referred to as a black-box or behavioural model (such as neural networks). At the other extreme, a model may be developed from the application of first principles (conservation laws) to the process. Such models are called phenomenological or knowledge-based.

The knowledge-based models are further classified as:

- Lumped-parameter models in which the state variables have no spatial dependence, and therefore the models consist of ordinary differential equations (e.g. the classical continuous stirred tank reactor).
- Distributed-parameter models, in which the state variables are position-dependent and the models take the form of partial differential equations (e.g. a tubular reactor). Very often, a distributed-parameter model is discretized (division of a tubular reactor into  $n$  continuous stirred tank reactors) so as to transform the partial differential equations into a set of ordinary differential equations that are more tractable mathematically.

Furthermore, models can be linear or nonlinear. A process model is linear if all variables describing the process appear linearly in the equations. It is nonlinear in the opposite case. The advantage of linear models is that they can be easily transformed by mathematical mappings and their mathematical behaviour is well known.

Among the many forms of models that will be used in this book, the transfer functions (in the continuous  $s$  Laplace or discrete  $z$  domains) and the state-space models are of special significance.

A key point which must be remembered is that a model, however sophisticated it may be, remains an approximation of the real process. It will often differ according to the pursued objective.

## 1.5 State-Space Models

Generally, a state-space multivariable system is modelled by a set of algebraic and differential equations of the form

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}, t) \\ \mathbf{y} = \mathbf{h}(\mathbf{x}, t) \end{cases} \quad (1.1)$$

where  $\mathbf{x}$  is the state vector of dimension  $n$ ,  $\mathbf{u}$  is the input vector (or control variables vector) of dimension  $n_u$  and  $\mathbf{y}$  is the output vector of dimension  $n_y$  (in general,  $n_u \geq n_y$ ). The state  $\mathbf{x}$  of the system at any time  $t$  is described by a set of  $n$  differential equations, which are often non-linear. The states  $\mathbf{x}(t)$  depend only on initial conditions at  $t_0$  and on inputs  $\mathbf{u}(t)$  between  $t_0$  and  $t$ . At the initial time, the state variables are the initial conditions and later they represent the evolution of the state of the system.

A remarkable characteristic of the non-linear dynamic knowledge-based models in chemical engineering is that they are described by differential equations, either ordinary or partial, which are usually affine with respect to the input vector. Thus, the most common form of a non-linear state-space model is

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t) + \mathbf{g}(\mathbf{x}, t) \mathbf{u} \\ \mathbf{y} = \mathbf{h}(\mathbf{x}, t) \end{cases} \quad (1.2)$$

An important class is linear state-space models of the form

$$\begin{cases} \dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \\ \mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{u}(t) \end{cases} \quad (1.3)$$

which includes any process model described by a set of  $n$  linear ordinary differential equations.  $\mathbf{A}$  is the state matrix of dimension  $(n \times n)$ ,  $\mathbf{B}$  is the control matrix of dimension  $(n \times n_u)$ ,  $\mathbf{C}$  is the output matrix of dimension  $(n_y \times n)$ , and  $\mathbf{D}$  is the coupling matrix of dimension  $(n_y \times n_u)$  which is very often equal to zero. When  $\mathbf{D}$  is different from zero, it is said that the output is directly driven by the input.

The linearization of a set of differential equations of the most general form

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}, t) \quad (1.4)$$

around a steady-state operating level  $\mathbf{x}_0$  for a nominal input  $\mathbf{u}_0$  can be achieved by the following Taylor series expansion

$$\dot{x}_i = f_i(\mathbf{x}_0, \mathbf{u}_0, t) + \sum_{j=1}^n \left( \frac{\partial f_i}{\partial x_j} \right)_{\mathbf{x}=\mathbf{x}_0, \mathbf{u}=\mathbf{u}_0} \delta x_j + \sum_{k=1}^{n_u} \left( \frac{\partial f_i}{\partial u_k} \right)_{\mathbf{x}=\mathbf{x}_0, \mathbf{u}=\mathbf{u}_0} \delta u_k \quad (1.5)$$

with:  $\delta x_j = x_j - x_{j,0}$ ,  $\delta u_k = u_k - u_{k,0}$  where  $x_{j,0}$  is the  $j$  component of steady-state vector  $\mathbf{x}_0$  and  $u_{k,0}$  is the  $k$  component of the nominal input vector  $\mathbf{u}_0$ .  $\delta$  indicates any deviation with respect to the nominal operating condition, thus  $\delta x$  and  $\delta u$  are respectively deviations of the state and of the input with respect to the steady state of the process. One gets  $\dot{x}_i = \delta \dot{x}_i + \dot{x}_{i,0}$  and  $\dot{x}_{i,0} = f_{i,0}$ , so that the following set of linear ordinary differential equations is obtained

$$\delta \dot{x}_i = \sum_{j=1}^n \left( \frac{\partial f_i}{\partial x_j} \right)_{\mathbf{x}=\mathbf{x}_0, \mathbf{u}=\mathbf{u}_0} \delta x_j + \sum_{k=1}^{n_u} \left( \frac{\partial f_i}{\partial u_k} \right)_{\mathbf{x}=\mathbf{x}_0, \mathbf{u}=\mathbf{u}_0} \delta u_k \quad (1.6)$$

which can be easily written in a more condensed matrix form similar to Eq. (1.3). Similarly

$$\delta y_i = \sum_{j=1}^n \left( \frac{\partial h_i}{\partial x_j} \right)_{\mathbf{x}=\mathbf{x}_0, \mathbf{u}=\mathbf{u}_0} \delta x_j + \sum_{k=1}^{n_u} \left( \frac{\partial h_i}{\partial u_k} \right)_{\mathbf{x}=\mathbf{x}_0, \mathbf{u}=\mathbf{u}_0} \delta u_k \quad (1.7)$$

The form of Eqs. (1.6) and (1.7) is referred to as the linearized state-space model with the matrices of the linear state-space model indicated by their current element

$$\mathbf{A} = \left[ \frac{\partial f_i}{\partial x_j} \right] \quad ; \quad \mathbf{B} = \left[ \frac{\partial f_i}{\partial u_j} \right] \quad ; \quad \mathbf{C} = \left[ \frac{\partial h_i}{\partial x_j} \right] \quad ; \quad \mathbf{D} = \left[ \frac{\partial h_i}{\partial u_j} \right] \quad (1.8)$$

$\mathbf{A}$  and  $\mathbf{B}$  are respectively the Jacobian matrices of  $\mathbf{f}$  with respect to  $\mathbf{x}$  and  $\mathbf{u}$ , while  $\mathbf{C}$  and  $\mathbf{D}$  are respectively the Jacobian matrices of  $\mathbf{h}$  with respect to  $\mathbf{x}$  and  $\mathbf{u}$ .

Notions of controllability and observability in the state space will be specially studied in Chap. 7.

## 1.6 Examples of Models in Chemical Engineering

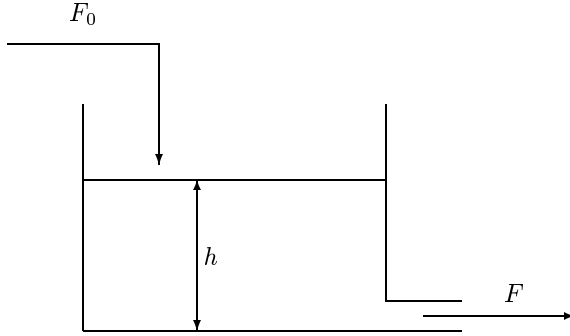
With the help of certain classical examples in chemical engineering, we will show how various chemical processes can be described in the state-space form.

### 1.6.1 Lumped-Parameter Systems

In lumped-parameter systems, the process variables depend only on time, which is the independent variable. The dynamic behaviour of the process is then described by a set of ordinary differential equations.

#### A Surge Tank

Consider a cylindrical tank fed by an incompressible liquid (Fig. 1.4) at a varying flow rate  $F_0$  ( $\text{m}^3/\text{s}$ ). The exit flow rate  $F$  is also time-dependent.



**Figure 1.4:** A surge tank with varying level

At steady-state, the level in the tank is constant and the mass balance requires equality of inlet and outlet mass flow rates

$$F_0 \rho_0 = F \rho \quad (1.9)$$

where  $\rho$  is the fluid density.

In transient regime, the liquid level  $h$  in the tank varies with time.

The general mass balance formulated as

$$\text{(inlet mass / unit time)} = \text{(outlet mass / unit time)} + \text{(time rate of change of mass in the system)}$$

gives the dynamic model of the tank

$$F_0 \rho_0 = F \rho + \frac{d(\rho V)}{dt} \quad (1.10)$$

This is the state-space equation of the process.

If the liquid density is constant ( $\rho = \rho_0$ ) and the tank cross-sectional area  $S$  does not depend on the liquid level, the previous mass balance will become

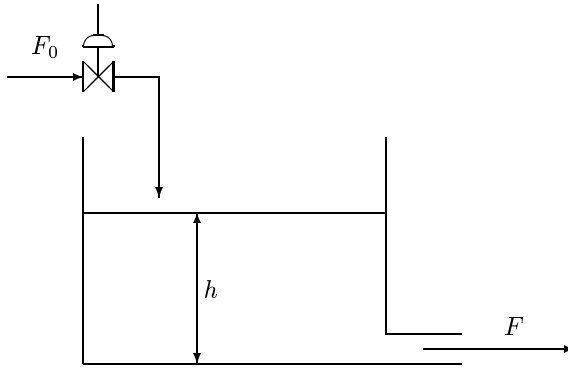
$$\frac{dh}{dt} = F_0/S - F/S \quad (1.11)$$

One notices that only the liquid level in the tank, the controlled variable, appears in the derivative. With the section area  $S$  being a constant parameter, this ordinary differential equation is linear. Equation (1.11) can be considered as the fundamental model of a level control system.

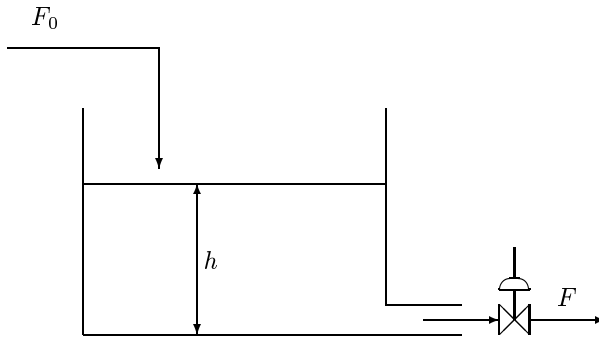
Assuming that a valve is placed on the inlet pipe (Fig. 1.5), the inlet flow rate  $F_0$  will become the control (manipulated) variable of the system. In state space, the system is single-input single-output (SISO), with an input  $u = F_0$ , an output  $y = h$  and only one state:  $x = h$ . The state-space model is

$$\begin{aligned} \dot{x} &= u/S - F/S \\ y &= x \end{aligned} \quad (1.12)$$





**Figure 1.5:** Surge tank with varying level with valve on the inlet stream



**Figure 1.6:** Surge tank with varying level with valve on the outlet stream

In this linear model, the cross-sectional area  $S$  is a constant parameter, and the flow rate  $F$  is an external disturbance acting on the system.

In the case where the valve is on the outlet stream (Fig. 1.6), the manipulated input is the outlet flow rate  $F$ , so that the state-space model becomes

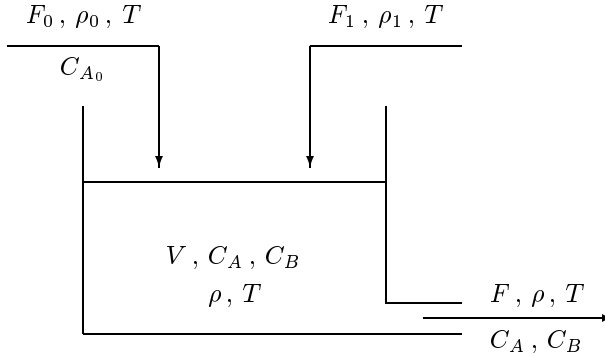
$$\begin{aligned}\dot{x} &= F_0/S - u/S \\ y &= x\end{aligned}\tag{1.13}$$

In this case, the flow rate  $F_0$  is a disturbance.

### An Isothermal Continuous Chemical Reactor

The cylindrical reactor (Fig. 1.7) is assumed to be perfectly mixed, i.e. the temperature  $T$ , the concentration of any given species, the pressure, etc. are identical at any location of the reactor and keep their value in the effluent stream. The reactor is fed by two streams, one having a flow rate  $F_0$  containing the reactant A, and the other one an inert stream with a flow rate  $F_1$ . Both streams have their temperature equal to that of the reactor contents. Fur-

thermore, we will assume that the heat of reaction is negligible so that there is no need to write the energy balance.



**Figure 1.7:** An isothermal continuous stirred tank reactor (CSTR)

The overall mass balance equation is similar to that of the previous tank

$$\frac{d(\rho h)}{dt} = F_0 \rho_0 / S + F_1 \rho_1 / S - F \rho / S \quad (1.14)$$

and we assume that the densities in different streams are equal.

The balance for component A in transient regime is given by the continuity equation for A:

$$(\text{rate of A entering}) = (\text{rate of A exiting}) - (\text{rate of A produced}) + (\text{rate of accumulation of A}),$$

giving

$$F_0 C_{A_0} = F C_A - R_A V + \frac{d(V C_A)}{dt} \quad (1.15)$$

noting that  $F'_{A_0} = F_0 C_{A_0}$  is the molar flow rate (mol/s) of component A in the inlet stream, and similarly  $F'_A$  is the outlet molar flow rate. Equation (1.15) can be written as

$$F'_{A_0} = F'_A - R_A V + \frac{d(V C_A)}{dt} \quad (1.16)$$

The term  $R_A$  represents the number of moles of A produced per unit volume and unit time; it can be called the production rate of A (Levenspiel, 1999; Villermaux, 1982). When  $R$  reactions designated by  $i$  occur simultaneously, the rate of production of a component  $A_j$  is equal to

$$R_j = \sum_{i=1}^R \nu_{ij} r_i \quad (1.17)$$

where each reaction rate  $r_i$  is in general positive. The stoichiometric coefficient  $\nu_{ij} > 0$  if  $A_j$  is produced by reaction  $i$ , and  $\nu_{ij} < 0$  if  $A_j$  is consumed by reaction

*i*. Note that this definition of reaction can be applied to either a continuous reactor, a batch reactor ( $F_0 = F = 0$ ) or a fed-batch reactor ( $F = 0$  and  $F_0 \neq 0$ ). The chemical advancement  $\xi$  (dimension: mol) and the generalized yield  $\chi$  (without dimension) are defined such that:

- For a closed reactor:

Taking  $n_0$  as the total number of moles of reacting species present at a reference state, in general the initial state, the number of moles of a component  $A_j$  at any other state is equal to

$$n_j = n_{j0} + \sum_{i=1}^R \nu_{ij} \xi_i = n_{j0} + n_0 \sum_{i=1}^R \nu_{ij} \chi_i \quad \text{with: } n_0 = \sum_j n_{j0} \quad (1.18)$$

given the rate of reaction *i*:

$$r_i = \frac{1}{V} \frac{d\xi_i}{dt} = \frac{n_0}{V} \frac{d\chi_i}{dt} \quad (1.19)$$

- For an open continuous stirred reactor:

The reference is in general the inlet molar flow rate  $F'_0$  including all entering reacting species *j* present in the reference state. So the molar flow rate  $F'_j$  of a component  $A_j$  at any point of the system is equal to

$$F'_j = F'_{j0} + \sum_{i=1}^R \nu_{ij} \dot{\xi}_i = F'_{j0} + F'_0 \sum_{i=1}^R \nu_{ij} \chi_i \quad \text{with: } F'_0 = \sum_j F'_{j0} \quad (1.20)$$

given the rate of reaction *i*:

$$r_i = \frac{F'_0}{V} (\chi_{i,out} - \chi_{i,in}) = \frac{F_0 C_0}{V} (\chi_{i,out} - \chi_{i,in}) \quad (1.21)$$

where *in* denotes the inlet stream and *out* the exit stream.  $C_0$  is the total concentration in the reference state of all the constituents. The residence time  $\tau$  is equal to

$$\tau = \frac{V}{F_0} = \frac{C_0 (\chi_{i,out} - \chi_{i,in})}{r_i} \quad (1.22)$$

In the general case of *R* simultaneous reactions, Equation (1.15) becomes

$$S \frac{d(h C_A)}{dt} = F_0 C_{A_0} - F C_A + \sum_{i=1}^R \nu_{iA} r_i V \quad (1.23)$$

In the case where only one first-order chemical reaction occurs:  $A \rightarrow B$ , the reaction rate  $r_A$  is equal to  $r_A = k C_A$ , and the production rate of A is equal to  $R_A = -r_A$ , as  $\nu_{iA} = -1$ . Equation (1.15) becomes

$$F_0 C_{A_0} = F C_A + k C_A V + \frac{d(V C_A)}{dt} \quad (1.24)$$

which can be transformed into

$$\frac{dC_A}{dt} = \frac{F_0}{S h} (C_{A_0} - C_A) - \frac{F_1}{S h} C_A - k C_A \quad (1.25)$$

This balance will be used as the fundamental model for the control of the concentration  $C_A$ .

The differential equation describing the variations in the concentration  $C_A$  is in general nonlinear, since the inlet and outlet flow rates  $F_0$  and  $F$  are time-varying and the reaction rate can be a complicated function with respect to concentration. Frequently, a chemical reaction is either endothermic or exothermic. Therefore, an energy balance equation should be added to the previous differential equations.

Assuming that the inputs are the inlet volumetric flow rate  $F_1$  and inlet concentration  $C_{A_0}$ , the control vector is  $\mathbf{u} = [F_1, C_{A_0}]^T$ . We wish to control the reactor level and concentration, thus the output vector is  $\mathbf{y} = [h, C_A]^T$ . The process is a  $2 \times 2$  multivariable system. The state vector is chosen to be equal to  $\mathbf{x} = [h, C_A]^T$ . The state-space representation of the isothermal reactor with a first-order reaction is

$$\begin{cases} \dot{x}_1 = F_0/S - F/S + u_1/S \\ \dot{x}_2 = \frac{1}{S x_1} [F_0 (u_2 - x_2) - x_2 u_1] - k x_2 \\ y_1 = x_1 \\ y_2 = x_2 \end{cases} \quad (1.26)$$

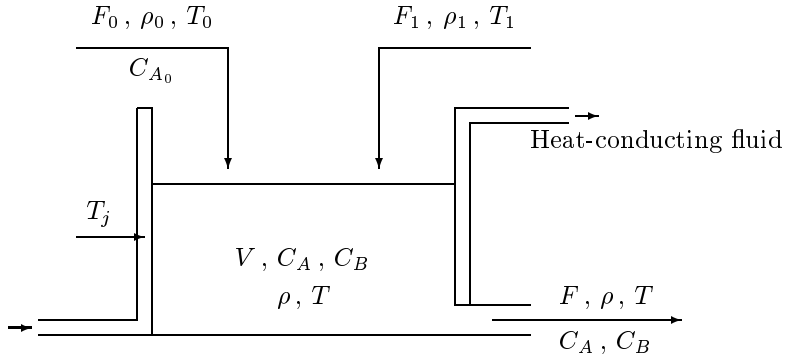
This multi-input multi-output (MIMO) model is nonlinear even if we assume that the level  $h$  is perfectly regulated by an independent controller because of the differential equation describing the concentration variations. Disturbances are flow rates  $F_0$  and  $F$ .

Frequently, when the main objective is concentration control, the influence of level variations is considered as secondary and the level can be regulated independently.

## A Non-isothermal Continuous Chemical Reactor

Figure 1.8 represents the schematics of a non-isothermal continuous chemical reactor with a heating/cooling jacket. The heating/cooling medium may also be supplied by means of a coil immersed inside the reactor. It is used for cooling in cases of exothermic reaction or desired temperature decrease, and for heating in cases of endothermic reaction or desired temperature increase. The rate of heat transfer transferred between the reacting mixture and the heating/cooling medium is  $\dot{Q}$ .  $\dot{Q}$  is positive for heating the reacting mixture and negative in the opposite case.  $\dot{Q}$  is given by

$$\dot{Q} = U S_{\text{ex}} (T_j - T) \quad (1.27)$$



**Figure 1.8:** A non-isothermal continuous stirred tank chemical reactor (CSTR)

where  $U$  is the overall heat transfer coefficient,  $S_{\text{ex}}$  is the available heat exchange area,  $T_j$  is the mean temperature in the jacket, and  $T$  is the temperature of the reactor.

Apart from the overall mass balance and component mass balance on A, the energy balance written in general terms as

$$\begin{aligned} & \text{(variation of internal energy / unit time)} = \\ & \text{(inlet enthalpy by convection / unit time)} - \\ & \text{(outlet enthalpy by convection / unit time)} + \\ & \text{(rate of heat transfer and mechanical energy)} \end{aligned}$$

must also be considered. The energy balance of the reactor is thus as follows

$$\frac{dU}{dt} = F'_{in} h_{in} - F'_{out} h_{out} + \dot{Q} \quad (1.28)$$

where  $F'_{in}$  is the total inlet molar flow rate and  $F'_{out}$  is the total outlet molar flow rate.  $h'$  is the specific molar enthalpy of each stream given by

$$h'_{in} = \sum_j x_{j,in} h'_{j,in} \quad h'_{out} = \sum_j x_{j,out} h'_{j,out} \quad (1.29)$$

where  $x_{j,in}$  and  $x_{j,out}$  are the inlet and outlet mole fractions respectively and  $h'_{j,in}$  and  $h'_{j,out}$  are the specific enthalpies of component  $j$  in the inlet and outlet streams respectively. The specific molar enthalpy  $h'$  of a pure component can be expressed with respect to its enthalpy of formation  $\Delta H_f(T_{ref})$  at a reference temperature  $T_{ref}$  according to

$$h' = \Delta H_f(T_{ref}) + \int_{T_{ref}}^T C'_p d\tau \quad (1.30)$$

provided that there is no change of state between  $T_{ref}$  and  $T$ . If, however, there is a change of state, the corresponding latent heat of transformation should be

accounted for.  $C'_p$  is the molar specific heat of the component at constant pressure.

The change of total internal energy  $U$  of the reactor contents can be expressed in terms of the specific molar internal energy by

$$\frac{dU}{dt} = \frac{d(nu)}{dt} = \frac{d(H - PV)}{dt} = \frac{d(nh)}{dt} - P \frac{dV}{dt} - V \frac{dP}{dt} \quad (1.31)$$

For isobaric operation and negligible pressure work, there remains

$$\frac{dU}{dt} = \frac{d(nh)}{dt} \quad (1.32)$$

The enthalpy change  $\Delta h_i$  due to reaction  $i$  is equal to

$$\Delta h_i = \sum_j \nu_{ij} h_j \quad (1.33)$$

which concerns only reacting and produced species, not inert ones. For  $R$  reactions, the total enthalpy contribution  $dh$  linked to the reactions is

$$dh = V dt \sum_{i=1}^R r_i \Delta h_i \quad (1.34)$$

The enthalpy of the reactor walls and its accessories such as the mixer should also be considered. Assuming that the mass of the reactor wall and its accessories is represented by  $m_r$  and the corresponding heat capacity is  $C_r$ , the overall thermal balance after some mathematical manipulation can be written as

$$(m C_p + m_r C_r) \frac{dT}{dt} = \sum_{in} F_{in} \rho_{in} C_{p,in} (T_{in} - T) + \dot{Q} - V \sum_{i=1}^R r_i \Delta h_i \quad (1.35)$$

where  $m$  is the mass of the reactor contents,  $C_p$  its mean specific heat calculated at the reactor temperature  $T$ , and the summation is carried out over all inlet streams to the reactor. Note that the reactor is perfectly mixed, therefore the exit temperature and concentration are identical to those in the reactor. The heats of reactions  $\Delta h_i$  are calculated at the reactor temperature.

Consider again the first-order chemical reaction  $A \rightarrow B$  with heat of reaction  $\Delta h_{A \rightarrow B}$ , taking place in the reactor shown in Fig. 1.8. The temperature dependency of the reaction rate is expressed by the Arrhenius equation  $r = k_0 \exp(-E/(RT)) C_A$ , which is a highly nonlinear term. When applied to the reactor shown in Fig. 1.8 with its two inlet streams, Eq. (1.35) becomes (assuming that densities  $\rho_0, \rho_1, \rho$  and heat capacities are constant)

$$(m C_p + m_r C_r) \frac{dT}{dt} = F_0 \rho_0 C_{p0} (T_0 - T) + F_1 \rho_1 C_{p1} (T_1 - T) + \dot{Q} - V r \Delta h_{A \rightarrow B} \quad (1.36)$$

where  $C_{p0}$  is the mean specific heat of the inlet stream with volumetric flow rate  $F_0$ . The densities are assumed to be identical and constant.

Notice that the differential equation describing the temperature variation is nonlinear. This model will be used for temperature control studies in the remainder of the book.

The behaviour of the chemical reactor shown in Fig. 1.8 is described by a set of three coupled ordinary differential equations.

In addition to the level and concentration in the case of the isothermal reactor, temperature must also be controlled. Moreover, it is assumed that a valve allows us to manipulate the thermal power  $\dot{Q}$  introduced in the jacket. This can be performed by a heat exchanger. Therefore, the output vector is  $\mathbf{y} = [h, C_A, T]^T$ , the control vector is  $\mathbf{u} = [F_1, C_{A0}, \dot{Q}]^T$ , and the state vector is  $\mathbf{x} = [h, C_A, T]^T$ .

In this case, the state-space model obtained from balance equations is as follows

$$\left\{ \begin{array}{l} \dot{x}_1 = F_0/S - F/S + u_1/S \\ \dot{x}_2 = \frac{1}{S x_1} [F_0 (u_2 - x_2) - x_2 u_1] - k_0 \exp(-E/(R x_3)) x_2 \\ \dot{x}_3 = \frac{1}{\rho S C_p x_1 + m_r C_r} [F_0 \rho_0 C_{p0} (T_0 - x_3) + u_1 \rho_1 C_{p1} (T_1 - x_3) \\ \quad - k_0 \exp(-E/(R x_3)) S x_1 x_2 \Delta h_T + u_3] \\ y_1 = x_1 \\ y_2 = x_2 \\ y_3 = x_3 \end{array} \right. \quad (1.37)$$

The state-space model is multi-input multi-output and nonlinear because of the two differential equations describing respectively the variations of concentration and of temperature in the reactor. Nevertheless, this model is affine with respect to manipulated variables.

In general, this model will be too complicated for control system design and analysis. If one is primarily concerned with temperature control, only the energy balance will be taken into account.

## Staged Processes

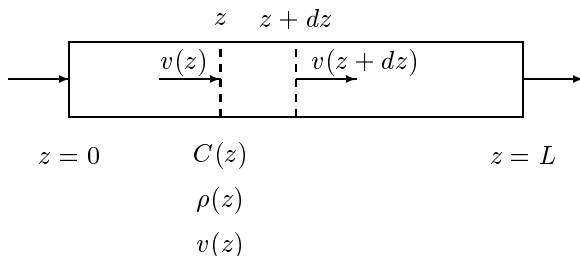
A tray distillation column is composed of a finite number of stages, similar to a tray absorption column or a multi-stage mixer-settler for liquid-liquid extraction. In a staged process, the overall mass balance, the component mass balance and the energy balance are applied to each stage separately. The full state-space model of a staged process is thus obtained by gathering the stage models and taking into account the relations between the stages and the environment. Therefore, the overall model of these processes consists of a large number of ordinary differential equations adequate for dynamic simulation but which pose difficult problems for control studies and implementation. The

number of differential equations (the model order), however, can be reduced by efficient model reduction techniques to obtain approximate low-order models. The reduced model must keep the main dynamic characteristics of the original high-order model. An example of model reduction for a distillation column is given in Chap. 20.

### 1.6.2 Distributed-Parameter Systems

When process variables depend simultaneously on time and spatial variables, the process is described by partial differential equations.

A chemical tubular reactor, chromatography column, packed absorption or distillation column are examples of distributed-parameter systems. Only one example will be presented here: an isothermal tubular reactor (Fig. 1.9). If noticeable heat exchange occurs in the reactor, the energy balance equations must be considered as previously with heat exchange occurring at the wall.



**Figure 1.9:** Schematics of a tubular reactor

The flow is assumed to be fully turbulent, which results in a flat velocity profile and justifies the plug flow assumption. For a plug flow reactor, the reaction rate and all the process variables are constant over a given cross-section, i.e. the radial variations are discarded and only the axial variations are considered. The chemical reaction is identical to the previous cases:  $A \rightarrow B$ , first-order, and the reaction rate  $r_A$  is given by  $r_A = k_0 \exp(-E/(RT)) C_A$ .

The conservation principles, in the case of distributed-parameter systems, are applied to an infinitesimal volume (control volume) in which the fluid properties may be assumed constant. The shape of the control volume depends on the geometry and the flow conditions in the reactor. For example, for a plug flow reactor, the control volume is a cylinder of thickness  $dz$  (example of Fig. 1.9), for a tubular reactor with both radial and axial variations in process variables, the control volume will be a ring with height  $dz$  and radial thickness  $dr$ , and for a tubular reactor with variations of process variables in radial, axial and angular directions, the control volume will be a sector of a ring.

Consider a cylindrical control volume between  $z$  and  $z + dz$  at time  $t$ . All the variables such as the density  $\rho$ , velocity  $v$  and concentration  $C_A$  depend on time  $t$  and axial dimension  $z$ . The mass balance is performed on the control



volume with thickness  $dz$ , and cross-sectional area  $S$ , giving

$$v(z) S \rho(z) = v(z + dz) S \rho(z + dz) + \frac{\partial(S dz \rho(z))}{\partial t} \quad (1.38)$$

which is simplified to

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v)}{\partial z} = 0 \quad (1.39)$$

Diffusion is related to the axial concentration gradient in the reactor.

The axial diffusive flux of component A (moles per unit time and unit cross-sectional area) is expressed by Fick's law

$$N_A = -\mathcal{D}_A \frac{\partial C_A}{\partial z} \quad (1.40)$$

where  $\mathcal{D}_A$  is the turbulent diffusion coefficient and the corresponding mass balance on A over the control volume is

$$v(z) S C_A(z) + S N_A(z) = v(z + dz) S C_A(z + dz) + S N_A(z + dz) + k C_A S dz + \frac{\partial(S dz C_A)}{\partial t} \quad (1.41)$$

which can be simplified as

$$\frac{\partial C_A}{\partial t} + \frac{\partial v C_A}{\partial z} + k C_A - \frac{\partial}{\partial z} \left( \mathcal{D}_A \frac{\partial C_A}{\partial z} \right) = 0 \quad (1.42)$$

Such equations, however, are too complex for control applications. It is well known that a tubular reactor can be represented as a series of  $n$  perfectly mixed continuous stirred tank reactors, where  $n$  is large (infinite in theory). For control purposes, an approximate dynamic model is often sufficient. For example, a tubular reactor can be modelled as a cascade of a few (possibly three) perfectly mixed continuous stirred tank reactors, i.e. for  $i$  ( $1 \leq i \leq 3$ ) the overall and component mass balances become

$$\begin{cases} \rho_{i-1} v_{i-1} = \rho_i v_i + \Delta z \frac{d\rho_i}{dt} \\ v_{i-1} C_{A,i-1} = v_i C_{A,i} + k/S C_{A,i} + \Delta z \frac{dC_{A,i}}{dt} \end{cases} \quad (1.43)$$

Note that a rigorous simulation model will need a much larger number of elementary reactors in series.

### 1.6.3 Degrees of Freedom

A state-space model can represent either the steady state or the transient behaviour of a system. The steady-state solution obtained by setting all time derivatives to zero constitutes the initialization of the dynamic regime. The following discussion on degrees of freedom could be applied to steady state, but is here devoted to control, thus to the dynamic model.

The number of degrees of freedom  $ndf$  of a system is equal to the number of variables minus the number of equations

$$ndf = \text{number of var.} - \text{number of eq.}$$

If the degrees of freedom  $ndf$  is zero, the system is fully determined (or specified) and there exists only a unique solution; if it is positive, the system is under-specified and  $ndf$  equations should be added; if it is negative, the system is over-specified and  $ndf$  equations should be removed to get a unique solution.

Each control loop adds an additional equation. Furthermore, the external disturbances are also specified to reduce the number of unknowns.

## 1.7 Process Stability

A process is said to be stable (asymptotically) when in response to a disturbance, the state variables converge towards a steady state (the system is said to be feedback-negative). Another definition of stability is that a process is said to be stable if any bounded input results in a bounded output. If a bounded input results in an unbounded output, the process is unstable.

The process is unstable when in response to a disturbance some state variables tend mathematically towards infinity (the system is feedback-positive). In practice, that means simply that the variables go out of the desired domain or do not tend to come back in a stable manner, but oppositely go far from it at least periodically.

Nearly all chemical processes are stable in open loop. However, a CSTR with an exothermic reaction can be unstable. Indeed, if the cooling is insufficient with regard to the heat of reaction, there may be three stationary states, one stable at low temperature and low conversion, one stable at high temperature and high conversion, a third unstable state at an intermediate temperature and conversion (see Sect. 3.2.3). Nearly all processes can be made unstable in closed loop. A major recommendation for the controller design is to avoid instability.

## 1.8 Order of a System

If a process is described by an ordinary differential equation of order  $n$ , the process is said to be of order  $n$

$$f(t) = a_0 x + a_1 \frac{dx}{dt} + a_2 \frac{d^2x}{dt^2} + \dots + a_n \frac{d^nx}{dt^n} \quad (1.44)$$

where  $f(t)$  represents an input or a forcing function. Note that an ordinary differential equation of order  $n$  is equivalent to a set of  $n$  first-order ordinary differential equations.

The first-order process model

$$f(t) = a_0 x + a_1 \frac{dx}{dt} \quad (1.45)$$

can be written as

$$f(t) = a_0 \left( x + \tau \frac{dx}{dt} \right) \quad (1.46)$$

where  $\tau$  is the process time constant.

The second-order process model

$$f(t) = a_0 x + a_1 \frac{dx}{dt} + a_2 \frac{d^2x}{dt^2} \quad (1.47)$$

can be written as

$$f(t) = a_0 (x + 2\zeta\tau \frac{dx}{dt} + \tau^2 \frac{d^2x}{dt^2}) \quad (1.48)$$

where  $\zeta$  is the damping coefficient.

## 1.9 Laplace Transform

The Laplace transform is an elegant mathematical method to solve *linear* or *linearized* differential equations. In control theory, it is used to develop simple continuous input-output models and thereby analyze the influence of external variables on a given process.

The Laplace transform of a function  $f(t)$  is defined by

$$\mathcal{L}[f(t)] = F(s) = \int_0^\infty f(t) \exp(-st) dt \quad (1.49)$$

assuming that the function or signal  $f(t)$  is zero for  $t < 0$ . This is the monolateral Laplace transform which is used throughout this book. Notice that the exponential term has no dimension, therefore the dimension of variable  $s$  is the inverse of time (frequency).

If function  $f(t)$  presents discontinuities at the boundaries, the Laplace transform is defined as

$$\mathcal{L}[f(t)] = F(s) = \lim_{\epsilon \rightarrow 0} \int_\epsilon^T f(t) \exp(-st) dt \quad (\epsilon \rightarrow 0, T \rightarrow \infty) \quad (1.50)$$

The bilateral Laplace transform for nonzero functions for negative  $t$  is defined as

$$\mathcal{L}[f(t)] = F(s) = \int_{-\infty}^\infty f(t) \exp(-st) dt \quad (1.51)$$

and is identical to the Fourier transform if we set  $s = j\omega$ . The Laplace transform exists only if the integral (1.49) is bounded: the function  $f(t) \exp(-st)$  is summable in Lebesgue's way. For example, consider the function  $f(t) = \exp(t)$ . This function is unbounded when  $t \rightarrow +\infty$ . However, let us try to calculate its Laplace transform. We get

$$\begin{aligned} \mathcal{L}[f(t)] &= \int_0^\infty \exp(t) \exp(-st) dt = \left[ \frac{1}{s-1} e^{(1-s)t} \right]_0^{+\infty} \\ &= \frac{1}{1-s} \quad \text{if: } \Re(s) > 1 \end{aligned} \quad (1.52)$$

Its Laplace transform would be defined only in a frequency domain excluding low frequencies. Its convergence region is the domain of  $s$  complex values such

that the Laplace transform exists, here the real part of  $s$  should be larger than 1.

If we consider the step function  $f(t) = 1$ , if  $t \geq 0$ ,  $f(t) = 0$  else, its Laplace transform is

$$\begin{aligned}\mathcal{L}[f(t)] &= \int_0^{\infty} 1 \exp(-st) dt = \left[ e^{(-s)t} \right]_0^{+\infty} \\ &= \frac{1}{s} \quad \text{if: } \Re(s) > 0\end{aligned}\tag{1.53}$$

Its convergence region is the complex right half-plane.

The inverse Laplace transform is defined as

$$f(t) = \mathcal{L}^{-1}[F(s)] = \frac{1}{2\pi j} \int_{\sigma-j\infty}^{\sigma+j\infty} F(s) \exp(ts) ds\tag{1.54}$$

This integral is defined on a complex domain with  $s = \sigma + j\omega$ .

The Laplace transformation is a linear mapping

$$\mathcal{L}[a_1 f_1(t) + a_2 f_2(t)] = a_1 \mathcal{L}[f_1(t)] + a_2 \mathcal{L}[f_2(t)]\tag{1.55}$$

To get the inverse Laplace transform of  $F(s)$ , it is in general useful to expand the function  $F(s)$  which very often takes the form of a rational fraction, as a sum of simple rational fractions, and then to operate the inverse transformation on each fraction separately.

### 1.9.1 Linearization and Deviation Variables

#### What is a Nonlinear Model?

Model linearization often poses problems for students. One reason may be that the analysis of the nonlinearity of the model is not clear. First, let us give some mathematical examples.

Consider a function of a single variable  $f(x)$ :

$f(x) = 4x$  and  $f(x) = 2x + 3$  are linear with respect to  $x$ ,

$f(x) = 3x^2$ ,  $f(x) = \frac{1}{2x+3}$ ,  $f(x) = \sqrt{3x}$ , are nonlinear with respect to  $x$ .

A function of a single variable is linear with respect to this variable when the derivative of this function is constant. Otherwise, it is nonlinear.

Consider a function of two variables  $f(x, y)$ :

$f(x, y) = 2y + 3$  is linear with respect to  $y$  and independent of  $x$ ,

$f(x, y) = 2x + 6y + 5$  is linear with respect to  $x$  and  $y$ ,

$f(x, y) = xy$  is nonlinear with respect to  $x$  and  $y$ ,

$f(x, y) = 2x^2 + 3y$  is nonlinear with respect to  $x$  and linear with respect to  $y$ ,

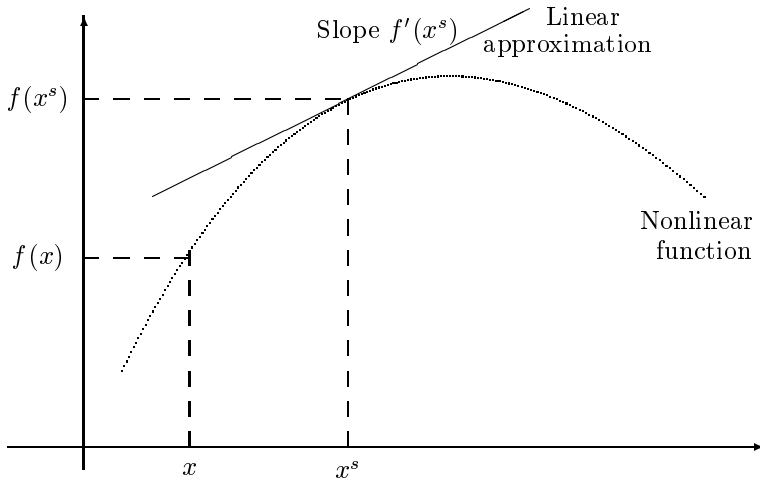
$f(x, y) = 4x + 2x^2 + 3y + 5y^2$  is nonlinear with respect to  $x$  and  $y$ .

A function of several variables is linear with respect to one of its variables when the partial derivative of this function with respect to the considered variable is constant. Otherwise, it is nonlinear with respect to that variable.

## Significance of Linearization in Process Control

Two cases can be considered: either a fixed set point is imposed on the process (case of regulation), or a reference trajectory is to be followed by the process (case of output tracking). Consider the simpler first case. We wish the process to be maintained in the neighbourhood of a set point, which will thus be the steady state. Due to imperfections of the control, the output and the state variables move around their steady-state values. The difference between the transient value of any variable and its steady-state value is called a deviation variable. When this latter remains small with respect to its absolute value, the behaviour of a function of this variable can be approximated by the tangent at the considered point (Fig. 1.10)

$$f(x) \approx f(x^s) + f'(x^s)(x - x^s) \quad (1.56)$$



**Figure 1.10:** Linear approximation of a nonlinear function by linearization of this function around steady state

## General Linearization

A nonlinear state-space model of a process must be linearized before applying the Laplace transform. The system thus obtained is called a linear time-invariant (LTI) system. Consider again the example of the chemical reactor (Eq. 1.15); the term  $FC_A$ , which appears in the differential equation in the component mass balance, is nonlinear as  $F(t)$  and  $C_A(t)$  both depend on time. As the Laplace transformation is a linear mapping, it is therefore necessary to linearize the balance ordinary differential equations around steady state (denoted by  $^s$ ); thus, the product  $F C_A$  becomes

$$F(t) C_A(t) = F^s C_A^s + F^s (C_A(t) - C_A^s) + C_A^s (F(t) - F^s) + o(\epsilon^2) \quad (1.57)$$

The term  $O(\epsilon^2)$  indicates that the Taylor series expansion in the neighbourhood of the steady state is truncated at the first order. Generally, for a function  $f$  of  $n$  variables  $x_1, \dots, x_n$ , by neglecting the higher-order terms, the Taylor series expansion leads to

$$f(x_1, \dots, x_n) \approx f(x_1^s, \dots, x_n^s) + \sum_i \left( \frac{\partial f}{\partial x_i} \right)^s (x_i - x_i^s) \iff \delta f \approx \sum_i \left( \frac{\partial f}{\partial x_i} \right)^s \delta x_i \quad (1.58)$$

It can be noticed that the linearization results in deviation variables (with respect to the steady state or a reference state) of the form  $\delta x_i = (x_i - x_i^s)$  which play an important role in Laplace transformation.

### 1.9.2 Some Important Properties of Laplace Transformation

- The Laplace transformation is a linear operation

$$\mathcal{L}[a_1 f_1(t) + a_2 f_2(t)] = a_1 \mathcal{L}[f_1(t)] + a_2 \mathcal{L}[f_2(t)] \quad (1.59)$$

- The Laplace transform of a first-order derivative of a function is

$$\mathcal{L}\left[\frac{df(t)}{dt}\right] = s F(s) - f(0) \quad (1.60)$$

If  $f(t)$  is a deviation variable with respect to the initial steady state, its initial value becomes zero:  $f(0) = 0$ , and the previous equation simply becomes

$$\mathcal{L}\left[\frac{df(t)}{dt}\right] = s F(s) \quad (1.61)$$

This assumption is used in general.

- The Laplace transform of the  $n^{\text{th}}$ -order derivative of a function is

$$\mathcal{L}\left[\frac{d^n f(t)}{dt^n}\right] = s^n F(s) - s^{n-1} f(0) - s^{n-2} f^{(1)}(0) \dots - f^{(n-1)}(0) \quad (1.62)$$

If  $f(t)$  is a deviation variable, its initial value and successive derivatives up to the  $(n-1)$ -th-order become zero so that the previous formula becomes

$$\mathcal{L}\left[\frac{d^n f(t)}{dt^n}\right] = s^n F(s) \quad (1.63)$$

- The Laplace transform of the integral of a function is

$$\mathcal{L}\left[\int_0^t f(x) dx\right] = \frac{1}{s} F(s) \quad (1.64)$$

- The initial value theorem is

$$\lim_{t \rightarrow 0} f(t) = \lim_{s \rightarrow \infty} s F(s) \quad (1.65)$$

- The final value theorem is

$$\lim_{t \rightarrow +\infty} f(t) = \lim_{s \rightarrow 0} s F(s) \quad (1.66)$$

Notice that the final value theorem cannot be applied in the case of a function corresponding to an unstable system. For example, consider the Laplace transform  $F(s) = 1/(s-1)$ , which would be the transform of function  $f(t) = \exp(t)$  if we strictly apply Table 1.1. Let us try to apply the final value theorem (1.66) to this function. It gives

$$\lim_{t \rightarrow +\infty} f(t) = \lim_{s \rightarrow 0} \frac{s}{s-1} = 0^- \quad (1.67)$$

One would wrongly conclude that the function  $f(t) = \exp(t)$  tends towards 0 when  $t \rightarrow +\infty$ . The mistake comes from the fact that one does not take into account the remark concerning Eq. (1.52).

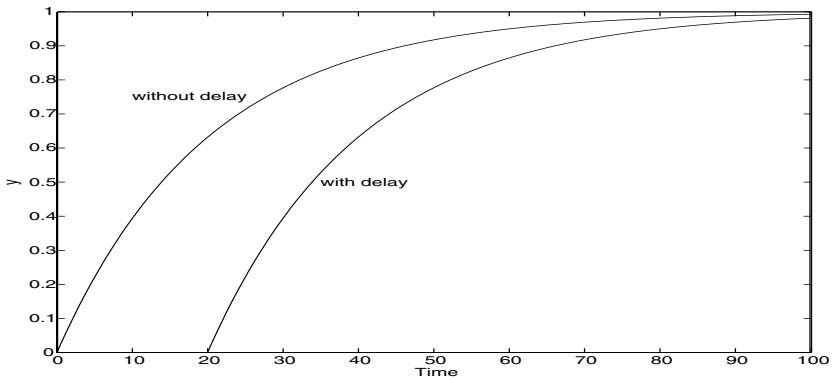
Consider the Laplace transform  $F(s) = 1/(s(s+1))$  corresponding to a stable system (we will later see that it is a first-order system subjected to an input step). The final value theorem gives

$$\lim_{t \rightarrow +\infty} f(t) = \lim_{s \rightarrow 0} \frac{s}{s(s+1)} = 1 \quad (1.68)$$

- The Laplace transform of a delayed function is

$$\mathcal{L}[f(t-t_0)] = \exp(-s t_0) \mathcal{L}[f(t)] \quad (1.69)$$

Note that the function  $f(t-t_0)$  is the same as  $f(t)$  delayed by  $t_0$ , which means that at time  $t_0$ , the delayed function is equal to  $f(0)$  (Fig. 1.11). The delay corresponds to a time translation of the function.



**Figure 1.11:** Illustration of the effect of a time delay of 20 time units on a response

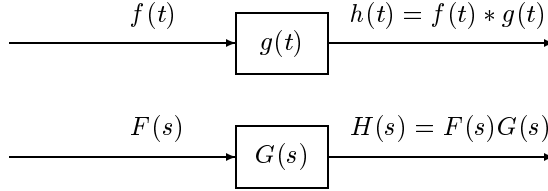
- The complex translation is

$$\mathcal{L}[f(t) \exp(at)] = F(s-a) \quad (1.70)$$

- The scale change is

$$\mathcal{L}[f(t/a)] = a F(as) \quad (1.71)$$

- Laplace transform of convolution



**Figure 1.12:** Convolution for a linear system. Top: time domain. Bottom: frequency domain

When a signal  $f(t)$  excites a linear time-invariant system with impulse response  $g(t)$  (Fig. 1.12), the response of the system  $h(t)$  is equal to the convolution product of  $f(t)$  by  $g(t)$  denoted by

$$h(t) = f(t) * g(t) = \int_{-\infty}^{\infty} f(\tau) g(t - \tau) d\tau \quad (1.72)$$

The Laplace transform  $H(s)$  of the output is equal to

$$\mathcal{L}[f(t) * g(t)] = F(s) G(s) \quad (1.73)$$

which is expressed as the Laplace transform of a convolution product being equal to the product of the Laplace transforms of the functions.

A consequence of this property is that when a signal  $f(t)$  excites two linear systems in series  $g_1(t)$  and  $g_2(t)$ , the response  $h(t)$  is equal to

$$h(t) = f(t) * (g_1(t) * g_2(t)) \quad (1.74)$$

and its Laplace transform  $H(s)$  is

$$\mathcal{L}[f(t) * (g_1(t) * g_2(t))] = F(s) G_1(s) G_2(s) \quad (1.75)$$

Thus, the Laplace transform of the impulse response of two linear systems in series is equal to the product of the Laplace transforms of the individual impulse responses.

- The complex convolution is

$$\mathcal{L}[f(t) g(t)] = \frac{1}{2\pi j} \int_{\sigma-j\infty}^{\sigma+j\infty} F(q) G(s - q) dq \quad (1.76)$$

- Parseval-Plancherel relation



This relation, classical in signal processing, expresses that the energy of a signal is equal to the sum of the energies of its constitutive signals

$$\int_{-\infty}^{+\infty} f^2(t) dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} |F(j\omega)|^2 d\omega \quad (1.77)$$

It is necessary that the signal  $f(t)$  be square-integrable, which means that the integral of  $f^2(t)$  must exist.

- Differentiation or integration with respect to a parameter

Consider the function  $f(t, \theta)$  which depends on parameter  $\theta$  as well as time  $t$  (both are independent variables) the Laplace transforms of the derivative or integral of the function with respect to  $\theta$  are

$$\mathcal{L} \left[ \frac{\partial f(t, \theta)}{\partial \theta} \right] = \frac{\partial}{\partial \theta} \mathcal{L}[f(t, \theta)] \quad (1.78)$$

and

$$\mathcal{L} \left[ \int_{\theta_1}^{\theta_2} f(t, \theta) d\theta \right] = \int_{\theta_1}^{\theta_2} \mathcal{L}[f(t, \theta)] d\theta \quad (1.79)$$

- Table 1.1 lists the Laplace transforms of some common functions.

### 1.9.3 Transfer Function

#### Definition of a Transfer Function

Consider a linear single variable system whose dynamic behaviour is described in terms of deviation variables by an ordinary differential equation of order  $n$  linking the input and the output

$$b_0 u(t) + b_1 \frac{du(t)}{dt} + \dots + b_m \frac{d^m u(t)}{dt^m} = a_0 y(t) + a_1 \frac{dy(t)}{dt} + \dots + a_n \frac{d^n y(t)}{dt^n} \quad , \quad m \leq n \quad (1.80)$$

where  $u(t)$  and  $y(t)$  are the system input and output respectively (Fig. 1.13). If we assume that the system is initially at steady state, the deviation variables and their successive derivatives are zero at initial state

$$\begin{aligned} \delta u(0) = 0, \left( \frac{du}{dt} \right)_0 = 0, \dots, \left( \frac{d^m u}{dt^m} \right)_0 = 0 \\ \delta y(0) = 0, \left( \frac{dy}{dt} \right)_0 = 0, \dots, \left( \frac{d^n y}{dt^n} \right)_0 = 0 \end{aligned} \quad (1.81)$$

The Laplace transformation of (1.80) gives

$$(b_0 + b_1 s + \dots + b_m s^m) U(s) = (a_0 + a_1 s + \dots + a_n s^n) Y(s) \quad (1.82)$$

The transfer function of the system results as the ratio of the Laplace transform of the output variable to the Laplace transform of the input variable, both expressed in terms of deviations from their steady states

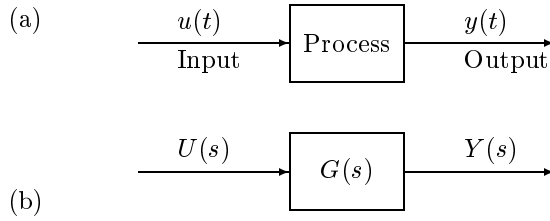
$$\frac{Y(s)}{U(s)} = G(s) = \frac{b_0 + b_1 s + \dots + b_m s^m}{a_0 + a_1 s + \dots + a_n s^n} \quad (1.83)$$

**Table 1.1:** Laplace transform of some common functions

Signal $f(t)$ ( $t \geq 0$ )	Transform $\mathcal{L}[f(t)] = F(s)$
Convolution product $f(t) * g(t)$	$F(s) G(s)$
Derivative: $\frac{df(t)}{dt}$	$s F(s) - f(0)$
Integral: $\int_0^t f(x) dx$	$\frac{1}{s} F(s)$
Delayed function: $f(t - t_0)$	$\exp(-s t_0) F(s)$
Dirac unit impulse: $\delta(t)$	1
Unit impulse of duration $\tau$ defined by $\delta_\tau(t) = 0$ if $t < 0$ or $t > \tau$ $\delta_\tau(t) = \frac{1}{\tau}$ if $0 < t < \tau$	$\frac{1}{\tau} \frac{1 - \exp(-s/\tau)}{s}$
Step of amplitude $A$	$\frac{A}{s}$
Exponential: $\exp(-a t)$	$\frac{1}{s + a}$
$\frac{1}{\tau} \exp(-t/\tau)$	$\frac{1}{\tau s + 1}$
Ramp: $a t$	$\frac{a}{s^2}$
$t \exp(-a t)$	$\frac{1}{(s + a)^2}$
$\frac{1}{n!} t^n \exp(-a t)$ ( $n \geq 1$ )	$\frac{1}{(s + a)^{n+1}}$
$\sin(\omega t)$	$\frac{\omega}{s^2 + \omega^2}$
$\cos(\omega t)$	$\frac{s}{s^2 + \omega^2}$
$\sin(\omega t + \phi)$	$\frac{\omega \cos(\phi) + s \sin(\phi)}{s^2 + \omega^2}$
$\exp(-a t) \sin(\omega t)$	$\frac{\omega}{(s + a)^2 + \omega^2}$
$\exp(-a t) \cos(\omega t)$	$\frac{s + a}{(s + a)^2 + \omega^2}$
$\frac{t^n}{n!}$	$\frac{1}{s^{n+1}}$
$\frac{1}{b - a} (\exp(-a t) - \exp(-b t))$	$\frac{1}{(s + a)(s + b)}$
$\frac{1}{\tau_1 - \tau_2} (\exp(-t/\tau_1) - \exp(-t/\tau_2))$	$\frac{1}{(\tau_1 s + 1)(\tau_2 s + 1)}$
$\sum_{i=1}^n \left( \frac{\exp(-a_i t)}{\prod_{j \neq i} (a_j - a_i)} \right)$	$\frac{1}{\prod_{i=1}^n (s + a_i)}$
$\frac{1}{\omega_p} \exp(-\zeta \omega t) \sin(\omega_p t)$ with: $\omega_p = \omega \sqrt{1 - \zeta^2}$ ( $0 \leq  \zeta  \leq 1$ )	$\frac{1}{s^2 + 2\zeta\omega s + \omega^2}$
$\frac{1}{a} (1 - \exp(-a t))$	$\frac{1}{s(s + a)}$

Thus, the transfer function is totally equivalent to the linear ordinary differential equation describing the linearized system and can be further used to find output solutions to a given input.

Most transfer functions take the previous form of a ratio of two polynomials,



**Figure 1.13:** Block diagram of a process (a) in the time domain, (b) in the Laplace domain (transfer function)

symbolized as

$$G(s) = \frac{N(s)}{D(s)} \quad (1.84)$$

A transfer function is said to be proper if

$$\text{degree of } N(s) \leq \text{degree of } D(s)$$

it is strictly proper if

$$\text{degree of } N(s) < \text{degree of } D(s)$$

A transfer function is said to be biproper if

$$\text{degree of } N(s) = \text{degree of } D(s)$$

A transfer function is said to be improper if

$$\text{degree of } N(s) > \text{degree of } D(s)$$

It will be shown that improper transfer functions, such as an ideal derivative, amplify high-frequency noise.

The following steps are followed to **derive the transfer function of a process from a theoretical model**:

- Using the conservation principles, write the dynamic model describing the system,
- Linearize equations using Taylor series expansion,
- Express the equations in terms of deviation variables by subtracting the steady-state equations from the dynamic equations
- Operate Laplace transformation on the linear or linearized equations,
- Obtain the ratio of the Laplace transform of the output over the Laplace transform of the input.

**Example 1.1: Application to the Surge Tank**

Equation (1.12) is linear with respect to all variables, and results simply in

$$X(s) = \frac{1}{Ss} U(s) - \frac{1}{Ss} \bar{F}(s) \quad (1.85)$$

which contains two transfer functions, both pure integrators. The process transfer function with respect to the input is

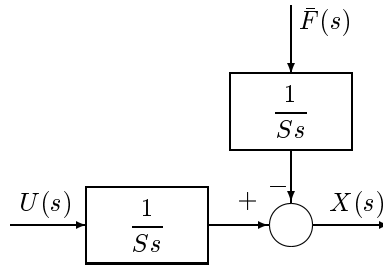
$$G_u(s) = \frac{1}{Ss} \quad (1.86)$$

and the load or disturbance transfer function with respect to the disturbance  $F$  is

$$G_d(s) = -\frac{1}{Ss} \quad (1.87)$$

where  $S$  is the cross-sectional area of the surge tank and  $s$  is the Laplace operator.

The block diagram (Fig. 1.14) represents the influence of the input and of the disturbance.



**Figure 1.14:** Block diagram of the surge tank

**Example 1.2: Application to the Isothermal Chemical Reactor**

The system of Eqs. (1.26) is nonlinear with respect to the variables. Using the superscript “ $s$ ” for the steady-state, linearizing the nonlinear terms, introducing the equations in terms of deviation variables and Laplace transforming results in

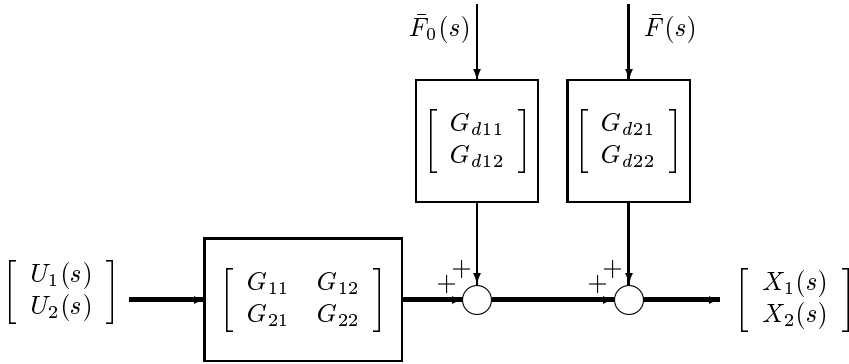
$$\begin{aligned}
 sX_1(s) &= \frac{1}{S} [\bar{F}_0(s) - \bar{F}(s) + U_1(s)] \\
 sX_2(s) &= -\frac{1}{S(x_1^s)^2} [F_0^s (u_2^s - x_2^s) X_1(s)] - k X_2(s) \\
 &\quad + \frac{1}{Sx_1^s} [(u_2^s - x_2^s) \bar{F}_0(s) + F_0^s (U_2(s) - X_2(s)) - x_2^s U_1(s) - u_1^s X_2(s)]
 \end{aligned} \quad (1.88)$$

The steady-state equations resulting from Eq. (1.26) are

$$\begin{aligned} 0 &= \frac{1}{S} [F_0^s - F^s + u_1^s] \\ 0 &= \frac{1}{S x_1^s} [F_0^s (u_2^s - x_2^s) - x_2^s u_1^s] - k x_2^s \end{aligned} \quad (1.89)$$

which yield

$$\begin{aligned} u_1^s &= F^s - F_0^s \\ u_2^s &= \frac{x_2^s F^s + S k x_1^s x_2^s}{F_0^s} \end{aligned} \quad (1.90)$$



**Figure 1.15:** Block diagram of the linearized isothermal chemical reactor tank

The final system of transfer functions, the transfer function matrix, expresses the state vector with respect to the input vector and the disturbances

$$\begin{aligned} \begin{bmatrix} X_1(s) \\ X_2(s) \end{bmatrix} &= \begin{bmatrix} \frac{1}{S s} & 0 \\ -\frac{1}{S s} \frac{x_2^s}{S (x_1^s)^2} (F^s + S k x_1^s - F_0^s) - \frac{x_2^s}{S x_1^s} & \frac{F_0^s}{S x_1^s} \end{bmatrix} \begin{bmatrix} U_1(s) \\ U_2(s) \end{bmatrix} \\ &+ \begin{bmatrix} \frac{1}{S s} \frac{x_2^s}{S x_1^s} \left( \frac{1}{F_0^s} - \frac{1}{S s x_1^s} \right) (F^s + S k x_1^s - F_0^s) \\ \frac{1}{S s} \frac{x_2^s}{S (x_1^s)^2} \frac{F^s + S k x_1^s - F_0^s}{s + \frac{F^s}{S x_1^s} + k} \end{bmatrix} \bar{F}_0(s) \\ &+ \begin{bmatrix} -\frac{1}{S s} \frac{x_2^s}{S (x_1^s)^2} \frac{F^s + S k x_1^s - F_0^s}{s + \frac{F^s}{S x_1^s} + k} \end{bmatrix} \bar{F}(s) \end{aligned} \quad (1.91)$$

Note that the states  $x_1$  and  $x_2$  are coupled by this system of equations. The first state  $x_1$  is influenced only by input  $u_1$ , while the second state  $x_2$  is influenced by both inputs. With the system being multi-input multi-state, matrices of transfer functions relate the inputs and disturbances to the states. The linearized system described by the previous equation can be symbolized by the block diagram in Fig. 1.15.

The non-isothermal chemical reactor could be treated in the same manner with added complexity.

### Impulse Response and Transfer Function of a System

Consider a linear system in which the input and output are linked by the convolution product (Fig. 1.16)

$$y(t) = u(t) * g(t) \quad (1.92)$$

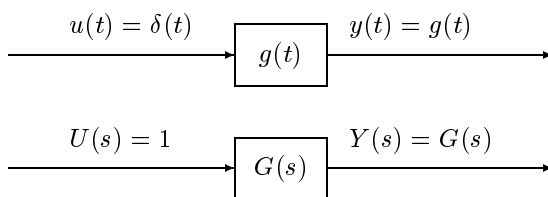
If this system is excited by a Dirac impulse:  $u(t) = \delta(t)$ , the output becomes

$$y(t) = g(t) \quad (1.93)$$

thus  $g(t)$  is the impulse response of the system and is equal to the inverse Laplace transform of the system transfer function as the Laplace transform of the convolution product is

$$\mathcal{L}[y(t)] = \mathcal{L}[u(t) * g(t)] = U(s) G(s) = G(s) \quad (1.94)$$

with  $U(s) = 1$  for a unit impulse input.



**Figure 1.16:** Time and frequency responses for a linear system subjected to a Dirac impulse input

Although obtaining a system transfer function in this manner seems attractive, it suffers from several drawbacks:

- A Dirac impulse is not realizable in practice, only an impulse of finite duration is possible.
- A simple impulse input contains poor characteristics with respect to frequency excitation and introduces difficulty in process identification as will be shown later in this book.

In experimental characterization of the flow pattern in chemical processes, in particular reactors, however, the impulse response technique is used to get the residence time distribution. A tracer is injected over a short time at the process inlet and its evolution is recorded at the reactor outlet. The analysis of the output response is often complicated but it enables us to characterize the system as a combination of perfectly mixed CSTRs, tubular reactors placed in parallel or in series with possible bypass and/or dead volume (Levenspiel, 1999; Villiermaux, 1982).

### Principle of superposition

When the input can be decomposed into a sum of inputs (e.g. a rectangular pulse is the sum of a positive and a negative step, occurring at different times, see Figs. 1.17 and 1.18), the global output is the sum of the responses to the individual inputs

$$U(s) = \sum_i U_i(s) \implies Y(s) = G(s) U(s) = \sum_i G(s) U_i(s) = \sum_i Y_i(s) \quad (1.95)$$

The principle of superposition results directly from the properties of linearity of the Laplace transform. The principle of superposition is not valid for a nonlinear system.

For example, a rectangular pulse can be seen as the sum of a positive and a negative step (in Fig. 1.17,  $u_3$  is the sum of  $u_1$  and  $u_2$ ). The respective responses to the three inputs for a given transfer function are given in Fig. 1.18.

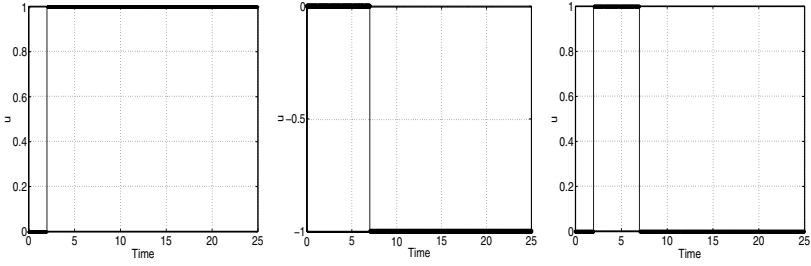
### Experimental Determination (Identification) of a System Transfer Function

Consider a general system whose dynamics in the time domain can be described in terms of the following ordinary differential equation

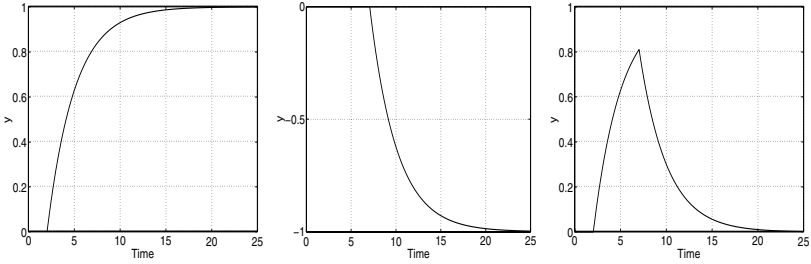
$$\frac{dy}{dt} = f(y(t), u(t), d) \quad (1.96)$$

where  $y$  is the output,  $u$  is the input, and  $d$  is the disturbance. To determine the system transfer function  $G(s)$ , several possibilities exist depending on the choice of the applied input to the system:

- For a Dirac impulse input, the output is equal to  $g(t)$ , i.e. the inverse transform of the system transfer function  $G(s)$ . The drawback of this technique is that the frequency content (the information content) of the input signal is not rich and results in poor identification.
- For a step input or a succession of small amplitude positive and negative steps such as a pseudo-random binary sequence (PRBS), the information content of the input signal is adequate for yielding a satisfactory identification. This technique is particularly well adapted to discrete-time identification. In the continuous-time domain, often a single step or a succession



**Figure 1.17:** Inputs from left to right:  $u_1$ ,  $u_2$ ,  $u_3$



**Figure 1.18:** Outputs from left to right:  $y_1$ ,  $y_2$ ,  $y_3$  as responses of the transfer function  $G(s) = \frac{1}{3s+1}$  to respective inputs  $u_1$ ,  $u_2$ ,  $u_3$

of positive and negative steps is applied. System nonlinearities are demonstrated by dissimilar responses to positive and negative step changes in the input. For example, a furnace often shows a different time constant for a step increase or decrease in the heat rate.

- For a sinusoidal input (Fig. 1.19), the identification is performed in the frequency domain. In this latter method, the Laplace variable  $s$  is replaced by  $s = j\omega$  (where  $\omega$  is the angular frequency in rad/s and is related to the frequency in Hz,  $\nu$ , by  $\omega = 2\pi\nu$ ). If a linear system is excited by a sinusoidal input  $u(t) = \exp(j\omega t)$ , after a transient period, the output will also be a sinusoidal wave with the same frequency, a different amplitude and a phase difference, i.e.

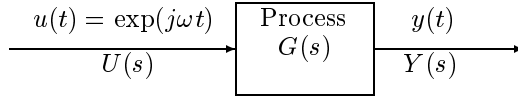
$$y(t) \approx G(j\omega) \exp(j\omega t) = G(s) \exp(st) \quad \text{for sufficiently large } t \quad (1.97)$$

which, when combined with Eq. (1.96), gives

$$s G(s) \exp(st) = f(G(s) \exp(st), \exp(st), d) \quad (1.98)$$

Complex exponential functions (such as sines and cosines) are proper functions for the Laplace operator. In order to obtain a rich information for the experimental determination of the transfer functions, it is sufficient to vary the frequency  $\omega$  of the input signal over a large range.





**Figure 1.19:** Experimental determination of a process transfer function by sinusoidal excitation

Provided the function  $f$  is known, one analytically deduces from Eq. (1.98) the transfer function  $G(s)$  as the ratio of the output transform  $Y(s)$  over the input transform  $U(s)$ .

### 1.9.4 Poles and Zeros of a Transfer Function

Consider a system described by the differential equation

$$a_0 y(t) + a_1 \frac{dy(t)}{dt} + \dots + a_n \frac{d^n y(t)}{dt^n} = b_0 u(t) + b_1 \frac{du(t)}{dt} + \dots + b_m \frac{d^m u(t)}{dt^m} \quad (1.99)$$

In the absence of an input excitation, the output Laplace transform is given by

$$D(s) Y(s) = 0 \quad (1.100)$$

where  $D(s) = a_0 + a_1 s + \dots + a_n s^n$ . The shape of the response curve depends on the roots of  $D(s)$  which are called the system modes.

The system transfer function describes the response when the initial state is zero (refer to the relation between the transfer function and the state-space model) or when we refer to deviation variables. In general, the transfer function can be expressed as the ratio of two polynomials

$$G(s) = \frac{N(s)}{D(s)} = \frac{b_0 + b_1 s + \dots + b_m s^m}{a_0 + a_1 s + \dots + a_n s^n} \quad \text{with: } n \geq m \quad (1.101)$$

where the denominator degree  $n$  is higher than or equal to the numerator degree  $m$ .

The roots of the numerator polynomial  $N(s)$  are called the system zeros or zeros of the transfer function, since the transfer function is equal to zero for these values.

If the numerator  $N(s)$  and the denominator  $D(s)$  have common roots, after cancellation of these common roots, the remaining roots of  $D(s)$  are referred to as the poles of the transfer function; they determine the response for zero initial state.

If no common roots exist between  $N(s)$  and  $D(s)$ , then the system can be completely characterized by its transfer function, and the sets of poles and the modes are the same. The transfer function  $G(s)$  becomes infinite when  $s$  is equal to one of the poles.

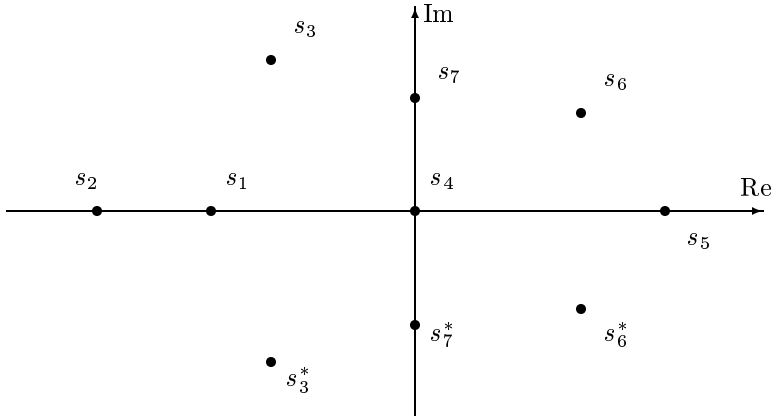
If  $N(s)$  and  $D(s)$  have common factors, the latter form a polynomial noted  $R(s)$ . The roots of  $R(s)$  are called system nodes, but are not poles for  $G(s)$ . For that reason, they are called missing poles of the transfer function. In this case, the system is not completely characterized by its transfer function.

### 1.9.5 Qualitative Analysis of a System Response

The response of a system to a given input  $u(t)$  can be determined from its Laplace transform

$$Y(s) = G(s) U(s) \quad (1.102)$$

If the transfer function  $G(s)$  and the input transform  $U(s)$  are given, the system response  $y(t)$  can be obtained by inverse Laplace transformation of  $Y(s)$ .



**Figure 1.20:** Different types of poles represented in the complex  $s$ -plane

The behaviour of a system, such as its stability and the the shape of the system response, is largely determined by the poles of its transfer function. Let us consider a general transfer function with poles as depicted in Fig. 1.20

$$G(s) = \frac{N(s)}{D(s)} = \frac{N(s)}{(s - s_1)(s - s_2)^m (s - s_3)(s - s_3^*)(s - s_4)(s - s_5)(s - s_6)(s - s_6^*)(s - s_7)(s - s_7^*)} \quad (1.103)$$

where  $s_1$  is a negative real pole

$s_2$  is a negative real multiple pole of order  $m$

$s_3$  is a complex pole with negative real part

$s_3^*$  is the conjugate complex pole ( $D$  being a real polynomial, all complex poles must appear as a pair in conjugate form)

$s_4$  is a pole at the origin

$s_5$  is a positive real pole

$s_6$  is a complex pole with positive real part

$s_6^*$  is the complex conjugate pole of  $s_6$

$s_7$  is a pure imaginary pole

$s_7^*$  is the conjugate of the imaginary pole  $s_7$

The transfer function  $G(s)$  can be expanded as a sum of rational fractions

$$G(s) = \frac{c_1}{s-s_1} + \left( \frac{c_{21}}{s-s_2} + \frac{c_{22}}{(s-s_2)^2} + \dots + \frac{c_{2m}}{(s-s_2)^m} \right) + \frac{c_3}{s-s_3} + \frac{c_3^*}{s-s_3^*} + \frac{c_4}{s} + \frac{c_5}{s-s_5} + \frac{c_6}{s-s_6} + \frac{c_6^*}{s-s_6^*} + \frac{c_7}{s-s_7} + \frac{c_7^*}{s-s_7^*} \quad (1.104)$$

If poles are distinct, to find the coefficients in the numerators (residuals), it suffices to multiply  $G(s)$  by  $(s-s_i)$  and set  $s=s_i$

$$c_i = [(s-s_i)G(s)]|_{s=s_i} = \frac{N(s)}{(s-s_1)\dots(s-s_{i-1})(s-s_{i+1})\dots(s-s_n)} \Big|_{s=s_i} \quad (1.105)$$

In the case of multiple poles, e.g. if  $s_i$  is a multiple pole of order  $m$ , the residuals are calculated by multiplying  $G(s)$  by  $(s-s_i)^m$  and differentiating successively with respect to  $s$  and setting  $s=s_i$  after differentiation. Consider the following transfer function with a multiple pole  $s_i$  of order  $m$

$$\begin{aligned} G(s) &= \frac{N(s)}{(s-s_1)\dots(s-s_{i-1})(s-s_i)^m(s-s_{i+1})\dots(s-s_n)} \\ &= \frac{c_1}{s-s_1} + \dots + \frac{c_{i-1}}{s-s_{i-1}} + \frac{c_{i,1}}{s-s_i} + \frac{c_{i,2}}{(s-s_i)^2} + \dots + \frac{c_{i,m}}{(s-s_i)^m} \\ &\quad + \frac{c_{i+1}}{s-s_{i+1}} + \dots + \frac{c_n}{s-s_n} \end{aligned} \quad (1.106)$$

Let us define a new transfer function having the same poles as  $G(s)$  except for the multiple pole  $s_i$

$$Gt(s) = \frac{N(s)(s-s_i)^m}{D(s)} \quad (1.107)$$

The residuals are calculated by the following expression

$$c_{i,m-j} = \frac{1}{j!} \frac{d^{(j)}Gt(s)}{ds^j} \Big|_{s=s_i} \quad ; \quad j = 0, 1, \dots, m-1 \quad (1.108)$$

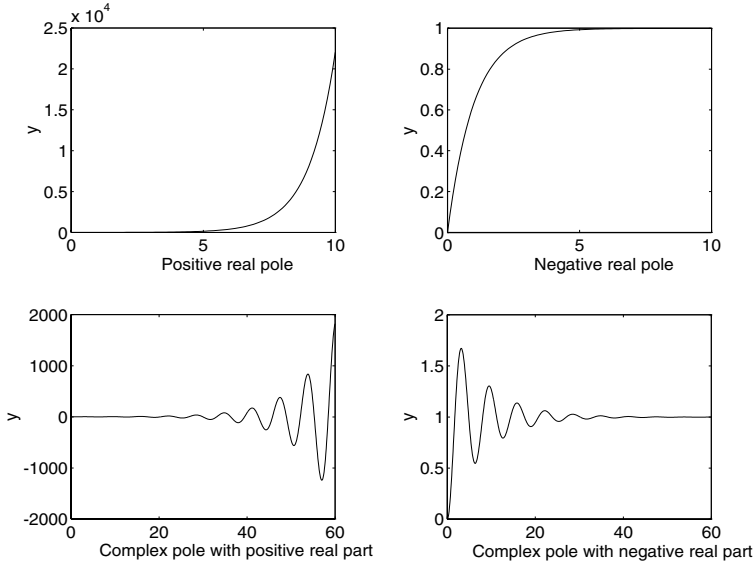
Note that multiple poles are more frequently encountered in physical modelling than in identification.

When a process having a transfer function  $G(s)$  of the form given by Eq. (1.106) is subjected to a unit impulse, the Laplace transform of the process output is equal to the process transfer function. To determine the time response to this impulse input, the inverse Laplace transformation is performed.

- Simple real poles such as  $s_1$  and  $s_5$  result in exponential responses (Fig. 1.21)

$$y(t) = c_i \exp(s_i t) \quad (1.109)$$

If the pole is negative real, the exponential tends towards 0:  $s_1$  is a stable pole. The closer the pole to the origin, the slower the response will be. If the pole is positive real such as  $s_5$ , the response increases exponentially with time and tends towards infinity:  $s_5$  is an unstable pole.



**Figure 1.21:** Impulse response of transfer functions with different types of poles

- A multiple real pole with order  $i$  such as  $s_2$  results in the following responses:

$$y(t) = \frac{t^{i-1} \exp(s_2 t)}{(i-1)!} \quad (1.110)$$

The response increases towards infinity if the pole is positive or zero, and decreases towards zero if the pole is negative.

- A complex pole  $s$  is represented by its real part and its imaginary part:  $s = s_R + j s_I$ , and the impulse response of a transfer function presenting a complex pole will be

$$y(t) = \exp(s_R t) \exp(j s_I t) = \exp(s_R t) [\cos(s_I t) + j \sin(s_I t)] \quad (1.111)$$

The imaginary part is responsible for the oscillatory behaviour while the stability depends only on the sign of the real part.

Conjugate complex poles with negative real part such as  $s_3$  and  $s_3^*$  (Fig. 1.21) result in damped oscillatory behaviour: they are stable poles. The closer the poles are to the imaginary axis, i.e. the nearest to 0 their real part is, the slower the decay of their exponential part.

When poles are complex conjugate with positive real part such as  $s_6$  and  $s_6^*$  (Fig. 1.21), they induce an oscillatory undamped response: they are unstable poles.

- A pole at the origin such as  $s_4$  results in a constant term.

- Pure imaginary poles  $s = \pm j\omega$  such as  $s_7$  and  $s_7^*$  result in a sinusoidal response with a frequency  $\omega$  equal to the imaginary part of the poles. Under these conditions the system is said to be on the verge of stability or marginally stable.

## 1.10 Linear Systems in State Space

### 1.10.1 General Case

Consider the single variable linear system (single-input single-output). Its state-space model is

$$\begin{cases} \dot{\mathbf{x}}(t) = \mathbf{A} \mathbf{x}(t) + \mathbf{B} u(t) \\ y(t) = \mathbf{C} \mathbf{x}(t) + D u(t) \end{cases} \quad (1.112)$$

where  $\mathbf{A}$ ,  $\mathbf{B}$ ,  $\mathbf{C}$ ,  $D$  are matrices of respective dimensions  $n \times n$ ,  $n \times 1$ ,  $1 \times n$  and  $1 \times 1$ . The initial state of the system is  $\mathbf{x}(0)$ . For a system which can be represented by a strictly proper transfer function, i.e. whose numerator degree is strictly lower than the denominator degree, the matrix  $D$  is zero. This is the case for most physical systems.

As this system is linear, it is possible to apply the Laplace transformation

$$s X(s) - \mathbf{x}(0) = \mathbf{A} X(s) + \mathbf{B} U(s) \iff (s \mathbf{I} - \mathbf{A}) X(s) = \mathbf{x}(0) + \mathbf{B} U(s) \quad (1.113)$$

where  $\mathbf{I}$  is the identity matrix of dimension  $n \times n$ . Provided that the matrix  $(s \mathbf{I} - \mathbf{A})$  is invertible, the Laplace transform of the states can be obtained

$$X(s) = (s \mathbf{I} - \mathbf{A})^{-1} \mathbf{x}(0) + (s \mathbf{I} - \mathbf{A})^{-1} \mathbf{B} U(s) \quad (1.114)$$

and the Laplace transform of the output is

$$Y(s) = \mathbf{C} X(s) + D U(s) = \mathbf{C} (s \mathbf{I} - \mathbf{A})^{-1} \mathbf{x}(0) + [\mathbf{C} (s \mathbf{I} - \mathbf{A})^{-1} \mathbf{B} + D] U(s) \quad (1.115)$$

This response is composed of two terms, the first called response for a zero input and the second called response for a zero state.

Given

$$\exp(\mathbf{A} t) = \mathcal{L}^{-1} [(s \mathbf{I} - \mathbf{A})^{-1}] \quad (1.116)$$

the output response can be deduced from (1.115)

$$y(t) = \mathbf{C} \exp(\mathbf{A} t) \mathbf{x}(0) + \mathbf{C} \exp(\mathbf{A} t) \int_0^t \exp(-\mathbf{A} \tau) \mathbf{B} u(\tau) d\tau + D u(t) \quad (1.117)$$

and the state of the process is given by

$$\mathbf{x}(t) = \exp(\mathbf{A} t) \mathbf{x}(0) + \exp(\mathbf{A} t) \int_0^t \exp(-\mathbf{A} \tau) \mathbf{B} u(\tau) d\tau \quad (1.118)$$

To obtain  $y(t)$  as in (1.117), it is possible to integrate the differential equation of the system given by (1.112) by using the following properties of the matrix exponential

$$\exp(\mathbf{A} t) = \mathbf{I} + t \mathbf{A} + \frac{t^2}{2!} \mathbf{A}^2 + \dots + \frac{t^n}{n!} \mathbf{A}^n + \dots \quad (1.119)$$

$$\frac{d}{dt}(\exp(\mathbf{A} t)) = \mathbf{A} \exp(\mathbf{A} t) \quad (1.120)$$

The system transfer function is obtained, assuming that all initial conditions are zero, and consequently the initial states are zero:  $\mathbf{x}(0) = 0$ . The output Laplace transform is

$$Y(s) = [\mathbf{C} (s \mathbf{I} - \mathbf{A})^{-1} \mathbf{B} + D] U(s) \quad (1.121)$$

and the system transfer function is

$$G(s) = \mathbf{C} (s \mathbf{I} - \mathbf{A})^{-1} \mathbf{B} + D \quad (1.122)$$

This transfer function can be written in a different form using the determinant “det” and the adjoint matrix “adj”:

$$G(s) = \mathbf{C} \frac{1}{\det(s \mathbf{I} - \mathbf{A})} [\text{adj}(s \mathbf{I} - \mathbf{A})] \mathbf{B} + D \quad (1.123)$$

The determinant of  $(s \mathbf{I} - \mathbf{A})$  is called the characteristic polynomial of  $\mathbf{A}$  (dimension  $n \times n$ ). Its  $n$  roots are the eigenvalues of  $\mathbf{A}$ .

## 1.10.2 Analog Representation

### First Case

Consider a second-order system having the following transfer function

$$G_1(s) = \frac{K}{(\tau_1 s + 1)(\tau_2 s + 1)} \quad (1.124)$$

This transfer function is equivalent to the second-order ordinary differential equation

$$\tau_1 \tau_2 \frac{d^2 y}{dt^2} + (\tau_1 + \tau_2) \frac{dy}{dt} + y = K u(t) \quad (1.125)$$

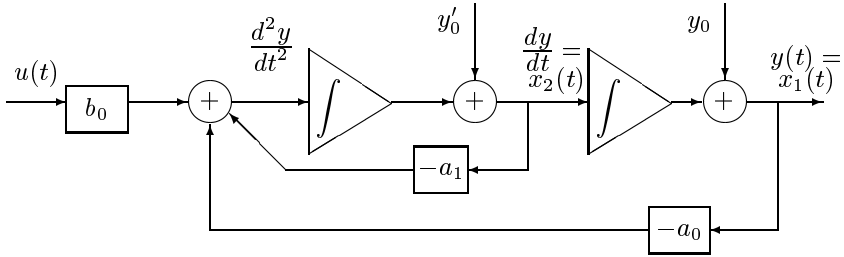
which can be rewritten, in view of its further use in the analog block diagram, as

$$\frac{d^2 y}{dt^2} = -a_0 y(t) - a_1 \frac{dy}{dt} + b_0 u(t) \quad (1.126)$$

with:

$$a_0 = 1/(\tau_1 \tau_2), \quad a_1 = (\tau_1 + \tau_2)/(\tau_1 \tau_2), \quad b_0 = K/(\tau_1 \tau_2).$$

Note that the above differential equation is in terms of the deviation variables in the same way as for the transfer function. Let us assume that at



**Figure 1.22:** Analog block diagram of the state-space representation

time  $t = 0$  the steady state prevails,  $y(t = 0) = y(0)$  and  $(dy/dt)_{t=0} = y'(0)$ . The analog circuit representation of the above ordinary differential equation is shown in Fig. 1.22. The input  $u(t)$  passes through a potentiometer (gain  $b_0$ ), a summator, an integrator and another summator (supplying the initial condition  $y'(0)$ ). The output from the second summator is passed through a second integrator and a third summator (supplying the initial condition  $y(0)$ ). The final output is  $y(t)$ .

Designating  $x_2(t)$  as the output of the first integrator and  $x_1(t)$  as the output of the second integrator, the above system can be represented by the following state-space model

$$\begin{aligned}\dot{x}_1(t) &= x_2(t) \\ \dot{x}_2(t) &= -a_0x_1(t) - a_1x_2(t) + b_0u(t) \\ y(t) &= x_1(t)\end{aligned}\tag{1.127}$$

or, using matrix form

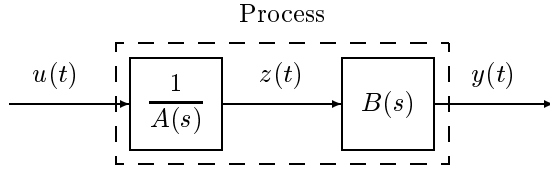
$$\begin{aligned}\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \end{bmatrix} &= \begin{bmatrix} 0 & 1 \\ -a_0 & -a_1 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} + \begin{bmatrix} 0 \\ b_0 \end{bmatrix} u(t) \\ y(t) &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}\end{aligned}\tag{1.128}$$

where  $x_1(t)$  and  $x_2(t)$  are the system state variables. The number of state variables is equal to the order of the differential equation or the order of the transfer function. The state of the system at any time  $t$  depends only on the initial conditions at  $t_0$  and on the input  $u(t)$  between  $t_0$  and  $t$ . At initial time, the state variables are equal to the initial conditions and, in the following, they represent the evolution of the system.

## Second Case

Consider a different second-order system having the following transfer function

$$G_2(s) = \frac{B(s)}{A(s)} = \frac{b_0 s^2 + b_1 s + b_2}{a_0 s^2 + a_1 s + a_2}\tag{1.129}$$



**Figure 1.23:** Representation of the partial state  $z(t)$

This transfer function is not strictly proper. It is equivalent to the second-order ordinary differential equation

$$a_0 \frac{d^2 y}{dt^2} + a_1 \frac{dy}{dt} + a_2 \delta y(t) = b_0 \frac{d^2 u}{dt^2} + b_1 \frac{du}{dt} + b_2 \delta u(t) \quad (1.130)$$

The transformation into an analog form is not as straightforward as in the first case. We introduce the partial state  $z(t)$  (Fig. 1.23) such that

$$Y(s) = B(s) Z(s) \quad \text{and} \quad Z(s) = \frac{1}{A(s)} U(s) \quad (1.131)$$

As previously, we assume that  $u(t)$ ,  $z(t)$  and  $y(t)$  are deviation variables. From the previous equations, we deduce

$$\begin{aligned} y(t) &= b_0 \frac{d^2 z}{dt^2} + b_1 \frac{dz}{dt} + b_2 z(t) \\ u(t) &= a_0 \frac{d^2 z}{dt^2} + a_1 \frac{dz}{dt} + a_2 z(t) \end{aligned} \quad (1.132)$$

Set

$$\begin{aligned} x_1(t) &= \frac{dz}{dt} \\ x_2(t) &= z(t) \end{aligned} \quad (1.133)$$

The state representation follows

$$\begin{aligned} \begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \end{bmatrix} &= \begin{bmatrix} \frac{-a_1}{a_0} & \frac{-a_2}{a_0} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} + \begin{bmatrix} \frac{1}{a_0} \\ 0 \end{bmatrix} u(t) \\ y(t) &= \begin{bmatrix} \frac{-b_0 a_1}{a_0} + b_1 & \frac{-b_0 a_2}{a_0} + b_2 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} + \frac{b_0}{a_0} u(t) \end{aligned} \quad (1.134)$$

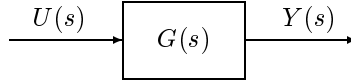
which allows to easily obtain the analog representation.

## 1.11 Dynamic Behaviour of Simple Processes

Initially, simple processes without a controller are considered (Fig. 1.24) and their open-loop behaviour is studied.

Let us consider the response of the system to two types of inputs  $u(t)$ :





**Figure 1.24:** Open-loop block diagram of a process

- A unit step:  $u = 1$  for  $t > 0$ ,  $u = 0$  for  $t \leq 0$ ; the response of the system to this input is referred to as the step response.
- A Dirac unit impulse:  $u = \delta$  (theoretical Dirac<sup>1</sup>); the response of the system to such an input is referred to as an impulse response.

Let  $G(s)$  be the system transfer function subject to an input  $U(s)$ . Except for possible time delays,  $G(s)$  is a rational fraction. For any physical input (impulse, step, ramp, sinusoidal, ...),  $U(s)$  can also be expressed as a rational fraction, therefore

$$G(s) = \frac{N_g(s)}{D_g(s)} \quad ; \quad U(s) = \frac{N_u(s)}{D_u(s)} \quad (1.135)$$

The Laplace transform  $Y(s)$  of the output can be decomposed into

$$Y(s) = G(s) U(s) = \frac{N_g(s) N_u(s)}{D_g(s) D_u(s)} = \frac{N_1(s)}{D_g(s)} + \frac{N_2(s)}{D_u(s)} = Y_n + Y_f \iff$$

Response = Natural response + Forced response

(1.136)

provided that the product  $(G(s) U(s))$  is strictly proper and that denominators  $D_g(s)$  and the  $D_u(s)$  have no common roots.

The response  $y_n(t)$  depends on the modes of  $G(s)$  and is called the natural response of the system, while  $y_f(t)$  depends on the modes of  $U(s)$  (linked to the input type) and is referred to as the forced response of the system.

---

<sup>1</sup>The Dirac function  $\delta(t)$  is defined by physicists as

$$\begin{aligned} \delta(t) &= 0 & \forall t \neq 0 \\ \delta(0) &= +\infty \\ \int_{-\infty}^{+\infty} \delta(t) &= 1 \end{aligned}$$

which is the limit of a real pulse function centred around 0 with unit area (strength or energy) and zero duration.

Mathematicians define the Dirac distribution such that the convolution of a function  $f(x)$  by the Dirac distribution is equal to

$$f(x) * \delta(x) = f(x)$$

An important property of a Dirac distribution is

$$\int_{-\infty}^{+\infty} f(t) \delta(t - t_0) = f(t_0)$$

The Dirac distribution is equal to the derivative of a unit step function (Heaviside function).

### 1.11.1 First-Order Systems

A first-order system is described by a first-order differential equation of the form

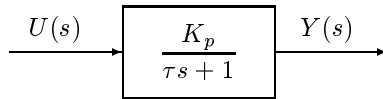
$$\tau \frac{dy}{dt} + y(t) = K_p u(t) \quad (1.137)$$

The corresponding transfer function is equal to

$$G(s) = \frac{K_p}{\tau s + 1} \quad (1.138)$$

where  $\tau$  is the time constant and  $K_p$  is the steady-state gain, or asymptotic gain of the process.

A first-order system can be represented by the block diagram shown in Fig. 1.25.



**Figure 1.25:** Block diagram of a first-order system

If the input  $u$  of the process is a step function with amplitude  $A$ , the Laplace transform of the input is

$$U(s) = \frac{A}{s} \quad (1.139)$$

Using the definition of the transfer function, the Laplace transform of the output is obtained

$$Y(s) = G(s) U(s) = \frac{K_p}{\tau s + 1} \frac{A}{s} = \frac{A K_p}{s} - \frac{A K_p \tau}{\tau s + 1} = Y_f(s) + Y_n(s) \quad (1.140)$$

and the time domain response (Fig. 1.26) is

$$y(t) = A K_p (1 - \exp(-t/\tau)) \quad (1.141)$$

The forced and natural parts of the response are respectively equal to

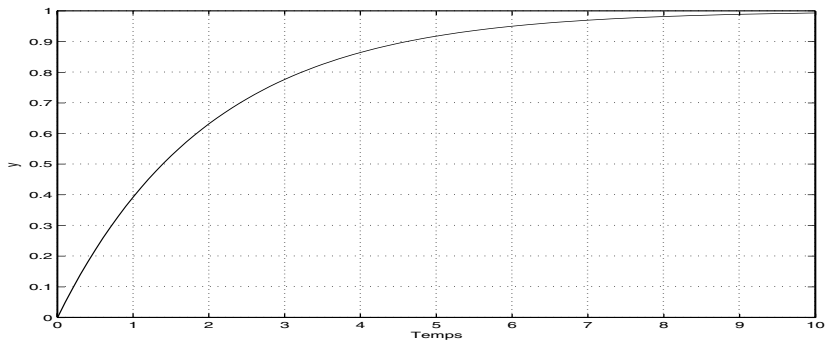
$$y_f(t) = A K_p \quad ; \quad y_n(t) = -A K_p \exp(-t/\tau) \quad (1.142)$$

With respect to the input of amplitude  $A$ , the asymptotic output (when  $t \rightarrow \infty$ ) is thus multiplied by the gain of the process  $K_p$ . A first-order process is also called a “first-order lag”.

The time constant  $\tau$  corresponds to the time necessary for the system response to reach 63.2% of its asymptotic value for a step input. After  $2\tau$ , the response reaches 86.5% and after  $5\tau$  it reaches 99.3% (Table 1.2).

Several real physical systems have first-order dynamics. Examples of such systems are:

- Systems storing mass, energy or momentum,
- Systems showing resistance to the flow of mass, energy or momentum.



**Figure 1.26:** Response of a first-order system ( $K_p = 1, \tau = 2$ ) to a unit step function

**Table 1.2:** Response of a first-order system to a unit step function expressed in percentage of the asymptotic value

Time	Percentage of the asymptotic value
0	0
$\tau$	63.21%
$2\tau$	86.47%
$3\tau$	95.02%
$4\tau$	98.17%
$5\tau$	99.33%
$6\tau$	99.75%
$7\tau$	99.91%

### 1.11.2 Integrating Systems

Integrating or pure capacitive processes are those whose dynamics only contain the first-order derivative of  $y(t)$

$$\frac{dy}{dt} = K_p u(t) \tag{1.143}$$

The corresponding transfer function is

$$G(s) = \frac{K_p}{s} \tag{1.144}$$

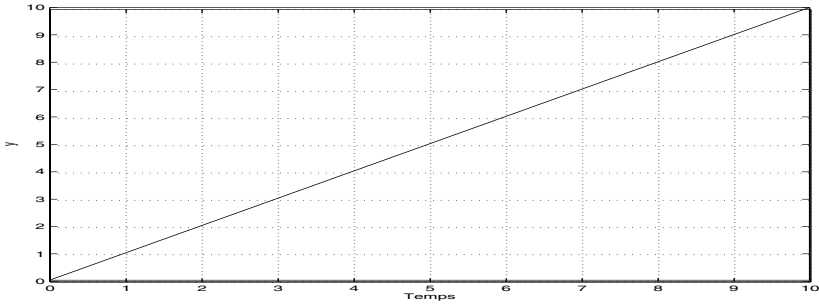
The Laplace transform of the output of such a system to a step function with magnitude  $A$  is

$$Y(s) = \frac{A K_p}{s^2} \tag{1.145}$$

The time domain response  $y(t)$  (Fig. 1.27) is thus equal to

$$y(t) = A K_p t \tag{1.146}$$

The process is referred to as a “pure capacitive” or a “pure integrator”. The term “capacitive” signifies the accumulation of electrical charges, energy or mass. A surge tank can behave as a pure capacitive process.



**Figure 1.27:** Response of a pure capacitive system ( $K_p = 1$ ) to a unit step input

### 1.11.3 Second-Order Systems

A second-order system is described by a second-order differential equation written in the classical form as

$$\tau^2 \frac{d^2 y(t)}{dt^2} + 2\zeta\tau \frac{dy(t)}{dt} + y(t) = K_p u(t) \quad (1.147)$$

with the corresponding transfer function

$$G(s) = \frac{K_p}{\tau^2 s^2 + 2\zeta\tau s + 1} \quad (1.148)$$

where  $\tau$  is the natural period of oscillation of the system which determines the stabilization time of the system,  $\zeta$  is the damping coefficient and  $K_p$  is the steady-state gain of the system.

The notions of natural period of oscillation and of damping factor are related to the damped or undamped oscillators. For  $\zeta = 0$ , the expression (1.155) shows that the response to a step input oscillates continuously with a frequency  $1/\tau$  in radians/time unit.

The transfer function of a second-order system is sometimes written as

$$G(s) = \frac{K_p \omega_n^2}{s^2 + 2\zeta\omega_n s + \omega_n^2} \quad (1.149)$$

where  $\omega_n = 1/\tau$  is the natural undamped frequency and  $\sigma = \zeta\omega_n$  is the damping parameter.

Several real physical processes exhibit second-order dynamics, among them are:

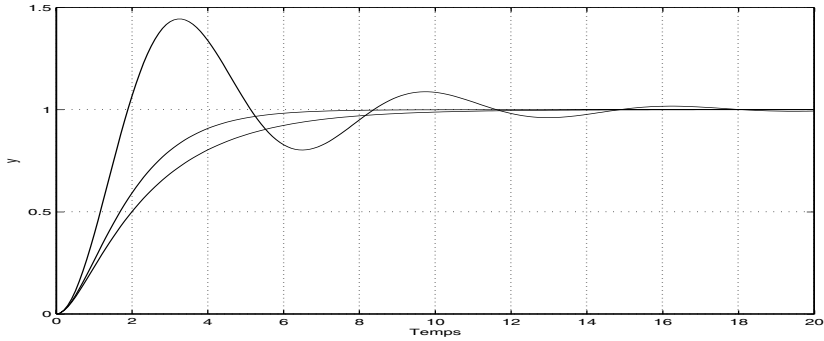
- Two first-order systems in series.

- Intrinsic second-order systems, e.g. mechanical systems having an acceleration.
- Feedback or closed-loop transfer function of a first-order process with a PI controller.

Note that the transfer function  $G(s)$  defined by Eq. (1.148) has two poles, roots of:  $\tau^2 s^2 + 2\zeta\tau s + 1 = 0$ , which are equal to

$$\left\{ \begin{array}{ll} s_i = \frac{1}{\tau} (-\zeta \pm \sqrt{\zeta^2 - 1}) & \text{if: } \zeta \geq 1 \\ s_i = \frac{1}{\tau} (-\zeta \pm j\sqrt{1 - \zeta^2}) = \omega_n(-\zeta \pm j\sqrt{1 - \zeta^2}) = -\sigma \pm j\omega_a & \text{if: } 0 \leq \zeta \leq 1 \end{array} \right. \quad (1.150)$$

If the natural period of oscillation  $\tau$  is fixed, then the position of the poles depends only on the damping coefficient  $\zeta$ . The shape of the open-loop response to a given input is determined by the location of these poles on the  $s$ -plane. For  $0 \leq \zeta \leq 1$ , the natural frequency  $\omega_n$  is equal to the distance of the poles from the origin, the damped frequency  $\omega_a$  is equal to the distance of the poles from the real axis, and the damping parameter  $\sigma$  is equal to the distance of the poles from the imaginary axis.



**Figure 1.28:** Normalized response of a second-order system to a unit step function for different values of the damping coefficient  $\zeta$  ( $= 0.25; 1; 1.3$  resulting in oscillatory underdamped response to overdamped response) ( $K_p = 1, \tau = 1$ )

If the input is a step function with magnitude  $A$ , the output Laplace transform is equal to

$$Y(s) = A \frac{K_p}{s(\tau^2 s^2 + 2\zeta\tau s + 1)} \quad (1.151)$$

which can be decomposed into

$$Y(s) = \frac{AK_p}{s} - \frac{AK_p\tau^2 s + 2\zeta\tau}{\tau^2 s^2 + 2\zeta\tau s + 1} = Y_f(s) + Y_n(s) \quad (1.152)$$

The overall response consists of the forced and the natural responses

$$y(t) = y_f(t) + y_n(t) \quad (1.153)$$

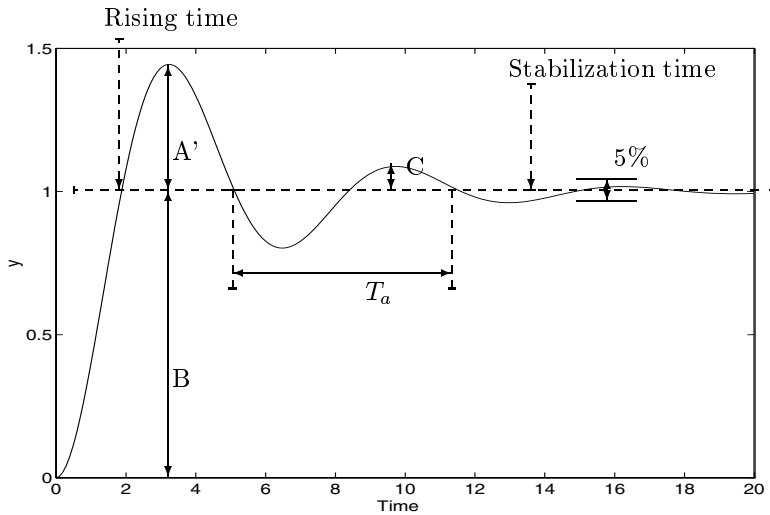
The forced response is equal to

$$y_f(t) = AK_p \quad (1.154)$$

and the overall response is

$$y(t) = \begin{cases} AK_p \left\{ 1 - \exp(-\zeta t/\tau) \left[ \cos \left( \frac{\sqrt{1-\zeta^2}}{\tau} t \right) + \frac{\zeta}{\sqrt{1-\zeta^2}} \sin \left( \frac{\sqrt{1-\zeta^2}}{\tau} t \right) \right] \right\} & \text{if: } 0 \leq \zeta < 1 \\ AK_p [1 - (1 + \frac{t}{\tau}) \exp(-t/\tau)] & \text{if: } \zeta = 1 \\ AK_p \left\{ 1 - \exp(-\zeta t/\tau) \left[ \cosh \left( \frac{\sqrt{\zeta^2-1}}{\tau} t \right) + \frac{\zeta}{\sqrt{\zeta^2-1}} \sinh \left( \frac{\sqrt{\zeta^2-1}}{\tau} t \right) \right] \right\} & \text{if: } 1 < \zeta \end{cases} \quad (1.155)$$

The forced response is constant and equal to  $AK_p$  while the natural response tends towards 0 when  $t \rightarrow \infty$ . The natural response takes into account the natural modes of the system and thus depends on the value of  $\zeta$  (Fig. 1.28):



**Figure 1.29:** Response of a second-order system to a unit step input

- For  $\zeta > 1$ , there will be two real and distinct poles. The response is overdamped (multi-capacitive systems) with no overshoot.
- For  $\zeta = 1$ , there will be one multiple second-order pole. The response is critically damped, which corresponds to the faster overdamped response.
- For  $0 < \zeta < 1$ , there will be two complex conjugate poles with negative real part. The response is underdamped. This response is initially faster than the critically damped and overdamped responses, which are sluggish; the drawback is the resulting overshoot.

With reference to the underdamped response of Fig. 1.29, the following terms are defined:

- Overshoot

$$\text{overshoot} = \frac{A'}{B} = \exp\left(\frac{-\pi\zeta}{\sqrt{1-\zeta^2}}\right) \quad (1.156)$$

- Decay ratio =  $C/A' = (\text{overshoot})^2$
- Natural period of oscillation is defined for a system with a damping coefficient  $\zeta$  equal to zero. Such a system oscillates continuously with the natural period  $T_n = 2\pi\tau = 2\pi/\omega_n$  and the undamped natural frequency  $\omega_n$ .
- Actual period of oscillation  $T_a$ , which is the time between two successive peaks, characterized by its damped frequency  $\omega_a$

$$\omega_a = \omega_n \sqrt{1-\zeta^2} = \frac{\sqrt{1-\zeta^2}}{\tau} = \frac{2\pi}{T_a} \quad (1.157)$$

- Rise time: this is the time necessary to reach the asymptotic value for the first time

$$t_m = \frac{1}{\omega_n \sqrt{1-\zeta^2}} \arctg\left(-\frac{\sqrt{1-\zeta^2}}{\zeta}\right) \quad (1.158)$$

It can also be defined as the time necessary to go from 10% to 90% of the asymptotic value and, in that case, it can be approximated (Goodwin and Sin, 1984) by

$$t_m \approx \frac{2.5}{\omega_n} \quad (1.159)$$

- First peak reach time: the time necessary for the response to reach the first peak

$$t_p = \frac{\pi}{\omega_d} = \frac{\pi}{\omega_n \sqrt{1-\zeta^2}} \quad (1.160)$$

- Settling time: time necessary for the response to remain in an interval between  $\pm\epsilon$  ( $\pm 5\%$ , or  $\pm 2\%$ ) of the asymptotic value. For  $\pm\epsilon = \pm 1\%$ , according to Goodwin and Sin (1984), the settling time is

$$t_s \approx \frac{4.6}{\zeta\omega_n} \quad (1.161)$$

For ( $0 < \zeta < 1$ ), the time domain response can be written as

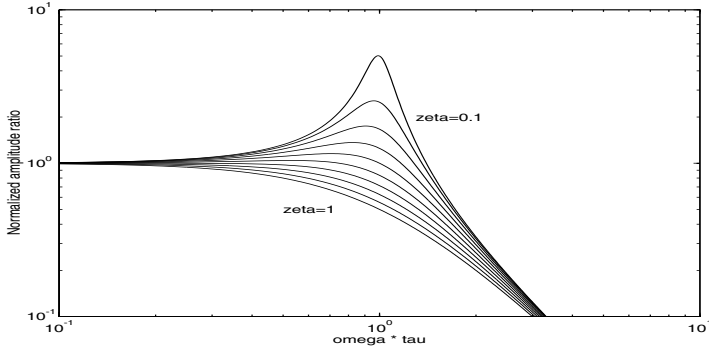
$$y(t) = AK_p - AK_p \frac{\omega_n}{\omega_a} \exp(-\sigma t) \sin(\omega_d t + \theta) \quad (1.162)$$

with

$$\theta = \arccos\zeta = \arctan\left(\sqrt{\frac{1-\zeta^2}{\zeta}}\right) = \arcsin(\sqrt{1-\zeta^2}) \quad (1.163)$$

and the envelope of the undamped sinusoidal response is

$$\exp(-\sigma t) \sin(\omega_d t + \theta) \quad (1.164)$$



**Figure 1.30:** Normalized amplitude ratio for a sinusoidal input with varying damping coefficient  $\zeta$  between 0 and 1 per increment of 0.1

The time domain response of a second-order system subjected to a sinusoidal input:  $u(t) = A \sin(\omega t)$ , after the transient response decays, will take the form

$$y_{\infty}(t) = \frac{K_p A}{\sqrt{[1 - (\omega\tau)^2]^2 + (2\zeta\omega\tau)^2}} \sin(\omega t - \arctan\left[\frac{2\zeta\omega\tau}{1 - (\omega\tau)^2}\right]) \quad (1.165)$$

and the normalized amplitude ratio is equal to

$$RA_n = \frac{1}{\sqrt{[1 - (\omega\tau)^2]^2 + (2\zeta\omega\tau)^2}} \quad (1.166)$$

which is maximum at a frequency  $\omega_{\max}$  given by

$$\omega_{\max} = \sqrt{(1 - 2\zeta^2)}/\tau \quad (1.167)$$

The normalized amplitude ratio has a maximum equal to  $1/(2\zeta\sqrt{1 - \zeta^2})$  for  $0 \leq \zeta \leq 0.707$ . This maximum increases very quickly when  $\zeta$  becomes small (Fig. 1.30).

Large oscillations are not desired, therefore small damping coefficients  $\zeta$  must be avoided. In controlled processes, a damping coefficient around  $\zeta = 1$  (conservative) or  $\zeta = 0.7$  (low overshoot, fast response), is often recommended.

#### 1.11.4 Higher-Order Systems

Three types of higher-order systems will be described:

- $n$  First-order processes in series (multi-capacitive).
- Processes with time delay.
- Processes with inverse response.



### $n$ First-Order Processes in Series

The transfer function of  $n$  first-order processes in series is obtained by multiplying the transfer functions of  $n$  first-order systems

$$G(s) = \prod_{i=1}^n \frac{K_{pi}}{\tau_i s + 1} \quad (1.168)$$

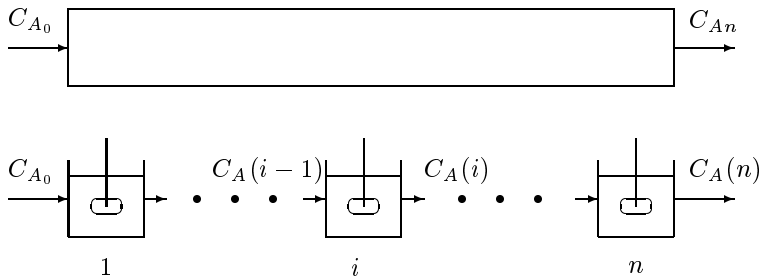
#### Example 1.3: Tubular Plug Flow Reactor

Consider a tubular plug flow reactor with a mean residence time equal to  $\tau_1$ . In the absence of reaction, for a simple flow, the outlet concentration is equal to the inlet one, just delayed by the residence time  $\tau_1$ . Suppose now that a first-order reaction  $A \rightarrow B$  with a reaction rate  $r_A = k C_A$  is carried out in the reactor, the reactor being fed with a reactant stream at inlet concentration  $C_{A_0}$ . This represents a distributed-parameter system whose model is given by a partial differential equation. Another approach to model the reactor is to discretize it into  $n$  elementary reactors (Fig. 1.31) with a residence time given by

$$\tau_n = \frac{\tau_1}{n} \quad (1.169)$$

The component mass balance on each element is given by

$$\frac{dC_A(i)}{dt} = \frac{1}{\tau_n} [C_A(i-1) - C_A(i)] - k C_A(i) \quad (1.170)$$



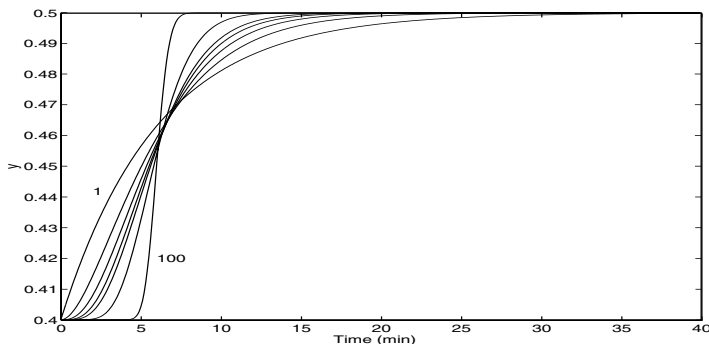
**Figure 1.31:** Decomposition of a tubular reactor into a series of  $n$  continuous perfectly stirred tank reactors

In the absence of reaction, the flow is simply represented by  $n$  first-order systems in series with unit gain

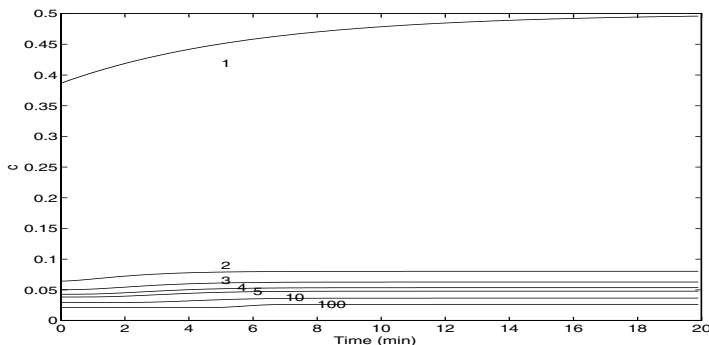
$$\frac{\bar{C}_A(i)}{\bar{C}_A(i-1)} = \frac{1}{\tau_n s + 1} \quad (1.171)$$

The observed response at the reactor exit is similar to an overdamped system with a sluggish sigmoidal shape. Figure 1.32 represents the response of the system to a step increase in  $C_{A_0}$  from 0.4 to 0.5, using different numbers of

discretization elements  $n$  ranging from 1 to 100. Note that as  $n$  approaches 100, the response looks like the input step with a delay time equal to the mean residence time of the tubular plug flow reactor (assumed 6 min. in this simulation).



**Figure 1.32:** Response of the discretized plug flow reactor to a step increase in the inlet concentration from 0.4 to 0.5 with the number  $n$  of discretized elements, ranging from 1, 2, 3, 4, 5, 10 and 100 (in the absence of reaction)



**Figure 1.33:** Response of the discretized plug flow reactor to a step increase in the inlet reactant concentration from 0.4 to 0.5 in the presence of a first-order reaction

In the case where a chemical reaction occurs, each element represents a CSTR. Except in the simple case where the reaction is first-order, the model is in general nonlinear and would need a linearization around a steady state. For a first-order reaction, the transfer function is

$$\frac{\bar{C}_A(i)}{\bar{C}_A(i-1)} = \frac{1}{\tau_n s + 1 + k \tau_n} \quad (1.172)$$

Note that the process gain is no longer unity due to the depletion of reactant by chemical reaction. The process response to a unit increase in the inlet concen-

tration of reactant  $C_{A_0}$  from 0.4 to 0.5 in the presence of reaction is shown in Fig. 1.33. Due to the chemical reaction, the asymptotic outlet concentrations decrease with the number of elements of discretization in a similar manner to a tubular reactor. In comparison with Fig. 1.32, the response is more sluggish.

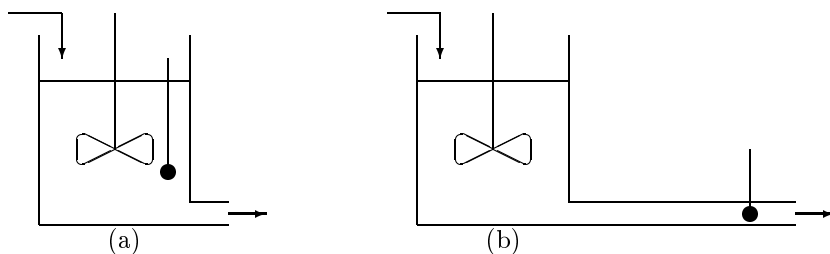
Another example of a series of elementary systems resulting in an overall higher order system is the staged processes such as a tray distillation column. Each tray of a distillation column can be often considered as a first-order interacting process.

A packed column (distillation, absorption or chromatography) can be modelled by partial differential equations and could be discretized in a similar manner to a tubular reactor.

The dynamics of distributed-parameter systems and higher-order systems are often approximated by a first- or second-order overdamped model with time delay. For example, in a distillation column, a set of plates such as the stripping or the enrichment section is often identified as first-order with delay.

### Processes with Time Delay

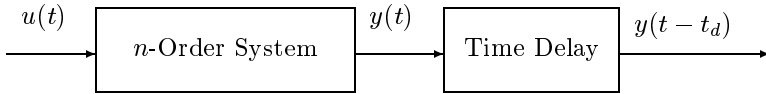
Time delay may be an inherent dynamic characteristic of a process or due to the measurement. In the former case, the process input does not immediately affect the process output. In the latter case, the measured signal received by the controller does not correspond to the contemporary process information and suffers from delay. A common example of time delay is the transportation lag, which may be either due to the process or measurement or both. Consider, for example, the concentration measurement in a reactor which frequently is not done in situ (Fig. 1.34). The measuring device is mounted on a sampling loop. The sample is pumped through the loop and experiences some transportation lag  $t_d$  to reach the sensor.



**Figure 1.34:** Case (a): In situ sensor. Case (b): sensor placed in the exit pipe, inducing a transportation lag

In the case of a distillation column, in general distillate and bottom concentrations are controlled by manipulating, for example, the reflux flow and the steam

flow to the reboiler. Measurements are typically the levels in the reboiler and in the condenser, temperatures at different points of the column, and distillate and bottom concentrations. Temperature and level measurements can be considered as instantaneous. This is not the case for concentration measurement, e.g. in the case of refineries, a chromatograph some distance away from the distillation column is often used. In such cases, the delay time will consist of a transportation lag to pump the sample from the process to the analyzer and an additional time for the analysis of the sample, which in the case of a chromatograph could be in the order of several tens of seconds. A sample is taken from the distillation column at time  $t_1$  and the result is available at time  $t_2$ , where  $t_2 - t_1 = t_d$ . During the measurement, the process continues to evolve.



**Figure 1.35:** Representation of a system with time delay

The time delay poses a problem in process control. The time delay between an input and an output (Fig. 1.35) means that the input variations have no immediate influence on the output.

For a first-order system with a time delay, the transfer function linking the input  $u(t)$  and the delayed output  $y(t - t_d)$  is

$$\frac{\mathcal{L}[y(t - t_d)]}{\mathcal{L}[u(t)]} = \frac{K_p \exp(-t_d s)}{\tau s + 1} \quad (1.173)$$

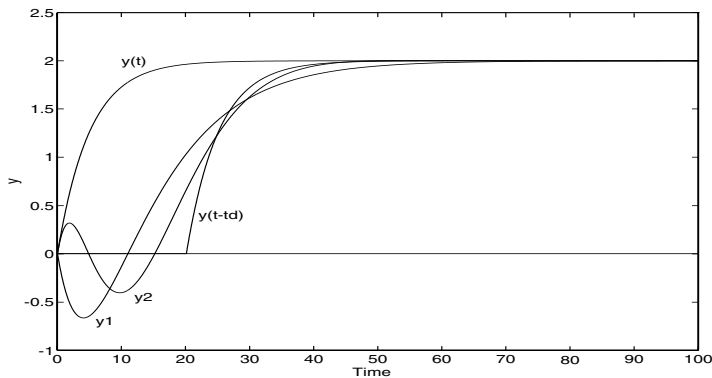
The exponential term is a nonlinear term. It is often approximated, for example, by a Padé approximation (here a first-order approximation), which converts the delay term to a rational fraction

$$\exp(-t_d s) \approx \frac{1 - \frac{t_d}{2} s}{1 + \frac{t_d}{2} s} \quad (1.174)$$

A more accurate approximation of the time delay is realized by the second-order Padé approximation.

$$\exp(-t_d s) \approx \frac{1 - \frac{t_d}{2} s + \frac{t_d^2}{12} s^2}{1 + \frac{t_d}{2} s + \frac{t_d^2}{12} s^2} \quad (1.175)$$

Figure 1.36 shows the unit step response of a first-order system without time delay  $y(t)$ , with exact time delay  $y(t - t_d)$ , with first-order Padé approximation  $y_1$  and with second-order Padé approximation  $y_2$ . Note that the approximations are valid for times much larger than the time delay. Initially both first- and second-order approximations exhibit inverse response due to the zeros of

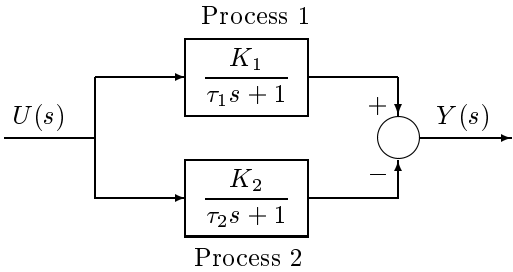


**Figure 1.36:** Response of a first-order system ( $K_p = 2, \tau = 5$ ) with a time delay of 20 s to a step input:  $y(t)$  (without time delay),  $y(t - t_d)$  (with time delay),  $y_1$  (Padé first-order),  $y_2$  (Padé second-order)

the rational transfer functions introduced by Padé approximations. The number of intersections of the approximated response with the time axis is equal to the order of Padé approximation and corresponds to the number of positive real zeros or complex zeros with positive real part of the transfer function, i.e. for the first-order Padé approximation, there is one real positive zero and for the second-order Padé approximation, there are two conjugate complex zeros with positive real part.

There exists no perfect approximation for the time delay. However, digital computers handle time delays with relative ease, in particular in the case of digital control.

### Processes with Inverse Response



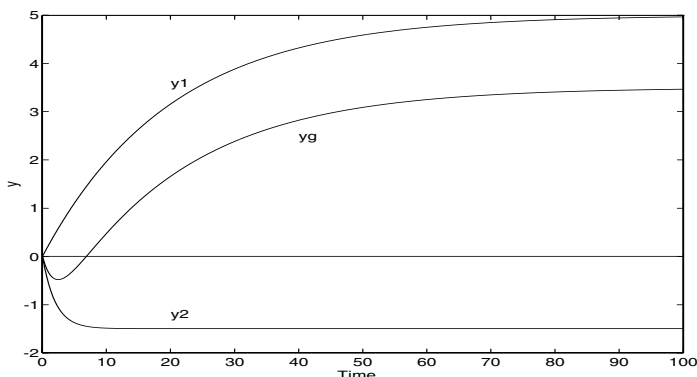
**Figure 1.37:** Representation of a system with inverse response

In a system with inverse response such as that represented in Fig. 1.37, the overall response  $y_g$  (Fig. 1.38) initially moves in a direction opposite to its

final direction. This behaviour is caused by the addition of two opposing subprocesses. At the beginning, process 2, which has a smaller time constant, is dominant. Subsequently, process 1, which has a higher gain ( $K_1 > K_2$ ), becomes dominant. The overall process is thus composed of two competitive processes having different time constants and different gains.

To produce an inverse response, it is necessary and sufficient that the plant transfer function exhibits a positive real zero or a complex zero with a positive real part. For the example shown in Fig. 1.37, the overall transfer function will have a positive zero if

$$\frac{K_2}{\tau_2} > \frac{K_1}{\tau_1} \quad (1.176)$$



**Figure 1.38:** Inverse response of the system shown in Fig. 1.37 to a unit step input ( $K_1 = 5$ ,  $\tau_1 = 20$ ,  $K_2 = 1.5$ ,  $\tau_2 = 2$ )

Chemical processes which exhibit an inverse response are not rare. For example, an increase in the vapour boil-off (increase in the steam flow rate to the reboiler) in a distillation column results in an inverse response in the liquid level in the bottom of the column. The increase in the vapour boil-off, initially, decreases the liquid level in the bottom of the column. Subsequently, due to the increased vapour flow rate and frothing on the trays immediately above the reboiler, the liquid level may eventually increase.

Another example is the response in the liquid level in a boiler due to an increase in the inlet water flow rate. The initial increase in the water flow rate decreases the liquid level because of the collapse of the vapour bubbles. However, if the steam production is maintained at a constant rate, the liquid level will eventually increase.

A third example is the response in the exit temperature of a fixed-bed reactor with exothermic reactions to a step increase in the feed temperature. If the feed temperature increases, the rate of reactions at the reactor inlet will increase and the reactants are consumed close to the reactor inlet. This will move the hot spot closer to the reactor entrance and consequently the exit re-

actor temperature decreases. However, eventually the reactor exit temperature will increase as a result of the increase in the inlet temperature.

### 1.11.5 Process Identification in the Continuous Domain

#### General Principles

It is possible to develop a model for an existing process using only the input-output data. This empirical technique for developing process models is referred to as process or system identification (Sinha and Rao, 1991; Unbehauen and Rao, 1987; Walter and Pronzato, 1997; Young, 1981). System identification for complex processes requires less engineering effort compared to the theoretical model development. Of course, the application field of such an identified model is more limited. In open-loop system identification, the controller is switched to manual, the controller output is changed by a step function or a series of pseudo-random-binary-signal (PRBS) or any other exciting input sequence, and the process response is monitored. The input-output data are used to develop the system model. This model will represent the dynamics of the combination of the final control element (the control valve), the process, and the measuring element. Measurement noise will generally be superposed on the actual process response. Sophisticated process identification techniques are capable of distinguishing the process model from the noise model.

Often, a low-order linear model based on the a priori information of the process is assumed, i.e. the structure of the model is fixed. Under these conditions, process identification is reduced to the determination of the unknown model parameters, i.e. a parameter estimation problem. Let us assume that the process model is given by

$$y(t) = f(t, \boldsymbol{\theta}) \quad (1.177)$$

where  $\boldsymbol{\theta}$  is the unknown parameter vector. In order to determine the unknown parameter vector, one may use the least-squares technique by minimizing the following objective function, which is the sum of the squares of errors between the measured output  $y_i$  at time  $t_i$  and the output predicted by the model  $\hat{y}_i$

$$J(\boldsymbol{\theta}) = \sum_i (y_i - \hat{y}_i)^2 \quad (1.178)$$

Other criteria can be introduced in particular by the use of weighting factors.

Two main cases are distinguished depending on whether the model is linear or nonlinear. In the case of a linear model with respect to  $m$  parameters  $\theta_j$ , the model can be written as

$$y(\mathbf{x}) = \sum_{j=1}^m \theta_j \phi_j(\mathbf{x}) \quad (1.179)$$

A set of  $n$  input-output observations can be collected in a matrix  $\Phi$  such that

$$\Phi_{ij} = \phi_j(\mathbf{x}_i) \quad ; \quad 1 \leq i \leq n \quad ; \quad 1 \leq j \leq m \quad (1.180)$$

The parameter vector estimated by minimization of the criterion (1.178) is equal to

$$\hat{\boldsymbol{\theta}} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y} \quad (1.181)$$

where  $\mathbf{y}$  is the measured vector.

#### Example 1.4: Identification of a Linear Model

Consider the example of determining the parameters in the model of the heat capacity of a fluid expressed with respect to temperature by

$$C_p = a + bT + cT^2 \quad (1.182)$$

This model is nonlinear with respect to temperature but linear with respect to the coefficients  $a$ ,  $b$ ,  $c$ . As we wish to determine the coefficients, we must realize at least three experiments. In the case where only three experiments are performed, the coefficients are the solution of a perfectly determined system which can be solved by the Gauss method, for example. In the case where more than three experiments are performed, it becomes a least-squares problem. Assume that we perform  $n > 3$  experiments which give heat capacities  $C_{p,i}$  at temperatures  $T_i$ . The matrix  $\Phi$  and vector  $\mathbf{y}$  of Eq. (1.181) are equal to

$$\Phi = \begin{bmatrix} 1 & T_1 & T_1^2 \\ 1 & T_2 & T_2^2 \\ \vdots & \vdots & \vdots \\ 1 & T_n & T_n^2 \end{bmatrix} \quad ; \quad \mathbf{y} = \begin{bmatrix} C_{p,1} \\ C_{p,2} \\ \vdots \\ C_{p,n} \end{bmatrix} \quad (1.183)$$

The vector of estimated parameters is then

$$\begin{bmatrix} \hat{a} \\ \hat{b} \\ \hat{c} \end{bmatrix} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y} \quad (1.184)$$

---

In the case of a nonlinear model, which is most common in practice, more general optimization methods such as direct search or gradient-type methods such as the generalized reduced gradient method or the quasi-Newton method (Fletcher, 1991; Gill et al., 1981), must be employed. Powerful algorithms exist for solving such problems as the BFGS method (Byrd et al., 1995; Zhu et al., 1994) or sequential quadratic programming (SQP) under NLPQL form (Schittkowski, 1985). It is also possible to linearize the non-linear model with respect to the parameter vector and then use a linear parameter estimation method.

#### Example 1.5: Identification of a Nonlinear Model

Consider the example of determining the parameters in the model of the saturated vapour pressure of a fluid expressed with respect to temperature by Antoine's law

$$\ln(P_{sat}) = A - \frac{B}{C + T} \quad (1.185)$$



We can make remarks similar to the previous case. This model is nonlinear with respect to the temperature and nonlinear with respect to the coefficients  $A$ ,  $B$ ,  $C$ . In the case where only three experiments are performed, the coefficients are the solution of a perfectly determined system which is now nonlinear and could be solved by the Newton-Raphson method (Carnahan et al., 1969). In the case where more than three experiments are performed, it becomes a least-squares problem. Assuming that we make  $n$  experiments which give vapour pressures  $P_i$  at temperatures  $T_i$ , a least-squares criterion to be minimized is written as

$$J = \sum_{i=1}^n \left( \ln(P_i) - A + \frac{B}{C + T_i} \right)^2 \quad (1.186)$$

whose minimization with respect to parameters can be performed by a quasi-Newton method.

---

### A First-Order Model

If a time delay is present, first it must be estimated and then the system is examined without this delay. The steady-state gain  $K_p$  is also estimated from the asymptotic response. The time constant  $\tau$  can be evaluated by using Table 1.2, for example, by searching the time at which 63.2% of the asymptotic value is reached. For a step change with magnitude  $A$  in the input, the time domain response is given by

$$\ln\left(1 - \frac{y}{K_p A}\right) = -\frac{t}{\tau} \quad (1.187)$$

which corresponds to a straight line with a slope  $-1/\tau$ .

### A Second-Order Model

Similar to a first-order model, the time delay must be estimated first, then the steady-state gain  $K_p$ .

If the second-order system is overdamped, its transfer function can be written as

$$G(s) = \frac{K_p}{(\tau_1 s + 1)(\tau_2 s + 1)} \quad (1.188)$$

with two unknown time constants. Harriott's method offers a simple graphical method for the determination of the unknown time constants based on the measurements of process outputs at two points during its evolution. A more accurate method is the numerical non-linear optimization using the entire process output response to a step change in the input

$$y(t) = A K_p \left[ 1 + \frac{\tau_1}{\tau_2 - \tau_1} \exp(-t/\tau_1) + \frac{\tau_2}{\tau_1 - \tau_2} \exp(-t/\tau_2) \right] \quad (1.189)$$

When plotted versus time, this function has a sigmoidal shape with an inflection point at

$$t = \frac{\tau_1 \tau_2}{\tau_1 - \tau_2} \ln\left(\frac{\tau_1}{\tau_2}\right) \quad (1.190)$$

If the second-order system is underdamped, its transfer function is

$$G(s) = \frac{K_p}{\tau^2 s^2 + 2\zeta \tau s + 1} \quad (1.191)$$

Two parameters must be estimated, the damping coefficient and the time constant  $\tau$ . Graphical methods can be used to determine the decay ratio or the overshoot to estimate the unknown parameters.

However, a better approach is the nonlinear optimization using the response given by Eq. (1.155) to minimize a criterion such as the one given in Eq. (1.178). Consider the response of the model denoted by  $y_{mod,i}$  and the experimental response denoted by  $y_{exp,i}$  at  $n$  different instants  $t_i$ . The nonlinear optimization problem is expressed as

$$\min_{\tau, \zeta, K_p} \sum_{i=1}^n (y_{exp,i} - y_{mod,i})^2 \quad (1.192)$$

which again can be solved by a quasi-Newton-type method. The response of the model depends analytically on the parameters and the criterion can be analytically differentiated. If this differentiation seems too difficult, it may be performed numerically.

### The Method of Moments

The advantage of the method of moments is that it can be used with any type of input.

This method is based on the definition of the Laplace transform of the impulse response  $g(t)$  of a system, which is its transfer function

$$G(s) = \int_0^\infty \exp(-s t) g(t) dt \quad (1.193)$$

As the  $n$ -th-order moment of a function  $f(x)$  is defined by

$$\mathcal{M}_n(f) = \int_0^\infty x^n f(x) dx \quad (1.194)$$

it can be noticed that the first two derivatives of  $G(s)$  with respect to  $s$

$$G'(s) = - \int_0^\infty t \exp(-s t) g(t) dt \quad ; \quad G''(s) = \int_0^\infty t^2 \exp(-s t) g(t) dt \quad (1.195)$$

are related to the moments of the impulse response function by

$$G(0) = \int_0^\infty g(t) dt \quad ; \quad G'(0) = - \int_0^\infty t g(t) dt \quad ; \quad G''(0) = \int_0^\infty t^2 g(t) dt \quad (1.196)$$

Thus  $G(0)$ ,  $-G'(0)$ ,  $G''(0)$  are respectively the zero-, first- and second-order moments of the impulse response  $g(t)$ .

Note that the above three integrals can be calculated by using the measured output response. Consider the following systems for the application of this method:

- A first-order model with time delay

$$G(s) = \frac{K_p \exp(-t_d s)}{\tau s + 1} \quad (1.197)$$

giving

$$G(0) = K_p \quad ; \quad G'(0) = -K_p (\tau + t_d) \quad ; \quad G''(0) = K_p (2\tau^2 + 2\tau t_d + t_d^2) \quad (1.198)$$

from which the three unknown parameters  $K_p$ ,  $\tau$  and  $t_d$  can be determined.

- An overdamped second-order model with time delay (previously determined)

$$G(s) = \frac{K_p \exp(-t_d s)}{(\tau_1 s + 1)(\tau_2 s + 1)} \quad (1.199)$$

from which

$$\begin{aligned} G(0) &= K_p \quad ; \quad G'(0) = -K_p (\tau_1 + \tau_2 + t_d) \\ G''(0) &= K_p [(\tau_1 + \tau_2 + t_d)^2 + \tau_1^2 + \tau_2^2] \end{aligned} \quad (1.200)$$

The time delay can be obtained by inspection of the response curve and the other parameters are obtained from the moments.

- An underdamped second-order model with time delay (previously determined)

$$G(s) = \frac{K_p \exp(-t_d s)}{\tau^2 s^2 + 2\zeta\tau s + 1} \quad (1.201)$$

from which

$$\begin{aligned} G(0) &= K_p \quad ; \quad G'(0) = -K_p (2\zeta\tau + t_d) \\ G''(0) &= K_p [t_d^2 + 4\zeta\tau t_d - 2\tau^2 + 8\zeta^2\tau^2] \end{aligned} \quad (1.202)$$

Note that in this method, it is possible to use any type of input. We have, in general

$$\begin{aligned} Y(s) &= G(s) U(s) \quad ; \quad Y'(s) = G'(s) U(s) + G(s) U'(s) \\ Y''(s) &= G''(s) U(s) + G(s) U''(s) + 2G'(s) U'(s) \end{aligned} \quad (1.203)$$

from which the following equations are deduced

$$\begin{aligned} Y(0) &= G(0) U(0) \quad ; \quad Y'(0) = G'(0) U(0) + G(0) U'(0) \\ Y''(0) &= G''(0) U(0) + G(0) U''(0) + 2G'(0) U'(0) \end{aligned} \quad (1.204)$$

These quantities can be calculated by the following equations:

$$U(0) = \int_0^\infty u(t) dt \quad ; \quad U'(0) = - \int_0^\infty t u(t) dt \quad ; \quad U''(0) = \int_0^\infty t^2 u(t) dt \quad (1.205)$$

and

$$Y(0) = \int_0^\infty y(t) dt \quad ; \quad Y'(0) = - \int_0^\infty t y(t) dt \quad ; \quad Y''(0) = \int_0^\infty t^2 y(t) dt \quad (1.206)$$

In order to determine the characteristic parameters of the system, the moments method uses the entire input and output curves and can be applied to any type of the input signal. This method should be preferred to any method based on only two given points of an output response.

## References

- R.B. Bird and E.N. Lightfoot. *Transport Phenomena*. Wiley, New York, 1960.
- P. Borne, G. Dauphin-Tanguy, J.P. Richard, F. Rotella, and I. Zambetakis. *Commande et Optimisation des Processus*. Technip, Paris, 1992a.
- P. Borne, G. Dauphin-Tanguy, J.P. Richard, F. Rotella, and I. Zambetakis. *Modélisation et Identification des Processus*, volume 1, 2. Technip, Paris, 1992b.
- P. Borne, G. Dauphin-Tanguy, J.P. Richard, F. Rotella, and I. Zambetakis. *Analyse et Régulation des Processus Industriels. Tome 1. Régulation Continue*. Technip, Paris, 1993.
- P. Borne, G. Dauphin-Tanguy, J.P. Richard, F. Rotella, and I. Zambettakis. *Commande et Optimisation des Processus*. Technip, Paris, 1990.
- R.H. Byrd, P. Lu, J. Nocedal, and C. Zhu. A limited memory algorithm for bound constrained optimization. *SIAM J. Scientific Computing*, (5):1190–1208, 1995.
- B. Carnahan, H.A. Luther, and J.O. Wilkes. *Applied Numerical Methods*. Wiley, New York, 1969.
- C.T. Chen. *One-dimensional Digital Signal Processing*. Marcel Dekker, New York, 1979.
- C.T. Chen. *Analog and Digital Control System Design: Transfer-Function, State-Space, and Algebraic Methods*. Harcourt Brace Jovanovich College, Fort Worth, 1993.
- D.R. Coughanowr and L.B. Koppel. *Process Systems Analysis and Control*. McGraw-Hill, Auckland, 1985.
- R. Fletcher. *Practical Methods of Optimization*. Wiley, Chichester, 1991.
- P.E. Gill, W. Murray, and M.H. Wright. *Practical Optimization*. Academic Press, London, 1981.

- G.C. Goodwin and K.S. Sin. *Adaptive Filtering, Prediction and Control*. Prentice Hall, Englewood Cliffs, 1984.
- D.M. Himmelblau and K.B. Bischoff. *Process Analysis and Simulation*. Wiley, New York, 1968.
- R. Isermann. *Digital Control Systems*, volume I. Fundamentals Deterministic Control. Springer-Verlag, 2nd edition, 1991a.
- R. Isermann. *Digital Control Systems*, volume II. Stochastic Control, Multivariable Control, Adaptive Control, Applications. Springer-Verlag, 2nd edition, 1991b.
- T. Kailath. *Linear Systems Theory*. Prentice Hall, Englewood Cliffs, New Jersey, 1980.
- H. Kwakernaak and R. Sivan. *Linear Optimal Control Systems*. Wiley-Interscience, New York, 1972.
- O. Levenspiel, editor. *Chemical Reaction Engineering*. Wiley, 3rd edition, 1999.
- W.S. Levine, editor. *The Control Handbook*. CRC Press, Boca Raton, Florida, 1996.
- C.F. Lin. *Advanced Control Systems Design*. Prentice Hall, Englewood Cliffs, New Jersey, 1994.
- D.G. Luenberger. *Introduction to Dynamic Systems. Theory, Models and Applications*. Wiley, New York, 1979.
- W. L. Luyben. *Process Modeling, Simulation, and Control for Chemical Engineers*. McGraw-Hill, New York, 1990.
- T.E. Marlin. *Process Control. Designing Processes and Control Systems for Dynamic Performance*. McGraw-Hill, Boston, 2000.
- R.H. Middleton and G.C. Goodwin. *Digital Control and Estimation*. Prentice Hall, Englewood Cliffs, 1990.
- K. Ogata. *Discrete-Time Control Systems*. Prentice Hall, Englewood Cliffs, New Jersey, 1987.
- K. Ogata. *Modern Control Engineering*. Prentice Hall, Englewood Cliffs, New Jersey, 1997.
- R.H. Perry. *Perry's Chemical Engineers' Handbook*. McGraw-Hill, New York, 6th edition, 1973.
- W.H. Ray and B.A. Ogunnaike. *Process Dynamics, Modeling and Control*. Oxford University Press, 1994.
- W.H. Ray and J. Szekely. *Process Optimization with Applications in Metallurgy and Chemical Engineering*. Wiley, New York, 1973.

- K. Schittkowski. NLPQL: A Fortran subroutine solving constrained nonlinear programming problems. *Ann. Oper. Res.*, 5:485–500, 1985.
- D.E. Seborg, T.F. Edgar, and D.A. Mellichamp. *Process Dynamics and Control*. Wiley, New York, 1989.
- S.M. Shinnars. *Modern Control System Theory and Design*. Wiley, New York, 1992.
- F.G. Shinskey. *Process Control Systems*. McGraw-Hill, New York, 1979.
- N.K. Sinha and G.P. Rao, editors. *Identification of Continuous Time Systems. Methodology and Computer Identification*. Kluwer Academic Publishers, Dordrecht, 1991.
- G. Stephanopoulos. *Chemical Process Control, an Introduction to Theory and Practice*. Prentice Hall, Englewood Cliffs, New Jersey, 1984.
- H. Unbehauen and G.P. Rao. *Identification of Continuous Time Systems*. North Holland, Amsterdam, 1987.
- J. Villermaux. *Génie de la Réaction Chimique*. Lavoisier, Paris, 1982.
- E. Walter and L. Pronzato. *Identification of Parametric Models from Experimental Data*. Communications and Control Engineering. Springer-Verlag, London, 1997.
- K. Watanabe. *Adaptive Estimation and Control*. Prentice Hall, London, 1992.
- W.A. Wolovich. *Automatic Control Systems, Basic Analysis and Design*. Holt, Rinehart and Winston, New York, 1994.
- P.C. Young. Parameter estimation for continuous time models. A survey. *Automatica*, 17:23–39, 1981.
- C. Zhu, R.H. Byrd, P. Lu, and J. Nocedal. L-BFGS-B: a limited memory FORTRAN code for solving bound constrained optimization problems. Technical report, NAM-11, EECS Department, Northwestern University, 1994.



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