Dynamic system modeling for control and diagnosis

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Contents

Chapter 1

Introduction

Most of the advanced control and diagnosis methods are based on dynamic models of different kinds, therefore the efficient construction of dynamic models is a key limiting factor in these activities. Despite of this fact, there has often been a lack of modeling expertise, because model building requires a strongly interdisciplinary background that includes not only a deep understanding of the application field and systems and control theory but also some knowledge of applied mathematics and numerical analysis.

Not only the process of constructing a "good" dynamic model is difficult, but either there exists no general agreement on what "good" means in this context. That is why the "best engineering practice" in model development has been worked out for process system models [7], and adopted to the wide class of dynamic models based on first engineering principles in this book. Here we discuss (thermal) energy, mechanical, electrical and (bio)chemical dynamic system models and the combination of these, like thermo-mechanical models.

Because of its inherent complexity and difficulty, model building on an advanced level is sometimes considered as art. This highlights that teaching someone how to construct a good model is even more difficult and cannot be done by giving simple instructions. Instead, the principle of "learning by doing" and following an expert's activity in one's model building process is to be followed [1]. Therefore, this book provides numerous worked out examples of constructing simple dynamic models for energy, mechanical, electrical, (bio)chemical and mixed (like thermo-mechanical, bio-mechanical etc.) systems.

This book is written as a textbook for an MSc course in constructing dynamical models for control and diagnostic processes, where students in information technology take part. Therefore, basic knowlege in systems and control theory and applied mathematics is expected, and only a solid background in highschool physics is assumed. The material consists of a general part dealing with dynamic system modeling for control and diagnosis in all application fields (this includes chapters 2-5, and chapters 8-9), while the material presented in chapters 6 and 7 can be included or omitted depending on the focus of the course and its audience. Some of the more complex examples are given only for the sake of the

most interested and motivated students, they can also be omitted or replaced by simple ones when needed.

We hope that not only the students will find our book a useful help in their course work and self-study, but also our colleagues can use the book or its parts in their teaching activity, too.

The material in this book is based on joint work with a number of colleagues over the years who are (in alphabetical order) Piroska Ailer, Ian Cameron, Dávid Csercsik, Csaba Fazekas, Attila Fodor, Attila Gábor, Attila Magyar, Erzsébet Németh and Gábor Szederkényi. Their contribution and support is gratefully acknowledged.

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Chapter 2

Dynamic modeling based on first engineering principles

Although it is widely believed that constructing a good model is "an art", but there are powerful aid the modeler can rely on. If one wants to build a model of an engineering object, a so called engineering system, that the basic principles that govern the behavior of the system can be and should be used.

Furthermore, model building is also an engineering activity, a construction, for which "best engineering practices" have already been developed and successfully applied (see for example [7]).

This chapter provides an introduction to the modeling problem itself by describing and discussing its basic ingredients, and gives a brief introduction to the notions and tools of systems and control theory that will be used throughout the book.

2.1   The modeling problem

It is intuitively clear that one should give the object to be described if a model is to be constructed. It is less obvious that one should in addition specify the intended use of the model, that is the *modeling goal*. This section describes the basic ingredients of the modeling problem specification that are based on the notion of the model.

This implies that a *general problem statement* should include two given items

- the object (system) to be modeled,

- the modeling goal.

2.1.1   The notion of model

Real objects – for example trains, large equipment, the Sun or a lake – are most often too large, too expensive or simple unique to perform experiments on them

if one wants to understand their sometimes complex behavior or to design an action or a controller for a given purpose. Therefore, we apply substitutes – these are called *models* – that are

- simpler, less complex, less expensive and more handy, but

- describe only certain aspects of the behavior that are relevant for the given purpose.

It is important to emphasize that there is no point in constructing a model that describes the original object in full details, but we have to extract those properties of the object that we are interested in and model only those.

Models can have very different nature. *Physical models* implement the behavior of the original object, for example a locomotive, using different physical phenomena. This is the case, when an electrical circuit model of the locomotive is constructed. *Mathematical models* use different mathematical objects, for example equations or graphs, to describe the behaviour of a physical object.

Different models of the same object   Fig. 2.1 shows a picture of an old fashioned a coffee machine that can be modeled for different purposes.

Figure 2.1: The coffee machine

Some of these models are shown in Fig. 2.2. The first model in the sub-figure 2.2(a) is a flow-sheet that describes the coffee machine qualitatively from the viewpoint of its operation, the inlet of the cold (with the flow rate v_I) and outlet of the hot water (with the flow rate v_O) and the electrical heating (coil icon). The second model in the sub-figure 2.2(b) is even more simplified. Here the model is in the form of a graph that shows the effects between the variables (temperature T, level h, valve positions k_I and k_O and heating switch k_H). The most widespread form of mathematical models – that is also used almost exclusively in this book – is the form of differential and algebraic equations. Fig. 2.2(c) shows a simple mathematical model of the coffee machine. Here

the details of the nice shape of the coffee machine and its sub-equipment are completely neglected, but a cylinder shape with constant cross-section A is assumed.

(a) flow-sheet

(b) structure graph

(c) mathematical model

$$\frac{dh}{dt} = \frac{v_I}{A}k_I - \frac{v_O}{A}k_O$$
$$\frac{dT}{dt} = \frac{v_I}{Ah}k_I(T_I - T) + \frac{Q_H}{c_P\rho Ah}k_H$$
$$h(0) = h_0, T(0) = T_0$$
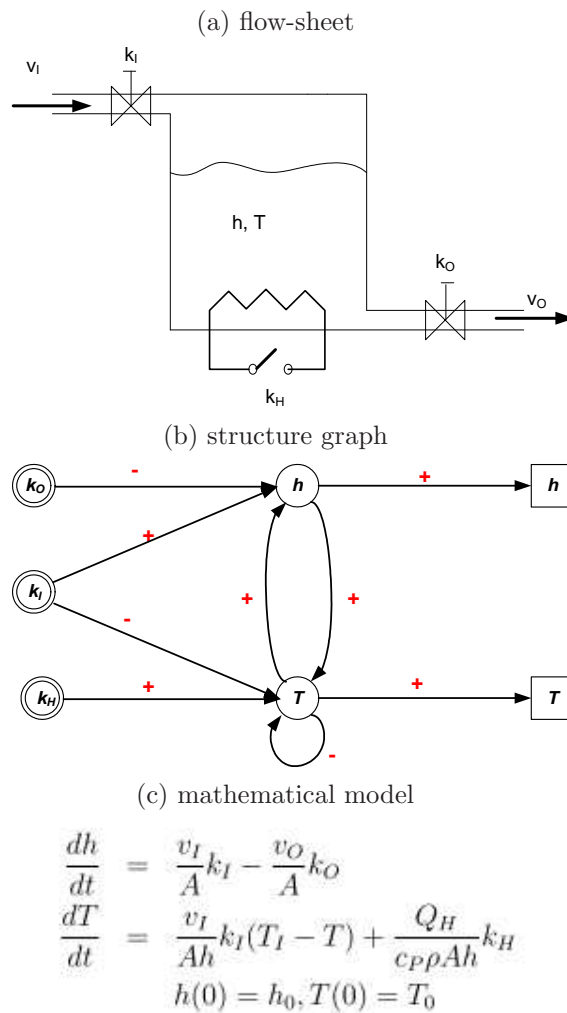
Figure 2.2: Different models of the coffee machine

2.1.2 Specification of the object to be modeled

The object to be modeled is usually described in a verbal way. However, a more precise specification is required in most of the cases. This is especially needed when we develop models *for control and/or diagnostic purposes*, when the time-
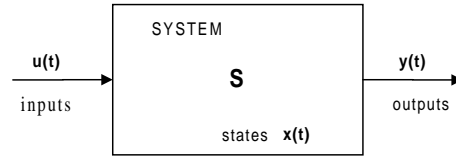
Figure 2.3: The signal flow diagram of dynamic systems

dependent, i.e. dynamic behavior of the object is of primary importance. In this case the notions and descriptor forms of systems theory [9] can be applied and *the object is simply regarded as a system.*

"System" is a basic notion in system theory that means an object that has a time-dependent behavior. A system is specified by giving its boundaries, that is used to decide if anything belongs to the system or (alternatively) to its environment: a similar concept to the specification of a set.

A system interacts with its environment through *signals*, that are time-dependent functions. The *input signals* of the system describe the effect of the environment to the system, and act as cause for the system behavior. The reaction (i.e. back-effect) of the system to its environment is described by the *output signals*. Usually, a set of auxiliary signals called *state signals* used for the mathematical descriptions are also defined.

Fig. 2.3 depicts the *signal flow diagram* of a system, where the system is denoted by a rectangle, and signals are denoted by arrows.

The above implies that a *system specification includes not only the system boundary definition, but also the description of the potential system inputs and outputs*, that is the interaction with its environment.

2.1.3   The modeling goal

As it has been emphasized before, the modeling goal constitutes an important part of the modeling problem description together with the system specification.

In various engineering sciences one can find quite similar and typical *modeling goal type*s. The most important and relevant modeling goals are listed below.

- *Dynamic and static (steady-state) simulation*
  Simulation is a "classical" modeling goal, that is applied when one wants to make experiments with the model to test its behavior in different circumstances. Here we assume that a complete and validated system model is available. The static simulation is used for determining the steady-state static values of some (state and output) signals if the input signal values are given. In the dynamic cases it includes dynamic prediction and also "what-if" type dynamic analysis with different given hypothetical inputs to the system. Dynamic simulation is also used as an auxiliary sub-task in process control problems.

- *System design*
  This is also a traditional task, the inverse problem of simulation in a wide sense. Here one assumes that the set of possible system elements are given with their parameters (such as types or sizes) to be determined during the design, such that the design specification, i.e. expected input-output behavior of the system is met.

- *Process control*
  This type of modeling goal requires having a complete and *validated dynamic system model* together with a control aim, i.e. an expected way of system behavior. These are used to develop a method (algorithm, procedure etc.) that makes the system behave as expected, i.e. to fulfill the control aim. As a complete and validated dynamic model is rarely available or it may change in time or under disturbances, there are auxiliary tasks – that generate corresponding modeling goals – in process control [9]. These include dynamic prediction, regulation, optimal control, identification, diagnosis, etc.

More about the process control related modeling goals follow in subsections 2.2.2 and 2.2.3.

The importance of modeling goal becomes apparent, if one considers the effect of the modeling goal on the properties of the model to be developed.

- The modeling goal determines the (validity) domain of the model.

- In addition, the modeling goal influences the following model properties.

  - It indicates which mechanisms should be taken into account.
  - It determines the mathematical form (algebraic equations, differential equations, graphs, etc.) of the model.
  - The accuracy of the model, that is, the accuracy of the characteristic variables is also determined by the modeling goal.

2.2 Control or diagnosis as a modeling goal

This section describes the required model properties that control or diagnosis put on the model as a modeling goal. For this purpose, first we briefly recall some basic notions in systems and control (see e.g. [9] for more details), thereafter the specialties of control and diagnosis as modeling goal are given.

2.2.1 Basic notions in systems

The basic notions about systems and their signals have already appeared in subsection 2.1.2, when the specification of the modeling object as system were described.

Dynamic model types

Systems can be classified according to the type of their signals, and to the type of the signal transformation they represent. A signal $u(t)$ can be

- continuous time signal if $t \in \mathcal{T} \subseteq \mathbb{R}$ or discrete time signal if $t \in \mathcal{T}_Z \subseteq \mathbb{Z}$,

- scalar $(u(t_0) \in \mathbb{R})$ or vector-valued $(u(t_0) \in \mathbb{R}^n)$,

- a function of position, too, e.g. $u(x, t)$.

In this book we only consider position-independent (i.e. purely time-dependent) signals, that give rise to *concentrated parameter systems*.

State space models   State space models are widely used in model-based control and diagnosis. This type of dynamic models uses all the three categories of signals belonging to a system: its inputs, outputs and states.

A state space model consists of two equation types:

- *state equations* are dynamic (differential or difference) equations that describe the evolution of the state variables as functions of input variables,

- *output equations* are algebraic equations, they give the value of the output signals at any given time as a function of the state and input variables at the same time.

The simplest state space model of concentrated parameter continuous time linear time-invariant (LTI) systems shows the above structure

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) \qquad \textit{(state equations)} \\ y(t) &= Cx(t) + Du(t) \qquad \textit{(output equations)} \end{aligned} \tag{2.1}$$

with

- given initial condition $x(t_0) = x(0)$ and $x(t) \in \mathbb{R}^n$,

- $y(t) \in \mathbb{R}^p$, $u(t) \in \mathbb{R}^r$, and

- system parameters

$$A \in \mathbb{R}^{n \times n} , \ B \in \mathbb{R}^{n \times r} , \ C \in \mathbb{R}^{p \times n} , \ D \in \mathbb{R}^{p \times r}$$

Most of the engineering systems, however, are not linear and not necessarily time-invariant, therefore nonlinear state space models of concentrated parameter systems are used in the following general form

$$\begin{aligned} \dot{x}(t) &= \widetilde{f}(x(t), u(t)) \qquad \textit{(state equations)} \\ y(t) &= \widetilde{h}(x(t), u(t)) \qquad \textit{(output equations)} \end{aligned} \tag{2.2}$$

with the state, input and output vectors x, u and y and with the smooth nonlinear mappings

$$\widetilde{f} \ : \ \mathbb{R}^n \times \mathbb{R}^r \mapsto \mathbb{R}^n \quad , \quad \widetilde{h} \ : \ \mathbb{R}^n \times \mathbb{R}^r \mapsto \mathbb{R}^p \ .$$

Note that *most of the controller design and diagnosis problems require a state space model* of the investigated system.

Input-output models If the dynamic model of a system is expressed as a relationship between the input and output signals and their derivatives, we call it an input-output model.

The simplest case of an input-output model arising, when one constructs a model for a discrete time linear time-invariant (LTI) single-input single-output system, is in the form of a linear difference equation:

$$y(k) + a_1 y(k-1) + ... + a_{n_a} y(k-n_a) = b_0 u(k-d) + ... + b_{n_b} u(k-d-n_b) \quad (2.3)$$

where the discrete time instance t_k is abbreviated as an integer k, and $d = n_a - n_b > 0$ is the *pole excess (time delay)*.

The above LTI input-output model can be generalized to the nonlinear case assuming a unit time delay, i.e. $d = 1$ to get the following general model form.

$$y(k) = \mathcal{F}\left(y(k-1), ..., y(k-n_a), u(k-1), ..., u(k-n_b)\right) \quad (2.4)$$

where $\mathcal{F}$ is a nonlinear function.

Note that input-output type dynamic models are used for identification (i.e. model structure and parameter estimation), and for prediction-based diagnosis (see later).

2.2.2 Problem statements and model requirements for control

The problem statement of control

If one wants to specify a control design task, two items should be given:

- *a dynamic model* of the system to be controlled,

- *a control aim*, that is an expected behavior of the system.

Based on these items the general control task is to design the input of the system in such a way that it fulfills the control aim.

Control aims The control design problems can be classified based on the control aim, that can be

- to keep the system output(s) constant at a desired level, this is called *regularization*,

- to move the state of the system from an initial point to a given target one in a time or energy optimal way, this is an *optimal control* task,

- to follow a given reference trajectory with the output(s) of the system, that is called *servo-control*, etc.
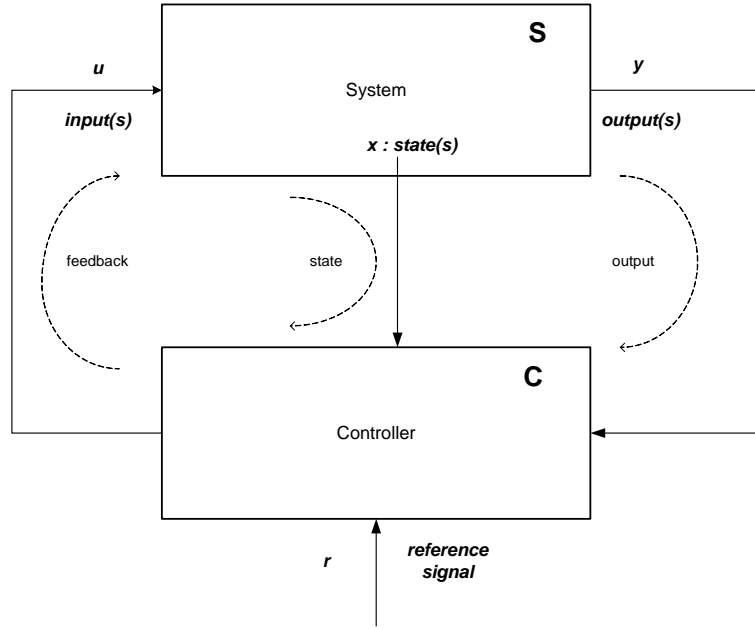
Figure 2.4: The signal flow diagram of state and output feedbacks

Feedback controllers

In the general control problem statement one has to design the complete time-dependent trajectory to the input(s) to achieve the control aim, that is a difficult mathematical task in the general case. Alternatively, one may choose to compute the value of the control input as a static or dynamic function of the state and/or the output of the system, such that

$$u(t) = \mathcal{F}_x(x(t)) \quad \text{or} \quad u(t) = \mathcal{F}_y(y(t)) \tag{2.5}$$

where $\mathcal{F}_x$ or $\mathcal{F}_y$ is a static or dynamic (containing the time derivatives of its arguments) function of a given functional form with unknown parameters. Then the controller design simplifies to computing the values of these parameters, that is usually simpler. The controllers which are based on these principles are called *state or output feedback controllers*, respectively.

Figure 2.4 illustrates the notion of state and output feedback on a signal flow diagram of the system and its feedback controller.

Model requirements

As we have seen before one needs a dynamic model for the system to be controlled together with a control aim to design a controller. Besides of its dynamic

character, the following properties are important if the model will be used for control design.

- The model should be as simple as possible, in particular the number of state variables should be kept at a minimum.

- Only approximately 5-10 % accuracy is required in the values of the signals, but the dominant time constants should be modeled in a 2-5 % accuracy.

2.2.3 Problem statements and model requirements in diagnosis

Diagnosis is a special problem class in process control, that is of great practical importance. Here we assume to have

G1: a dynamic model of the fault-less (i.e. healthy) system

G2: possibly other dynamic models that describe the system's behavior at different faulty modes,

G3: measured data from the system in unknown faulty mode.

The task is to estimate

T1: if the system is fault-less or not (this is called *fault detection* and requires only the given items G1 and G3)

T2: the faulty mode of the system (*fault isolation*).

One can use dynamic models for diagnostic purposes in two different ways. The model is either used for predicting future model outputs that is compared to the measured ones (*prediction-based diagnosis*), or the model parameters are estimated form measured data and these are compared to reference values (*identification-based diagnosis*).

Prediction-Based Diagnosis

The general problem statement of prediction-based diagnosis can be formulated as follows.

Given:

- *The number of faulty modes n_F The index $i = 0$ corresponds to the fault-free normal case.*

- *A set of **predictive system models** $(Fi, i = 1, ..., n_F)$ for the various faulty modes*

$$y^{(Fi)}(k+1) = \mathcal{M}^{(Fi)}(\mathcal{D}[1, k]) \ , \quad k = 1, 2, \ldots$$
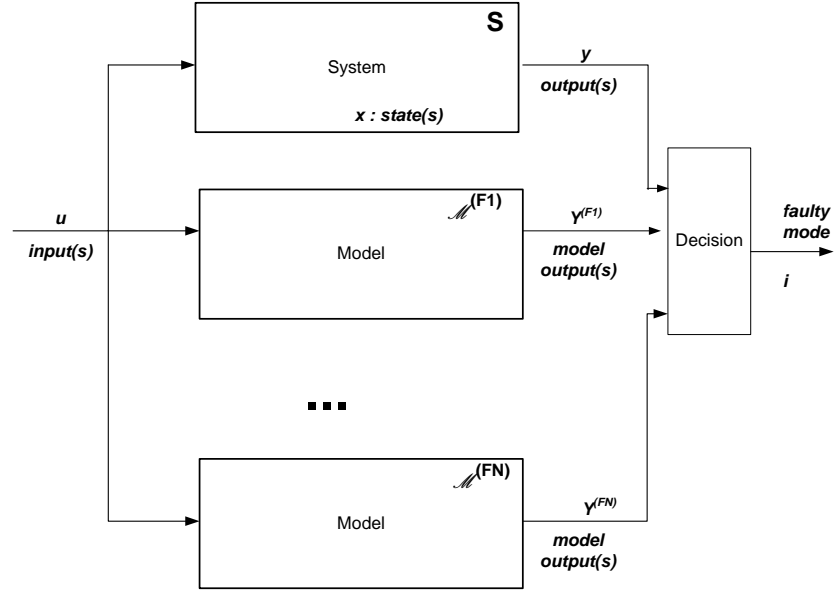
Figure 2.5: The principle of prediction-based diagnosis

- A *measurement record* containing a finite set of measured input-output pairs

$$D[1, k] = \{ (u(\tau), y(\tau)) \mid \tau = 1, \ldots, k\}$$

- A *loss functional* $J^{(Fi)}$, $i = 0, \cdots, n_F$

$$J^{(Fi)}(r^{(i)}, u) \;\; = \;\; \sum_{\tau=1}^{k} [\; r^{(i)T}(\tau) Q r^{(i)}(\tau)\;]$$

with $r(\tau) = y(\tau) - y^{(Fi)}(\tau)$ being the *residual* signal, and Q is a positive symmetric weighting matrix.

Compute:
The faulty mode of the system being the model index i that minimizes the loss function subject to model equations.

The principle of prediction-based diagnosis is depicted in Fig. 2.5 as a signal flow diagram.

Identification-Based Diagnosis

The identification-based diagnosis uses the estimated model parameters to derive diagnostic conclusions therefrom according to the following problem statement.

Given:

- *The number of faulty modes n_F* The fault index $i = 0$ corresponds to the normal operation.

- *A set of predictive **parametrized system models** for the various faulty modes*
$$y^{(Fi)}(k+1) = \mathcal{M}^{(Fi)}(\mathcal{D}[1,k];\ p^{(Fi)})\ , \quad k = 1, 2, \ldots$$

- A *measurement record* with the measured input-output pairs
$$D[1,k] = \{\ (u(\tau), y(\tau) \mid \tau = 1, \ldots, k\}$$

- A *loss functional $J^{(Fi)}$, $i = 0, \ldots, n_F$* depending on the parameters $p^{(Fi)}$
$$J^{(Fi)}(p^{(estFi)} - p^{(Fi)})\ =\ \rho^{(i)T}Q\rho^{(i)}\ , \quad \rho^{(i)} = p^{(estFi)} - p^{(Fi)}$$

Compute:
The faulty mode of the system being the model index i that minimizes the loss function subject to model equations.

2.3 Mechanisms and related phenomena

Dynamic models can be constructed in two principally different ways that define the basic model categories.

- Models can be *based on first engineering principles*, when the model equations are constructed from the usual equations of the engineering disciplines, such as thermodynamics, mechanics, electrical engineering etc. Here we collect all of the important (from the viewpoint of the modeling goal) physical and chemical phenomena – that are called *mechanisms* – and describe them individually assuming some basic additivity among them.

- There are also *data-driven* models, that use a general descriptive model form – such as polynomials, for example – the parameters of which are estimated using measured data.

The first category of models is also called *white-box models*, while the second is the category of *black-box models*.

Mechanisms and system classes   Within the category of models based on first engineering principles we shall form different model classes based on the main and most important mechanisms taking place in them. This way we should distinguish

- mechanical systems (chapter 6),

- thermodynamical (process, energy) systems (chapter 5),

- electrical systems (chapter 6),

- chemical systems (chapter 7),

- biological systems, etc.

There are also "mixed" system classes, such as bio-chemical or thermo-mechanical systems, that will also be included in the material of this book.

The above system classes and their modeling specialties will be described in details in separate chapters that are indicated in brackets in the above list.

Chapter 3

The modeling procedure

This chapter gives a birds' eye overview of the "good engineering practice" of how dynamic models based on first engineering principles are constructed. This is given in the form of a modeling procedure [7] that consists of seven steps.

3.1   The steps in the 7 step modeling procedure

The modeling process is started when a modeling problem is given by describing the object of the modeling and the modeling goal (see in section 2.1).

Fig. 3.1 depicts the steps of the modeling procedure in the form that also indicates the workflow of the modeling procedure itself. The steps can be grouped into three phases of the modeling process as follows.

- *Preparatory steps*
  These prepare the model construction by formalizing the modeling problem statement, by exploring the mechanisms to be included in the model and by collecting data for the model.

- *Model construction and solution*
  These related steps are only considered traditionally as parts of the modeling procedure.

- *Model refinement and checking*
  The steps of model verification, calibration and validation belong here, that are essential to ensure that the model fits to the modeling goal. These steps control the quality of the model, and as a result - in the case of any problems - the revisit of previous steps may be needed.

It is apparent from Fig. 3.1, that the steps of the procedure are usually not executed in a purely sequential way. The results of a particular step may require revisiting an earlier step and improving its outcome. Therefore, the modeling is rather an iterative activity that gradually improves the model than a "one shot" sequential procedure.
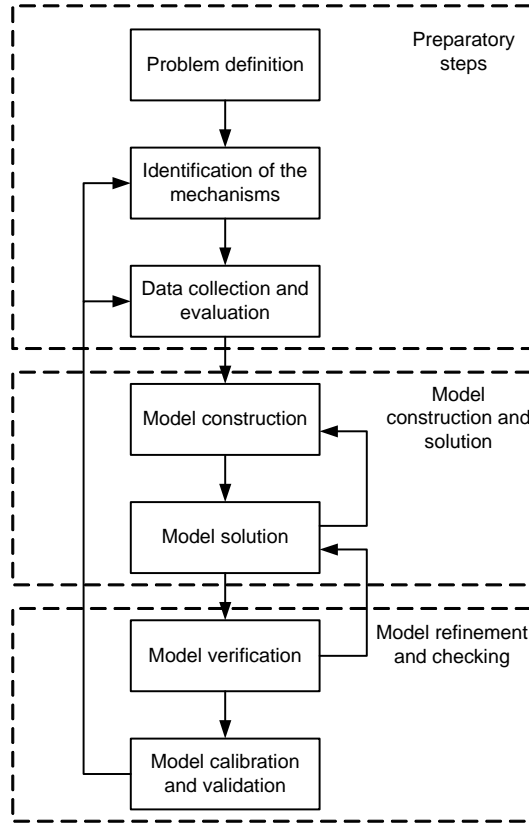
Figure 3.1: The 7 step modeling procedure

3.2 Brief description of the steps

In this subsection we briefly describe in some more details the activity or sub-steps that are needed when performing a certain step of the modeling procedure. The naming of the steps follows the box labels of the steps in Fig. 3.1.

1 Problem definition
This step is dedicated to the formal description of the modeling problem statement and results in the

- system specification
- modeling goal determination
- flow-sheet construction (indicating the equipment and the major variables)

2 Mechanisms identification
Based on the system specification and taking into account the modeling

goal, we should collect the list of phenomena (e.g. convection, transfer, reaction, evaporation) that will be described by the model.

3 Data collection and evaluation
This is a key preparatory step, the result of which may determine the level of details and/or the mechanisms that one can include into the model by excluding certain model elements we do not have any information about. Here we search for and collect any data about the system to be modeled in the following data sources.

- *Constants from data tables* are often available either on the web (see for example [13]) or in engineering handbooks or reference sources (e.g. [10]). Here the key aspect is the accuracy of the available data that may be as large as 50 % for some of the data types (for example reaction kinetic data).

- *Properties of equipment and operation* are contained in equipment documentation and operating manuals. These are also valuable data sources containing sizes and types of the equipment and data of their normal and faulty operation.

- Often there are preliminary *measured data* available that are measured on laboratory size or pilot plant equipment. While these contain valuable information about the modeled system, these should be taken with care of the differences between the real and this preliminary operation circumstances.

4 Model construction
This is perhaps the most critical step that is directed towards constructing a complete model that is well specified (i.e. mathematically solvable) and contains all ingredients that document the modeling decisions. The next chapter 4 is fully devoted to the sub-steps of this step and to the description of the ingredients of a properly developed model. Briefly, the sub-steps that are necessary to perform here are as follows:

- determination of balance volumes,

- formulation of modeling assumptions,

- construction of model equations (conservation balances, constitutive equations),

- determination of initial and boundary conditions.

5 Model solution
In this step one needs to find (or in the worst case develop) a mathematical method or procedure that provides the solution of the complete and mathematically well posed model originating from the previous step. The sub-steps of this step are as follows:

- *Implementation of or recasting a solution method* is relatively straight-forward for concentrated parameter dynamic models that are in the mathematical form of ordinary differential and algebraic equations that form an initial value problem. More details about solving this model class are given in [5].

- Together with finding a model solution method, one needs to perform rough *model checking* to collect information about the plausibility (for example positivity of the variable trajectories) and the accuracy of the solution. Problems found in this sub-step may require to revisit the model construction step 4, in order to correct possible mistakes or to find an alternative, more favorable model form.

6 Model verification
Model verification constitutes an important draft checking of the newly developed model to find out if its properties correspond to that of the modeling object. Here we may

- verify qualitative model behavior against engineering intuition (for example the qualitative properties of step responses),

- check dynamic properties (e.g. stability, controllability or observability) on the model.

Chapter 8 is devoted to the methods and possible results of model verification.

7 Model calibration and validation
The methods of model calibration and validation are strongly related, as they both use measured data from the modeled system and a system model to conclude on some properties of the model.

- *Model calibration* deals with *estimating unknown/uncertain model parameters using measured data.*

- *Model validation* compares the final model and the real system (measured data) using statistical methods in order to decide if it fits to the modeling goal, i.e. it is able to predict or compute the value of the important key variables in a satisfactory manner. This is also a control step, that may require revisiting some of the earlier steps in the case of unsatisfactory results.

The problems and applicable methods of model calibration and validation are described completely in chapter 9.

Chapter 4

Model equations and their construction

A key step in the 7 step modeling procedure (see in section 3.1) is the 4th step "Model construction". Because of its importance, we devote a separate chapter to this step that presents a sub-procedure of how to construct the equations and other ingredients of a mathematical model based on first engineering principles.

4.1 Conservation balances

Dynamic models based on first engineering principles are built upon the principles of conservation. From elementary physics we know that certain quantities, such as the overall mass or the internal energy of a closed system remain unchanged: this is stated by the corresponding *principle of conservation*, for example mass conservation. It is called principle, because we cannot prove it (neither experimentally, nor theoretically), but no counter-example has ever been found.

4.1.1 Balance volumes and equations

Balance volumes We start developing conservation balance equations by defining the so called *balance volumes*. These are fixed or variable size parts of the system over which conservation balances can be constructed. These are

- most often with *constant volume*, and

- usually *perfectly stirred*, that result in concentrated parameter or lumped systems. The conservation balance equations for this type of balance volumes are in the form of ordinary differential equations.

Conserved (extensive) quantities It is well known that only extensive quantities, that are added together when joining separate sub-systems are con-
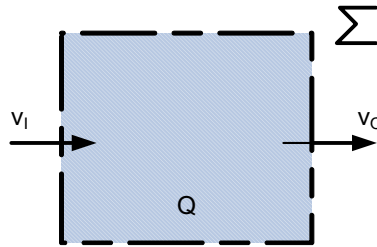
Figure 4.1: A simple balance volume with a convective in- and out-flow and a source

served. Some of the extensive quantities for which conservation principles can be applied are as follows:

- overall mass,

- energy (enthalpy, internal energy),

- component masses,

- momentum, angular momentum,

- electric charge, etc.

Note that the different types of engineering systems (such as energy or chemical systems) have characteristic conserved quantities associated to them.

Dynamic conservation balance   Assume a single perfectly stirred balance volume that is *not closed*, but has convective in- and out-flows as connection with its environment. The convective flows are characterized by the property, that their center of mass is moving with time. Then the general form of the conservation balance equation for a conserved quantity can be written as

$$
\left\{ \begin{array}{c} rate\ of \\ change \end{array} \right\} = \left\{ \begin{array}{c} in\text{-} \\ flow \end{array} \right\} - \left\{ \begin{array}{c} out\text{-} \\ flow \end{array} \right\} \begin{array}{c} + \\ - \end{array} \left\{ \begin{array}{c} source\ \} \\ \{\ sink\ \} \end{array} \right. \tag{4.1}
$$

A simple example of a balance volume with a convective in- and out-flow and the source can be seen in Fig. 4.1

Given the problem statement and the flowsheet of the modeling task, it is usually a simple sequential procedure to identify the relevant balance volumes. The steps of the determination procedure of the possible balance volumes in case of a simple example are shown in details in the animation

balance volume determination

4.1.2 Intensive quantities

Beside of extensive quantities for which balance equations are conserved, intensive quantities are also playing a fundamental role in model development. *Intensive quantities* are not added but they *equilibrate when joining sub-systems.*

The following characterizing properties make the intensive variables important for modeling.

- Intensive quantities (such as temperature, pressure, concentrations) are usually easily *measurable.*

- They are potential (driving force) type quantities that drive diffusive flows and transfer between phases (see details later in chapter 5 dealing with energy systems).

- There exist pairs of extensive and intensive variables that are related to each other algebraically, and the intensive variable acts as a driving force variable for the flow of its extensive variable pair. These pairs are as follows:

    – overall mass $m \leftrightsquigarrow$ pressure p

    – energy $U \leftrightsquigarrow$ temperature T

    – component mass $m_X \leftrightsquigarrow$ concentration c_X (or more generally chemical potential)

Extensive - intensive relationships   As mentioned before, there exist algebraic relationships between the extensive and intensive variables of such pairs. These relationships form an important class of the algebraic constitutive equations (see later in section 4.2). Below we list the two most important ones in their most simple form that are used to develop the intensive variable form of conservation balance equations:

- $U = c_p m T + U_0$ (where c_p is the specific heat, U_0 is the reference value at $T = 0^o C$ and the temperature T is measured in $[^o C]$)

- $m_X = \frac{m}{\rho} c_X$ (where ρ denotes the density and the concentration c_X is measured in $[kg/m^3]$ component)

4.1.3 Dynamic conservation balance for the overall mass

The overall mass balance is the basic conservation balance equation of any dynamic system. Some of its terms may induce related terms in other conservation balance equations, for example convective in- or outflow terms require the presence of corresponding convective in- or outflow terms in energy balance equations.

The special properties of the overall mass balance equation are as follows:

- There is **no source/sink** term in the equation if the underlying balance volume has only boundaries with the environment, otherwise mass transfer through phase boundaries (such as evaporation, for example) may appear as a source/sink term.

- The overall mass m is measurable (e.g. through level measurement), therefore there is usually no need to transform it to its intensive variable form. In some cases, however, we transform it to the intensive variable form using e.g. the ideal gas law to have the pressure p as its characterizing intensive variable pair.

- For perfectly stirred balance volumes the in- (v_I) and out-flows (v_O) are mass flows measured in e.g. $[kg/s]$.

Example   The simplest example is the mass balance equation for the perfectly stirred balance volume in Fig. 4.1:

$$\frac{dm}{dt} = v_I - v_O \qquad (4.2)$$

4.1.4   Dynamic conservation balance for energy

Energy conservation balance equations are characteristic to thermodynamical and energy systems, but they play role in almost every system model. They are closely related to mass balance equations through their convective terms in these systems. In the case of "mixed" type systems, such as thermo-mechanical ones, the models are usually coupled through the joint energy balance equation.

The characteristic properties of dynamic energy conservation balances are as follows:

- There are usually source/sink terms present in the equation that correspond to external (e.g. electrical) heating/cooling, heat transfer Q ($[J/s]$), chemical reaction enthalpy, etc.

- For perfectly stirred balance volumes the convective in- ($c_{pI}v_I T_I$) and out-flows ($c_p v_O T$) are energy flows expressed in unit $[J/s]$.

- The energy U is directly **not** *measurable*, we use the temperature T instead of it in the equation. Therefore, there is a need to transform the equation into an intensive variable form.

A more detailed discussion of the energy conservation balance equation and its transformation to intensive variable form can be found later in section 5.3.

Example   The related energy balance equation to the mass balance equation (4.2) for the perfectly stirred balance volume in Fig. 4.1 can be written in the following form:

$$\frac{dU}{dt} = c_{pI}v_I T_I - c_p v_O T \pm Q \ . \qquad (4.3)$$

4.2 Constitutive equations

As it has already appeared before, there are usually algebraic equations that we can use to develop a more useful form of the balance equations (for example their intensive variable form). In addition, the describing equations of various mechanisms that appear as source/sink terms in the balance equations are also in algebraic form.

These different, usually algebraic further equations that are *necessary to complete the model are called constitutive equations*. According to their origin, the constitutive equations can be of the following most common types:

- extensive-intensive relationships,

- transfer rate equations,

- thermodynamical relationships,

- balance volume relations,

- equipment and control relations.

As most of the constitutive equations are associated with a certain family of mechanisms, the different classes of engineering systems (e.g. energy, mechanical, electrical etc.) have a characteristic set of constitutive equations. Therefore, the more detailed description of the above constitutive equation types will follow in later chapters.

4.3 Modeling assumptions

Modeling assumptions are very important ingredients of dynamic models as they *document the decisions that are taken when developing the model* from the problem statements and from first engineering principles. These assumptions are not expressed in the form of equations, but in the form of logical statements about the model equations, their terms, variables and parameters.

It is important to emphasize, that these assumptions are closely related to the set of model equations, and part of them can in principle be reconstructed from the developed model, but they are an integrated part of the model itself.

As we will see later, the list of modeling assumptions should be *collected incrementally* during the modeling procedure.

Modeling assumption types There are general type modeling assumptions that are applicable to any modeling problem, but the great majority of them are strongly problem and system type specific. Below is the list of the most common modeling assumption types together with a few examples:

- assumptions on the *time-dependent behavior* of the (sub)systems or mechanisms
  (e.g. the behavior of the liquid is dynamic, the gas phase is in steady-state)

- assumptions on the *balance volumes*
  (e.g. the tank contains only fluid phase, there is both vapor and liquid phase present in the container)

- assumptions on the *spatial distributions*
  (e.g. the balance volume is perfectly stirred or concentrated parameter)

- assumptions on the *presence/absence of properties or mechanisms*
  (e.g. there is no evaporation, linear heat transfer is assumed)

- assumptions on the *negligible effects*
  (e.g. the density depends only on the temperature T but not on the pressure p, the specific heat c_P is constant)

- assumptions on the domain of state variables, and on the required accuracy
  (e.g. the temperature T is between 30 and 40 ^oC)

4.4   Ingredients of a model

The above sections gave the description of the various ingredients of a model (conservation balance equations, constitutive equations, modeling assumptions) in details. This section summarizes the list of the necessary ingredients of a model and the way how these are collected.

Sub-procedure for developing the model ingredients   Fig. 4.2 depicts the steps and connections of developing a dynamic model from the problem statement and from first engineering principles. The sub-procedure is sequential in its steps except for the development of the modeling assumptions that are made and collected incrementally at each sub-procedure steps.

The list of model ingredients   As the result of the above model constructing sub-procedure and that of the preliminary modeling procedure steps one can develop a complete dynamic model that consists of the following elements:

S1: System description (flow-sheet, variables)

S2: Modeling goal description

Me: List of considered mechanisms

Bv: Balance volumes description that are indicated on the flow-sheet

As: List of modeling assumptions

Me: Model equations (conservation balance equations, constitutive equations, initial and boundary conditions)

Vp: List of model variables and parameters

Da: List of model data (with describing the data, its unit, source and accuracy)
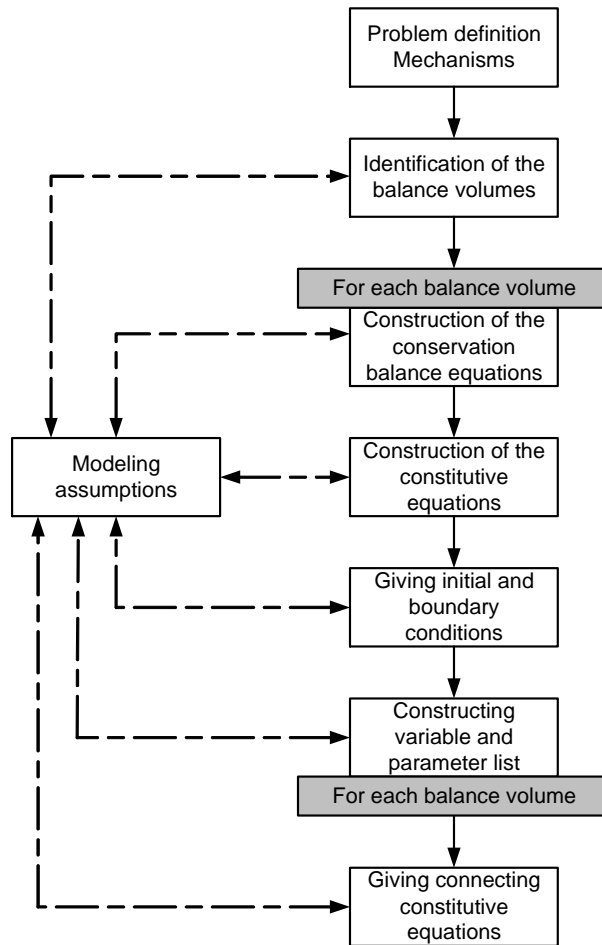
Figure 4.2: The sub-procedure of developing the model equations
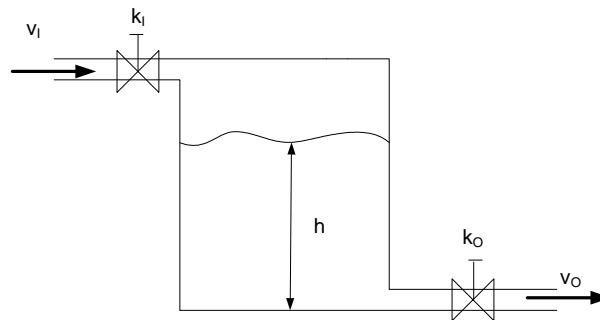
Figure 4.3: Flowsheet of the tank

4.5   Example: tank with gravitational outflow

In this section a simple dynamic model is developed for a tank in order to illustrate how the ingredients of a model look like.

4.5.1   Problem description

Given a tank with constant cross section that is used for storing water. The water flows into the tank through a binary input valve, the outflow rate is driven by gravitation, i.e. depends on the water level in the tank, but it is controlled by a binary output valve.

Construct the model of the tank for diagnostic purposes if we can measure the water level and the status of the valves.

The flow-sheet of the tank with the most important variables is shown in Fig. 4.3.

4.5.2   Mechanisms and modeling assumptions

Mechanisms

- in- and out-flow (v_I and v_O are mass flow-rates measured in $[kg/s]$)

- gravitational outflow (driven by the hydro-static pressure)

Modeling assumptions

F1 one balance volume (the tank) perfectly stirred (see in Fig. 4.4)

F2 only water is present (only overall mass balance is considered)

F3 gravitational outflow

F4 constant cross-section A

F5 density (ρ) is constant
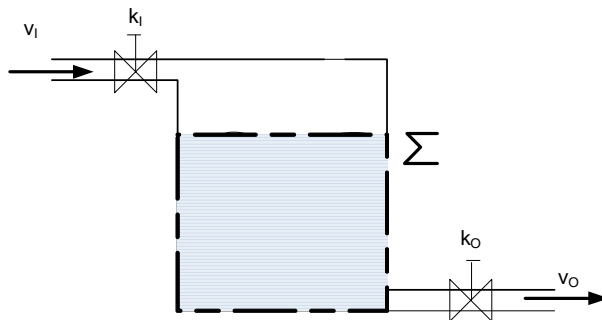
Figure 4.4: The balance volume for the tank model

4.5.3   Model equations

Conservation balance equation   It is constructed for the overall mass m

$$\frac{dm}{dt} = v_I - v_O \tag{4.4}$$

Constitutive equations

- $m = A \cdot h \cdot \rho$ (water level h is measurable)

- $v_I = v_I^* k_I$ (v_I^* is the maximal constant mass flow-rate, valve status k_I is measurable)

- $v_O = k_O \cdot \sqrt{2gh}$ (gravitational outflow, g is the gravitation constant, valve status k_O is measurable)

Model equation with measurable variables

$$\frac{dh}{dt} = \frac{v_I^*}{A\rho} k_I - \frac{\sqrt{2g}}{A\rho} \sqrt{h} \cdot k_O \tag{4.5}$$

State-space model form

- state variable: water level h

- input variables: status of the valves k_I and k_O

- output variable: water level h

The steps of the sub-procedure of developing the model ingredients are shown in details in the animation

developing the model of the tank with gravitational outflow

Chapter 5

Dynamic models of energy systems

5.1 Energy systems

The main function of energy systems in a wide sense is to generate, transfer, distribute and store energy in various forms. Thermal energy – commonly called as heat – plays a central role in energy processes, therefore, this chapter focuses on the modeling aspects of thermal energy systems.

Some practically important systems fall within the class of thermal energy systems, that include power plants, buildings, heating and cooling systems etc. Therefore, the modeling case studies were mainly chosen from this application area.

The foundations of modeling thermal energy systems can be found in thermodynamics augmented with the principles of engineering heat processes. Therefore, the basic principles of thermodynamics are briefly summarized after giving a short characterization of thermal energy systems.

5.1.1 Characterization of thermal energy systems

Naturally, the processes and mechanisms related to mass and energy conservation are of great importance in thermal energy systems. Conservation balances are constructed for balance volumes that are the objects to be modeled: these are parts of the dynamic system with homogeneous phase conditions (e.g. containing only water, or steam etc.).

In thermal energy systems we usually *assume that the chemical composition of the system and its subsystems remain unchanged during the dynamics.* If this is not the case, then the principles of modeling chemical systems should be applied that will be discussed in a later chapter (see chapter 7).

Modeling objects

The objects of the modeling process are the *balance volumes* for which conservation balances are constructed.

The simplest elementary modeling objects are the **perfectly stirred** balance volumes. The models based on perfectly stirred balance volumes result in concentrated parameter models: these are called *concentrated parameter or lumped systems*. Because of simplicity, we only consider perfectly stirred balance volumes in this chapter.

It is important to note that spatially distributed balance volumes are also widespread in energy systems, these have distributed parameter system models [7]. There is a widely known procedure called *lumping* that can be used for approximating a distributed balance volume by a set of perfectly stirred ones.

Mechanisms

The mechanisms related to thermal energy systems include a broad variety of physical and thermal engineering processes listed below. The describing equations of these phenomena are used to construct the constitutive equations in the developed model.

- The most widespread are the convective and diffusive *transport* phenomena. In both cases the transport of mass is the primary process that may cause an "induced" transport of energy. Only convective transport can be present in lumped systems.

- *Energy transfer* takes place between balance volumes where their boundary prevents their mass to mix, i.e. it prevents any mass transport. The direct energy transfer (heating or cooling) between the balance volume and the environment belongs to this group, too.

- *Phase change processes*, like evaporation, boiling, melting, freezing etc. are also thermodynamical mechanisms.

5.2   Basic principles of thermodynamics

The basic principles important from the viewpoint of constructing dynamic models of thermal energy systems are briefly summarized in this section. The interested Reader can find a more detailed discussion of the area in e.g. [2].

5.2.1   Thermodynamical variables

The simplest situation in thermodynamical description arises when one wants to characterize a system that contains only one phase (for example gas phase or liquid phase) and this is in equilibrium. The variables that characterize this system can be of two kinds:

1. extensive quantities, that are additive when joining two subsystems of the same phase: such as mass, energy etc.

2. intensive quantities, that equilibrate when joining two subsystems of the same phase: such as pressure, temperature etc.

The so-called *canonical set of variables* is necessary and sufficient to describe the thermodynamical state of a single phase system, each such set consists of one extensive and some intensive variables. For the purpose of dynamic model building the canonical set

$$\{m, p, T, c_i, i = 1, ..., K\} \tag{5.1}$$

is most often used, where m is the overall mass of the system (an extensive quantity), p is the pressure, T is the temperature, and $c_i, i = 1, ..., K-1$ are the concentrations (in mass fraction, for example) of the K components (different chemicals) in the system.

5.2.2 The laws of thermodynamics

The foundations of describing thermal energy systems lie in the laws of thermodynamics. Thermodynamics is the discipline for studying energy, the conversion of energy between various forms and the ability of energy to do work. Four laws of it has been postulated that are numbered from the 0th to the 3rd [2]. From the viewpoint of model building the 1st and 2nd law are of importance.

The first law states that energy or matter can neither be created nor destroyed. This is a version of mass and energy conservation for thermodynamical systems that has been formulated to heat conversion machines. Equivalently the first law states, that perpetual motion machines of the first kind are impossible. Another form of the 1st law postulates that the internal energy of a system can be changed (ΔU) only by providing heat (Δq) to, or performing work (ΔW) on the system, i.e. $\Delta U = \Delta q + \Delta W$.

The second law postulates the conditions of thermal equilibrium. It states that the entropy - an extensive property of a thermodynamical system - of any isolated system not in thermal equilibrium almost always increases (i.e *never* decreases). Isolated systems spontaneously evolve towards thermal equilibrium – the state of maximum entropy of the system – in a process known as "thermalization". Equivalently, perpetual motion machines of the second kind are impossible.

5.2.3 Non-equilibrium processes

Non-equilibrium thermodynamics is a branch of thermodynamics that deals with systems that are not in thermodynamic equilibrium [11]. Note that dynamic energy systems are not in equilibrium, since they are continuously and

discontinuously subject to flux of matter and energy to and from other systems and to chemical reactions. Non-equilibrium thermodynamics is concerned with transport processes and with the rates of chemical reactions.

The second law of thermodynamics postulates the change of entropy in isolated systems, and the first step towards the realistic situation is to assume that the system is not far from its equilibrium. This approximation is used in the so called classical *irreversible thermodynamics*, and it is used to derive relationships for flows of extensive variables between subsystems that are not in equilibrium. To each of the characterizing conserved extensive quantity (overall mass, internal energy and component masses) an intensive type "driving force" or potential variable is associated, a difference of which causes a flow or transfer of its extensive counterpart. As we have seen before, the conserved extensive - potential intensive pairs are as follows:

- overall mass $m \leftrightsquigarrow$ pressures p

- energy $U \leftrightsquigarrow$ temperature T

- component mass $m_X \leftrightsquigarrow$ concentration c_X (or more generally chemical potential μ)

In classical irreversible thermodynamics a linear relationship is assumed between the flow vector of conserved extensive variables and the difference of their potentials because of the close-to-equilibrium assumption. In the simplified practical cases, however, usually a linear approximation without any cross-effects is used. This linear relationship is utilized in the transfer rate expressions (see later in sub-section 5.4.4) when constructing model of thermal energy systems.

5.3   Balance equations in energy systems

As we have already seen earlier in section 4.1, the differential equations in a dynamic model originate from conservation balances constructed for conserved extensive quantities. In energy systems these variables are the *overall mass and the internal energy for each balance volumes.*

For the sake of simplicity, *we only consider lumped parameter models here*, that is, we assume to have only *perfectly stirred balance volumes*. Furthermore, we assume constant physical properties (such as density, heat capacity etc.) in this section to make the presentation as simple as possible. The flow-sheet of the simple balance volume that will be used for illustrating the construction of balance equations for energy systems is shown in Figure 5.1.

5.3.1   Mass balances

As we have already seen in sub-section 4.1.3, the overall mass balances have the following properties in the perfectly stirred balance volume case.
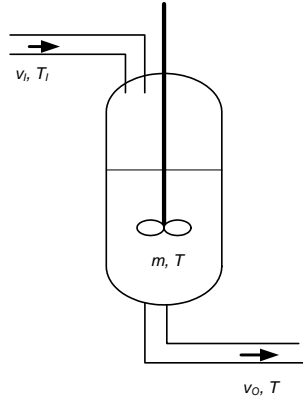
Figure 5.1: The simple balance volume for energy systems

- They have no source or sink term if the balance volume is connected to the environment only. Otherwise, the phase changes (evaporation, boiling, melting, etc.) may generate a mass source or sink through the interphase boundary.

- Their convective terms are the in- and out-flows entering or leaving the balance volume, that are mass flows $[kg/s]$.

It is important to note that the overall mass is the conserved extensive quantity that is most often measurable using level measurements. Therefore, the mass balances are transformed to have this variable by assuming constant cross section, for example.

5.3.2 Energy balances

The dynamic balance equation for internal energy is the characterizing equation for an energy system. In the perfectly stirred balance volume case this equation has the following properties.

- The convective energy flows are induced by the convective mass flows of a balance volume, such that each v_I inflow induces an energy inflow $c_{pI}v_IT_I$ measured in $[J/s]$, where c_{pI} is the specific heat and T_I is the temperature of the flow. Similarly, the mass out-flow v_O results in an energy flow c_pv_OT.

- The source or sink term can be external (e.g. electrical) heating/cooling or heat transfer Q (again in unit $[J/s]$).

The energy U is directly **not** *measurable*, therefore we use the temperature T instead in the model equations. This is achieved by transforming the energy balance equation into its intensive form, that is discussed in details in subsection 5.5.1.

5.4 Constitutive equations in energy systems

As we saw in section 4.2, constitutive equations augment the set of conservation balance equations, and make the set of model equations complete. They are usually algebraic equations that describe the actual form of various mechanisms, such as transfer rates, for example, or establish relationships between model variables, such as extensive-intensive relationships. This section is devoted to the most important classes of constitutive equations that appear in the dynamic models of lumped parameter energy systems.

5.4.1 Extensive-intensive relationships

The most important extensive-intensive relationship in energy systems is the dependence of the internal energy on temperature. Earlier in section 5.2.3 the conserved extensive variables and their intensive "potential" pairs were described, that includes the pair (internal energy $U \leftrightsquigarrow$ temperature T). In the general case there is a nonlinear static relationship in the form of $U = \mathcal{U}(T, p)$ between the internal energy and the temperature, that depends on the pressure (and may depend on the composition), too.

In the simplest case, when constant pressure is assumed (or it is assumed that the internal energy does not depend on the pressure), the reference point of the internal energy is chosen to be zero at the reference temperature ($U_0 = U(T_0) = 0$), and the reference temperature is $T_0 = 0^oC$, a simple algebraic equation describes a relationship between them in the form

$$U = c_p \cdot m \cdot T \tag{5.2}$$

in a perfectly stirred balance volume, where m is the overall mass, c_P is the specific heat measured in unit $[J/kg/K]$ that may depend on temperature, pressure and component concentrations, (see in subsection 5.4.2 later).

Sometimes the relationship between the intensive variable density (ρ) and the extensive mass (m) is also used, mainly for fluid phases in the form

$$m = V \cdot \rho \tag{5.3}$$

where V is the volume of the balance volume.

5.4.2 Property relations

The material in a balance volume has thermodynamical properties, such as density, specific heat, etc., that depend both on the nature of the material and on the intensive thermodynamical state variables, temperature T, pressure p and compositions c_i, $i = 1, ..., K$. The property relations are algebraic relations that describe these dependencies.

In energy systems the most important property relations that appear in dynamic models in the case of constant compositions are as follows:

- density relation: $\rho(p, T)$,

- specific heat relation: $c_p(p, T)$,

- dependence of equilibrium saturated pressure on the temperature $p^*(T)$

It is important to emphasize that a substantial part of modeling assumptions concern property relations: most often constant (i.e. temperature and pressure independent) properties are assumed.

5.4.3 Thermodynamical state equations

Thermodynamical state equations establish algebraic relationship between the canonical state variables (mass m, pressure p, temperature T and volume V) of a balance volume. These are mainly used for balance volumes with gas phases.

Ideal gas law This is applicable when the pressure of the gas is low compared to its saturation pressure in the temperature of interest, i.e. the average distance of the gas molecules is large compared to their size. The ideal gas law is written in the following form:

$$p \cdot V = \frac{m}{M} \cdot R \cdot T \tag{5.4}$$

where M is the molecular weight of the gas, and R is the universal gas constant ($R = 8.31 \ J/mol/K$).

Nonideal gas laws Under relatively high pressure, the ideal gas law is not applicable, therefore we have to resort to various nonideal gas laws. The most common is the so called Van der Waals equation, but there are dosens of state-equations for various gases under different conditions.

The water The state equations and thermodynamical properties of the water are of primary importance, because this is the most frequently used material in the industries. Here we can use the data collected in *steam tables* (see e.g. [13]), that contain the properties of water and steam in different regions. This is the most accurate source of information about water and steam that outperforms any state equation.

Simple interactive illustration of the state equations The effect of the temperature and pressure on the state and phase of matter can be investigated by interactive simulation using the "Phase Changes" tab of the interactive states of matter simulator.

The simulator has been created in the framework of the PhET^{TM} project [12] at the University of Colorado PhET project.

5.4.4 Transfer rates

The locally linear approximation of the fluxes of conserved extensive thermodynamical variables as functions of their driving force potential variables applied

in irreversible thermodynamics (see in section 5.2.3) gives rise to the widely accepted expression for the energy transfer term between two balance volumes with different temperatures T_1 and T_2

$$Q_{transfer} = K_T \cdot A \cdot (T_1 - T_2) \qquad (5.5)$$

where A is the heat transfer area in $[m^2]$, K_T is the heat transfer coefficient measured in $[J/m^2/K/s]$, and the energy transfer rate $Q_{transfer}$ is measured in units $[J/s] = [W]$. Note that in engineering models one often assumes that the heat transfer coefficient K_T is not a constant, but a function of the temperatures, pressures and flow conditions of the two balance volumes, respectively.

Note that mass can also be transferred between balance volumes with different phases (such as liquid and its vapor) in a mechanism called *evaporation*. The evaporation mass flow rate $Q_{mevap}^{(m)}$ (measured in units $[kg/s]$) is driven by the difference between the actual partial pressure p of the vapor phase and the saturated vapor pressure at the vapor temperature $p^*(T)$, therefore

$$Q_{mevap}^{(m)} = K_m \cdot A \cdot (p^*(T) - p) \qquad (5.6)$$

5.4.5   Energy source terms caused by phase changes

Phase changes, such as evaporation, boiling, freezing, melting etc. appear as source terms both in the overall mass and the energy balance equations. There is always a substantial internal energy change in the balance volume (phase) from which the material leaves for the other balance volume (phase), that is proportional to the mass flow leaving the phase.

The internal energy change associated with the phase change of unit mass is called phase change energy (and measured in $[J/kg]$ accordingly), for example *evaporation energy* E_{evap} or *melting energy* $E_{melting}$. This implies that an evaporation mass flowrate $Q_{mevap}^{(m)}$ (see above in subsection 5.4.4) induces an energy source term in the energy balance equation of the liquid in the form

$$Q_{Eevap} = E_{evap} \cdot Q_{mevap}^{(m)} \qquad (5.7)$$

where the unit of Q_{Eevap} is $[J/s]$.

A special type of evaporation is the case of *boiling*. The boiling point is the temperature when the pressure of saturated vapor in equilibrium with its liquid phase reaches the pressure of the gas phase, thus vapor is produced not only on the surface but in the bulk liquid. It is important to know that the temperature remains at the boiling point irrespectively of how much energy is injected into the liquid phase until all liquid transfers to the gas phase.

5.5   State space model form of dynamic energy models

For control and diagnostic applications one needs to transform the developed dynamic model based on engineering principles into its state space model form.

This section is devoted to this problem in the case of lumped parameter energy system models that are based on perfectly stirred balance volumes. As we have seen before, an engineering model consists of conservation balance equations that are ordinary differential equations in the lumped case, and algebraic constitutive equations. In order to have a state space model form one needs to perform two substantial steps on the model equations

- The conservation balance equations should be transformed to have measurable (mostly intensive) quantities in them.

- The constitutive algebraic equations should be substituted into the differential ones (if possible).

5.5.1 Energy balance equations in intensive variable form

The procedure of how to construct the intensive variable form of an energy balance equation from the mass balance and from the original extensive form of the energy equation is discussed in the simplest case with the following assumptions.

F1 A single perfectly stirred balance volume is considered with overall mass m and internal energy U.

F2 One in- (v_I) and one out-flow (v_O) is assumed, that are mass flows $[kg/s]$.

F3 Constant thermodynamical properties (specific heat c_p) are assumed.

Original conservation balances We start from the usual balance equations below.
Mass balance

$$\frac{dm}{dt} = v_I - v_O \tag{5.8}$$

Energy balance

$$\frac{dU}{dt} = c_{pI} v_I T_I - c_p v_O T + Q \tag{5.9}$$

where T_B is the temperature and c_{pB} is the specific heat of the in-flow, and Q is the energy source term.

Internal energy - temperature relationship The internal energy - temperature relationship in the form $U = c_p m T$ is used for expressing the non-measurable internal energy with the measurable temperature T and mass m. Using assumption F3 above, the energy balance equation (5.9) can be rewritten in the following form

$$c_P m \frac{dT}{dt} + c_P T \frac{dm}{dt} = c_{pI} v_I T_I - c_p v_O T + Q \tag{5.10}$$

The intensive variable form   We can now substitute the overall mass balance (5.8) into the second term of the left-hand side of Eq. (5.10) and rearrange the expression to have the intensive variable form

$$\frac{dT}{dt} = \frac{v_I}{c_p m}(c_{pI}T_I - c_p T) + \frac{Q}{c_p m} \qquad (5.11)$$

This is now in the form of a *state equation originating from the energy balance.*

5.5.2   State and output equations, system variables

State equations   In a state space model of a lumped parameter system, the state equations are ordinary differential equations, therefore they are constructed from the dynamic conservation balances in an energy system with perfectly stirred balance volumes. Above in subsection 5.5.1 we saw that the intensive variable form of an energy balance equation is in the form of a state equation, therefore, we can have *at most two state equations for each balance equation, one originates from the mass balance, the other one is from the energy balance.*

As the constitutive equations make the set of balance equations mathematically complete, we should substitute the constitutive equations into the differential ones to obtain a complete set of state equations. This is straightforward for the transfer rate equations and other source terms, and for the property relations, as they are explicit for the variables present in the balance equations. We have also seen in subsection 5.5.1 the use of the extensive-intensive relationships to obtain the intensive form of the energy balance equation. The only constitutive equation that may cause problems is the thermodynamical state equation (for example the ideal gas law).

State variables   It follows from the discussion on the potential state equations above, that the set of state variables of an energy system consisting of perfectly stirred balance volumes may include the overall mass (or a derived extensive variable, for example a level) and the temperature of each balance volume, i.e.

$$x = [\ m_i, T_i \mid i = 1, ..., N]^T \qquad (5.12)$$

Output equations and output variables   The output equations relate the state and input variables to the ones we can directly measure, therefore, they strongly depend on the instrumentation conditions of the system to be modeled. As the intensive variable form of the energy balance equation is normally used as a state equation, we can expect to have at least some of the state variables to be directly measurable, i.e. to be an output variable.

5.6 Modeling of typical operating units in power systems

Power systems are an important subclass within energy systems, that are used to produce electrical energy (power) from other energy sources, such as renewables, nuclear or fossil energy. Most often (but with exceptions such as photovoltaic panels) the electric power is produced by large industrial generators that are attached to turbines, mostly steam turbines.

Therefore, the most important utility operating units in power plants are heat exchangers and steam generators, the modeling of which is the subject of this case study section.

An example: the operating units in the primary circuit of a pressurized water nuclear power plant

Because of safety reasons, pressurized water reactors use two closed circuits to transfer the energy generated by their nuclear reactor into the steam turbines. The (radioactive) water in the so called primary circuit acts as both the moderator of the nuclear reactions and the heat transfer media that produces steam from the secondary circuit water in the steam generator such, that the water in the two circuits are not mixing. The primary circuit high pressure ensures that the coolant is not boiling, this gives the name "pressurized water reactor" to this type of technology.

Figure 5.2 shows the operating units and their connections that can be taken into account in a simplified model of the primary circuit. For more details we refer to the paper [17]. The sensors that provide on-line measurements are also indicated in the figure by small full rectangles. The controllers are denoted by double rectangles, their input and output signals are shown by dashed lines.

The steady-state values of the system variables in the normal 100 % power operating point are also indicated in Fig. 5.2.

In the following subsections simple models of the operating units above will be described with their ingredients (see section 4.4).

5.6.1 A simple heat exchanger model

Heat exchangers are one of the simplest units in power industries – they can be found in almost every plant. As their name suggests, heat exchangers are used for energy exchange between at least two fluid phase (gas or liquid) streams, a hot and a cold stream.

The simplest model of a heat exchanger describes a so called *heat exchanger cell*. A heat exchanger cell is a primitive dynamic unit which consists of two perfectly stirred (lumped) balance volumes (called *lumps*) connected by a heat conducting wall. The lumps with their variables are shown in Fig. 5.3.
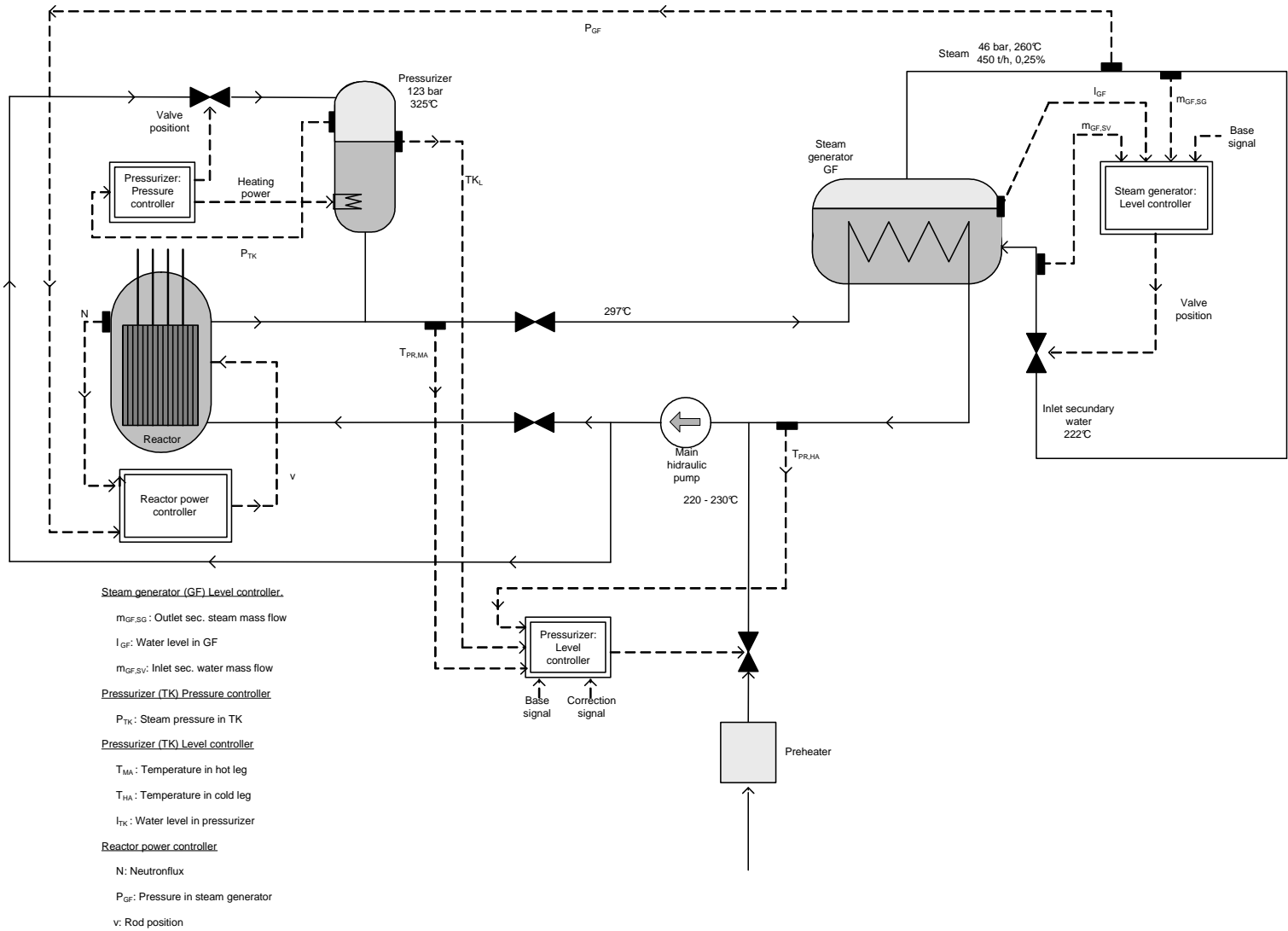
Figure 5.2: Process flowsheet with the operating units of the simplified model
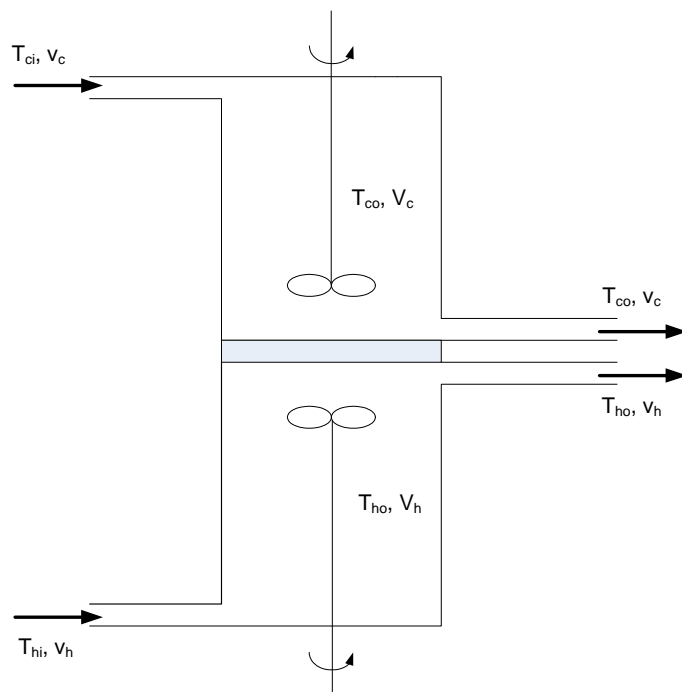
Figure 5.3: A heat exchanger cell

Modeling assumptions

In order to obtain a simple model with only two state equations, the following simplifying modeling assumptions are used:

F1 Constant volume and mass hold-up is assumed in both lumps ($j = c, h$).

F2 Constant physico-chemical properties are assumed for the density: ρ_j and the specific heat: c_{Pj} in both lumps, i.e. for $j = c, h$.

F3 Constant heat transfer coefficient (K_T) and area (A) is considered.

F4 We assume completely observable states, i.e. $y(t) = x(t)$.

Conservation balances

The continuous time state equations of the heat exchanger cell above are the following energy conservation balances in their intensive variable form:

$$\dot{T}_{co}(t) = \frac{v_c(t)}{V_c}(T_{ci}(t) - T_{co}(t)) + \frac{K_T A}{c_{pc}\rho_c V_c}(T_{ho}(t) - T_{co}(t)) \qquad (5.13)$$

$$\dot{T}_{ho}(t) = \frac{v_h(t)}{V_h}(T_{hi}(t) - T_{ho}(t)) + \frac{K_T A}{c_{ph}\rho_h V_h}(T_{co}(t) - T_{ho}(t)) \qquad (5.14)$$

where T_{ji} and T_{jo} are the inlet and cell temperatures (that are equal to the outlet temperatures because of the perfectly stirred assumption), V_j is the volume and v_j is the volumetric flow rate (measured in units $[m^3/s]$) of the two sides ($j = c, h$) respectively.

System variables

The *state vector* is therefore composed of the two outlet temperatures:

$$x_1 := T_{co}, \quad x_2 := T_{ho} \qquad (5.15)$$

There are a number of possibly time-dependent variables on the right-hand side of the above equations which may act as manipulable *input variables* or disturbances, depending on the measurement and actuator settings and on any additional modeling assumptions we may have. These are as follows:

- the inlet temperatures: T_{ci} and T_{hi},

- the volumetric flowrates: v_c and v_h.

The special cases of the heat exchanger cell models are obtained by specifying assumptions on their variation in time. For every case, the output equation is

$$y(t) = x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} \qquad (5.16)$$

5.6.2 A simple steam generator model

The steam generators connect the primary and secondary circuit and transfer the energy generated by the reactor to the secondary steam flow. The steam generator is an operating unit of the primary circuit that was shown in Fig. 5.2. The steam generator itself is a vessel that contains water of the secondary circuit. The vapor is produced from this secondary circuit water by heating the liquid phase using the energy coming from the circulating primary circuit liquid as it can be seen in Fig. 5.4.
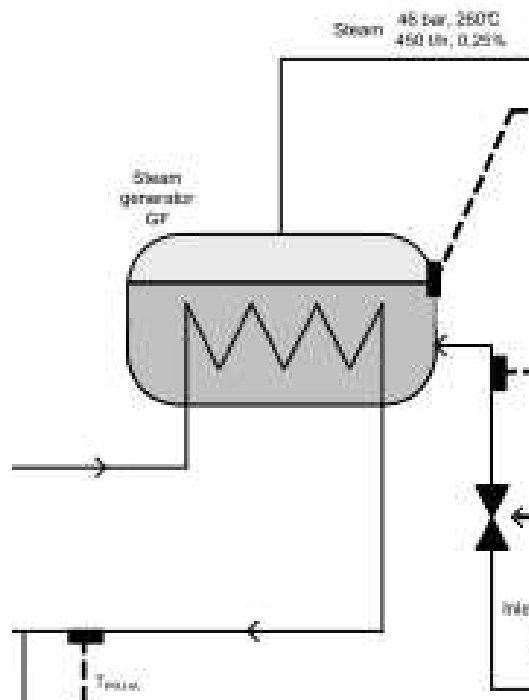
Figure 5.4: Simplified flowsheet of the steam generator

Modeling assumptions

Because the focus of our model is the primary circuit and its controllers, the following simplifying assumptions are made for the steam generators:

1. The dynamics of the primary side of the steam generators is very quick compared to that of the secondary side, therefore it is assumed to be in a quasi steady state and no conservation balances are constructed for it.

2. The dynamics of the secondary side vapor phase in the steam generators

is also assumed to be very quick compared to that of the secondary side liquid, equilibrium is assumed between the water and the vapor phases.

3. Constant physical properties are assumed for the secondary side of the steam generators.

4. All the controllers acting on the secondary side (including the liquid level controller and the secondary steam pressure controller) are assumed to be ideal.

Conservation balances

There is only a single balance volume in the steam generators, the liquid of the secondary side, where the overall mass balance is simplified to an algebraic equation $M_{SG} = const$ (M_{SG} is the liquid mass), because the inlet secondary water mass flow rate $m_{SG,SW}$ and the outlet secondary steam mass flow rate $m_{SG,SS}$ is kept to be equal by the ideal water level controller of the steam generators

$$m_{SG,SW} = m_{SG,SS} = m_{SG}$$

Then the energy balance for the secondary water in the steam generators is in the form

$$\begin{aligned} \frac{dU_{SG}}{dt} &= c_{p,SG}^L m_{SG} T_{SG,SW} - c_{p,SG}^V m_{SG} T_{SG} - m_{SG} E_{evap,SG} + \\ &\quad + K_{T,SG}(T_{PC} - T_{SG}) - W_{loss,SG} \end{aligned} \quad (5.17)$$

where U_{SG} is the internal energy, $c_{p,SG}^L$ is the water specific heat, $c_{p,SG}^V$ is the vapor specific heat, $T_{SG,SW}$ is the inlet temperature, T_{SG} is the temperature, $E_{evap,SG}$ is the evaporation energy, and $W_{loss,SG}$ is the heat loss.

Constitutive equations

The algebraic constitutive equations describe the relationships between physical properties and temperature:

$$U_{SG} = c_{p,SG}^L M_{SG} T_{SG} \quad (5.18)$$

$$p_{SG} = p_*^T(T_{SG}) \quad (5.19)$$

where p_{SG} is the pressure, and p_*^T is a quadratic function that approximates the values obtained from the steam table [13].

5.6.3   A simple pressurizer model

A widespread type of nuclear power plants operates pressurized water reactors, which means that in the primary circuit high pressure ensures that the coolant is not boiling. The task of the pressurizer is to keep the pressure within a
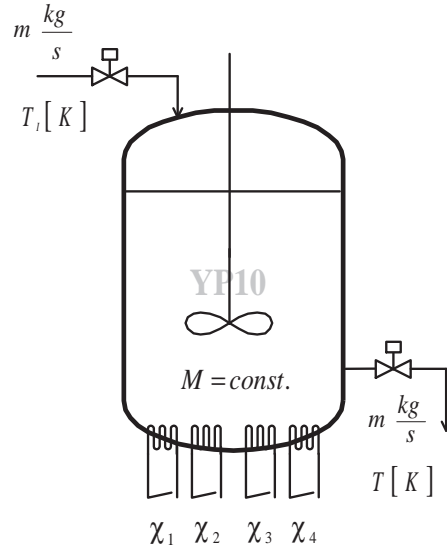
Figure 5.5: Simplified flowsheet of the pressurizer

predefined range. The pressurizer is a vertical tank shown in Fig. 5.5, and also in Fig. 5.2 as one of the operating units in the primary circuit. Inside this tank there is hot water at a temperature of about 325°C and steam above. If the primary circuit pressure decreases, electric heaters switch on automatically in the pressurizer. Due to the heating more steam will evaporate and this leads to a pressure increase.

Unlike steam boilers or steam generators, where the purpose of the equipment is producing steam, the purpose of the pressurizer is to keep the pressure constant, while there is no vapor withdrawal from the tank. The heating is mainly used to compensate for the heat losses through the wall and to heat the infiltrated cold water. The intended use of the model is controller design in *normal operating mode where the vapor can be considered to be in equilibrium with the liquid phase (saturated vapor)*, i.e. the dynamics of the vapor phase is infinitely quick compared to the other dynamic effects and the mass of the vapor phase is negligible compared to the other masses.

Modeling assumptions

In order to have a simple model, the following modeling assumptions have been used:

F1 There are two perfectly stirred balance volumes, one for the water and another for the wall, and no balance volume for the vapor.

F2 There is a single component in each of the balance volumes (water and iron, respectively).

F3 Constant overall mass is assumed in both balance volumes.

F4 We assume constant physico-chemical properties.

F5 Vapor-liquid equilibrium is assumed in the tank.

Balance and constitutive equations

Thus, the simplified model consists of two energy balances: one for the water and another one for the wall of the tank as balance volumes.

Water energy balance

$$\frac{dU}{dt} = c_p m T_I - c_p m T + K_W (T_W - T) + \sum_{i=1}^{4} W_{HE} \cdot \chi_i \qquad (5.20)$$

Wall energy balance

$$\frac{dU_W}{dt} = K_W (T - T_W) - W_{loss} \qquad (5.21)$$

Extensive-intensive relationships   These equations describe the relationship between the internal energies and the corresponding temperatures, and complete the model. These are

$$U = c_p M T, \qquad (5.22)$$
$$U_W = C_{pW} T_W. \qquad (5.23)$$

Variables and parameters

The variables and parameters of the above model and their units of measure are the following

T	water temperature	°K
T_W	tank wall temperature	°K
c_p	specific heat of water	$\frac{J}{kg °K}$
U	internal energy of water	J
U_W	internal energy of the wall	J
m	mass flow rate of water	$\frac{kg}{s}$
T_I	inlet water temperature	°K
M	mass of water	kg
C_{pW}	heat capacity of the wall	$\frac{J}{°K}$
W_{HE}	power of one electric heater	W
K_W	wall heat transfer coefficient	$\frac{W}{°K}$
χ_i	on/off (1/0) state of the ith heater	–
W_{loss}	heat loss of the system	W

Input variables The manipulable input to the system is the external heating, all the other input variables are regarded as disturbances. Then we can list the disturbances with physical meaning as follows:

- *Cold water infiltration*
  This effect is taken into account with the in-convection term $c_p m T_I$ in the water energy conservation balance (5.20), where the in- and outlet mass flowrate m is controlled to be equal (but might change in time) and the inlet temperature T_I can also be time-varying.

- *Energy loss*
  This effect is modeled as a loss term W_{loss} in the wall energy balance (5.21).

Nonlinear dependence between temperature and pressure The pressure of saturated vapor in the gas phase of the tank depends strongly on the water temperature in an exponential, i.e. nonlinear way. The experimental measured data found in the literature [10] have been used to create an approximate analytic function to describe the dependence. The function has the form

$$p = h(T) = \frac{e^{\varphi(T)}}{100},$$
$$\varphi(T) = c_0 + c_1 T + c_2 T^2 + c_3 T^3$$

(5.24)

For the parameters of φ, the following values were obtained

$$c_0 = 6.5358 \cdot 10^{-1}, \; c_1 = 4.8902 \cdot 10^{-2}$$
$$c_2 = -9.2658 \cdot 10^{-5}, \; c_3 = 7.6835 \cdot 10^{-8}$$

(5.25)

The *pressure of saturated vapor is the output variable* of the model.

State variables As usual for the energy systems, the state variables are the two temperatures T and T_W of the water and wall balance volumes, respectively.

The validity range of the model is the usual operating domain of the pressurizer, i.e. $315°C \le T \le 350°C$. In pressure terms, this means 105.65 bar $\le p \le 137.09$ bar.

Chapter 6

Dynamic models of mechanical and electrical systems

Mechanical and electrical systems occur often in practice both in their "clean" form, i.e. without additional mechanisms, or in a combined form when the characterizing mechanisms of mechanical or electrical systems play a major role in developing a dynamic model.

Therefore, besides of presenting the basic principles and some simple examples of modeling mechanical and electrical systems, we present a thermo-mechanical (a gas turbine), a bio-mechanical (a simple limb), and a bio-electrical (a simple neuron) – i.e. three mixed type – modeling case studies in this chapter, too.

6.1 Mechanical systems

In mechanical systems the dynamics of different motion and deformation types are of modeling interest.

6.1.1 Characterization of mechanical systems

When constructing a dynamic model for a mechanical system, one takes into account the properties of motions (such as rectilinear motions, rotating motions, for example) and that of the mechanical deformations (elastic, quasi-elastic etc.).

Here we usually assume that both the composition and the thermodynamical properties (for example pressure or temperature) in the system are constant, or not of modeling interest. If this is not the case, we have a mixed-type system, and should also use the mechanisms and modeling principles of chemical (see chapter 7) or energy (see chapter 5) systems.

We can characterize a mechanical system through its mechanisms and modeling objects.

Modeling objects

The modeling objects in mechanical systems are called "bodies" for which momentum and energy conservation balances are constructed. These are classified as follows:

- The elementary object is the so called ***mass point***, that has a fixed mass m but no spatial extent, therefore, its position can be characterized by a point in the three dimensional space.

- The so called *mass-point systems* consist of a set of mass points the distance of which may be time-varying or fixed. The dynamic model of mass point systems is in the form of concentrated parameter system models.

- Rigid bodies have a fixed spatial extent (form), but no deformation is considered. Rigid bodies can be approximated (lumped) by a set of mass points with fixed spatial distances.

- Deformable bodies are the most general types, they have a spatial extent that may suffer from elastic or non-elastic deformation. Their approximating mass point system model consists of a set of mass points with variable spatial distances.

In order to keep the treatment simple, *we only consider mass point type mechanical systems in this chapter.*

Mechanisms

The mechanisms we consider in mechanical systems are the ones that affect the motion and deformation, and for which constitutive equations are available. These include

- forces originating from a potential field, e.g. *spring* or gravitation,

- friction, drag,

- torsion, deformation (elastic, non-elastic), etc.

6.1.2   Basic principles

The basic principles of modeling mechanical systems were laid down by Newton in his famous Principia Mathematica Phylosophiae Naturalis in 1687, and these are as follows.

Newton's 1st Law
Each object (body) keeps its steady-state position or its rectilinear motion with constant velocity unless an external effect forces it to change.
From the modeling point of view it implies that (i) the external effects should be described by *forces*, and (ii) the equivalent coordinate systems move with constant relative velocity.

Newton's 2nd Law
*The change of **momentum** is proportional to the effect of the force and takes place in the direction of the force.*
Because *momentum is a conserved extensive quantity*, the above principle gives direction of how to construct the momentum balance equations in modeling. Thus the conservation equation takes the form $\frac{dp}{dt} = \sum_i F_i$, where p is the momentum and F_i are the forces.
It is important to consider, that *both the momentum and the force are vectors*, thus they have magnitude and direction.

Newton's 3rd Law
The effect is equal to the reaction, that is, the effect of two bodies to each other is of equal magnitude but of adverse direction.

6.1.3 Rectilinear motions

Newton's 1st Law states that rectilinear motion takes place whenever there are only such external effects (forces) that act in the direction of the motion, i.e. in its orbit.

Mass-point systems

The simplest case of mass point systems is only considered here. We have already seen in chapter 4, that we need to construct both the conservation balance and the constitutive equations to obtain a complete model.

Conservation balances   The conservation balance equations for a mass-point type mechanical system with rectilinear motion are formed from the momentum balances in each considered direction (for example x, y, z) for each mass point i. These equations have the form for the direction x and the mass point i

$$\frac{dp_{x,i}}{dt} = \sum_j F_{x,i,j} \tag{6.1}$$

where $p_{x,i}$ is the momentum of the mass point in the x-direction, and $F_{x,i,j}$ the jth force acting on the mass point i in the x-direction.
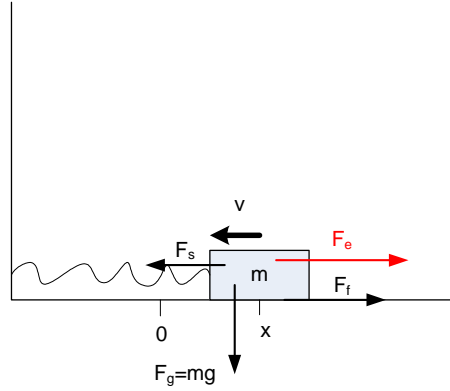
Figure 6.1: Mass and spring system

Constitutive equations   The constitutive equations are of two types. The first type is *static equation(s) for each force* from the physics of its underlying mechanism, such as

- *gravitation*: $F_g = m \cdot g$
  where g is the gravitational constant, $g = 10 \ \frac{m}{s^2}$

- *friction*: $F_f = \mu \cdot m \cdot g$
  where μ is the friction coefficient, a number $0 \leq \mu \leq 1$

- *elastic force* (e.g. in spring): $F_s = -k \cdot \Delta x$
  where k is the spring constant and Δx is the distance from the equilibrium position.

- other position dependent forces (e.g. from a potential, electrical forces)

The other type of constitutive equation is a *dynamic position-momentum equation* (if needed). In the x direction for the ith mass point such an equation is in the form of

$$p_{x,i} = m_i \frac{dx_i}{dt} \tag{6.2}$$

where x_i is the position and m_i is the mass of the mass point.

Example: mass and spring

Problem description
Given a mass point m connected to the wall by an elastic spring with spring coefficient k and moving along a horizontal line. The mass is under the influence of an external force F_e and there is a friction with a coefficient μ. Construct the model of the mass-spring system for control purposes if we can measure the position of the mass point x and the external force F_e.

Mechanisms   The following mechanisms are considered:

- elastic force in the spring

- friction generated by the gravitational force

- external force F_e

Modeling assumptions   The mechanical system with its variables are depicted in Fig. 6.1.

F1 one mass-point with mass m

F2 rectilinear motion

F3 elastic ideal spring with coefficient k (force F_s)

F4 friction with constant coefficient μ (force F_f)

F5 position origin $x = 0$ is at the equilibrium point

Conservation balance equation   It is constructed for the momentum $p = m \cdot v$, where only one spatial direction (horizontal) is needed.

$$\frac{dp}{dt} = F_f + F_s + F_e \tag{6.3}$$

Constitutive equations   These are written for the acting forces and for the momentum-velocity relationship.

- $F_f = \mu \cdot m \cdot g$ (friction)

- $F_s = -k \cdot x$ (spring)

- $p = m \cdot v = m \cdot \frac{dx}{dt}$ (position is measurable)

State-space model form   The above model equations can be re-arranged to obtain a state-space model

$$\frac{dp}{dt} = \mu \cdot m \cdot g - k \cdot x + F_e \tag{6.4}$$

$$\frac{dx}{dt} = \frac{1}{m}p \tag{6.5}$$

where the state variables are the position x and momentum p (but alternatively the velocity v can also be used), the input variable is the external force F_e and the output variable is the position x.
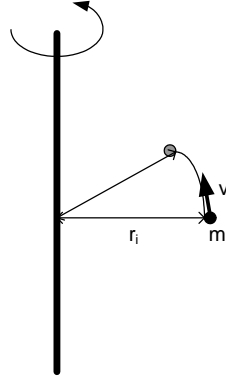
Figure 6.2: Rotating motion

6.1.4   Rotating motions

A rotating motion arises if an external force constrains the body (or bodies) to move along a circular orbit. Then we usually *restrict the description to the motion along this circular orbit*: this way a motion with a single spatial degrees of freedom will arise.

Again the simplest case of mass-point systems is only considered.

Characteristic variables and parameters   The variables and parameters that are applicable for describing rotating motions are as follows for a single mass point and for a given rotating axis (centerline):

- angular momentum N (analogue to the momentum p)

- angle velocity (angular frequency) ω (measured in units $[\frac{rad}{s}]$)

- moment of inertia Θ (for mass point m_i: $\Theta_i = m_i \cdot r_i^2$)

- torque $M = F \cdot r$ in $[Nm]$, where r is the distance from the rotating axis

The mechanical system with its variables is shown in Fig. 6.2.

Conservation balances   For a mass-point type mechanical system with a rotating motion the angular momentum balance in each considered direction for each rotating mass point forms the set of conservation balance equations in the form

$$\frac{dN}{dt} = \sum_k M_k \tag{6.6}$$

where M_k are the external torques that act on the system (the analogue of forces in rectilinear motion).
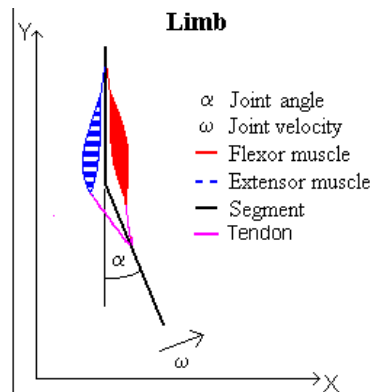
Figure 6.3: Mechanical structure of a simple limb

6.2 A bio-mechanical example: a simple limb model

A simple bio-mechanical example is presented here for illustrating the modeling of rotating motions. The detailed model derivation can be found in [15].

6.2.1 Problem statement

Given a simple limb consisting of two segments (bones) and two muscles (flexor and extensor) that move the lower segment around the joint axis. The considered mechanical structure can be seen in Fig. 6.3.

Construct the model of the simple limb system for control purposes if we can measure the position of lower segment and the external excitations u^f and u^e causing contraction in the flexor and extensor muscles, respectively.

Mechanisms

- muscle force generation,

- muscle contraction by activation,

- rotation.

6.2.2 Modeling assumptions

F1 one mass point with mass m for the lower segment

F2 the upper segment is fixed vertically

F3 fixed distance l_{COM} from the rotating axis

F4 activation state equations with fixed parameters (τ activation time, β decreasing factor)

F5 activation determines the torque of the muscles M

6.2.3   Model equations

Conservation balance equations

The conservation of the angular momentum $N = \Theta^{(total)} \cdot \omega$ is considered in the form

$$\frac{dN}{dt} = M(q_1, q_2, \alpha, \omega) + m \cdot l_{COM} \cdot \cos(\alpha - \frac{\pi}{2}) \cdot g \qquad (6.7)$$

Two more conservation balances are also present for the activation states q_1 and q_2 that originate from a bioelectrical model:

$$\frac{dq_1}{dt} = \left(\frac{1}{\tau_{act}} (\beta + [1 - \beta] u^f(t)) \right) q_1 + \frac{1}{\tau_{act}} u^f(t) \qquad (6.8)$$

$$\frac{dq_2}{dt} = \left(\frac{1}{\tau_{act}} (\beta + [1 - \beta] u^e(t)) \right) q_2 + \frac{1}{\tau_{act}} u^e(t) \qquad (6.9)$$

where u^f and u^e are the external exitations coming from the nervous system.

Constitutive equations

These are of the following form and origin:

- $\frac{d\alpha}{dt} = \omega$ (velocity equation)

- the actual form of $M(q_1, q_2, \alpha, \omega)$ (from biology)

System variables

- The state variables are the joint angle and velocity (α and ω), together with the two activation states q_1 and q_2.

- The two external excitation signal u^f and u^e form the set of input variables.

- The measurable output variable is the joint angle α.

6.3   Thermo-mechanical systems

Quite often, one has both mechanical and thermal phenomena in the system to be modeled, when a thermo-mechanical system description arises. For this purpose we need to describe the two set of mechanisms in a unified framework. This mainly concerns the set of balance equations, because in the thermal energy systems we use internal energy balances, but for mechanical systems we

considered the conservation of momentum. The first step to couple the thermal and mechanical description is to consider the energy-based description of mechanical systems.

6.3.1 Energy-based description of mechanical systems

As before, we consider the simplest case of a mechanical system, the class of mass-point systems. It will turn out, that the conventional momentum-based description of mechanical systems that uses the momentum balances is in most cases equivalent to the energy-based description.

Rectilinear motion

Assume the simplest mechanical system consisting of a single mass point with mass m. It has a potential (position dependent) and kinetic (momentum dependent) energy term in its total energy

$$E_{total} = V(x) + \frac{1}{2m}p^2 \tag{6.10}$$

The change of the total energy in a finite time interval is caused by the effect of the work done by the external forces F ($\Delta E_{total} = \Delta W = F\Delta x$). Therefore, the time-derivative of the total energy is driven by the power provided by the force F:

$$\frac{dE_{total}}{dt} = F \cdot \frac{dx}{dt} = F \cdot v \tag{6.11}$$

In the case of a constant (i.e. position independent) external force and no potential energy ($V(x) = 0$), one can perform the differentiation of Eq. (6.10) to obtain

$$\frac{d}{dt}\left(\frac{1}{m}p^2\right) = \frac{1}{m}p\frac{dp}{dt} = v \cdot \frac{dp}{dt} = F \cdot v$$

that is exactly the momentum conservation balance equation in this case. This shows the *equivalence of the energy-based description with the momentum-based one*.

Simple interactive illustration of various energy components in springs
The effect of stiffness of the springs, the friction and the gravitation on the various energy components of the rectilinear motion can be investigated by interactive simulation using an interactive mass spring simulator.

The simulator has been created in the framework of the PhET^{TM} project [12] at the University of Colorado PhET project.

Rotating motion

Here we consider the kinetic energy for a rotating body with moment of inertia Θ as the total energy E_{rot} of the system

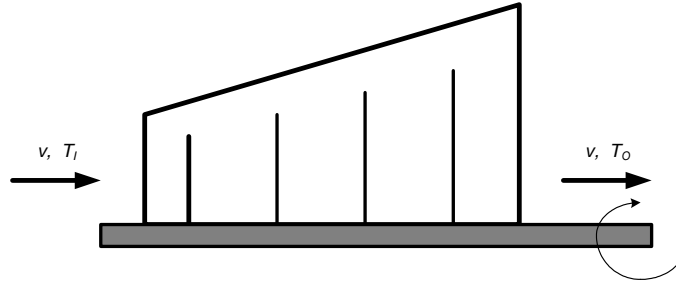$$E_{rot} = \frac{1}{2}\Theta\omega^2 \tag{6.12}$$

Figure 6.4: A simple steam turbine

The time-derivative of the total energy here is driven by the power provided by a torque M:

$$\frac{dE_{rot}}{dt} = M \cdot \omega \tag{6.13}$$

Similarly to the above derivation, we can again show the *equivalence of the energy-based description with the momentum-based one* here, too.

6.3.2   Example: a simple gas turbine

Gas turbines are important energy conversion machines that are present in almost every power plant (see section 5.6). A gas turbine converts the internal energy of the gas (most often steam) into the mechanical energy of a rotating shaft, that is usually converted further to electrical energy by a generator. Therefore, it is a *thermo-mechanical system* based on the mechanisms that are to be taken into account when developing its dynamic model.

The simplest version of a steam turbine is presented briefly here, that is a simplified version of a gas turbine model in [14].

Problem description
Given a simple gas turbine that moves a rotating shaft around a given axis. The steam enters and leaves the turbine with a given mass flow rate v, the inlet temperature is T_I, the outlet temperature is T_O. The flowsheet of the turbine is shown in Fig. 6.4.

Construct the model of the simple turbine for control purposes if we can measure the external load torque M_{load} and the angular velocity ω.

Mechanisms   The following mechanisms are taken into account:

- thermal energy conversion

- rotation

Modeling assumptions

F1 one rotating body (shaft) with moment of inertia Θ

F2 equal and given mass flow rate v for inlet and outlet

F3 given inlet T_I and outlet T_O temperatures (no condensation, i.e. phase change is assumed)

F4 the mechanical efficiency factor χ is given and constant

F5 constant gas specific heat c_P

F6 given the external load torque M_{load} (input)

Conservation balance equation The energy conservation balance for the rotation energy is used

$$\frac{dE_{rot}}{dt} = P_{steam} - M_{load}\omega \tag{6.14}$$

Constitutive equations Two algebraic constitutive equations are considered:

- $E_{rot} = \frac{1}{2}\Theta\omega^2$ (rotation energy)

- $P_{steam} = \chi \cdot c_P \cdot v \cdot (T_I - T_O)$ (power generated by the gas temperature drop)

We can substitute these into the energy conservation balance equation to obtain a model equation with measurable quantities

$$\frac{d\omega}{dt} = \frac{1}{\Theta\omega}\left(\chi \cdot c_P \cdot v \cdot (T_I - T_O) - M_{load}\omega\right)$$

6.4 Electrical systems

Electrical systems are very widespread in modeling practice, electrical circuits or electrical machines (motors, generators) are the most common types.

Furthermore, electrical sub-systems are also widely present in mixed type systems, such as bio-electrical or electro-chemical systems. Here we present a simple bio-electrical example, a simple cell model in the next section 6.5.

6.4.1 Characterization of electrical systems

The characterization can be performed through the modeling objects, that are elementary components called *two-pole*s. The poles of a two-pole are its input and output ports, respectively that connect it to the environment, and through which electrical current may flow.

The set of connected two-poles form an *electrical network*, that is the simplest electrical system, that has a concentrated parameter system model.
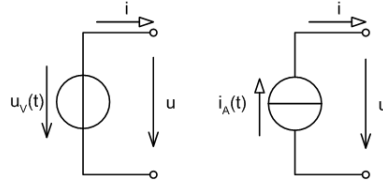
Figure 6.5: Voltage and current source two-poles

Source two-poles

Two types of source two-poles are in use in electrical network models that are seen in Fig. 6.5. A voltage source produces a given constant voltage u_S, it corresponds to an ideal voltage source (an accumulator, for example) without any internal resistance. Similarly, a current source is an ideal constant source i_S of current.

Resistors, capacitors and coils

Resistors, capacitors and coils form three categories of non-source two-poles with different dynamic behavior. They form the basic modeling elements of electrical network models.

Resistor types   A two-pole is called a resistor, if there is a static relationship between its power $u(t)$ and current $i(t)$ values, i.e.

$$u(t) = \rho(i(t)) \tag{6.15}$$

where $\rho(.)$ is the *resistance function*. The resistor is linear, if $u(t) = R(t) \cdot i(t)$ with $R(t)$ is the resistance, and linear and time-invariant when $R(t) = R$, i.e. the resistor is of constant resistance.

The inverse of the resistance function is called the *inductance function*, and the reciprocal value of the resistance is called inductance:

$$i(t) = \gamma(u(t)) \quad , \quad i(t) = g(t) \cdot u(t) \tag{6.16}$$

Capacitor types   Capacitors are also two-poles that have a dynamic behavior described by the equations

$$i(t) = \frac{dq(t)}{dt} \tag{6.17}$$

where $q(t)$ is the electrical charge, and

$$q = \varphi(u), \quad \text{or} \quad u = h(q) \tag{6.18}$$

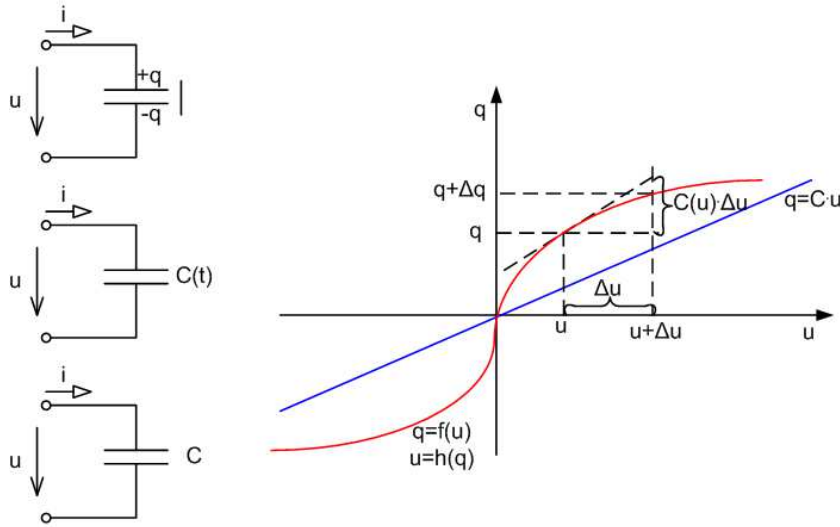where φ is the characteristic function of the capacitor.

Figure 6.6: General, linear and linear time-invariant capacitors

Figure 6.6 shows an example of a nonlinear characteristic function, together with different capacitor types. The linear capacitor has a linear characteristic function in the form $q(t) = C(t) \cdot u(t)$ with $C(t)$ being the *capacitance*, and a linear time-invariance capacitor has a constant capacitance C.

In the simplest LTI case the relationship between the power and the current of a capacitor is as follows

$$i(t) = C \cdot \frac{du(t)}{dt} \tag{6.19}$$

Coil types   A coil is a two-pole that has a dynamic behavior, too. Its describing equations are as follows:

$$u(t) = \frac{d\Psi(t)}{dt} \tag{6.20}$$

where $\Psi(t)$ is the magnetic flux, and

$$\Psi = \psi(i), \quad \text{or} \quad i = h(\Psi) \tag{6.21}$$

where ψ is the characteristic function of the coil.

A nonlinear characteristic function together with different coil types can be seen in Fig. 6.7. The linear coil has a linear characteristic function in the form $\Psi(t) = L(t) \cdot i(t)$ with $L(t)$ being the *inductance*, and a linear time-invariance coil has a constant inductance L.

In the simplest LTI case the relationship between the power and the current of a coil is as follows

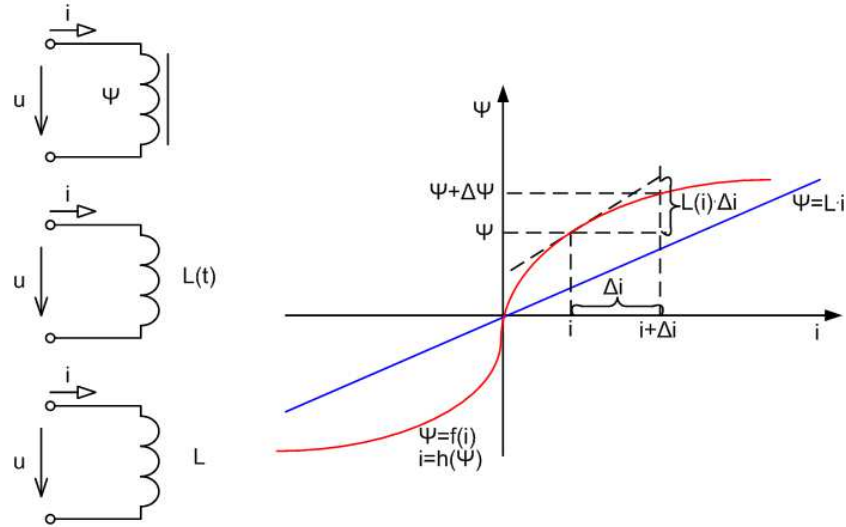$$u(t) = L \cdot \frac{di(t)}{dt} \tag{6.22}$$

Figure 6.7: General, linear and linear time-invariant coils

6.4.2   Basic principles: Kirchhoff's laws

The elements or two-poles of an electrical network form a graph where the vertices are the connection points of more than two two-poles connected by edges called branches.

Kirchhoff's laws express the conservation of electrical charge and energy within electrical networks.

Kirchhoff's vertex law

Kirchhoff's vertex law applies to any vertex of the electrical network and expresses the conservation of electrical charge. As current i is the time-derivative of charge, this law has the form

$$\sum_{k}^{K} i_k(t) = 0 \tag{6.23}$$

in every time instant for a vertex joining K branches.

Kirchhoff's circle law

This applies to any of the circles in an electrical network, and states that the signed sum of voltage along the circle is zero
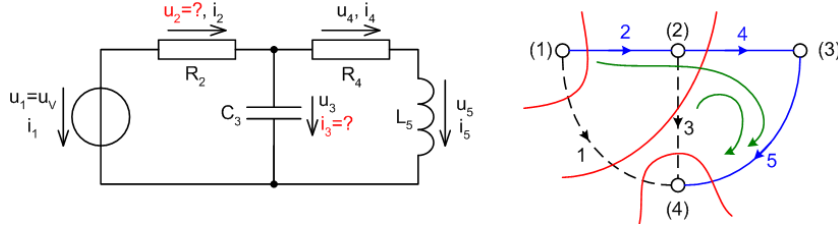
$$\sum_{k} u_k(t) = 0 \tag{6.24}$$

Figure 6.8: A simple circuit

in every time instance.

Example of Kirchhoff's laws

In order to show how to apply the Kirchhoff's laws, a simple electrical network is depicted in the left sub-figure of Fig. 6.8. The right sub-figure shows the underlying graph, where the vertices are numbered, and the independent circles are also indicated.

The *two-pole describing equations* relate the currents and powers of the elements in the networks as follows.

$$
\begin{aligned}
u_1 &= u_V \\
u_2 &= R_2 \cdot i_2 \\
i_3 &= C_3 \cdot \frac{du_3}{dt} \\
u_4 &= R_4 \cdot i_4 \\
u_5 &= L_5 \cdot \frac{di_5}{dt}
\end{aligned}
\tag{6.25}
$$

Three vertex and two circle type *Kirchhoff equations* can be constructed

$$
\begin{aligned}
i_1 + i_2 &= 0 \\
i_1 + i_3 + i_4 &= 0 \\
-i_1 - i_3 - i_5 &= 0 \\
-u_1 + u_2 + u_4 + u_5 &= 0 \\
-u_3 + u_4 + u_5 &= 0
\end{aligned}
\tag{6.26}
$$

6.4.3 Example: simple harmonic oscillator

The example of a simple harmonic oscillator is used to illustrate how to develop a dynamic system model of an electrical system based on the above first principles.

The electrical network form of the harmonic oscillator is shown in Fig. 6.9. The system consists of a power source, a resistor, a capacitor and a coil.

Modeling assumptions

F1 Simple LTI two-poles are assumed.

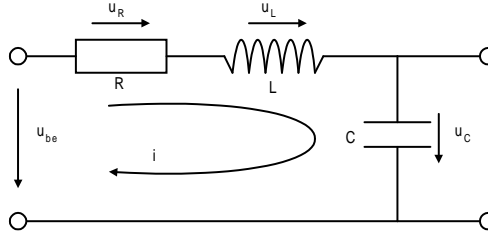F2 The power source u_{be} is the external input.

Figure 6.9: The simple harmonic oscillator

Model equations The two-pole description equations are as follows:

- resistor: $U_R = R \cdot i$

- capacitor: $i = C \cdot \frac{dU_C}{dt}$

- coil: $u_L = L \cdot \frac{di}{dt}$

The Kirchhoff's circle law applies to the only circle

$$-u_{be} + u_R + u_L + u_C = 0 \tag{6.27}$$

The two-pole description equations together with Eq. (6.27) form the set of model equations.

State space model Let us choose the current of the circuit i and the power of the capacitor u_C as state variables. Then we can differentiate Eq. (6.27) and substitute the two-pole equations into it to obtain the following state equations.

$$\frac{di}{dt} = -\frac{R}{L} \cdot i - \frac{1}{L} u_C + \frac{1}{L} u_{be}$$
$$\frac{du_C}{dt} = \frac{1}{C} \cdot i$$

6.5   Bio-electrical system example: a simple neuron model

Neurons are interesting dynamical systems where a combination of physico-chemical reactions and bio-physical (electrical) phenomena are taking place. Dynamical modeling and parameter estimation of neurons is a challenging and quickly developing area with great importance in understanding the operation of certain physiological processes and potential use in research, therapy and drug design.

6.5.1 A simple Hodgin-Huxley neuron model

The electrical properties of a cell are described by using the so called ionic channels present in the cell membrane. Each ironic channel acts as an element that affects the transmission of a specific ion to and from the cell to its environment.

Simple description of ionic channels   The current in an ionic channel is realized by the movement of some ion type X (for example $X = Ca^{2+}$) through the cell membrane. This movement is influenced by the voltage difference between the internal and external volume of the cell V, and by the electrochemical potential difference E_X that is caused by the concentration difference of the given ion X between the internal and external solution. Therefore, each ion channel is represented by *an element of the model that is a nonlinear conductance that describe the electrical conductance of the membrane with respect to the ionic current with a sequential power source that corresponds to the electrochemical potential difference.* The ionic channel sub-model described the ionic current resulted in the channel.

The Hodgin-Huxley model   A Hodgin-Huxley (abbreviated as HH) model is a modular electrical circuit type model of the cell membrane. Here each ionic channel produces its ionic current independently of the others driven by the overall voltage of the cell membrane and by the concentration difference of the corresponding ion, so it is a perfectly modular model.

The model presented here is the simplified version of the one described in [16], where more details can be found.

6.5.2 The electrical circuit model

The electrical circuit HH model consists of the following elements:

- A Na^+ channel is assumed with standard characteristics. The ionic current related to this channel will be denoted with I_{Na1}.

- A rapid K^+ channel is also taken into account, responsible for the rapid, transient component of the outward K^+ current (I_{K1}).

- A voltage gated delayed outward rectifier K^+ channel can be assumed, which contributes to the more slowly activating, sustained component of the outward K^+ current (I_{K2}).

- We consider a T-type voltage gated Ca^{2+} channel (I_{Ca1}).

- A high voltage gated Ca^{2+} channel is also assumed (I_{Ca2}).

- Static leakage currents are described with constant conductance (I_L).

The **equivalent electric circuit** of a simple GnRH neuron model in the case when all of the above conductances are taken into account is shown in Fig. 6.10.
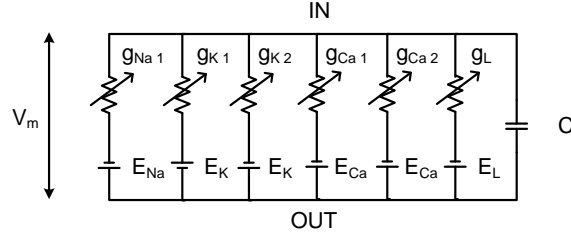
Figure 6.10: Parallel conductance model with different ion channels

6.5.3   Dynamic model equations

The model depicted in Fig. 6.10 can be described with the following equations:

$$\frac{dV_m}{dt} = -\frac{1}{C}(I_{Na1} + I_{K1} + I_{K2} + I_{Ca1} + I_{Ca2} + I_L) + \frac{1}{C}I_{ex}$$

$$\frac{dm_i}{dt} = \frac{m_{i\infty} - m_i}{\tau_{mi}} \quad , \quad \frac{dh_i}{dt} = \frac{h_{i\infty} - h_i}{\tau_{hi}}$$

where V is the notation for the membrane voltage, C is the membrane capacitance, I_{Na1} denotes the sodium current, I_{Ki} denotes the various potassium currents, I_{Cai} stands for the calcium currents, I_L for the leakage. The m_i and h_i variables are the activation and inactivation variables of the corresponding currents. $m_{i\infty}, h_{i\infty}$ and $\tau_{mi/hi}$ values are nonlinear Boltzmann and Gauss -like functions of the membrane potential:

$$m_{\infty}, h_{\infty}(V_{half}, k) = \frac{1}{1 + e^{\frac{V_{half} - V}{K}}}$$

$$\tau(V, V_{max}, \sigma, C_{amp}, C_{base}) = C_{base} + C_{amp} \; e^{\frac{-(V_{max} - V)^2}{\sigma^2}}$$

I_{ex} refers to the external injected current, and the indices refer to: $i = 1$ - I_{Na1}, $i = 2$ - I_{K1}, $i = 3$ - I_{K2}, $i = 4$ - I_{Ca1}, $i = 5$ - I_{Ca2}.

$$I_{Na1} = \bar{g}_{Na1}m_1^3 h_1(V - E_{Na}) \quad I_{K1} = \bar{g}_{K1}m_2^4 h_2(V - E_K)$$

$$I_{K2} = \bar{g}_{K2}m_3 h_3(V - E_K) \quad I_{Ca1} = \bar{g}_{Ca3}m_5 h_5(V - E_{Ca})$$

$$I_{Ca2} = \bar{g}_{Ca2}m_6^2 h_6(V - E_{Ca}) \quad I_L = \bar{g}_L(V - E_L)$$

where the E_{Na}, E_K, E_{Ca} and E_L values denote the reversal potentials of the corresponding ions and the leakage current.

Chapter 7

Dynamic chemical and biochemical models

In the earlier chapters it was assumed that the composition of the material in the various balance volumes is unchanged during the dynamics. This chapter is devoted to dynamic chemical and biochemical models, where the primary focus is the change of the composition in various parts of the system.

The underlying engineering disciplines of modeling dynamic chemical systems are thermodynamics, together with chemical and biochemical reaction kinetics. The basic principles of reaction kinetics are briefly summarized in section 7.3. Because of the thermal effect induced by the chemical reactions, the methods of modeling thermal energy systems discussed earlier in chapter 5 are also important here.

7.1 Characterization of chemical systems

Chemical systems are characterized by the presence of chemical reactions, that affect both the composition of the system and its energy. Therefore, besides of the overall mass and energy conservation balances, we shall consider component mass balances, too.

Modeling objects

Together with the class of thermal energy systems that are also governed by the laws of thermodynamics, chemical and biochemical systems belong to the class of *process systems*. As before in the book, we only consider the simplest case when the *model is based on **perfectly stirred balance volumes***, therefore, lumped parameter dynamic system models are resulted.

As a consequence, the basic modeling object is a perfectly stirred balance volume that is single phase and homogeneous in its composition and other thermodynamical state variables (temperature and pressure).

Mechanisms

Besides of the mechanisms that characterize thermal energy systems (see in section 5.1.1), the mechanisms that are important in a chemical or biochemical model are as follows:

- *Chemical reactions* are the most widespread mechanism in chemical systems that are described by reaction rate equations in the component mass balances. The rate expression is a polynomial function of the concentrations for chemical reactions with mass action law, and it is a rational function of the concentration for biochemical kinetics.

- *Chemical reactions have a thermal effect* associated with them that is twofold. Firstly, the reaction rate depends on the temperature through the temperature dependence of the reaction rate coefficient k (a physico-chemical property). This dependence is commonly described by the so called Arrhenius law, that is an exponential type relationship.

  Secondly, chemical reactions produce/consume energy that is proportional to the reaction rate, that is an induced energy term in the energy balance equation.

- In chemical systems we may have mixing and separation mechanisms, such as distillation, dissolution, crystallization, etc., but we do not discuss them in this book.

7.2 Conservation balance equations

In the general case three types of conservation balance equations are applicable in chemical and biochemical system models: the overall mass, the component mass and the energy balance equations.

As we have seen before, there are relationships between terms in the different balance equations that belong to the same mechanism. In order to show this, we discuss the above three types of balance equations in a logical order for only a single balance volume with only a single chemical reaction $A \rightarrow B$ with *reaction rate r* (measured in units $[mol/s]$), where A and B are the so called *chemical components* or species (such as H_2O, for example).

We recall that only perfectly stirred balance volumes are considered. Furthermore, we assume constant physical properties (such as density, heat capacity etc.) to make the presentation as simple as possible. The flow-sheet of the simple balance volume that will be used for illustrating the construction of balance equations for chemical systems is shown in Figure 7.1.

7.2.1 Overall mass balances

For the sake of simplicity let us assume that we have only a single mass inflow with rate v_b and a mass outflow with rate v_k, both are in units $[kg/s]$. Then
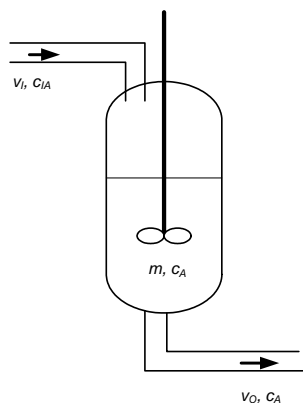
Figure 7.1: The simple balance volume for chemical systems

the overall mass balance is in the following simple form

$$\frac{dm}{dt} = v_I - v_O \tag{7.1}$$

7.2.2   Component mass balances

Assume we have K chemical components in the balance volume that are connected with chemical reactions. Because of the overall mass balance equation, we can only have $K-1$ independent component mass balance equations, therefore, we can only construct a single independent component mass balance for the component A when only a single chemical reaction $A \to B$ is present.

Because reaction rates are usually given in units $[mol/m^3/s]$ (or $[mol/kg/s]$), it is common to use the unit $[mol/m^3]$ (or $[mol/kg]$) for component concentrations. Therefore, if the concentration of component A is c_A (in units $[mol/kg]$), its component mass is $m_A = m \cdot c_A$ in the overall mass of the balance volume. Similarly, the component mass inflow of the mass inflow v_I with the inlet concentration c_{IA} is $m_{IA} = v_I \cdot c_{IA}$. Then the component mass analogue of the overall mass balance (7.1) can be written in its extensive form as

$$\frac{d(m \cdot c_A)}{dt} = v_I \cdot c_{IA} - v_O \cdot c_A - m \cdot R \tag{7.2}$$

where R is the reaction rate.

It is important to note that the first and second terms in the above equations are *induced component in- and out-flow terms*, that are the consequences of the in- and out-flow terms in the overall mass balance equation (7.1).

7.2.3   Energy balances

The energy balance of the above simple balance volume with a single in- and out-flow and a chemical reaction will account for the induced energy terms for the convective in- and out-flow and that of the chemical reaction in the following form:

$$\frac{dU}{dt} = c_{pI}v_I T_I - c_p v_O T - \Delta H \cdot m \cdot R \tag{7.3}$$

where c_{pI} and c_p are the specific heat of the in- and out-flow, respectively, T_I is the inlet temperature, T is the temperature and U is the internal energy of the balance volume and ΔH is the reaction enthalpy, a chemical property measured in units $[J/mol]$. Note that, by convention, the reaction enthalpy is negative for exothermic (i.e. energy generating) reactions.

It is important to note, that the above form of the energy balance equations is only valid when there is a large amount of inert (i.e. non-reacting) component present in the system such that the specific heat of the material in the balance volume can be assumed to be constant, i.e. independent of the composition.

7.3   Constitutive equations

In addition to the constitutive equation types present in thermal energy systems (see section 5.4) earlier, there are some characteristic constitutive equation classes present in chemical and biochemical system models. These are the chemical and biochemical reaction rate equations, and some special property relations related to reaction rate coefficients and reaction enthalpy relations.

7.3.1   Extensive-intensive relationships

Earlier we have already seen the extensive and intensive relationship between the internal energy U and temperature T that is present in energy balances and in energy systems (see Eq. (5.2)) in subsection 5.4.1.

Besides of this, there is another characteristic extensive intensive relationship between component concentration c_A and component mass m_A of component **A** that is in the simple form

$$m_A = m \cdot c_A \tag{7.4}$$

where m is the overall mass of the balance volume, and the concentration is measured in units $[mol/kg]$.

7.3.2   Mass action law reaction rate equations

The simplest, widely used and powerful way of describing how the reaction rate depends on component concentration is the use of mass action law. Physically, it originates from the ***molecular collision picture***, that states that the rate of a chemical reaction is proportional to the number of collisions of the reacting molecules in unit time. This implies that the reaction rate is a product of

the concentration of the reacting components taken on integer exponents, the maximum of which is 2.

Simple interactive illustration of the molecular collision picture The effect of the temperature and pressure on the rate of chemical reactions and on chemical equilibriums when molecular collisions result in chemical reaction can be investigated by interactive simulation using the "Rate Experiments" tab of the interactive reactions and rates simulator.

The simulator has been created in the framework of the PhET^{TM} project [12] at the University of Colorado PhET project.

Elementary reaction steps

Each reaction is assumed to be built from elementary reaction steps, that are *irreversible reactions* in the following form:

$$\sum_{i=1}^{K} \alpha_{ij} \mathbf{X}_i \rightarrow \sum_{i=1}^{K} \beta_{ij} \mathbf{X}_i \quad j = 1, ..., r \tag{7.5}$$
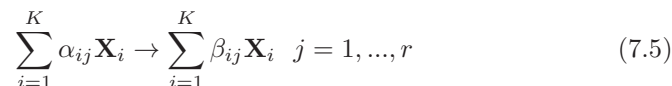
where $\mathbf{X}_i$ denotes a *chemical component* (for example water H_2O), K is the number of components and the *stoichiometric coefficients* α_{ij} and β_{ij} are always *non-negative integers*. Chemical components are also called *species* in chemical reaction kinetics.

Complexes

A multi-set of chemical components is C_k $(k = 1, ..., m)$ associated to the left-hand sides (describing the reacting components) of the reaction steps in the form of

$$C_j = \{ \alpha_{ij} \mathbf{X}_i \mid \text{for } \alpha_{ij} \neq 0, \ i = 1, ..., K \} \tag{7.6}$$

Reaction rate expression

If a reaction step $\sum_{i=1}^{K} \alpha_{ij} \mathbf{X}_i \rightarrow \sum_{i=1}^{K} \beta_{ij} \mathbf{X}_i$ obeys the mass action law, then its reaction rate R_j (measured in units $[mol/m^3/s]$ or $[mol/kg/s]$) is in the following form

$$R_j = k_j \prod_{i=1}^{n} c_i^{\alpha_{ij}} \tag{7.7}$$

where c_i is the concentration in $[mol/m^3]$ (or $[mol/kg]$) of component $\mathbf{X}_i$ and $k_j > 0$ is the *reaction rate constant* of the jth reaction, that is *always positive*.

Simple linear example Let us assume a simple reaction kinetic system with two irreversible steps and three components

$$\mathbf{X}_1 \rightarrow \mathbf{X}_2 \rightarrow \mathbf{X}_3$$

Then the reaction rate equations are

$$R_1 = k_1 c_1 \quad , \quad R_2 = k_2 c_2$$

Simple nonlinear example Now we consider a simple elementary reaction step

$$2\mathbf{A} + \mathbf{B} \rightarrow \mathbf{C}$$

Then the reaction rate equation is

$$R = k c_A^2 c_B$$

7.3.3 Biochemical rate equations

Biochemical rate equations usually have a more complicated algebraic form than the ones implied by mass action law (7.7). The reason for this lies in the fact that biochemical reactions do not obey the mass action law but they are described by an overall reaction rate expression that includes possibly many elementary reaction steps.

The most widespread reaction rate expression is the so-called "monod" kinetic rate that describes the concentration change of the components $\mathbf{X}_B$ and $\mathbf{X}$ as a consequence of a biochemical reaction

$$R(c, c_B) = k \cdot c \cdot \frac{c_B}{k_B + c_B} \tag{7.8}$$

where c_B is the concentration of the biologically active component (e.g. the biomass), c is that of the substrate with k and k_B being constant coefficients.

A more complicated expression also in the form of a rational function is also often used in the form of

$$R(c, c_B) = k \cdot c \cdot \frac{c_B}{k_B + c_B + k_{B1} c_B^2} \tag{7.9}$$

where k_{B1} is also constant.

7.3.4 Chemical property relations

There are two physico-chemical properties that are directly related to chemical reactions: the reaction rate coefficients k and the reaction enthalpies ΔH, that have a dependence on the thermodynamical state variables, on the temperature T, pressure p and composition. *Usually we assume that they only depend on the temperature but not on the pressure and composition.*

Reaction rate coefficient relations

It is widely assumed that the reaction rate coefficient depends exponentially on the temperature T (measured in units $[^oK]$) in the balance volume

$$k = k_0 \cdot e^{-\frac{E}{RT}} \tag{7.10}$$

where $k_0 > 0$ is the pre-exponential factor, $E > 0$ is the activation energy and R is the universal gas constant. The above expression is the celebrated *Arrhenius law*.

Reaction enthalpy relations

The reaction enthalpy is the factor in the energy balance equation (7.3) that gives the thermal effect of a chemical reaction. This is a physico-chemical property that - in principle - can be computed from the specific enthalpies of the components participating in the chemical reactions, if the temperature, pressure and composition dependence of these enthalpies are also taken into account.

If we assume constant specific enthalpies and/or a large amount of inert (non-reacting) component is present in the system, the reaction enthalpy can be used for describing the thermal effect.

Similarly to the case of reaction rate coefficients above, only the temperature dependence of the reaction enthalpy is usually taken into account, that is $\Delta H(T)$. Although this temperature dependence is exponential in nature, most often one resorts to an approximating polynomial function, such as

$$\Delta H = H_0 \cdot \left(1 + c_{H1}(T - T_0) + c_{H1}(T - T_0)^2\right) \qquad (7.11)$$

where T_0 is a suitable reference temperature, H_0 is the reaction enthalpy at the reference temperature, and $c_{Hi}, i = 1, 2$ are constants.

7.4 State space model form of chemical and biochemical models

As we have already seen in the case of energy systems (see section 5.5) one should transform the engineering model originating from first principles into a form that corresponds to the usual state space models. Therefore, one should substitute the algebraic constitutive equations into the differential ones and construct the intensive variable form of the conservation balance equations.

7.4.1 Intensive variable form of component mass balances

Similarly to the transformation of the energy balance equations to its intensive variable form (see subsection 5.5.1) we illustrate the procedure of transforming the component mass balance equation into its intensive variable form using the following simplifying assumptions

F1 A single perfectly stirred balance volume with a single $\mathbf{A} \to \mathbf{B}$ type chemical reaction is considered with overall mass m and internal energy U.

F2 One in- (v_I) and one out-flow (v_O) is assumed, that are mass flows $[kg/s]$.

F3 Constant thermodynamical properties are assumed.

F4 The component concentrations c_A and c_B are measured in $[mol/kg]$, and the unit of the reaction rate R is $[mol/kg/s]$, accordingly.

The component mass - concentration relationship in the form $m_A = mc_A$ is used for expressing the non-measurable component mass with the measurable concentration c_A and mass m. Using assumption F3 above, the component mass balance equation (7.2) can be rewritten in the following form.

$$m\frac{dc_A}{dt} + c_A\frac{dm}{dt} = v_I \cdot c_{IA} - v_O \cdot c_A - m \cdot R \qquad (7.12)$$

Now we can substitute the overall mass balance equation (7.1) into the above equation, that - after rearrangement - can be written in the following *intensive variable form*

$$\frac{dc_A}{dt} = \frac{v_I}{m} \cdot (c_{IA} - c_A) - R \qquad (7.13)$$

This is now in the form of a *state equation originating from the component mass balance.*

7.4.2   State and output equations, system variables

As we have already seen before in subsection 5.5.2, the state equations originate from conservation balances. Therefore, we may have $K + 1$ state equations in a chemical system, that originate from the overall mass, energy, and from the $K - 1$ independent component mass balances for each balance volume.

State variables   It follows from the discussion on the potential state equations above, that the set of state variables of a chemical system consisting of N perfectly stirred balance volumes may include the overall mass (or a derived extensive variable, for example a level) and the temperature of each balance volume, together with the component concentrations, i.e.

$$x = [\, m_i, \ T_i \ , c_{i,k}, k = 1, ..., K \mid i = 1, ..., N]^T \qquad (7.14)$$

as state variables.

7.5   Example: a simple fed-batch fermenter

Fermenters are special bio-reactors of great practical importance. They are mostly regarded as continuous stirred tank reactors (CSTRs) in which special fermentation reactions take place. Fermentation reaction rate expressions are usually quite complex and highly nonlinear. They are often the main source of nonlinearity in dynamic fermenter models.
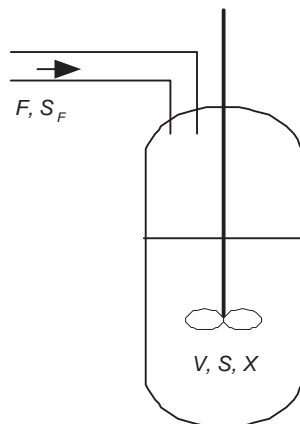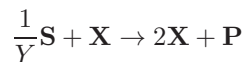
Figure 7.2: The simple fed-batch fermenter

System description

Consider a simple perfectly stirred tank in which a fermentation reaction

$$\frac{1}{Y}\mathbf{S} + \mathbf{X} \rightarrow 2\mathbf{X} + \mathbf{P}$$

takes place that consumes the substrate $\mathbf{S}$ and produces biomass $\mathbf{X}$ and products $\mathbf{P}$. The yield coefficient Y is smaller than 1.

Figure 7.2 shows the flow-sheet of the system. The fermenter is operating in a fed-batch mode, i.e. we continuously feed a solution of solvent to the system with a feed flow rate F measured in $[kg/s]$.

The goal is to construct a simple lumped dynamic model for dynamic analysis and control purposes.

Modeling assumptions

The following simplifying modeling assumptions are used:

F1 Here we assume that the fermenter is operating under isothermal conditions, so that no energy balance is needed.

F2 Constant physico-chemical properties are considered.

F3 The biomass growth rate is described by a nonlinear static function μ, that is of the biochemical reaction rate type (7.9).

F4 Initially a solution containing both substrate and biomass is present in the fermenter.

F5 During the operation we feed a solution of substrate with a given constant feed concentration S_f to the reactor.
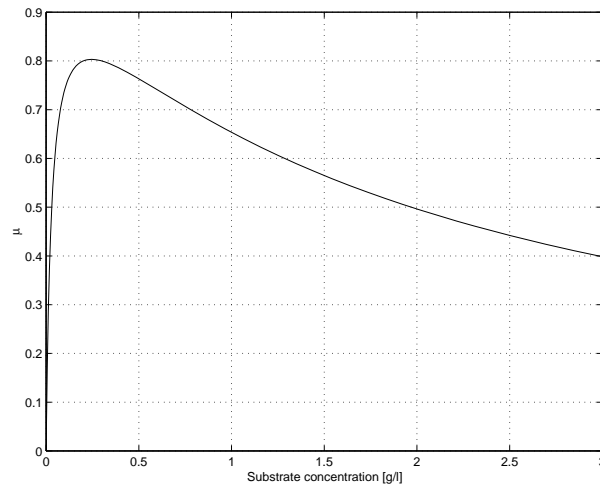
Figure 7.3: The μ function

The particular nature of a fermentation model appears in this so-called biomass growth rate function, which is highly nonlinear and non-monotonous in nature. Figure 7.3 shows the shape of this function. The maximum type character of the curve, i.e. the non-monotonous property, is the one which makes the system difficult to control. The following algebraic form of the function in Fig. 7.3 is used

$$\mu(x_2) = \frac{\mu_{max}x_2}{k_1 + x_2 + k_2 x_2^2} \tag{7.15}$$

where x_2 is the substrate concentration.

The variables and parameters used in the model are given later in subsections **System variables** and **Model parameters**.

Model equations

The simplest dynamic model of a fed-batch fermenter consists of three conservation balances for the biomass **X** (*e.g.* yeast to be produced), that of the substrate **S** (*e.g.* sugar which is consumed by the cells) and for the overall mass in the following form.

Overall mass Assuming constant physical properties and the same density of the feed as the bulk fluid in the tank we obtain

$$\frac{dV}{dt} = F \tag{7.16}$$

Component mass balances These are constructed for the substrate with concentration x_2 and for the biomass with concentration x_1 such that the substrate source of the inlet, and the effect of the reaction is taken into account. The extensive variable form of the component mass balances is as follows.

$$\frac{d(x_1 V)}{dt} = V\mu(x_2)x_1 \tag{7.17}$$

$$\frac{d(x_2 V)}{dt} = -V \cdot \frac{1}{Y}\mu(x_2)x_1 + S_f F \tag{7.18}$$

The intensive variable form of the above component mass balances is constructed by performing the derivation of the products on the left-hand sides, and substituting the overall mass balance (7.16) into them.

State equations

Under the above assumptions the nonlinear state-space model of the fermentation process can be written in the following input-affine form [20]:

$$\dot{x} = f(x) + g(x)u \tag{7.19}$$

where

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} X \\ S \\ V \end{bmatrix}, \quad u = F \tag{7.20}$$

$$f(x) = \begin{bmatrix} \mu(x_2)x_1 \\ -\frac{1}{Y}\mu(x_2)x_1 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{\mu_{max}x_2 x_1}{k_1+x_2+k_2 x_2^2} \\ -\frac{\mu_{max}x_2 x_1}{(k_1+x_2+k_2 x_2^2)Y} \\ 0 \end{bmatrix}, \quad g(x) = \begin{bmatrix} -\frac{x_1}{x_3} \\ \frac{S_f - x_2}{x_3} \\ 1 \end{bmatrix} \tag{7.21}$$

System variables

The variables of the model and their units are the following:

$x_1 = X$ biomass concentration (state)   [g/l]
$x_2 = S$ substrate concentration (state)   [g/l]
$x_3 = V$ volume (state)   [l]
$u = F$ feed flow rate (input)   [l/h].

Model parameters

A typical set of constant parameters and their values is as follows:

$Y = 0.5$ yield coefficient   [–]
$\mu_{max} = 1$ maximum growth rate   [h^{-1}]
$k_1 = 0.03$ Monod constant   [g/l]
$k_2 = 0.5$ kinetic parameter   [l/g]
$S_f = 10$ influent substrate concentration   [g/l]
$X_f = 0$ influent cell concentration   [g/l]
c_1, c_2 reaction enthalpy coefficients   [–] .

7.6   Chemical reaction networks

Chemical reaction networks (CRNs) form a special class of positive nonlinear systems, where the state variables (component concentrations) are positive in nature [3], [4].

The following modeling assumptions are usually applied when constructing the model of a CRN.

F1 A single perfectly stirred balance volume is considered, that is closed, and operates under isothermal and isobaric conditions. This implies constant total mass m, temperature T and pressure p.

F2 n chemical components or species $\mathbf{X}_i$, $i = 1, ..., n$ take part in r chemical reactions.

F3 The chemical reaction obeys the mass action law (MAL).

F4 Constant thermodynamical properties are assumed.

Because the system is assumed to be thermodynamically closed, its total mass (and its volume because of the constant density) is also constant.

7.6.1   The formal description of the reaction system

As the validity of the mass action law is assumed for the chemical reactions (see assumption F3 above), we can use the reaction rate forms in Eq. (7.7) described in subsection 7.3.2. Then the reaction rates are described using the so-called *reaction monomials* associated to the complexes in the form

$$\varphi_j(x) = \prod_{i=1}^{n} c_i^{\alpha_{ij}} \tag{7.22}$$

The stoichiometric matrix Y   The elements of the stoichiometric matrix Y are the stoichiometric coefficients of the components i, $i = 1, ..., n$ in the complexes j, $j = 1, ..., m$, such that the stoichiometric vector of the jth complex forms the jth column of matrix Y

$$[Y]_{ij} = \alpha_{ij} \quad , \quad j = 1, .., m; \ i = 1, ..., n \tag{7.23}$$

The reaction graph   The structure of the chemical reactions are described by a weighted directed graph, called the *reaction graph*, where

- the vertices correspond to the complexes,

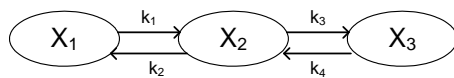- the directed edges describe reactions.

Figure 7.4: The reaction graph of the simple linear example

The *Kirchhoff matrix of the reaction graph* $A_k \in \mathbb{R}^{m \times m}$

$$[A_k]_{ij} = \begin{cases} -\sum_{l=1}^{m} k_{il} & \text{if} \quad i = j \\ k_{ji} & \text{if} \quad i \neq j \end{cases}$$

contains the reaction rate coefficients, and it is a column conservation matrix, that is, the sum of the elements in each of its columns are zero.

Dynamic state equations   These are ODEs in the following simple form

$$\frac{dx}{dt} = Y \cdot A_k \cdot \varphi(x) = N \cdot \varphi(x)$$

7.6.2   A simple linear example

Let us assume a simple reaction kinetic system with two reversible first order steps (i.e. 4 irreversible elementary reaction steps) and three components

$$\mathbf{X}_1 \rightleftarrows \mathbf{X}_2 \rightleftarrows \mathbf{X}_3$$

The dynamic state equations are linear ODEs

$$\frac{dc_1}{dt} = -k_1 c_1 + k_2 c_2$$

$$\frac{dc_2}{dt} = k_1 c_1 - k_2 c_2 - k_3 c_2 + k_4 c_3$$

$$\frac{dc_3}{dt} = k_3 c_2 - k_4 c_3$$

The stoichiometric and Kirchhoff matrices are

$$Y = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad A_k = \begin{bmatrix} -k_1 & k_2 & 0 \\ k_1 & -(k_2 + k_3) & k_4 \\ 0 & k_3 & -k_4 \end{bmatrix}$$

The reaction graph of this simple linear example can be seen in Fig. 7.4.

7.6.3   The Michealis-Menten kinetics

The Michaelis-Menten kinetics is the simplest example of an enzyme kinetic reaction that is widely used for kinetic and model reduction studies. The overall reaction equation is
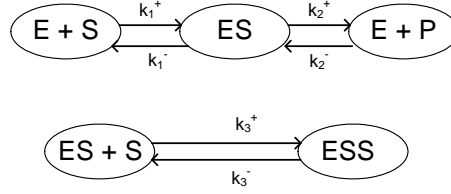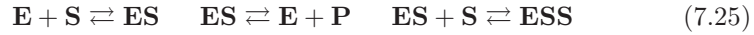
$$\mathbf{E} + \mathbf{S} \rightleftarrows \mathbf{E} + \mathbf{P} \tag{7.24}$$

Figure 7.5: Reaction graph of the Michaelis-Menten kinetic scheme

where $\mathbf{E}$ is the enzyme, $\mathbf{S}$ is the substrate and $\mathbf{P}$ is the product of the reaction. The enzyme acts as a catalyst. The mechanism assumes that the substrate forms a complex $\mathbf{ES}$ with the enzyme in a reversible reaction step that can react further to form the product $\mathbf{P}$ and giving back the unchanged enzyme $\mathbf{E}$. There is a substrate inhibition step in the scheme, too.

The kinetic scheme consists of three reversible reactions

$$\mathbf{E} + \mathbf{S} \rightleftarrows \mathbf{ES} \quad \mathbf{ES} \rightleftarrows \mathbf{E} + \mathbf{P} \quad \mathbf{ES} + \mathbf{S} \rightleftarrows \mathbf{ESS} \tag{7.25}$$

The dynamic model   The reaction kinetic model now consists of the component mass balances for the species $\mathbf{S}$, $\mathbf{E}$, $\mathbf{ES}$, $\mathbf{ESS}$ and $\mathbf{P}$. These can be written in the following ODE form with $x = [c_1, c_2, c_3, c_4, c_5]^T$.

$$\frac{dc_1}{dt} = -k_1^+ c_1 c_2 + k_1^- c_3 - k_2^- c_1 c_5 + k_2^+ c_3 \tag{7.26}$$

$$\frac{dc_2}{dt} = -k_1^+ c_1 c_2 + k_1^- c_3 - k_3^+ c_2 c_3 + k_3^- c_4 \tag{7.27}$$

$$\frac{dc_3}{dt} = +k_1^+ c_1 c_2 - k_1^- c_3 + k_2^- c_1 c_5 - k_2^+ c_3 - $$
$$- k_3^+ c_2 c_3 + k_3^- c_4 \tag{7.28}$$

$$\frac{dc_4}{dt} = +k_3^+ c_2 c_3 - k_3^- c_4 \tag{7.29}$$

$$\frac{dc_5}{dt} = -k_2^- c_1 c_5 + k_2^+ c_3 \tag{7.30}$$

The reaction graph   The reaction graph consisting of two connected components can be seen in Fig. 7.5.

Characterizing matrices The stoichiometric and Kirchhoff matrices are in the form

$$
Y = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} \;,\;\; A_k = \begin{bmatrix} -k_1^+ & k_1^- & 0 & 0 & 0 \\ k_1^+ & -(k_1^- + k_2^-) & k_2^- & 0 & 0 \\ 0 & k_2^- & -k_2^- & 0 & 0 \\ 0 & 0 & 0 & -k_3^+ & k_3^- \\ 0 & 0 & 0 & k_3^+ & -k_3^- \end{bmatrix}
$$
$$(7.31)$$

The procedure of constructing the formal description of a CRN Given the chemical reaction equations (7.25), one can construct the reaction graph, the dynamic model equations and the characterizing matrices in a simple algorithmic way that is illustrated in details in the animation

formal description of a chemical reaction network

Chapter 8

Model analysis and verification

The next step after constructing the dynamic model equations is to analyze the model equations and their solution. This can only be performed in a qualitative way, because usually not all of the model parameter values are known due to the fact, for example, that the simplifying modeling assumptions may cause that the parameters loose their exact physical meaning.

The aim of the model analysis is to perform a first rough checking of the model against engineering intuition: this is called model verification. Here we check if the model behaves - at least qualitatively - the way we expect: if it is stable, for example.

This chapter is devoted to the notions, methods and tools of the qualitative analysis of the models and their solution.

8.1   Analysis of dynamic models

First we recall, that lumped dynamic models developed from first engineering principles are mathematically in the form of ordinary differential equations (abbreviated as ODE) originating from the conservation balance equations, and from algebraic constitutive equations. This model form is called a differential-algebraic equations system, abbreviated as a DAE system in the general form

$$\frac{dx}{dt} = \tilde{F}(x, z) \quad , \quad x(t_0) = x_0$$

$$\tilde{G}(x, z) = 0$$

(8.1)

where x is the vector of differential, and z is the vector of algebraic variables, and $\tilde{F}$ and $\tilde{G}$ are nonlinear functions. In order to compute the solution, one needs to provide suitable initial conditions for the differential variables, as well.

Most often the function $\tilde{G}(x, z)$ can be made explicit for the algebraic variables, when $z = G(x)$, and this is substituted into the differential equations to

have a purely ODE model

$$\frac{dx}{dt} = \tilde{F}(x) \quad , \quad x(t_0) = x_0 \tag{8.2}$$

For the sake of simplicity we restrict our attention to this case.

For the sake of dynamic analysis one needs to identify the input, output and disturbance variables in the system to be modeled and augment the model in Eq. (8.2) with these variables and an output equation (see section 2.2.1) to have a nonlinear state space model in the form

$$\begin{aligned}\frac{dx}{dt} &= F(x,u) \quad , \quad x(t_0) = x_0 \\ y &= H(x,u)\end{aligned} \tag{8.3}$$

8.1.1   Steady states

The first important property of interest, that jointly characterizes the dynamic model and its solution is the set of the steady states. This can be formally obtained by equating the time-derivative of the differential variables to zero ($\frac{dx}{dt} = 0$) in the model equations (8.2) or in the state equation of the state space model in Eq. (8.3) assuming constant values of the input variables.

Then one needs to solve the resulting - usually nonlinear - set of algebraic equations for obtaining the steady state values x^*. The set of nonlinear algebraic equations may not have any solution, or may have more than one. *The existence and multiplicity of the steady states is a characterizing qualitative property of a developed dynamic model.*

8.1.2   Linearized model equations

If a dynamic model has a steady state point x^* for a given steady state input u^*, then the steady state value of the output y^* can also be easily computed from the model in Eq. (8.3). Then the *local dynamical behaviour* around the steady state point (u^*, x^*, y^*) can be characterized using a *locally linearized state space model around a steady state point* that is in the usual LTI form (see section 2.2.1)

$$\begin{aligned}\frac{d\tilde{x}}{dt} &= A\tilde{x} + B\tilde{u} \quad \text{(state eq.)} \\ \tilde{y} &= C\tilde{x} + D\tilde{u} \quad \text{(output eq.)}\end{aligned} \tag{8.4}$$

where the state, input and output variables are deviation variables, i.e.

$$\tilde{x}(t) = x(t) - x^*, \quad \tilde{u}(t) = u(t) - u^*, \quad \tilde{y}(t) = y(t) - y^*,$$

and the LTI model matrices A, B, C and D can be obtained as

$$\begin{aligned}A &= \left.\frac{\partial F}{\partial x}\right|_* \quad & B &= \left.\frac{\partial F}{\partial u}\right|_* \\ C &= \left.\frac{\partial H}{\partial x}\right|_* \quad & D &= \left.\frac{\partial H}{\partial u}\right|_*\end{aligned}$$

with x being the real state variable, and the Jacobian matrices (e.g. $\frac{\partial F}{\partial x}$) are taken at the steady state point that is denoted by $|_*$.

Using the above linearized LTI state space model, the local dynamic properties, such as local stability, local controllability and observability can be easily investigated. The *local dynamical properties form the second important qualitative characteristics of a dynamic model.*

It is important to note that the locally linearized model itself together with its local dynamical properties is strongly steady state point dependent. The dependence - that can be analyzed varying the steady state input value u^* - is also a characteristic qualitative property of the model.

8.1.3 Solution of dynamic models

Because of the nonlinear character of the model equations (8.3) or (8.2), there is not much hope to find an analytical solution in a closed form. Instead, numerical methods of computing the solution of ODEs (see e.g. [5]) are applied for obtaining a solution for a given initial value and the input signal values given for the integration interval. Usually a program implemented in a simulation environment (for example MATLAB) is used to construct a *dynamic simulator* of the model, that can be applied for the analysis of the solution properties, and later for control and diagnostic studies.

Problem statement of model solution

In order to collect the necessary ingredients that are needed for computing the solution of a dynamic model, we give a formal problem statement below.

Given

- the model equations: systems of ordinary differential and algebraic equations (DAEs),

- the initial values,

- the parameter values,

- the time interval of interest.

Construct the solution of the model, i.e. the time dependent value of the variables in the system model.

Numerical solution methods

Most often numerical solution methods of ODEs based on finite difference approximations, e.g. various versions of Runge-Kutta methods [5] are applied, for which there are ready subroutines in most of the simulation environments (e.g. MATLAB). The following properties are important if one wants to find or select a proper solution method

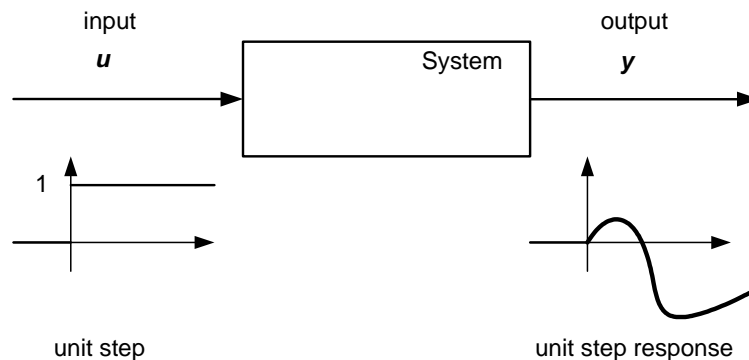- numerical stability (explicit versus implicit methods)

Figure 8.1: Unit step response

- the ability to handle stiff models

- accuracy (the order of the method)

- the way and flexibility of automatic selection of the integration steps

8.1.4   Response to test signals

The response of a system to the widely applied test signals - such as to a sinusoidal harmonic input, or to a unit step signal - characterizes the system behaviour and may serve as an input-output model for an LTI system (see [9]).

At the same time, such a response can be obtained easily both experimentally from a real system and by numerical computations using its dynamic simulator.

Therefore, these responses to the usual test signals are characteristic qualitative properties of the developed dynamic model.

Unit step response

The unit step is a simple, easily implementable test signal, that is zero until $t = 0$ and jumps to 1 thereafter. This is the most widespread characteristics of both linear and nonlinear systems.

The notion of the unit step response function is depicted in Fig. 8.1 in the case of a single-input single-output (SISO) system.

Impulse response

The unit impulse, also known as Dirac-delta function is the time-derivative of the unit step function, that can only be realized approximately.

Despite of this, the *impulse response function* (or weight function) is a widely accepted and used model form of continuous time SISO LTI systems, that is defined as the system response to a unit impulse input signal.

8.2 The structure and structural analysis of dynamic models

As it has been emphasized before, a newly developed dynamic model is most often incomplete in the sense, that the value of some of its parameters is not known, it is to be determined in the next step of the 7 step modeling procedure during the model calibration. This means, that only the functional form or the structure of the dynamic model is given, that can be and should be used for model analysis.

This section deals with the formal characterization of the dynamic model structure, and with the methods and procedures that can be used to derive structural dynamic properties (such as structural controllability, for example) therefrom.

8.2.1 The structure of state space models

The formal description of the structure of dynamic models is based on the notion of *signed structure matrices*. The matrix with sign-valued elements $[A]$ is a signed structure matrix of a numerical matrix A, when

$$[A]_{ij} = \begin{cases} + & \text{if} \quad a_{ij} > 0 \\ 0 & \text{if} \quad a_{ij} = 0 \\ - & \text{if} \quad a_{ij} < 0 \end{cases} \tag{8.5}$$

Structure graph

The so-called structure graph is associated with a concentrated parameter non-linear state space model in Eq. (8.3) in the following way. The structure graph is a signed (sign-weighted) directed graph (abbreviated as SDG) $S = (V, E; w)$ - where V is the set of vertices, E is the set of edges, and w is the edge weight function - with the following properties.

- The partitioned *vertex set* V corresponds to the state (X), input (U) and output (Y) variables

$$V = X \cup U \cup Y$$
$$X \cap U = X \cap Y = U \cap Y = \emptyset$$

- The *directed edges* in the set E correspond to *direct* effects between variables, an edge starts at the cause variable and ends at its consequence.

- The *edge weights* w describe the *sign* of the effect, where "+" corresponds to increasing and "-" to decreasing effect.

The occurrence matrix of a structure graph   An o_{ij} entry in the occurrence matrix O is computed from the edge weight values w_{ij} of the edges (v_i, v_j)

$$o_{ij} = \begin{cases} w_{ij} & \text{if} \qquad (v_i, v_j) \in E \\ 0 & \text{otherwise} \end{cases}$$

For a linear(ized) LTI state space model (in Eq. (8.4)) with the parameters (A, B, C, D) and the variable order (u, x, y) the following occurrence matrix is obtained.

$$O = \begin{pmatrix} 0 & 0 & 0 \\ [B] & [A] & 0 \\ [D] & [C] & 0 \end{pmatrix}$$

where the 0-s here denote zero matrices of appropriate dimensions.

Paths in the structure graph   A *directed path* $P = (v_1, v_2, ..., v_n)$, $v_i \in V$, $e_{i,i+1} = (v_i, v_{i+1}) \in \mathcal{E}$ in the structure graph corresponds to the *indirect effect* of variable v_1 on variable v_n.

The *value* of the path is defined as

$$W(P) = \prod_{i=1}^{n-1} w(e_{i,i+1})$$

i.e. the value is the product of all signs along the paths.

8.2.2   Example: the structure of a heat exchanger cell model

In order to illustrate the notion of the structure graph, the SDG model form of the simple heat exchanger cell model developed in subsection 5.6.1 is given here.

The LTI version   The state space model equations (5.13) and (5.14) are used with assuming that

1. the flow rates v_c and v_h are constant, and

2. the inlet temperatures T_{ci} and T_{hi} are the manipulable input variables.

Furthermore, a simple $y = x$ output equation is assumed, i.e. we can directly measure both state variables.

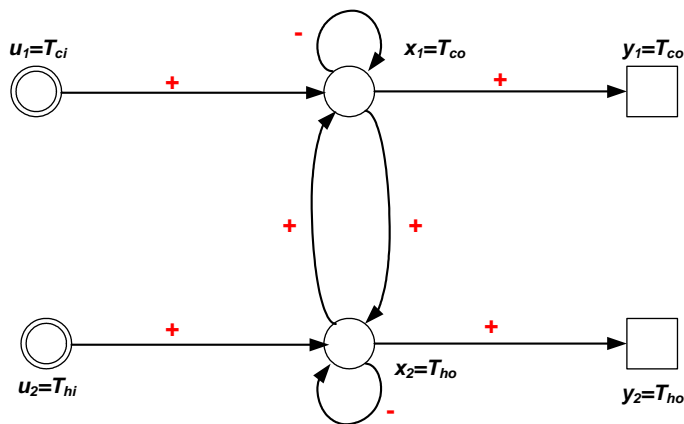Under the above assumptions the resulting state space model is LTI, and its SDG is depicted in Fig. 8.2.

Figure 8.2: The SDG of a heat exchanger cell model

The procedure of constructing the structure graph from the state space model equations The simple algorithmic way of how to construct the structure graph of a model given the LTI state space model equations is illustrated here in the animation

drawing the structure graph of the heat exchanger cell

using the simple heat exchanger cell example above with the state space model equations (5.13) and (5.14).

A nonlinear version A nonlinear (more precisely bilinear) version of the state space model is obtained, if we relax assumption 1. above, but assume instead, that the flow rate v_h is the time-dependent disturbance signal, and the other flow rate v_c remains constant.

Then the augmented version of the SDG model with a disturbance is depicted in Fig. 8.3.

8.2.3 Structural properties

Structural properties - such as structural stability, for example - *hold for a class of systems with the same structure.* This means, that the class members have a state space model, the structure graph of which is the same.

In other words we say that a system has a structural property if every element in the class of systems with the same structure - with a possible extension of a zero-measure set - has the property.

Relationship between the ordinary and structural version of the same property From the above formulation of structural properties it follows that
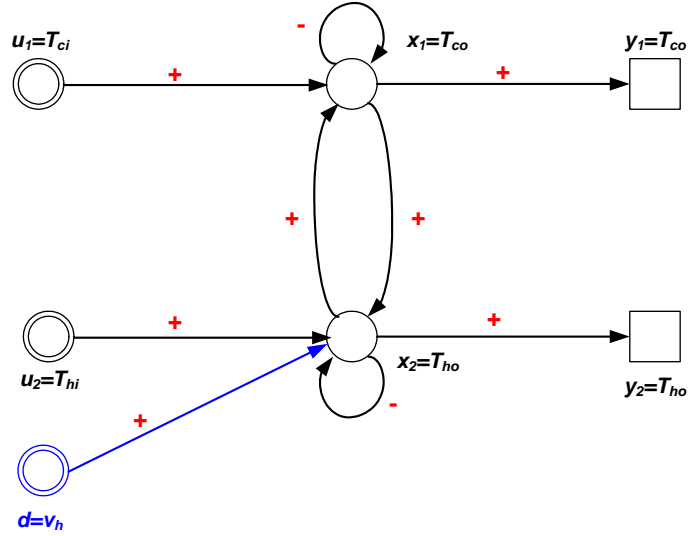
Figure 8.3: The SDG of a heat exchanger cell model with disturbance

the presence of a structural property for a class does not necessarily mean that every single member of the class holds the ordinary (i.e. non-structural) version of the property.

This is best illustrated on the example of the structural rank $(s - rank)$ of matrices. Assume we have a numerical matrix $A \in \mathbb{R}^{2 \times 2}$ with numerical rank 1. Then

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \ , \ \text{rank } A = 1 \ , \ \text{s} - \text{rank } A = \text{s} - \text{rank} \begin{bmatrix} + & + \\ + & + \end{bmatrix} = 2 \quad (8.6)$$

Structural dynamic properties   Usually, one investigates structural controllability, observability and structural stability as qualitative dynamic properties of a model.

The structural controllability and observability can be checked by computing the structural rank of the controllability or observability matrix [9], respectively.

Alternatively, necessary conditions for structural controllability and observability can be established by investigating the directed paths on the structure graph. A system is

- *structurally controllable* if there exists at least one path that ends at each state variable node and starts from any of the input nodes (*input connectivity*),

- *structurally observable* if there exists at least one path starting from each state variable node that ends at an output variable node (*output connectivity*).
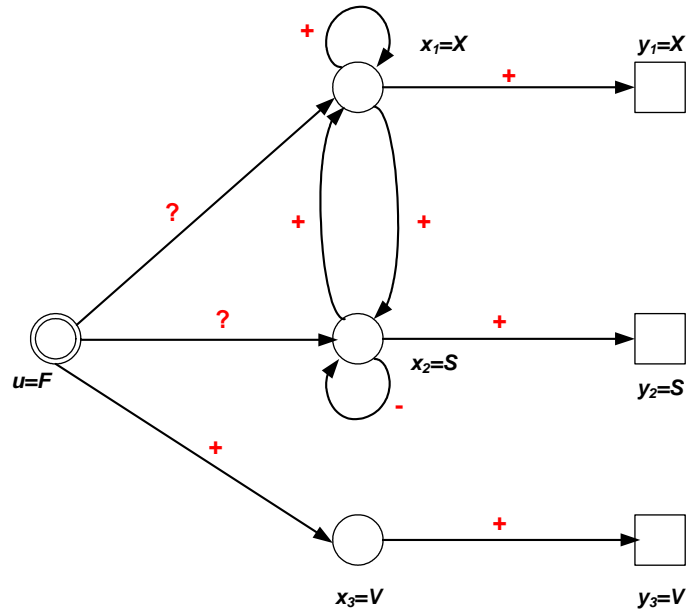
Figure 8.4: The SDG of the fed-batch fermenter model

8.2.4 Example: controllability and structural controllability

The using and meaning of the structural controllability analysis is illustrated here on the example of the simple fed-batch fermenter, the dynamic state space model of which is presented in subsection 7.5. The state equations are presented in Eqs. (7.19) that includes three state equations for the state variables X, S and V with the input variable F. A simple $y = x$ output equation is added to the model.

Structural controllability analysis

The SDG model of the fermenter is shown in Fig. 8.4. It can be seen that this model is structurally controllable, because we can reach each of the state variable nodes X, S and V from the input variable node F through directed paths. Note that the "?" sign weight on some directed arcs denotes an indefinite (unknown) sign.

Nonlinear controllability analysis

The structural controllability, however, does not mean that this particular nonlinear model is controllable indeed.
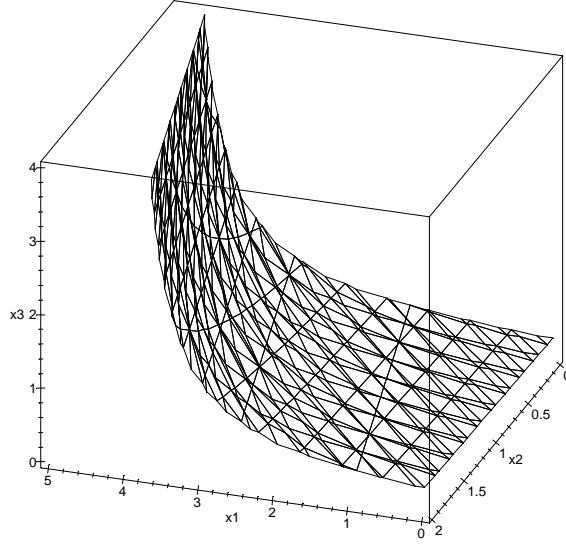
Figure 8.5: The controllability hypersurface of the fed-batch fermenter

By performing a nonlinear controllability analysis it has turned out that this model is not controllable, but there exists a two-dimensional manifold in the three dimensional state space determined by the initial conditions, on which the system moves for any input signal. This *controllability hyper-surface* of the fed-batch fermenter model for the *initial conditions* $x_1(0) = 2\frac{g}{l}$, $x_2(0) = 0.5\frac{g}{l}$, $x_3(0) = 0.5\frac{g}{l}$ is depicted in Fig. 8.5. The detailed analysis is available in [20].

8.2.5   Structural properties and the unit step response

Some qualitative properties of the unit step response function can also be related to the paths values in the structure graph that can also be used for model analysis and verification.

These qualitative properties of the step response functions are shown in Fig. 8.6: the sign of the initial deviation, and the steady state deviation.

The sign of the initial deviation   The sign of the initial deviation of the unit step response function between an input and an output signal can be computed as the sign-value of the shortest path or paths between the input and the output nodes in question.

The notion of the shortest path is illustrated in Fig. 8.7. If more than one path has the shortest length, i.e. the smallest number of connected directed arcs, then their sign values should be sign-added, that may result in an indefinite (unknown) sign value "?".
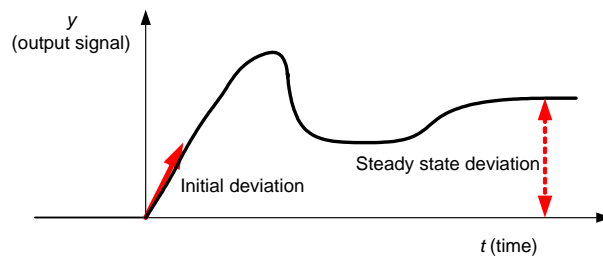
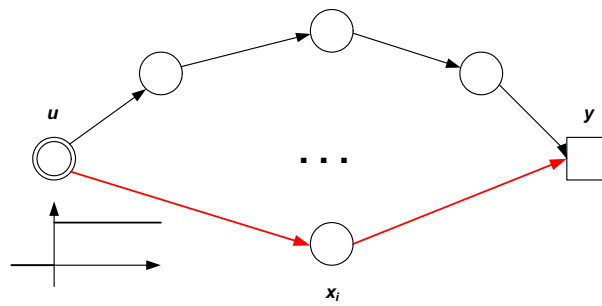Figure 8.6: Qualitative characterization of the unit step response

Figure 8.7: Shortest path(s)

8.2.6   The use of structural analysis results for model verification

If one has a newly developed model with possible unknown parameters, then the following steps can be performed to verify it using the methods of structural properties.

1. Develop the *SDG* form (signed structure graph) of the developed dynamic model that is in its state space model form.

2. Determine the *simple structural dynamic properties of the model*, and answer the following questions.

    (a) Is it structurally controllable?

    (b) What is the sign of the initial deviation of each of the outputs to each of the inputs?

3. Measure the unit step responses of each of the outputs to each of the inputs, and determine the sign of the initial deviations.

4. Compare the corresponding signs of steps 2.(b) to the experimentally obtained ones in step 3. If they are the same, then the model is verified, otherwise the model should be corrected.

5. Compare the structural controllability properties of the model to your engineering intuitions. If they coincide, then the model is verified, otherwise it needs to be improved.

Chapter 9

Model calibration and validation

Model calibration and validation form the last, but very important step of the model building process (see the 7 step modeling procedure in chapter 3). They are closely related by the methods and algorithms they use, because they both relate the developed model equations with measured data in order to come to certain basic conclusions about the model. This conclusion is different in two cases: it is the estimated value of some model parameters in the case of model calibration, and it is the suitability or acceptability of the developed model for model validation.

The methods and tools for model calibration and validation form a well defined and relatively independent area of systems and control theory called *identification* [9] for which there is wide literature (see e.g. [8]). Therefore we restrict ourselves to show briefly only the basic principles of this field, and a short case study in this chapter.

9.1   Model calibration

Dynamic models developed from first engineering principles are - in principle - "white-box" models, where all of the mechanism describing model elements (functions) and their parameters are known. However, one often formulates simplifying modeling assumptions during the model development, that not only make the model equations simpler, but may cause the appearance of model parameters with unknown physical value and/or model elements with unspecified functional form. Then the developed model is of "grey-box" nature, where most of the model is completely known with some unknown parts.

Then one can use measured data from the real system to be modeled to estimate the model parameters (or other unknown structural elements). Model calibration methods are used for this purpose.

Because we want to show only the basic principles of model calibration,

we only deal with the case when the model contains unknown parameters but no unknown structural elements. Then model calibration simplifies to model parameter estimation.

9.1.1   Problem statement of model parameter estimation

The general problem statement of model parameter estimation can be formulated as an optimization problem in the following form.

Given

- a parameterized sampled discrete time explicit dynamic system model in the following general form

$$y^{(M)} = \mathcal{M}(u;\; p^{(M)}) \tag{9.1}$$

- a *measurement record* containing a finite set of measured input and output data with possible measurement errors present with the measured output values $y(\tau)$

$$D[0, k] = \{\; (u(\tau), y(\tau) \mid \tau = 0, \ldots, k\; \}$$

- a *loss function L and signal norm* $||.||$ that characterize the "closeness" of the model-predicted output value $y^{(M)}(\tau)$ to the measured one, that is expressed as a function of the *residual signal r*

$$L(p) = ||r||\;\;,\;\; r(\tau) = y(\tau) - y^{(M)}(\tau)\;\;,\;\; \tau = 0, \ldots, k$$

Compute
An estimate $\hat{p}^{(M)}$ of $p^{(M)}$ such that $L(p)$ is minimum

$$||y - y^{(M)}|| \to \min$$

9.1.2   The methods of model parameter estimation

The model parameter estimation is a complex task that includes different other necessary sub-tasks besides the real parameter estimation itself. These sub-tasks form a model parameter estimation procedure that is depicted in Fig. 9.1.

The model parameter estimation procedure

The brief description of the sub-tasks is given below, where details can be found e.g. in [7].

1. *Model preparation*
   Majority of the dynamic models developed from first engineering principles are in the form of continuous time state-space models, that are not directly
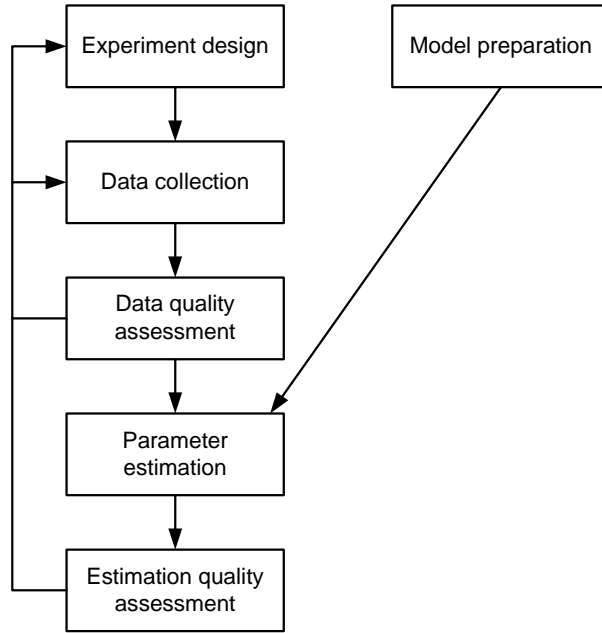
Figure 9.1: The model parameter estimation procedure

useful for model parameter estimation (see the problem statement above that requires discrete time models). Therefore, we need to apply at least sampling (see [9]) or transforming the model into its input-output form for some special parameter estimation methods.

2. *Experiment design*
Here we decide on the sampling rate (sampling time), on the number of measurements to be performed, on the necessary repetition number, on the applied input sequence to be applied (to ensure proper excitation, see [8]).

3. *Data collection*
This is a critical sub-task, where we do not only need to collect the measured data of interest according to the experiment design specification, but also carefully record any events or circumstances that may affect the quality of the measured data.

4. *Data quality assessment*
The aim of this sub-task is to decide if the collected data are suitable for model parameter estimation, that is, the data do not contain any bias, gross error, outliers etc. that may cause the deterioration of the estimated parameters. Here we use simple (i.e. not computationally intensive) procedures, such as visual inspection and screening, and simple statistical tests

either individually for the measured signal sequences, or for a collection of those.

If any problems with the data are detected, then one may improve their quality by data preprocessing, but usually it is much better if we either repeat the data collection or modify the experiment design and then repeat the measurements to get rid of the disturbing measurement errors.

5. *Parameter estimation*
   This is the essence of the whole parameter estimation procedure, the methods of which are described in more details below.

6. *Estimation quality assessment*
   This sub-task plays a key role also in model validation, therefore, it is discussed in a separate subsection 9.1.3.

Parameter estimation methods

The general case   In the most difficult and general case the parameter estimation method solves the optimization problem stated as the model parameter estimation problem in subsection 9.1.1. For this purpose we need

- a *dynamic simulator* that generates the model outputs $y^{(M)}(\tau), \tau = 0, ..., k$ in each iteration step k from the dynamic model with the current model parameter vector $p^{(M)}(k)$,

- an *optimizer* that changes the parameter vector in each step according to some strategy (for example using the gradient method) until the minimum value of the loss function is found,

- an initial value $p^{(M)}(0)$ for the parameter vector (or more plausible initial values if we expect local minima),

- a domain within which the physically meaningful parameter values can be found (most often they are positive, for example).

Unfortunately, the optimization problem is not convex in the general case, and more than one (local) optimum may be present, therefore, it is a difficult mathematical problem. In addition, the estimation procedure is an iterative method by nature, that only gives a point estimate but no information about the accuracy of the estimate (e.g. in terms of its covariance matrix).

The linear-in-parameters case   However, when the model is already in an input-output form that is linear in its parameters, when the discrete time predictive model is in the form of

$$y^{(M)}(j+1) = \left(p^{(M)}\right)^T \cdot \varphi\left(\ (u(j-\tau),\ y(j-\tau))\ |\ \tau = 0, ..., n\ \right) \qquad (9.2)$$

where φ is the residual vector, and the loss function is quadratic, then one can construct a least squares (LS) estimator [8] for the parameters that is in a
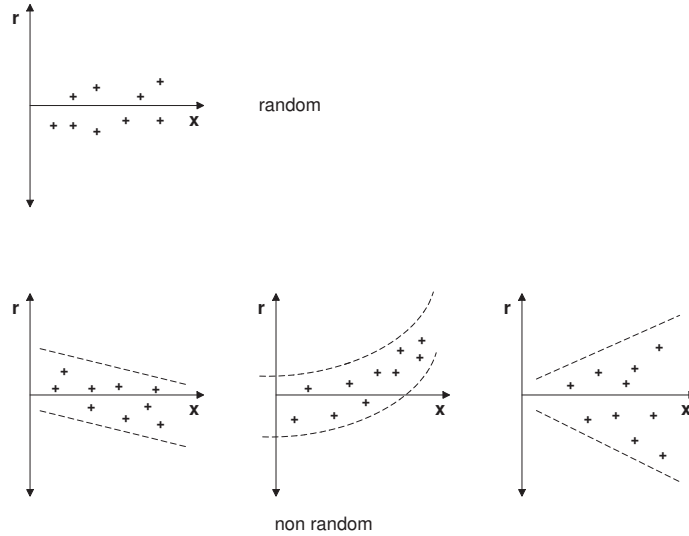
Figure 9.2: Typical residual patterns

closed form. The LS estimation procedure provides an estimate of the covariance matrix, too.

9.1.3 Assessing the quality of the estimates

The quality of the obtained parameter estimate can be assessed based on either the residual or on the covariance or confidence region pattern.

The residuals

Given the estimated parameter vector $\hat{p}^{(M)}$ we can generate the actual realization of the residual signal $r(\tau) = y(\tau) - y^{(M)}(\tau)$, $\tau = 0, \cdots, k$ using it for the model prediction. It is known from the theory of parameter estimation [8] that the residual signal is a white noise process (i.e. a sequence of zero mean independent random variables having the same distribution) when the estimate is asymptotically unbiased.

This condition can be checked either by statistical tests or by simple inspection of the sequence elements plotted against the time. Fig. 9.2 shows a few patterns that may arise, the only one on the top corresponds to the case of a "good", i.e. asymptotically unbiased estimate.

The covariance matrix and the confidence regions

As saw earlier in subsection 9.1.2 on the parameter estimation methods, an estimate of the parameter covariance matrix is rarely available, only when the
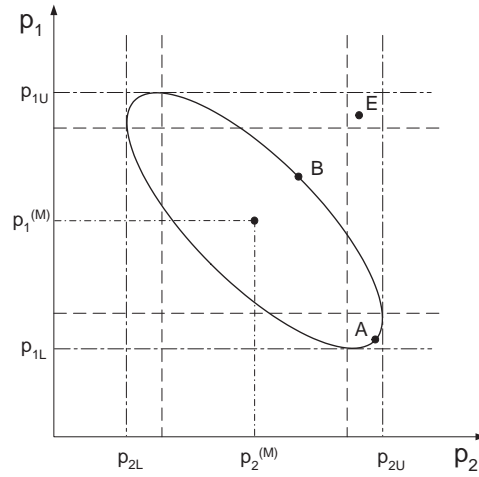
Figure 9.3: Ideal two parameter confidence region

model is in an input-output form and linear in its parameters (see Eq. (9.2)).

In the general case, however, the only information about the accuracy of the estimated values is available in the form of the shape of the loss function as a function of the model parameters. In the "ideal" LS estimate case, when the model is linear in its parameters and the loss function is quadratic, this shape is a paraboloid that has a definite unique minimum value, and its level sets are ellipses. Fig. 9.3 depicts a level set of such an ideal case in the case of two parameters.

Empirical confidence regions Following the analogy of the ideal case, one can construct an estimate of the parameter confidence region if the values of the loss function are known as a function of the parameters. This is readily available, if the parameter estimate is obtained by numerically optimizing the loss function in the parameter space.

Then the confidence region of the parameters can be obtained as a level set cut by the $100 + (100 - \epsilon)$ percent of the minimal value of the loss function in the parameter space, where ϵ is the confidence level (in percent). Note that it is usually not an ellipse, and does not keep its shape when changing the confidence level. However, the quality of the parameter estimate is regarded acceptable, if these regions are closed, bounded and of an close-to ellipse shape.

A very prolonged (in the worst case unbounded) region with multiple close-to minimal values indicates the presence of a deterministic relationship between some parameters, or the absence of sufficient excitation. Fig. 9.5 later in sub-section 9.2.2 shows such a non-satisfactory case.

9.2 Case study: model calibration of a steam generator model

As we saw in subsection 5.6.2, the steam generator is a vessel that contains water of the secondary circuit in a pressurized water nuclear power plant the vapor of which is produced by heating the liquid phase by the circulating primary circuit liquid.

This section illustrates the methods and procedures of model calibration on a steam generator model. The material is based on the paper [18], from where additional information can be obtained.

9.2.1 The dynamic model and the measured data

The state-space model is of the following form

$$\frac{dM_{SG}}{dt} = m_{SG,in} - m_{SG,out} \tag{9.3}$$

$$\frac{dT_{SG}}{dt} = \frac{1}{c_{p,SG}^L M_{SG}} \Big[c_{p,SG}^L m_{SG,in} \left(T_{SG,SW} - T_{SG} \right) - $$
$$- \left(c_{p,SG}^V - c_{p,SG}^L \right) m_{SG,out} T_{SG} - m_{SG,out} E_{evap,SG} + $$
$$+ K_{T,SG,2} \left(T_{PC} - T_{SG} \right) + W_{in,SG} \Big] \tag{9.4}$$

The output equations are as follows:

$$p_{SG} = p_*^T(T_{SG}) \tag{9.5}$$

where the input variable is $m_{SG,in}$, the disturbances are T_{PC}, $T_{SG,SW}$ and $m_{SG,out}$, the controlled output variable is T_{SG} (p_{SG}).

The estimated parameters in this subsystem were $K_{T,SG,2}$, $W_{in,SG}$, $c_{p,SG}^L$ and $c_{p,SG}^V$. Since the mass of the water in the secondary side of the steam generator is not measured, only the inlet water and the outlet vapor flow rate are known. It means that the initial water mass $M_{SG}(0)$ must also be estimated.

Measured data Measured data from units 1, 3 and 4 of the Paks Nuclear Power Plant were collected for parameter estimation purposes. In order to span a relatively wide operating domain, transient data of increasing and decreasing the power of the units when shifting from day to night load conditions and back have been used.

The following variables have been measured: $T_{PC}, m_{SG,in}, m_{SG,out}, T_{SG,SW}$, p_{SG}.

The parameter estimation method The steam generator model (Eqs. (9.3)-(9.4)) is nonlinear in its physical parameters and linear in the variables.

The dynamic model equation(s) is/are nonlinear in its/their parameters, an optimization-based parameter estimation method, the Nelder-Mead simplex method [19] available in MATLAB has been used.

The value of the objective function is given by the scaled 2-norm of the difference between the measured and the model-predicted output signals, i.e.

$$e = \sqrt{\frac{\int_0^T (\hat{y}(t) - y(t))^2 dt}{\int_0^T y^2(t) dt}} \tag{9.6}$$

where y is the measured output, $\hat{y}$ is the model-predicted (simulated) output signal and T denotes the time-span of the measurement/simulation. To use the simplex method, suitable initial values are needed. They could be found in [13, 10] and obtained from engineers from Paks NPP. In particular, the initial value of the initial mass in the steam generator is its normal value $M_{SG}(0) = 32000 \, kg$ known from a technical discussion.

9.2.2   Parameter estimation and its quality

The value of estimated parameters can be found in Table 9.1 for unit 1.

Parameter	Unit	unit 1 Time span: 4h
$M_{SG}(0)$	kg	34988
$c_{p,SG}^L$	$J/kg/K$	3922.2
$c_{p,SG}^V$	$J/kg/K$	2910.5
$W_{in,SG}$	W	$-1.1723 \cdot 10^5$
$K_{T,SG,2}$	W/K	$8.2939 \cdot 10^6$

Table 9.1: Results of the parameter estimation of the decomposed system

The fit can be assessed from the difference between the model-computed and measured temperatures that can be seen in Fig. 9.4, that shows an acceptable fit.

However, the estimated parameters are strongly correlated, as it is seen from the shape of the loss function as a function of two parameters c_{pPC} and $K_{T,SG,2}$.

More about this case study can be found in [18].

9.3   Model validation

Model validation is the final step in developing a dynamic model from first engineering principles. It requires a calibrated dynamic model, that is a model with all of its parameters known, and a set of measured data from the system to be modeled to decide if the model fits to the modeling goal specified in the beginning of the modeling procedure.
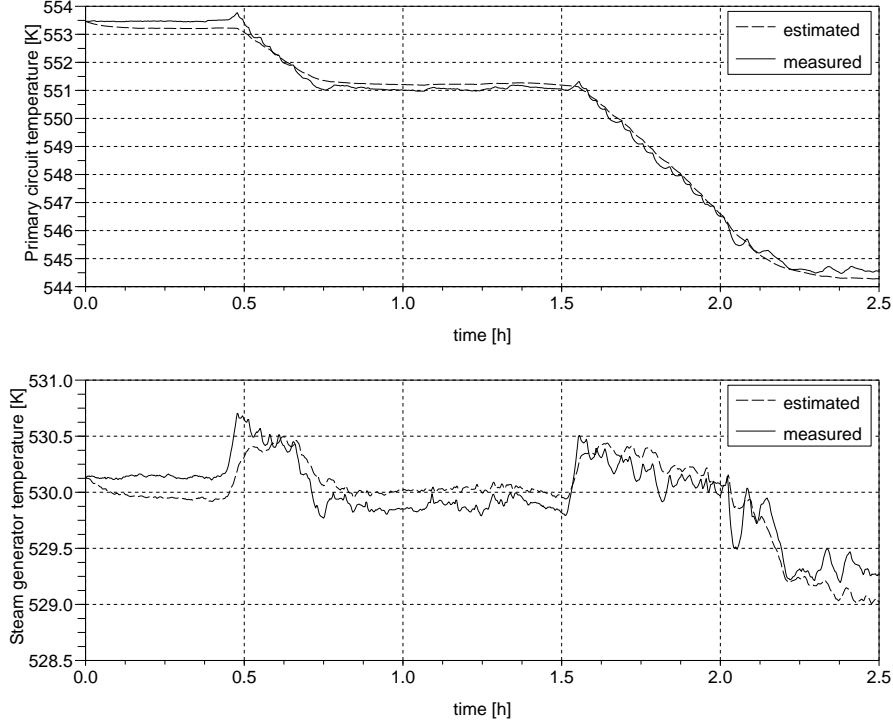
Figure 9.4: The temperatures in the steam generator model calibration

9.3.1 Problem statement of model validation

The general problem statement of model parameter estimation can be formulated as a decision problem in the following form.

Given

- a sampled discrete time explicit dynamic system model with all of its parameters $p^{(M)}$ known in the following general form

$$y^{(M)} = \mathcal{M}(u;\ p^{(M)})$$

where the *model outputs $y^{(M)}$ now include only those measurable signals that are relevant (important) with respect to the modeling goal*

- a *measurement record* containing a finite set of measured input and output data with possible measurement errors present with the measured output values $y(\tau)$

$$D[0, k] = \{\ (u(\tau), y(\tau) \mid \tau = 0, \cdots, k\ \}$$
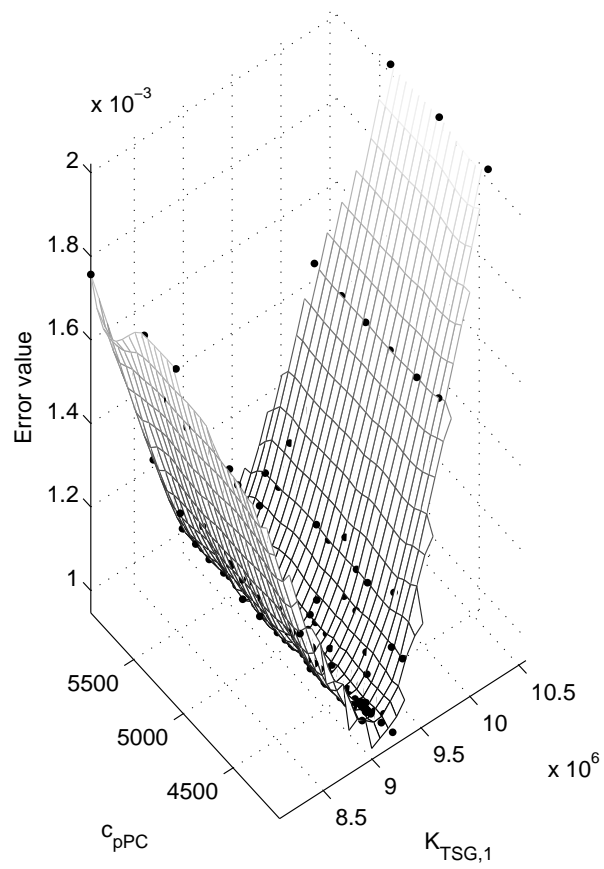
Figure 9.5: The relationship between the estimated values

- a *loss function L and signal norm* $||.||$ that characterize the "closeness" of the model-predicted output value $y^{(M)}(\tau)$ to the measured one, that is expressed as a function of the *residual signal r*

$$L(p) = ||r|| \quad , \quad r(\tau) = y(\tau) - y^{(M)}(\tau) \quad , \quad \tau = 0, \cdots, k$$

- *an expected accuracy ε* either globally for the loss function or element-wise for the components of the residual *that corresponds to the modeling goal*

Decide
if the model is acceptable for the modeling goal with respect to the loss function and the expected accuracy.

9.3.2   Model validation methods

Measured data for model validation

Similarly to the model calibration sub-step, here one needs measured data from the real system to perform model validation. It is important to emphasize, that one cannot use the same measured data as for model calibration, because the information contained in those data has already been incorporated into the estimated parameter values such that the fit is optimized. Instead, *additional measured data should be collected possibly using a slightly different experiment design and circumstances for validation purposes.*

The model validation procedure

At the same time, one has to perform all of the necessary auxiliary sub-tasks described already in subsection 9.1.2 when performing model validation, but just the model parameter estimation sub-task is replaced by the model validation, and the estimation quality assessment sub-task is substituted by the simple assessing the fit.

Therefore, the following sub-task is to be performed along the same logical connections as outlined in Fig. 9.1.

1. Model preparation

2. Experiment design

3. Data collection

4. Data quality assessment

5. Validation decision

6. Assessing the fit

The validation decision   The validation decision, i.e. the decision about the suitability of the developed model to the modeling goal, is taken by executing a simple decision specified in the validation problem statement (see subsection 9.3.1). As this is a Boolean (yes/no) decision that may require to revisit some of the earlier steps of the 7 step modeling procedure described in chapter 3, one needs to augment this decision with a more detailed assessment. This is usually based on assessing the fit of the developed model using the relevant methods described earlier in subsection 9.1.3.

Chapter 10

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Appendix A

Abbreviations and notations

Abbreviation	Explanation
CRN	cheamical reaction network
DAE	differential and algebraic equations
HH	Hodgin-Huxley
LTI	linear and time-invariant
LS	least square
ODE	ordinary differential equation
SDG	signed directed graph

Symbols	Meaning
$\mathbb{R}$	set of real numbers
$\mathbb{Z}$	set of integer numbers

List of Figures