Introduction to Systems Analysis

Dieter M. Imboden • Stefan Pfenninger

Introduction to Systems Analysis

Mathematically Modeling Natural Systems

Cartoons by Nikolas Stürchler

Springer

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Preface

Since the first publication of the German textbook *Systemanalyse: Einführung in die mathematische Modellierung natürlicher Systeme* by Dieter M. Imboden and Sabine Koch in 2003, many things have changed in the academic world. Others have remained firm and constant; one of them is the central role of the mathematical language as the common basis to express the ever more complex findings of scientific research. In fact, an introduction to the principles of mathematical modeling should still be part of the foundation of every university science curriculum.

At the same time, teaching is becoming more international, especially at the world's leading research universities (to which ETH Zürich proudly belongs). This in turn means that even in non-English-speaking countries, English has become firmly established as the lingua franca in the classroom. In fact, the first author (Dieter Imboden) was often asked for an English version of the book. Among those who contacted him was one of his former students and a young researcher, Stefan Pfenninger, at the time working at the International Institute for Applied Systems Analysis (IIASA) in Laxenburg, Austria. Dieter responded with his regrets over the lack of an English version of the book and spontaneously suggested to Stefan to help prepare one. Sabine Koch, the junior author of the German book and by now a successful ecological winemaker in Southern Germany, enthusiastically supported the idea and was happy to yield the junior author position to Stefan. The cartoonist Nikolas Stürchler, who had meanwhile joined the Swiss Diplomatic Service (where he is rumored to use his skills livening up drab international treaties), agreed to have his cartoons incorporated into the English version as well. Thus, cheeky Dang, muddle-headed Professor Dong, and clever dog Ding are still here to help the reader digest all the equations with humor and (sometimes) deep philosophical insight.

Since the concept of the book has been proven in the lecture hall time and again, we kept changes in the translated version to a minimum. With a few exceptions, the numbering of equations, figures, tables, examples, and problems correspond one-to-one to the German version. This will facilitate the use of the book for lectures in which students are using either version. The major exceptions to this are as follows. In Chap. 4, Example 4.13 has been moved before the explanation of the two extreme cases (slow/rapid fluctuation). The chapter ends with a new example on lake temperature (Example 4.14), which was taken from Problem 4.6 of the German edition.

Consequently, Problem 4.6 now refers to a modified situation of that lake temperature problem. The two other modifications are the addition of Problem 6.9 (competition for living space) and the replacement of Problem 8.7 by a more realistic example (transport and reaction in a lake's water column).

The book is firmly rooted in the algebraic formulation of mathematical models, their analytical solution, or—if solutions are too complex or do not exist—in a thorough discussion of the anticipated model properties. The reader will find neither mathematical proofs (just a summary of some useful equations in the Appendix) nor any specific reference to the many existing software tools. The latter make life easy for today's modelers, but they can also produce a false sense of security. We firmly believe that the user of such software should always be able to interpret the result of computer simulations, and that is only possible if she possesses at least a basic mathematical understanding. That being said, we also recognize the importance of connecting directly and visually to one's work and the ease with which modern software allows us to formulate and solve modeling problems. We therefore prepared interactive examples for several of the models presented in the book on the web as an additional aid in understanding the underlying principles (see the book website at `www.systems-analysis.org`).

Once again, the authors of the book were blessed with numerous favorable circumstances. After Dieter became President of the Research Council of the Swiss National Science Foundation, the principal Swiss public research funding agency, Nicolas Gruber succeeded him as environmental physics professor at ETH Zürich. Nicolas aided the development of the book in myriad ways: He graciously provided funding for travel and other expenses and provided feedback as well as new material.

Zürich, Switzerland — Dieter M. Imboden
Vienna, Austria — Stefan Pfenninger

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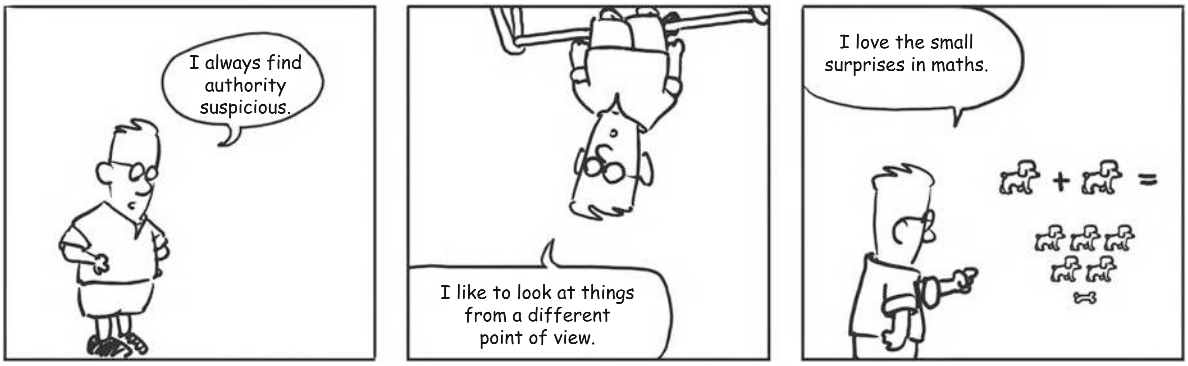
Introduction

Dang



Some Remarks Before We Begin

This book was originally developed alongside the lecture *Systems Analysis* at the Swiss Federal Institute of Technology (ETH) Zürich, on the basis of lecture notes developed over 12 years. The lecture, together with others on analysis, differential equations and linear algebra, belongs to the basic mathematical knowledge imparted on students of environmental sciences and other related areas at ETH Zürich.

The book was written to demonstrate practical applications of mathematics without becoming tedious and overly complex, in other words, how maths can be interesting and fun! Examples and exercises from various environmental sciences like limnology, population ecology and environmental chemistry demonstrate what the mathematical tools can be used for. A basic knowledge of environmental issues is beneficial for understanding these examples in their context.

The book aims to be more than a mathematical treatise on the analysis and modeling of natural systems, yet a certain set of basic mathematical skills are still necessary. We will use linear differential equations, vector

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and matrix calculus, linear algebra, and even take a glimpse at nonlinear and partial differential equations. Most of the mathematical methods used are covered in the appendices. Their treatment there is brief however, and without proofs. Therefore it will not replace a good mathematics textbook for someone who has not encountered this level of math before.

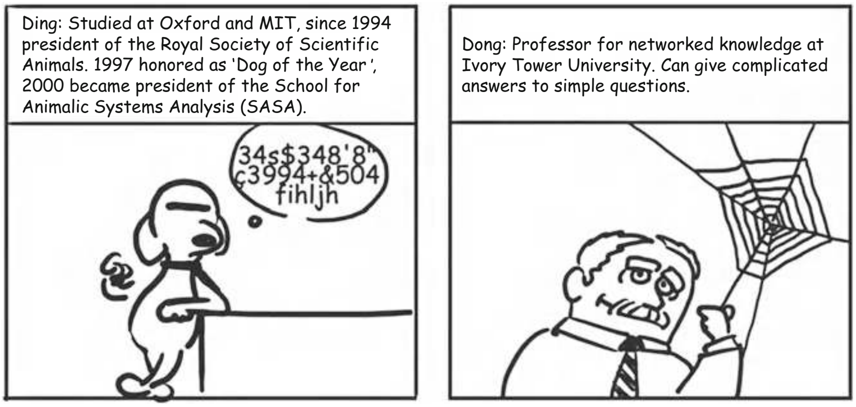
Although most of the examples used here are drawn from the environmental sciences, this book is not an introduction to the theory of aquatic or terrestrial environmental systems. Rather, a key goal of the book is to demonstrate the virtually limitless practical potential of the methods presented. Readers are encouraged to use the tools provided to tackle problems from their own areas of interest.

The first chapter is a short overview of the philosophy behind building models in science and does not use mathematical terms yet.

Book website

Visit the book website at `www.systems-analysis.org`. You’ll find interactive versions of several examples to help you understand the behavior of systems. You can also find additional resources there, such as a list of further recommended books.

Ding & Dong



1.1 Systems Analysis

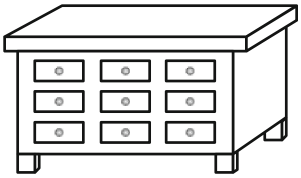
Heraclitus
(536–470 BC):
παντα ρει
panta rhei
gr.: “everything flows”

Everything flows, nothing remains constant. Science sees our world as a dynamic system. To describe and analyze this world, science has developed the remarkable ability to divide systems into ever smaller pieces, into subsystems which are again subdivided into sub-subsystems and so forth. The resulting entities are dynamic systems themselves, but they are brought down to a level of complexity understandable for the human mind. In most cases, the analysis of these systems is performed with the assistance of mathematical methods.

The principle underlying all of this is called reductionism. The reductionistic principle is not without its critics, and sometimes it is given responsibility for spawning a sort of technological progress which is blind to its negative consequences (environmental impacts such as biodiversity loss, climate change, as well as other effects such as the growing division between rich and poor).

We do not claim to be able to contribute to this important discussion. We do argue, however, that to criticize, improve or even transcend an idea, one must first understand it. On closer inspection, we discover that characterizing a scientific approach as reductionistic or on the contrary as holistic is always a question of one's point of view. A cell biologist would probably call a molecular biologist's work reductionistic. Cell biology, however, will appear as a holistic field to her. On the other hand, from a population ecologist's viewpoint, cell biology would itself appear reductionistic.

The division of science into different areas of expertise thus not only takes place through by putting different disciplines into different drawers of a chest (see illustration in the margin), but each drawer is again subdivided into further drawers. The chest of drawers depicted is therefore only *one* layer of reductionistic subdivision. In reality, many such chests would have to be drawn and each of their drawers would be subdivided further and further. Of course, this nested mass of drawers is not only a feature of biology—the reductionistic approach is used in every scientific field.



Reductionism can be thought of as a chest divided into drawers that are themselves further subdivided.

Even though it is not our aim to highlight this debate in principle, it will play a role indirectly throughout the book. The debate around reductionism forces us, time and again, to carefully examine the methods we develop here. As yet there are few concepts with which we could comprehend the world in a holistic way (whatever that may mean), without falling back to the method of subdividing it into smaller and more understandable parts. Even if we should develop such methods in the future, analyzing a system by dissecting its individual parts will always remain an important part of science. In any case, we want to think critically about our use of a reductionistic approach, and not lose track of the bigger picture.

In this book we want to convey how to model and analyze real-world systems. The underlying core principle is to construct simplified representations of such complex systems. These representations, called models,can often be expressed mathematically (e.g. through a system of equations). The construction of a mathematical model can be reduced to a few core ideas, in particular:

- The balancing of mass, energy or the number of objects (e.g. individuals of a biological species)
- The description of chemical or simple biological transformations through stoichiometric reaction equations
- The description of populations through equations describing growth, death and interaction between individuals

- The description of transport processes through exchange rates and processes of diffusion or advection
- The application of statistical methods to describe systems with many degrees of freedom

With this book you, the reader, should gain the ability to analyze real systems and make quantitative statements about their behavior. This requires the ability to translate empirically identified properties of these systems into a mathematical form, and to discuss the resulting equations (in particular, differential equations), in some cases even to solve them analytically. We will also delve into the behavior of more complex models, without specifically discussing how to solve them. Finally, we also want to demonstrate the limits of simulation and the emergence of mathematical artifacts.

Before we look at different mathematical models in more detail, we first have to clarify what exactly a system and a model are, and to understand the significance of modeling in science.

1.2 What is a System?

■ **The ant and the dung beetle**

A dung beetle watches an ant, desperately trying to lug a spruce needle onto a vast anthill. "Why waste your strength?" the beetle asks, "one needle more or less won't make a difference. What's the point?" "My work is part of building a system" the ant replies indignantly, and thinks to itself "You'll see that this is more than a pile of needles soon enough, when we carry you inside the anthill's vast tunnels after paralyzing you with our poison!"

A system is a set of objects between which relations exist.

The word system originates from Greek and means *configuration* or *composition*. The New Oxford American Dictionary gives the following definition: "a set of connected things or parts forming a complex whole". In a more abstract way, one could also say that a system is *a set of objects between which relations exist.*

A system is more than the sum of its parts.

What does this mean? A system is composed of different parts, the objects or system components. They are connected with each other through mutual interactions which we call *internal relations*.

A pile of metal parts is therefore not yet a system. The parts have to be connected in a meaningful manner. They might be connected to form the system *clockwork*. If one cog is removed from that system, it will entirely cease to function. This fact is reflected in the saying "a system is more than the sum of its parts".

Only through internal relations can the constituent parts become a system. This is not always as straightforward as in the clockwork example:

Example 1.1: Sand heap

Is a sand heap a system? Many will say that it is not. One can easily remove a grain of sand and what we call the *sand heap* remains nevertheless. Furthermore, from a mineralogical point of view one learns essentially the same whether looking at a couple of grains or at the whole heap. Others, however, will contend that a sand heap is indeed a system. Between the individual grains of sand, small gaps called *pore space* exist. These pores provide space for various organisms, they can store water, or in the case of sediments, provide information about the sand heap's formation through their structure.

Whether a number of objects constitute a system can therefore not be decided in a general way without taking into account the particulars of the specific question to be answered. For a construction firm a sand heap is a source of raw material, whereas for a geologist it is a system containing valuable information.

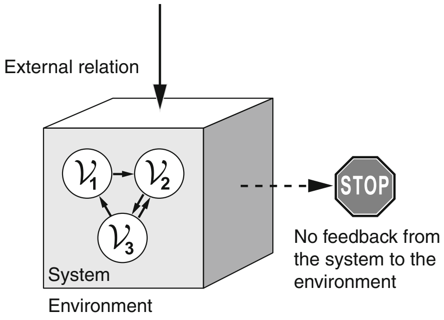


Fig. 1.1: *Schematic depiction of a system with three system variables $\mathcal{V}_1, \mathcal{V}_2$ and $\mathcal{V}_3$. The system boundary is the border between the system and the environment. The environment acts on the system (or rather, the system variables) through the external relation. The system variables are coupled through the internal relations. The feedback from the system to the environment is neglected*

Part of a system's definition is the system boundary, which forms the (often virtual) border between the system and its environment. This does not mean, of course, that there are no interactions between a system and the larger environment. On the contrary, it is these interactions across the boundary that make a system interesting. We assume here, however, that it is a one-way relationship: the system is influenced by the environment through what we call the external relations, but the environment is not influenced by the system. In other words, we assume that the environment is infinitely large and infinitely robust in comparison to the system we are looking at, therefore, any influence the system might have on the environment is so small that we can neglect it (Fig. 1.1).

The next example illustrates the hierarchy of interactions described above:

Example 1.2: The earth in the solar system

The earth is a subsystem of the solar system. It is influenced in particular by the energy reaching it from the sun, therefore, we can say it is driven by that external relation. On the other hand, we can assume that the earth has negligible influence on the sun. A sensible system boundary between the earth and the surrounding solar system would thus be drawn in the upper stratosphere (or maybe somewhat higher).

But setting the system boundary is not always as simple, as the next example demonstrates:

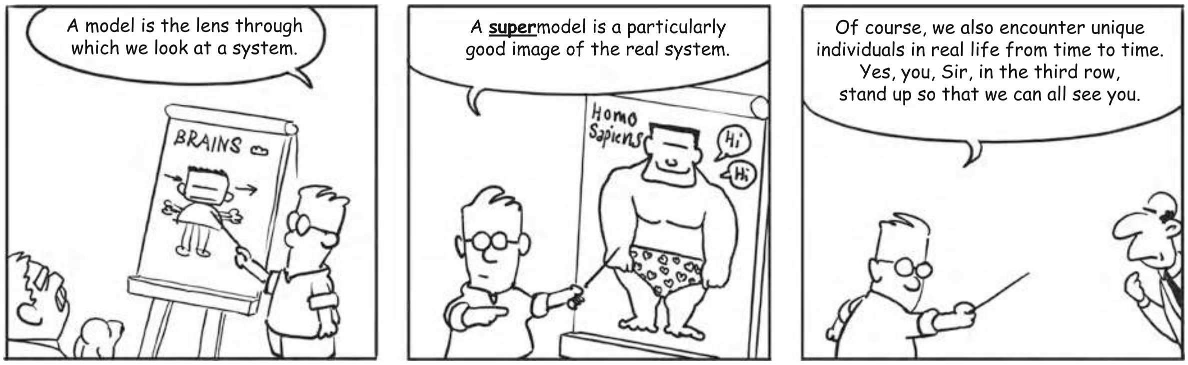
Example 1.3: A lake as a system

Let's look at a lake. Our goal is to describe the concentration of phosphorus in this lake. The lake's body of water is confined by the water surface and by the sediment. However, we will quickly realize that this system boundary makes little sense: the amount of phosphorus in the lake is also influenced by the dissolution of phosphorus from the sediment. As a result of prior phosphorus contaminations, a large amount of phosphorus is stored in the sediment body. So we choose as the system the body of water and the sediments combined. But then we further note that predicting the phosphorus concentration in the lake is impossible without knowing what happens in its upstream catchment area (population growth, construction of sewage treatment plants, agricultural policy, draining of wetlands, etc.). Therefore we choose as a system: the body of water, the sediment, as well as the catchment basin. By now, of course, our system is already a very complex entity with countless influences. In order to create a concise model, we would likely have to simplify or even neglect many of these influences.

Summing up, we can say that systems are theoretical constructs that help us in understanding a part of the world. There is no absolutely valid way to define a system's boundary. In fact, the exact choice of boundary depends on the question we are asking.

1.3 What is a Model?

Supermodel



We can trace the origin of our word *model* to ancient Rome, where small replicas of buildings were called *modulus*. Just as Roman architects needed replicas to assist them in designing large and complex buildings, if we want to analyze a natural system, we must first describe it in simplified terms. Whether this is as a drawing, a functional diagram, a mathematical equation or a verbal account, we can call such a description a model. So we can say that a model is always a simplified image of a real system.

Modulus is Latin for "small-scale replica of a building".

A model, therefore, does not necessarily have anything to do with maths at the outset. It is simply a concept with which we can describe a complex system in simplified terms. Models are used in architecture to plan buildings, or in chemistry to describe atoms as spheres and the molecular bonds as little rods between them (Fig. 1.2). Models are in use everywhere, whether they are physical models or purely mental constructs.

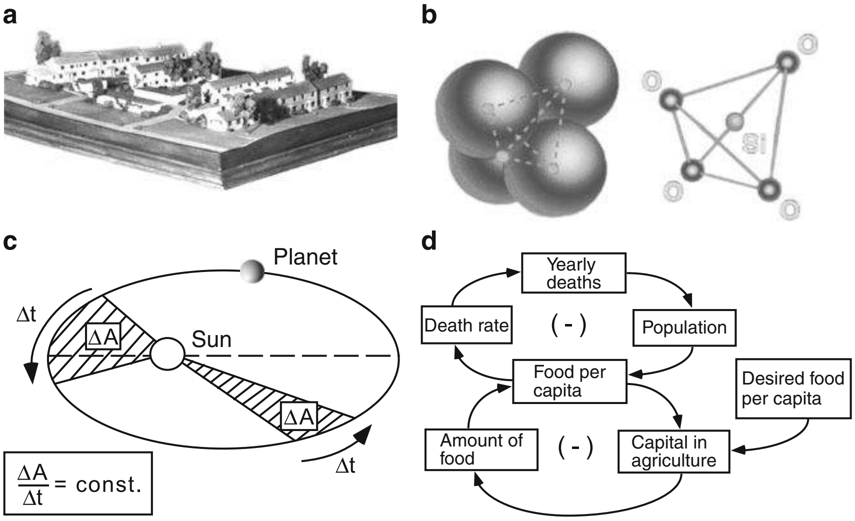
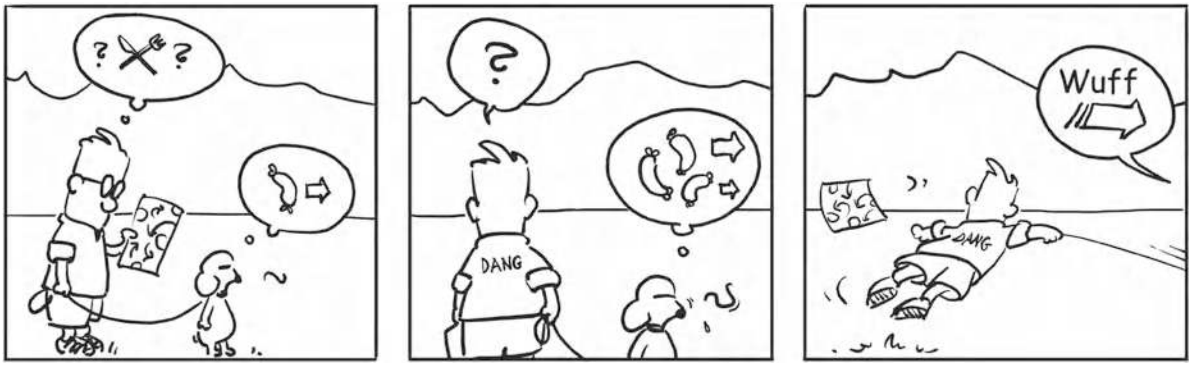


Fig. 1.2: *Examples of models: (**a**) Architectural model: Scaled-down execution of a planned or existing building. (**b**) Physical model: Model of chemical molecules. (**c**) Mathematical model: Kepler's second law of planetary motion. (**d**) Conceptional model: Excerpt from the World model by Forrester and Meadows (see Meadows et al. 1972)*

A model is the lens through which we look at the real system—it is not an exact copy of that system. For the same system, there can be completely different models. We could depict a landscape as a topographical map, or as an impressionistic painting. In both cases, the simplification of the system "landscape" is our explicit intention. It is impossible to say a priori which model is better. One model is not superior to another because it is more complex. Depending on the point of view that we want to emphasise and the question we intend to answer, we include certain properties of the system in the model while excluding others. You can think of it like a dog taken for a walk in a forest. The dog's model of the forest will be different than that of its owner; it might predominantly consist of scents, for instance. But he will be able to navigate the forest just as well or even better than his owner.

Good models allow us, through certain simplifications, to arrive at a readily comprehensible representation of the real world that can be described mathematically. Such models have a long tradition in science and engineering. The only way to apprehend and analyze a real system is with a model, that is, by framing it in terms that hold relevance for us. Often, an important motivation to construct a model is to make predictions about a system's future behavior. As we will see, however, making predictions is not the only role that models play.

Walking the dog



If a model is formulated with mathematical equations, it becomes a mathematical model. Mathematical models were developed primarily in the exact natural sciences and in engineering, above all in physics. They allow us to develop consistent theories about our physical surroundings. Under the influence of the phenomenal success these scientific disciplines had, more and more additional disciplines started using mathematical models throughout the twentieth century. This development did not stop short of the social sciences and humanities, although it was hindered there until the recent availability of immense amounts of data and with it the emergent "digital" social science and humanities. To date, the field beyond natural science in which mathematical modeling has seen the most success is economics.

The development of systems-oriented branches of science (such as ecology and environmental science) would not have been possible without models. More importantly, the models themselves would soon have been beyond reach of mathematical analysis if not for the enormous progress in information technology. The development of powerful computers now allows us to simulate models numerically which even in the 1990s were deemed to be unsolvable. On the other hand, some of the most influential ecological models, such as the famous predator-prey equations by Lotka (1924) and Volterra (1926) (see Sect. 6.2), were formulated more than 80 years ago, when computers did not yet exist.

To summarize: A model is a concept for the simplified description of a complex system. It serves to characterize the important features of a system and to leave aside the peripheral ones. If the model is a mathematical one, the interactions between the system variables (internal relations) and the ones between the system and its environment (external relations) are formulated mathematically. This way, the model can be analyzed by mathematical simulation.

A model is a concept for the simplified description of a complex system.

1.4 The Formation of Models in Natural Science

To develop theories in science one needs models: without models there is no generalizable or transferable insight. As we have seen above, "model" does not necessarily mean a complex computer program. Even just the assumption that in an electrical resistor current grows proportionally to voltage (Ohm's law) is a model.

Ohm's law:
$I = U/R$

A classic example of how scientific understanding comes about illustrates the pivotal role of model formulation better than a long explanation:

Example 1.4: Our model of the universe

The process of formulating a scientific model can be divided into the following phases:

1. **Collecting** Observations, measurements:
   Tycho Brahe (1546–1601) collects data on the movement of planets using his royally equipped observatory Uranienborg near Copenhagen.
2. **Arranging** The search for an underlying principle of order in the gathered data (model formation):
   Johannes Kepler (1571–1630) arranges Brahe's orbital data in such a way that he can describe it in terms of three mathematical equations (Kepler's laws).

3. Understanding	The search for an overarching principle, with which the empirically found order can be understood: *Isaac Newton (1643–1727) demonstrates that Kepler's laws can be explained through physical principles that are valid far beyond astronomy.*
4. Generalizing	Can the discovered laws be applied in other situations? *Albert Einstein (1879–1955) develops his theory of general relativity based on the equivalancy of inertial and gravitational mass already postulated by Newton.*
5. Predicting	Can the (possibly generalized) laws be used to predict observations or phenomena that have not yet been observed? *Einstein's theory of relativity remained a mathematical construct until the astronomical phenomena which he predicted were actually observed.*

Using this example, we can identify the two main tasks of systems analysis:

Model formation: The construction of a model begins with laying down the system boundary, the definition of the system variables, and the internal and external relations. The starting point is often empirical data, for instance from well-designed experiments. These data are analyzed in view of constructing a model. The model, usually a mathematical one, should explain the data in the simplest possible form, in terms of the internal model structure and the external relations. In other words: systems analysis looks for the (simplest) structure of the "black box" that can reproduce the postulated connection between the state of the environment and the system's state (Fig. 1.3).

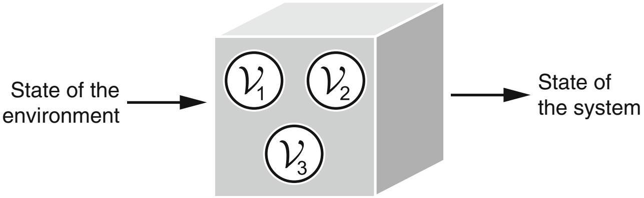


Fig. 1.3: *As a first step in mathematical model formation, the external relations (state of the environment) and the system variables ($\mathcal{V}_i$) have to be defined and quantified. The black box model attempts to describe the system variables from the external state as simply and meaningfully as possible*

In the end, therefore, gathering data only makes sense if further insight results from it, either as a generalizable statement, a prognosis, or as the formulation of new questions, that is, the planning of new experiments. To process observations in this manner, we need models.

Box model

Model validation: After constructing a model compatible with the data, and determining all model variables, we can use the model to predict the system's behavior under different conditions and compare these predictions with further measurements. Through these comparisons, we might be able to improve the model further. This process is called model validation.

In principle, the process of modeling is a process of infinite iteration, which we abort as soon as we reach sufficient accuracy (Fig. 1.4).

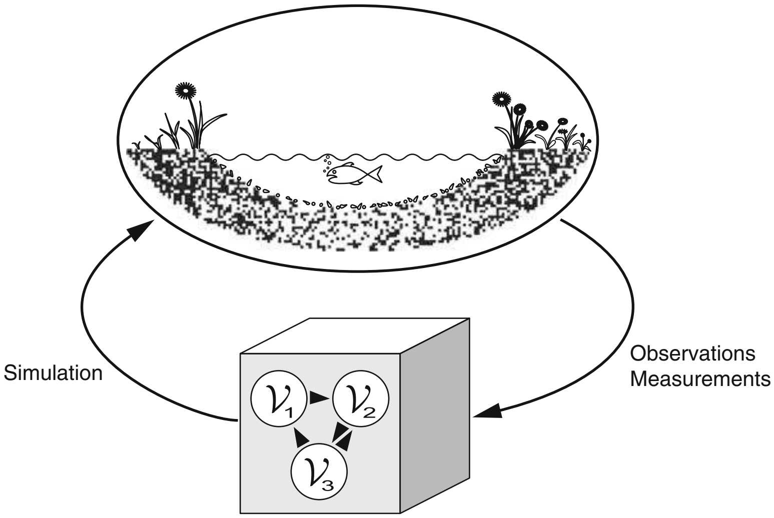


Fig. 1.4: *In model validation, observed data are repeatedly compared with adjusted model simulations until a satisfactory correspondence between model and observational data is achieved*

With this, we've reached the end of the first chapter, in which we looked at the importance of the modeling method in science. In the next chapter, we will get to know the fundamental tools with which we can actually build models.

At the end of each chapter, there is a set of questions and problems. In the questions, we recap the chapter's contents. They can usually be quickly and easily answered. The problems however require more in-depth work, but will greatly help with retaining and applying the key concepts and tools introduced in the chapter.

1.5 Questions and Problems

Question 1.1: Why is there no simple and unambiguous definition to differentiate between a reductionistic and a holistic description of a system?

Question 1.2: What is implied with the statement "The relation between a system and its environment is asymmetrical"?

Question 1.3: Give a short definition for each of the following terms: *system*, *model*, *mathematical model*.

Question 1.4: What distinguishes a model from reality?

Question 1.5: Give some of the most important decisions that have to be made when constructing a model.

Question 1.6: Which functions do models have in science?

Question 1.7: What does model validation mean?

Problem 1.1: Model formation

Look at the following three systems and try to formulate a model. Consider what system variables and external relations are important for the models. What can be neglected? Where is the system boundary?

(a) Population growth (nationally, i.e. in a specific country)

(b) Population growth (globally, i.e. for the entire planet)

(c) Carbon dioxide in the atmosphere

(d) Lead (a heavy metal) in a lake's sediment

Problem 1.2: Solar system

For a simplified description of the solar system, we choose the following variables: the location and speed of the sun and the eight planets.

(a) What are the internal relations?

(b) What external relations does the system have?

(c) How does our system deviate from the real solar system as part of the cosmos? Do our simplifications relate to the internal relations, the external relations, or both of them?

Problem 1.3: From chemical elements to nuclear physics

Characterize, like we did in Example 1.4 for our model of the cosmos, the path from the discovery of the chemical elements to the development of nuclear physics.

Chapter 2

Mathematical Models: A First Look

In the second chapter, we want to look more closely at mathematical models with which we can describe natural systems. Our aim is first and foremost to familiarize ourselves with a model's basic components, as well as with different types of models. We will learn how to construct a model on the basis of examples. For this, we will not yet need complex mathematics.

2.1 From System to Model

Before forming a model, we should think carefully about what we need the model for. What questions do we want to examine with it? Our research question helps us define the system, then select the system boundary and the relevant system variables.

For this first step of model formation, we can use some very simple tools. We draw our system as a box diagram. The boundary of the box corresponds to the system boundary. Inside the box we draw the system variables $\mathcal{V}_i$. From outside the box, the external relations $\mathcal{R}_i$ influence the system. In many cases, these external relations consist of mass flows from the environment into the system. Therefore, the external relations are also called input variables or mass input. But there could also be other kinds of external relations, for instance, solar radiation, atmospheric temperature, or a bank's interest rate. We connect the system variables with arrows that indicate the relations between them. These are the internal relations of the system. They could, for instance, be mass flows between the system variables.

One natural system that we will use as an example throughout this book is a lake. Figure 2.1 shows a first simple model to describe a chemical substance in a lake.

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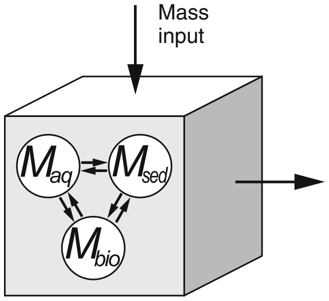

Fig. 2.1: *A lake as a box diagram with three variables*

Example 2.1: A lake as a black box

The model has three variables: the amount or mass of a chemical substance in the lake water M_{aq}, in the lake's sediment M_{sed} and in it's living organisms M_{bio} (for instance in fish). The substance to be modeled reaches the lake by a tributary river. This mass input represents the system's external relation. The loss of substance through the lake's outflow is symbolized by an arrow pointing out from the box. The exchange of substance between lake water, sediment and biomass is also symbolized by arrows connecting the three variables. These are the internal relations.

The dimension of a model equals the number of system variables.

The number of system variables is called the *dimension* of a model. The example above represents a *three-dimensional* model with the three system variables M_{aq}, M_{sed} and M_{bio}. In order to formulate the model mathematically, we must describe the internal relations (the mass flows between the three system variables) and the external relations. By doing so, we arrive at the system or model equations. They usually contain additional quantities: the model parameters. In the next section, we will illustrate the method to create the system equations step by step with an example.

2.2 Static Models

We will begin with a simple example: a static model of a lake. It might allow us to answer questions about the correlation between the influx of a substance through the lake's inlet and its average concentration in the lake. The substance we are interested in is phosphorus, which often enters surface waters from sewage and agricultural fertilisers.

Let's first think about how the system looks schematically (Fig. 2.2). Our model is one-dimensional, it has *one* system variable: the phosphorus concentration in the lake C_{aq} (unit: mg m^{-3}). The external relation of the system (the phosphorus input) is the influx of dissolved phosphorus into the lake J_{in} (unit: kg year^{-1}). It could either be constant or it could

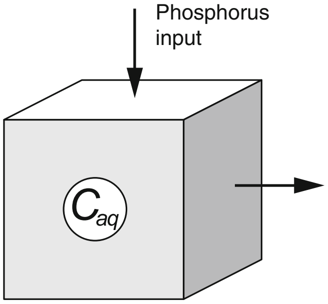

Fig. 2.2: *Static lake model: Average phosphorus concentration in the lake as a function of the current phosphorus input*

Is there a correlation between $J_{in}(t)$ and $C_{aq}(t)$?

fluctuate with time. In a first attempt, we assume that there is an *immediate* relation between the phosphorus input at time t and the average phosphorus concentration in the lake measured at the same time. Mathematically, this can be formulated as follows[1]:

$$C_{aq}(t) = \text{Function of } J_{in} = f\left[J_{in}(t)\right] \tag{2.1}$$

We assume that the lake in question has been under surveillance for several years and that a data set exists from which we can calculate $C_{aq}(t)$ and $J_{in}(t)$ for different times. To find the unknown function in Eq. (2.1), we can sketch the values of $C_{aq}(t)$ and $J_{in}(t)$ in a two-dimensional diagram. Let's look at a numerical example:

Example 2.2: Phosphorus in a lake — static model

In a lake, the nutrient load constantly increases over a period of many years. This so-called eutrophication of the lake is established through the following measurements. They demonstrate a correlation between the yearly phosphorus input $J_{in}(t)$ via inlets and wastewater treatment plants, and the average total phosphorus concentration in the lake that year $C_{aq}(t)$. The following data were measured in four not necessarily consecutive years.

$J_{in}(t)$ [kg year^{-1}]	1,500	2,100	2,800	4,200
$C_{aq}(t)$ [mg m^{-3}]	20	30	36	56

---

[1] With this example, we by no means suggest that this model is reasonable. It is merely a first attempt, the general validity of which we will later discuss in detail.

Figure 2.3 shows the pairs of data in a two-dimensional diagram. All data points lie roughly on a straight line. From that, we can conclude that the function in question is a linear relation of the form $f(x) = p \cdot x$. Now, we can mathematically formulate the linear relation between phosphorus input $J(t)$ and average phosphorus concentration $C_{aq}(t)$:

$$C_{aq}(t) = p \cdot J_{in}(t) \tag{2.2}$$

The coefficient p is is the model parameter. It can be calculated as the ratio between the pairs of data. The resulting average value is:

$$p = \overline{\left(\frac{C_{aq}(t)}{J_{in}(t)}\right)} = 1.33 \times 10^{-2} \, \frac{\text{mg m}^{-3}}{\text{kg year}^{-1}} \tag{2.3}$$

where the bar atop the quotient signifies the average of the data pairs.

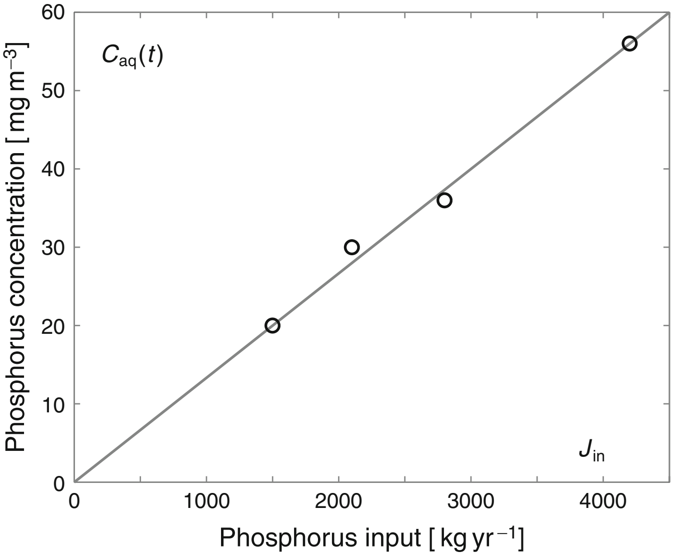

Fig. 2.3: *The data pairs $J_{in}(t)$ and $C_{aq}(t)$ in a two-dimensional space. The data points lie approximately on a straight line*

The above phosphorus model is called *static*, because for every value of the external relation $\mathcal{R}$ (in this example, the input $J_{in}(t)$) there is a precisely defined value of the system variable $\mathcal{V}$. Mathematically speaking, a static model with one system variable has the following form[2]:

$$\mathcal{V} = \text{Function of } \{\mathcal{R}\} = f(\mathcal{R}) \tag{2.4}$$

---

[2] Not in all cases can we explicitly describe the system variable $\mathcal{V}$ (as we did in Eq. 2.4). It can also be given through an implicit equation, such as $e^{a\mathcal{V}} = b\mathcal{V}$.

Equation (2.4) is called the system equation of the model. The function $f(\mathcal{R})$ can have an arbitrarily complicated form and can be defined by one or several model parameters p. If the function $f(\mathcal{R})$ is linear, as is the case in Eq. (2.2), the model is called linear.

We have described the system "phosphorus in a lake" with a linear, static model. By using Eq. (2.2), we can predict how the lake's phosphorus concentration changes in response to a changed phosphorus input. We cannot, however, make any statement about how long it takes until the phosphorus concentration reaches its new value after the input variable has been changed. In a static model, the change takes place instantaneously. A dynamic model is needed in order to describe the transition from one state to another.

A static model cannot adequately describe changes through time.

Before we delve deeper into dynamic models in Sect. 2.3, we will briefly discuss the importance of units and dimensions.

2.2.1 Handling Dimensions and Units

Mathematical models link model variables by mathematical relations. Model variables generally have a dimension (see Appendix B). In most cases, the combination of the three basic dimensions mass (M), time (T) and length (L) is sufficient to express the dimension of every variable. Units are formed by explicitly choosing a system of measurement for the dimensions; therefore, units are a specific representation of dimensions and should not be confused with them. As long as we only work with algebraical expressions, the choice of units is irrelevant. Only the dimensions have to match on both sides of an equation. Yet, as soon we give specific values to variables in an equation, a consistent set of units is needed.

Let's take another look at Eq. (2.3) in the example above. The unit of mass in the numerator (mg) is different from the one in the denominator (kg). It can be adjusted through the conversion 1 mg $= 10^{-6}$ kg. Then, the following holds:

$$\begin{aligned} p &= 1.33 \times 10^{-2}\, \frac{\text{mg m}^{-3}}{\text{kg year}^{-1}} \\ &= 1.33 \times 10^{-8}\, \frac{\text{mg m}^{-3}}{\text{mg year}^{-1}} \\ &= 1.33 \times 10^{-8}\, \text{year}\, \text{m}^{-3} \end{aligned}$$

The parameter p therefore has the dimension of an *inverse volume flow rate* (T L^{-3}). We will get to know the physical significance of this parameter in Sect. 4.2. For now, let's look at another example:

Example 2.3: Dimensions and units

A wastewater treatment plant with a water volume of 1,000 m^3 is accidentally contaminated with 10 kg of a toxic substance. How high is the concentration of that substance in the treatment plant after the accident?
The dimension of a concentration is (ML^{-3}), or mass (M) per volume (L^3). Therefore, we can calculate the average concentration C in the plant with the data we have. To do so, we insert the mass of the substance (in kg) and the plant's volume (in m^3). We then get the concentration in kg m^{-3}:

$$C = \frac{10 \text{ kg}}{1,000 \text{ m}^3} = 0.01 \text{ kg m}^{-3} \tag{2.5}$$

The units kg and m are so-called metric or SI units.[a] If possible, SI units should be used in scientific work. Often, however, it makes sense to convert the units into others that can more easily be visualized. The units of the average concentration in the sewage treatment plant, for instance, could be converted as follows:

$$0.01 \text{ kg m}^{-3} = 0.01 \times \frac{10^3 \text{ g}}{10^3 \text{ L}} = 0.01 \text{ g L}^{-1} = 10 \text{ mg L}^{-1} \tag{2.6}$$

Thus 10 mg of the toxic substance are dissolved in 1 L of water.

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[a] SI units were defined as the "système international d'unités" at a conference in Paris in 1960. They form the international standard units.

Most common spreadsheet and statistics software allows the user to graphically display the empirical relation between data pairs (like in Fig. 2.3) and to estimate the function by a regression. If we relate data pairs of two or more measured variables by a linear or nonlinear regression, a static model is produced where the regression equation becomes the model equation.

Since setting up model equations by regression analysis is very easy, one will often forget to verify whether the equation makes any physical sense. Even in literature, one occasionally finds model equations that have different dimensions on both sides. Furthermore, equations are often set up in a way that makes them valid only for a specific set of units.

In order to demonstrate this point, let's look at experimental data on the growth of an algae population under varying nitrate concentrations in water. The measurements were analyzed by a nonlinear equation.

Example 2.4: Nonlinear regression and the pitfall of units

A scientist determines the specific growth rate[a] G of an algae population at different nitrate concentrations C in water. A nonlinear fit of the data yields:

$$G = 0.1\ C^{0.6} \tag{2.7}$$

G	Specific growth (per hour)
C	Nitrate concentration

Unfortunately, the author of the model forgot to specify in which units the nitrate concentration should be inserted in Eq. (2.7). One user of the model may express nitrate concentration in $\mathrm{mol\,m^{-3}}$ and receives a value that is smaller by a factor of 4.9 than the result of another user who fills in the concentration C in $\mathrm{mgN\,L^{-1}}$. To make the formula compatible for both users, they would both have to use the same units. But which ones are the correct ones?

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[a] Specific growth rate (G) is the *relative* increase in biomass per unit of time. Independently of the dimension and unit in which biomass is given, the dimension of G is always $(\mathrm{T^{-1}})$.

For a serious modeler there are three ways to prevent this kind of confusion:

(1) The easiest, but not always the best way: We simply write the correct units in square brackets behind each variable:

$$G\ (\mathrm{h^{-1}}) = 0.1\ (C\ (\mathrm{mgN\,L^{-1}}))^{0.6} \tag{2.8}$$

This notation makes the equation confusing and difficult to read.

(2) A better way is to replace the numerical factor by the symbol p and to separately give the value of p together with the correct unit:

$$G = p\ C^{0.6}, \qquad \text{with } p = 0.1\ \mathrm{h^{-1}(mgN\,L^{-1})^{-0.6}} \tag{2.9}$$

G	$(\mathrm{h^{-1}})$	Specific growth rate
C	$(\mathrm{mgN\,L^{-1}})$	Nitrate concentration

If we would now like to insert the concentration in $\mathrm{mol\,m^{-3}}$, we have to keep in mind that $1\ \mathrm{mgN\,L^{-1}} = 1\ \mathrm{gN\,m^{-3}} = \frac{1}{14}\ \mathrm{mol\,m^{-3}}$. Thus, the parameter can be converted as follows:

$$\begin{aligned} p &= 0.1\ \mathrm{h^{-1}(mgN\,L^{-1})^{-0.6}} \\ &= 0.1\ \mathrm{h^{-1}}(\frac{1}{14}\mathrm{mol\,m^{-3}})^{-0.6} \\ &= 0.1\ \mathrm{h^{-1}}(14)^{0.6}(\mathrm{mol\,m^{-3}})^{-0.6} \\ &= 0.49\ \mathrm{h^{-1}}(\mathrm{mol\,m^{-3}})^{-0.6} \end{aligned}$$

Since this procedure is rather complicated, it may be better to transform the concentration values into the proper units and then apply Eq. (2.7).

(3) The safest way, however, is to use non-dimensional variables wherever fractional exponents could appear. Applied to Eq. (2.7), we should use the following expression:

$$G = G^0 \left(\frac{C}{C^0}\right)^{0.6} \tag{2.10}$$

G	(h^{-1})	Specific growth rate
C	$(\mathrm{mgN\,L}^{-1})$	Nitrate concentration

where G^0 is the "reference growth rate" at the "reference concentration" C^0. The pair of reference values can be chosen arbitrarily, preferentially somewhere in the middle of the range of available data. We can satisfy ourselves that for $C^0 = 1\ \mathrm{mgN\,L}^{-1}$, G^0 must be $0.1\ \mathrm{h}^{-1}$ for Eqs. (2.7) and (2.10) to be equivalent. Now, changing the units of concentration is much easier. One only has to adjust the units of the reference concentration accordingly.

Tabloid units

Editor: "You want a front page headline because of a laughable 10 Curies in RadonCorp's waste?"—Journalist: "How about 400 billion Becquerel?"[a]—"Much better. You've got journalism in your blood after all!"

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[a] Curie and Becquerel are both units for the radioactivity of a radiation source. 1 Becquerel corresponds to one decay per second. 1 Curie = 37 billion Becquerel.

Summing up, verifying the dimensions and units when we set up and solve system equations is one of the easiest and most efficient ways to prevent mistakes. The following rules may help:

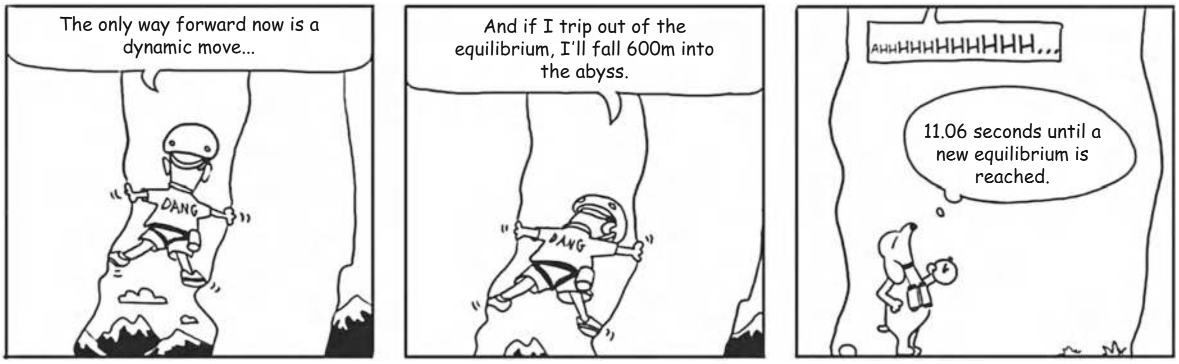
- The algebraic expressions to the left and right of the equals sign must always have the same dimension.
- Addition and subtraction are only possible if all algebraic terms have the same dimension.
- When inserting concrete numbers into an algebraic equation, their units have to be compatible. In other words, they have to be chosen so that the same combination of units results on both sides of the equals sign.
- Exponents in equations are non-dimensional (and therefore also without units). The same holds for arguments in transcendental functions

such as sin(..), cos(..) or exp(..). Ensure that you only have fractional powers or transcendental functions of *non-dimensional* variables in your equations.

Appendix B gives an overview of dimensions and units.

2.3 Dynamic Models

Equilibrium



In Sect. 2.2 we have described the system "phosphorus in a lake" with a static model. As we discovered, with such a model we can calculate the average concentration of phosphorus in the lake water as a function of the input concentration. However, the model neglects the fact that it takes some time for the system to adjust to the new input value. With a static model, we can make no statement about how rapidly the phosphorus concentration in the lake changes if there is a sudden change in the input concentration. If we want to describe a system's dynamics in time, static models are no longer sufficient: we need a dynamic model.

Often, adjustment processes to a change in the external relation are particularly important to understand natural systems, as is the case in the following example:

Example 2.5: Carbon dioxide in the atmosphere

Burning fossil fuels releases carbon dioxide into the atmosphere. The *current* atmospheric concentration of carbon dioxide (CO_2) does not directly depend on the *current* rate of fossil fuel consumption. Rather, the gradual increase of CO_2 mirrors the slow adjustment process of the global carbon cycle to the increased input of CO_2 into the atmosphere. The CO_2 concentration in the atmosphere will continue to rise even if the growth of fossil fuel consumption were to be reduced or halted completely. In Chap. 5, we will examine a dynamic model for the global carbon cycle (in Example 5.12).

A dynamic model describes the system's time-dependent answer to an external change.

In general terms, a dynamic model can describe how rapidly the system variable $\mathcal{V}$ changes when the external relation $\mathcal{R}$ varies. The dynamic model describes the time-dependent answer to the external change. Figure 2.4 shows the adjustment of a linear system to a disturbance that occurs suddenly at time $t = 0$. The solid line represents the simulation with a dynamic model. The system variable $\mathcal{V}(t)$ does not react immediately to the disturbance, but adjusts gradually to a new system state in equilibrium with the changed external relation $\mathcal{R}$. The static model, depicted as a dashed line, disregards this adjustment behaviour; the system variable immediately changes to the new system state.

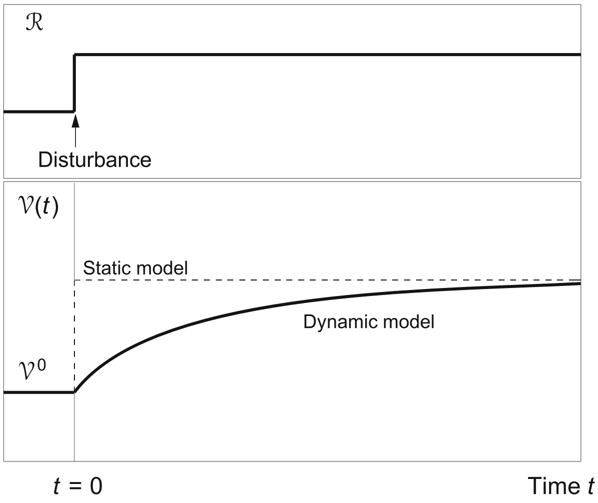


Fig. 2.4: *A dynamic model can describe the adjustment of the system variable $\mathcal{V}(t)$ to a changed external relation $\mathcal{R}$ (disturbance). The state $\mathcal{V}^0$ corresponds to the equilibrium of the system variable $\mathcal{V}$ with the external relation $\mathcal{R}$ before the disturbance occurred ($t < 0$)*

The system equation of a dynamic model is significantly different from Eq. (2.4). On the left-hand side of the equation we write the system variable's change with time:

$$\text{Temporal change of } \mathcal{V} = f(\mathcal{R}, \mathcal{V}) \tag{2.11}$$

If the temporal change of the system variable $\mathcal{V}$ is smooth, i.e. not made up by sudden jumps,[3] it can be described by the first derivative of the system variable with respect to time. The mathematical model is therefore

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[3] Mathematicians call such a function *differentiable*.

a first order differential equation[4] with respect to time:

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = f(\mathcal{R}, \mathcal{V}) \tag{2.12}$$

The function $f(\mathcal{R}, \mathcal{V})$ is called the change or velocity function of the system variable.

In order to calculate the adjustment of the model to a changed input variable, we have to integrate the differential equation (2.12). To do so, we need an initial value $\mathcal{V}^0$, that is, the value of the system variable at an arbitrary time t_0. The model calculation begins at time t_0. Usually, we set $t_0 = 0$. It is important to note that the solution of the differential equation (2.12) depends on the initial value $\mathcal{V}^0$. This is a crucial difference to the static model (Eq. 2.4), where there is no such dependency.

In many cases a dynamic model is developed to draw up a balance of a specific quantity, such as the mass of a chemical substance, the number of individuals of a specific species, or even just a quantity of money. In the resulting system equations we can characterize the temporal change of that quantity in the system as the difference between input and output. Let's look at an example:

Example 2.6: Phosphorus in a lake — dynamic model

The dynamic phosphorus model of a lake can be described as the mass balance of phosphorus in the lake water. First, let's describe the mass balance in words:

$$\begin{aligned}
&\left\{\begin{array}{c}\text{Temporal change of the}\\ \text{phosphorus mass in the lake}\end{array}\right\} = \\
&\left\{\begin{array}{c}\text{Inflow via inlet}\\ \text{per unit of time}\end{array}\right\} - \left\{\begin{array}{c}\text{Outflow via outlet}\\ \text{per unit of time}\end{array}\right\} \\
&- \left\{\begin{array}{c}\text{Net uptake through}\\ \text{biota per unit of time}\end{array}\right\} - \left\{\begin{array}{c}\text{Net uptake through}\\ \text{sediment per unit of time}\end{array}\right\}
\end{aligned}$$

To integrate this equation, we need to specify the terms on the right-hand side of the equals sign. We can either use explicit numerical values or algebraic expressions that create a link to the system variable. In addition, we need an initial value for the phosphorus mass in the lake. We will discuss this in more detail in Chap. 4.

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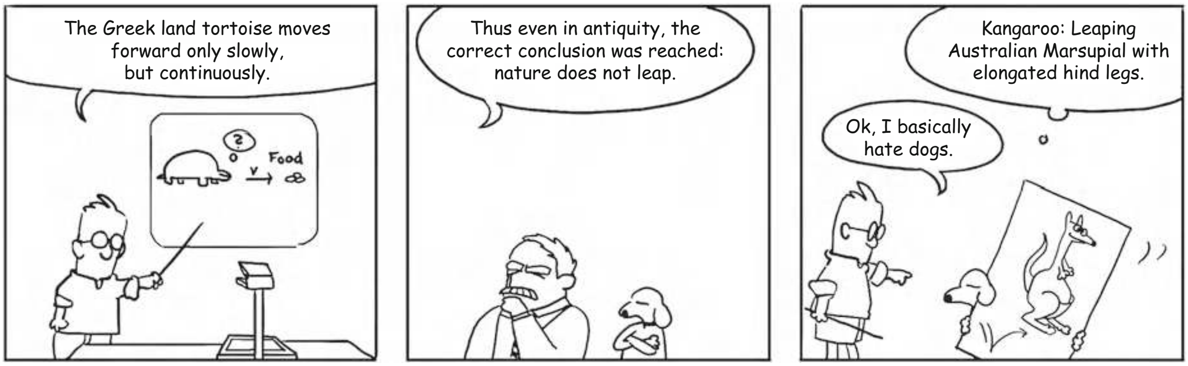
[4] In a first order (n-th order) differential equation, the function that constitutes its solution is no higher than in its first (n-th) derivative. The models we deal with here are usually first order with respect to time. In physics, particularly in classical mechanics, they are often second order with respect to time. For the solution of these differential equations this distinction is only marginally relevant, because one can convert an n-order differential equation into n first order equations.

2.4 Discrete Time Models

Leaps of nature



Before the discovery of quantum mechanics scientists were convinced that system variables such as temperature, velocity or concentration change continuously. It was postulated that *nature does not leap*. But at closer examination, this is also incorrect for many systems that have nothing to do with quantum mechanics. For instance, let's model an elephant herd in a national park in Africa. The herd's size changes with every birth and every death by a whole number—that is, the variable "number of individuals" leaps. There are also systems that only change at specific times. A typical example is a savings account that does not have its interest added continuously, but only once per year or once every quarter.

Not every variable changes continuously with time.

If a system variable doesn't change continuously, but—as shown in Fig. 2.5—only at discrete points in time $t_0, t_1, t_2, \ldots$, we can simulate the system with a *discrete time model* of the form

$$\mathcal{V}^{(k+1)} = f(\mathcal{R}^{(k)}, \mathcal{V}^{(k)}) \tag{2.13}$$

This means that the state $\mathcal{V}^{(k+1)}$ is calculated from $\mathcal{V}^{(k)}$ according to a specific "recipe". The superscript index k in parentheses indicates the system state at time t_k. Unlike in a differential equation Eq. (2.12), the system variable's change in time is not described infinitesimally by the first derivative, but by the change occurring during the time step $\left(t_{k+1} - t_k\right)$.[5] A more detailed description of these models follows in Chap. 7.

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[5] In order to show the connection of Eq. (2.13) to the differential equation (2.12) of the continuous model, the left-hand side of the former is often written as the difference between two consecutive time steps, $\mathcal{V}^{(k+1)} - \mathcal{V}^{(k)}$. In this way the differential equation (2.12) becomes a so-called difference equation. See Chap. 7 for details.

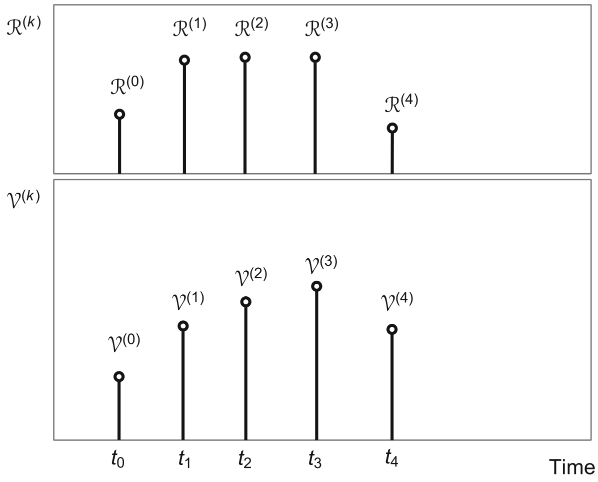


Fig. 2.5: *With a discrete model, the system variable* $\mathcal{V}^{(k)}$ *changes in "jumps" or discrete time steps* t_k*. It may be driven by a external relation* $\mathcal{R}$ *that changes with time*

2.5 Spatially Continuous Models

So far, we assumed that the system variable only depends on time. Yet, natural systems also have a spatial dimension. As long as we are only interested in the average phosphorus concentration and assume that it is distributed homogeneously in the lake, we do not need to consider any spatial variation of the system variable. Instead, we can think of the entire lake volume as one large box. We call such a spatially homogeneous model a *box model*.

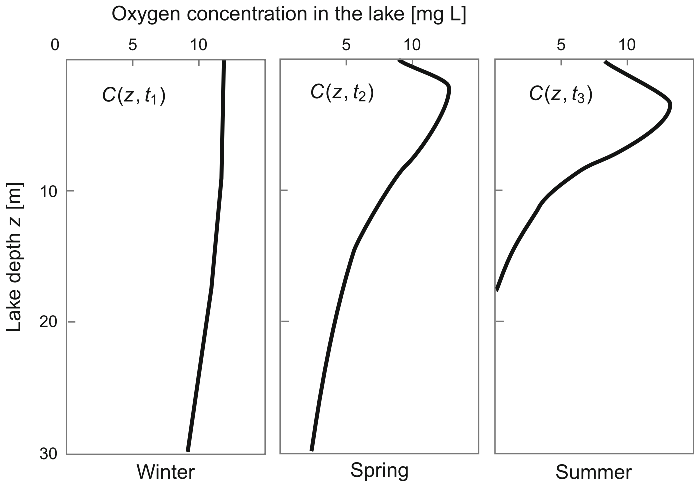
Often, however, the spatial distribution of a substance in the system is particularly important. For instance, we are interested in the oxygen distribution in different depths z of a lake. Figure 2.6 shows the oxygen profile in a lake at different times. To describe such a spatial distribution, we have to treat the lake as a spatial continuum in one or all three spatial dimensions. The oxygen distribution then appears in the system equation as a function of both time t and depth z, which we write as $C(z,t)$. The model equation thus becomes a *partial* differential equation. We call these models *spatially continuous* and distinguish them from box models. The analytic solution of partial differential equations is usually difficult—they are solved computationally. We will look at some simple examples in Chap. 8.

2.6 Stochastic Models

Solutions of differential equations have the property of being completely determined once the initial conditions are given. In other words: A system always develops in exactly the same way if it starts from the same initial state. Such behavior is called deterministic.

Our experience with a multitude of natural systems teaches us something different: many phenomena, from the weather to the dynamics of

Fig. 2.6: *The oxygen distribution in a lake can be described as a function of time t and depth z. The figure shows the vertical oxygen profile in a lake with a maximum depth of 30 m at three different times* t_1, t_2 *and* t_3



the stock exchange, appear to lie outside the possibility of deterministic analysis and prediction. In most cases—except in the case of very simple systems—we can at best predict the future within certain time limits. For instance, we may be able to predict that the system will develop into the state S_1 with a probability of p_1, into the state S_2 with the probability p_2, and so forth. This behavior is called stochastic.

There are many different reasons for the occurrence of stochastic processes. The most obvious reason is connected to quantum mechanics, which in several respects replaced our physical thinking over the course of the twentieth century. In quantum mechanics, the deterministic equations of classical mechanics are replaced with probability relations. For instance, we cannot predict when exactly a specific radioactive isotope will decay, that is, we cannot describe the isotope's behavior with a classical (deterministic) equation.

In many cases (but not in all), this kind of random process can be eliminated by assuming a macroscopical perspective. For instance, if we analyze a large number of identical isotopes, we can describe the behavior of the overall system relatively accurately through the half-life of the isotope. We can thus predict the time when half of the original isotopes will have decayed. The stochastic events at the microscopic scale can (at least approximately) be brought back to the deterministic scale by summing up many individual processes. We find similar examples in thermodynamics: The macroscopic variables *pressure* or *temperature* combine a large number of microscopic (stochastic) molecular processes. Example 2.7 illustrates by analogy the movement of atoms in an ideal gas: the movement is stochastic on the level of the single molecules (balls), but their overall behavior results in the macroscopic phenomenon of molecular diffusion (see Chap. 8).

Example 2.7: The bed of nails, a stochastic system

Figure 2.7 depicts schematically a classic toy made of nails fixed on an inclined wooden board—a bed of nails. A ball, starting from a fixed position $x = 0$, rolls down the slope and periodically hits a nail such that the ball's path either continues to the left or right with the same probability. The nails are depicted as squares, the numbers in the squares give the probability that an individual ball arrives at this nail. After n collisions (in the figure, $n = 6$) the ball lands with a specific probability in one of the final positions (seven in our example). The path of a specific ball cannot be predicted. But if a large number of balls is sent through the system, and if the entire setup is built perfectly symmetrically, we will find a characteristic distribution of balls in the final boxes. These probabilities are called Bernoulli numbers.

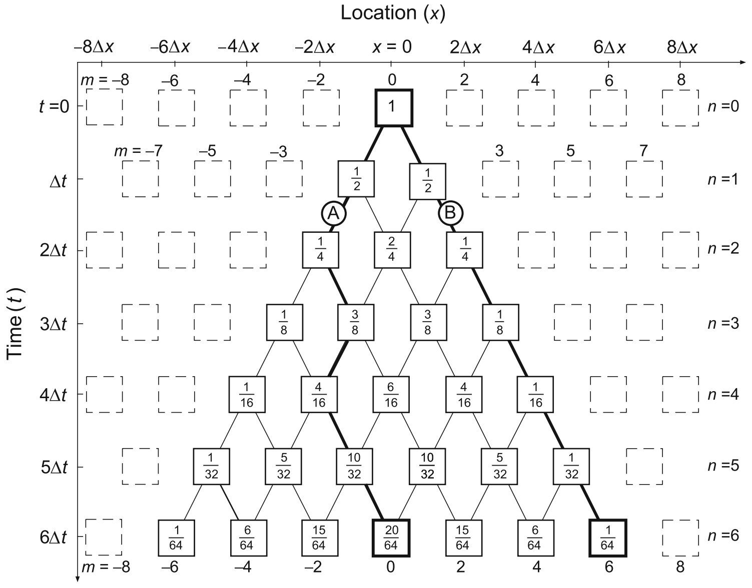


Fig. 2.7: *A schematic representation of the path of a ball through the bed of nails. The path of an individual ball cannot be predicted. If a large number of balls are successively sent through the system, we find a characteristic probability distribution in the final boxes. These probabilities are called Bernoulli numbers. Drawn in bold are two individual paths A and B. Path B leads to the right six times, it has a probability of* $2^{-6} = 1/64$*. The meaning of the variables labeled location* (x) *and time* (t) *will be discussed in Sect. 8.4*

In fact, we don't need to go all the way to quantum mechanics to explain the stochastic behavior of some natural systems. Even the classical equations of physics, using regular differential equations, contain the seed of randomness. As we will see in Chap. 6, three coupled differential equations are sufficient to introduce stochastics into models. Such systems of equations may have the special property that after a finite time, and starting from almost identical initial states, they develop states which are very different from each other. This happens even though the model equations themselves are entirely deterministic. Since every observation is subjected to some error, we are not able to determine the *absolute* equality of states.

With nonlinear differential equations, almost identical initial conditions can later lead to completely different system states.

Thus, apparently identical systems may develop differently. This is called deterministic chaos. The weather is a typical example for chaotic behavior. We are capable of predicting the weather over a period of a few days relatively well. But our limited knowledge of the atmosphere's state and other relevant factors means that a prognosis over 2 months will likely remain impossible.

When modeling, we can use various techniques to give essentially deterministic equations a whiff of stochastics. The simplest possibility is to introduce a randomly varying external relation. In this book, however, we will focus primarily on deterministic systems.

In this chapter, we got a general idea of some different model types and thereby encountered some properties with which we can characterize models. These properties include the pairs *static-dynamic*, *discrete-continuous* (either in space or in time) and *deterministic-stochastic*. In the following chapters, we will discuss the different model types in more detail.

Deterministic Chaos

2.7 Questions and Problems

Question 2.1: Explain the difference between internal and external relations.

Question 2.2: Most dynamic models implicitly contain a static model. The opposite is not true, however. Why?

Question 2.3: What is the difference between a dimension and a unit? Which of the two is unambiguously defined for every variable?

Question 2.4: What does the dimension of a model mean? (Note: Comparing questions 2.3 and 2.4 will make clear that *dimension* has a different meaning in mathematics than it does in physics.)

Question 2.5: Which of the following statements is correct?

- A box model is spatially discrete.
- A box model is always continuous in time.

Question 2.6: Look for some examples of systems that contain a stochastic component.

Question 2.7: Grubs live in the ground for 3 years and hatch as May beetles in spring of the fourth year. Sketch a simple regional model for May beetles. In particular, you should think about the following issues: choice of the system variables, type of model (dynamic or static, in space or in time, discrete or continuous).

Problem 2.1: Mass balance
A small lake has an inlet and an outlet. Establish the mass balance of a soluble substance in the lake, for the following two cases:

(a) A factory is built on the lake shore. From time t_0 onwards, it continuously discharges a substance into the lake. This substance is volatile, i.e. it can evaporate into the atmosphere, but is not degraded in the lake. It doesn't deposit in the sediment.

(b) Through an accident, a large amount of a toxic substance enters the lake at time t_0. This substance is degraded in the lake water and deposited in the sediment. After the accident, no more of the substance is added to the lake.

In both cases, you can assume that the substance's concentration in the inlet is zero.

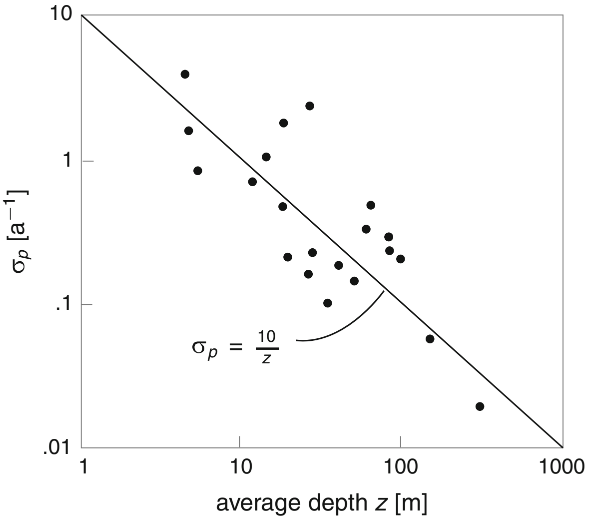


Fig. 2.8: *Phosphorus sedimentation, according to Vollenweider (1976)*

Problem 2.2: Determining the dimension of parameters

The following differential equation describes the progression through time of a substance's concentration profile in a vertical well shaft:

$$\frac{\partial C(z,t)}{\partial t} = -k_1 + k_2 \frac{\partial^2 C}{\partial z^2} + k_3 \frac{\partial C}{\partial z} + k_4 C(C^* - C)$$

Determine the dimensions (expressed by (M,L,T)) of the parameters k_1, k_2, k_3, k_4 and C^*. C is the concentration of a substance, z a length and t the time. Hint: How is the dimension of a first or second derivative of a variable determined?

Problem 2.3: Phosphorus sedimentation

Empirically established correlations should also be correct in terms of their dimensions. Figure 2.8 shows the relation between average lake depth z in meters and the specific phosphorus sedimentation rate $\sigma_p = \frac{10}{z}$ in year^{-1} for several lakes. What unit must the factor 10 have? What is the physical meaning of that factor?

Problem 2.4: Bed of nails

If we extend the bed of nails shown in Fig. 2.7 by two steps (to $n = 8$), the final boxes span from $m = -8, -6, \ldots, +6, +8$. What is the probability that a ball hits the box in the center ($m = 0$)? Calculate the Bernoulli numbers at level $n = 8$.

Chapter 3

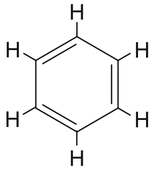
Static Models

Static accounts

Anne to Bill: “Yesterday, I brought 10 dollars to the bank, and the teller told me that I now had \$100 in my account.”—Bill: “Hmm. . . So, if I bring him 20 bucks tomorrow, my balance will be \$200!”

In this chapter we want to take a closer look at static models. In Chap. 2 we’ve seen that with a one-dimensional static model, the system variable $\mathcal{V}$ has an exactly defined value for a given external relation $\mathcal{R}$. A static model therefore simply describes the equilibrium state between $\mathcal{R}$ and $\mathcal{V}$ and does not give any indication about how rapidly $\mathcal{V}$ adjusts to changes in $\mathcal{R}$. Thus, static models are particularly useful when $\mathcal{V}$ quickly reacts to changes in $\mathcal{R}$ (that is, in cases where we can neglect the time that $\mathcal{V}$ takes to change).

In Chap. 2 we learned that pairs of data (such as the phosphorus concentration in a lake and the simultaneously measured phosphorus inflow) can be used to construct a static model through linear or nonlinear regression. Frequent applications of static models are generating calibration curves for analytical devices, stoichiometrically examining chemical equilibrium reactions, or describing the equilibrium distribution between two phases of a chemical substance in a reactor or the environment.



Benzene

In three examples, we now want to determine the distribution of benzene between the three phases *air*, *water* and *sediment*. In doing so we will get to know two frequently used static models: Henry’s law and the sorption isotherm. Benzene is a common solvent and is also contained in gasoline. It is a ring-shaped hydrocarbon with carcinogenic effects.

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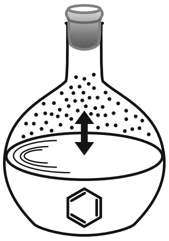
DOI 10.1007/978-3-642-30639-6_3,

3.1 Equilibrium Distribution Between Water and Air

In the first example we want to describe the equilibrium distribution of benzene between water and air. Let's imagine an experiment:



Example 3.1: Henry coefficient of Benzene

A flask is half filled with water. Some benzene is dissolved in the water. The flask is shaken for 5 min while kept closed with an airtight seal. Afterwards, the benzene concentration is measured in the water (C_{aq}) and in the air (C_{air}). If this experiment is repeated with a varying amount of benzene, the following series of measurements might be the result:

C_{aq}	[g L^{-1}]	1×10^{-2}	2×10^{-2}	6×10^{-2}	1×10^{-1}
C_{air}	[g L^{-1}]	1.9×10^{-3}	4.1×10^{-3}	1.1×10^{-2}	2×10^{-2}

The data pairs are plotted in Fig. 3.1. They lie approximately on a straight line, so we can formulate the following linear static model:

$$C_{air} = p \cdot C_{aq} \tag{3.1}$$

Through linear regression we obtain the non-dimensional model parameter $p = 0.196 \pm 0.004$.

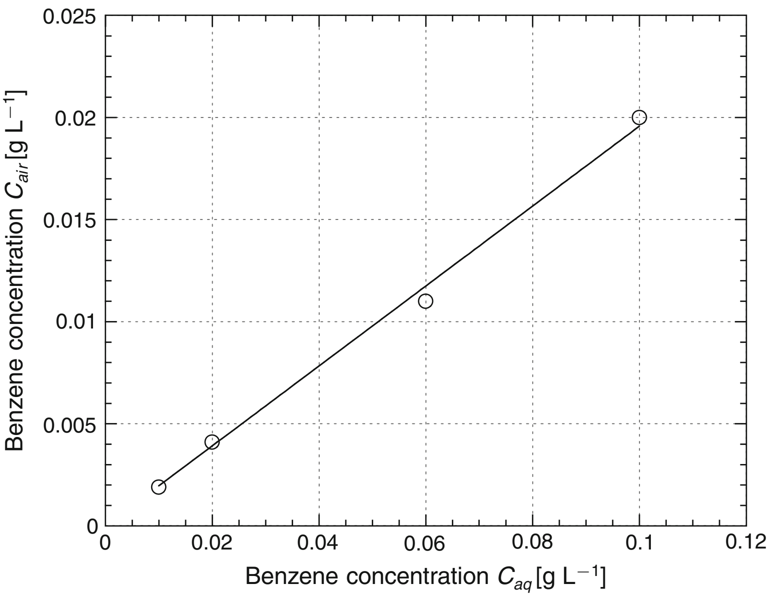


Fig. 3.1: *Two-dimensional diagram for determining the distribution coefficient $K_{a/w}$ of benzene between air and water. The linear regression yields $K_{a/w} = 0.196 \pm 0.004$*

We can repeat similar experiments with other soluble substances. The substance can initially exist in its gaseous form in air or dissolved in water. Through time, it will always be distributed throughout both the air and the water phases, and in describing this distribution we will obtain an approximately linear model (at least as long as the added substance mass is not too large or it is not a reactive substance). The model parameter p is the air-water distribution coefficient, or rather, the non-dimensional Henry coefficient $K_{a/w}$:

$$K_{a/w} = \frac{C_{air}}{C_{aq}} \tag{3.2}$$

The distribution coefficient $K_{a/w}$ is a substance-specific constant. Handbooks such as the CRC Handbook of Chemistry and Physics usually give the dimensional Henry coefficient K_H (more about this in Problem 3.1). Because the atmosphere is the most important transport medium for the global dispersal of many substances, the Henry coefficient is of substantial importance. In fact, many substances detected in surface waters originate from the atmosphere, within which they are rapidly transported from their point of emission and then dissolved into the water bodies where we measure them. As we will see later (Sect. 8.2), the Henry coefficient is also used to dynamically model the phase transition between air and water.

William Henry (1775–1836)

In 1803, he formulated the law named after him: At equilibrium, the concentration of a gas in water is proportional to its gas pressure over the liquid. William Henry was originally a physician. His own bad health eventually forced him to abandon that profession, and he turned his interest to chemistry instead.

William Henry
(1775-1836)

3.2 Equilibrium Distribution Between Water and Sediment

A substance dissolved in water also interacts with surfaces of solid materials. In this second example, we will therefore look at the distribution of benzene between water and suspended particles.

Example 3.2: Sorption isotherm of benzene

In this experiment we completely fill the flask with water and suspend a defined quantity of dried lake sediment within. Again, we add various amounts of benzene. The flask is then closed with an airtight seal and shaken for 1 h. Afterwards, the concentration of benzene in the water and on the sediment particles[a] is determined. We obtain the following data:

C_{aq} [g L^{-1}]	1×10^{-2}	2×10^{-2}	6×10^{-2}	1×10^{-1}
C_{sed} [g kg_{sed}^{-1}]	0.018	0.033	0.103	0.17

Once again we find an approximately linear relation between the data pairs C_{aq} and C_{sed}. This is illustrated as a two-dimensional diagram in Fig. 3.2. The average regression coefficient is $p = 1.7 \pm 0.008$ L kg_{sed}^{-1}:

$$C_{sed} = p \cdot C_{aq} \tag{3.3}$$

---

[a] The concentration on the sediment is given in the dimension *substance mass per sediment mass* [M M_{sed}^{-1}].

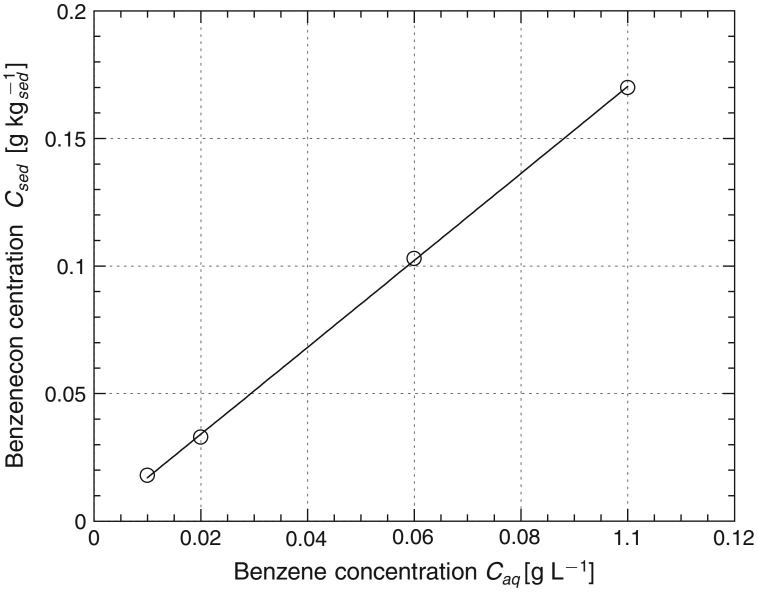


Fig. 3.2: *Sorption isotherm of benzene on a lake sediment: the distribution coefficient is* $K_d = 1.7 \pm 0.008$ *L* kg_{sed}^{-1}

This experiment can also be repeated with other chemicals and particles. The two-dimensional diagram representing the equilibrium distribution of a chemical substance between water and a solid phase is called *sorption isotherm*. In our example, the sorption isotherm is linear. The parameter p is the slope of the sorption isotherm and is called distribution coefficient K_d, with a dimension of [L^3M^{-1}]:

$$K_d = \frac{C_{sed}}{C_{aq}} \tag{3.4}$$

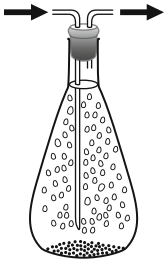
The distribution coefficient K_d depends on the properties of both the chemical substance and the solid phase. The concept of a constant distribution coefficient for the partition between a solution and a solid phase is also used in dynamic transport models for chemicals. One use of such models is to estimate the dispersion of a pollutant from a landfill site into an aquifer.[1]

3.3 Multi-dimensional Static Models

In the third example, we will couple the two models in order to describe the equilibrium concentration of benzene between water, air and sediment. In order to minimize the system's complexity, we look at a reactor (as shown in the margin illustration) instead of a natural lake.

Example 3.3: Benzene in a reactor with air, water and sediment

The reactor is filled with a specified amount of water and dried sediment. Air flows through the reactor's water volume, continuously mixing it. The benzene concentration in that air is constant at $C_{air} = 0.01$ g L^{-1}. Which benzene concentration will we measure after about 1 h (i.e., after equilibrium has been reached) in the water and on the sediment particles?



The system "reactor" has an input quantity $\mathcal{R}$ (the benzene concentration in the air C_{air}). It further has two variables $\mathcal{V}_1$ and $\mathcal{V}_2$: the benzene concentration in the water C_{aq} and the benzene concentration on the sediment particles C_{sed}.

$$\begin{aligned} C_{air} &\rightarrow \mathcal{R} \\ C_{aq} &\rightarrow \mathcal{V}_1 \\ C_{sed} &\rightarrow \mathcal{V}_2 \end{aligned}$$

To draw up the system equations, we use the relations derived in the two previous examples. This yields:

$$\mathcal{V}_1 = \frac{1}{K_{a/w}} \mathcal{R} \tag{3.5}$$

$$\mathcal{V}_2 = K_d \mathcal{V}_1 \tag{3.6}$$

---

[1] An aquifer is a water-carrying layer in the ground consisting of sand, gravel or permeable rock formations.

This is a two-dimensional, linear, static model with the system parameters:

$$\begin{aligned} \frac{1}{K_{a/w}} &\rightarrow p_1 \\ K_d &\rightarrow p_2 \end{aligned}$$

Because we know $\mathcal{R}$ and the two system parameters, we can calculate the benzene concentrations $\mathcal{V}_1$ and $\mathcal{V}_2$ directly with Eqs. (3.5) and (3.6). This gives us:

$$\begin{aligned} C_{aq} &\equiv \mathcal{V}_1 = \frac{1}{K_{a/w}}\mathcal{R} = \frac{1}{0.2} \times 0.01 \text{ g L}^{-1} = 0.05 \text{ g L}^{-1} \\ C_{sed} &\equiv \mathcal{V}_2 = K_d\mathcal{V}_1 = 1.7 \text{ L kg}_{sed}{}^{-1} \times 0.05 \text{ g L}^{-1} = 0.085 \text{ g kg}_{sed}{}^{-1} \end{aligned}$$

To calculate a model with two variables (a two-dimensional model), we need to solve a system of two coupled equations (Eqs. 3.5 and 3.6) with two unknown variables. Thus, in order to solve an n–dimensional model, an n–dimensional system of equations with n unknowns has to be solved. The system of equations for an n–dimensional static model has the following general form:

$$\mathcal{V}_i = f_i(\mathcal{R}_1, \ldots, \mathcal{R}_m, p_1, \ldots, p_q, \mathcal{V}_1, \ldots, \mathcal{V}_n) \qquad \text{for} \qquad i = 1, \ldots, n \tag{3.7}$$

Where:

$\mathcal{V}_i$	system variable, $i = \{1, \ldots, n\}$
$\mathcal{R}_j$	external relation, $j = \{1, \ldots, m\}$
p_k	model parameter, $k = \{1, \ldots, q\}$

In our case, the system of equations can be solved analytically by hand. In cases where this is not possible, software can solve the system computationally. One algorithm often used for this is the Gaussian elimination method.

In this chapter, we have used three static models to describe the equilibrium distribution of a chemical substance in the environment. We have thereby encountered two important parameters, the air-water and the sediment-water distribution coefficients, both of which we will utilize again for dynamic models.

However, all three examples have a weakness: we do not know how long it takes for an equilibrium to be established between the different phases. In the next chapter, dynamic models will let us investigate precisely that question.

3.4 Questions and Problems

Question 3.1: State the types of equations with which static and dynamic models are generally described.

Question 3.2: Which of the following laws and formulas from physics, chemistry and biology correspond to a static model?

Don't worry if you do not know some or all of these laws or can't clearly classify them. They are not necessary to understand the material. In addition, some of them will be discussed in detail later in the book.

(a) Ohm's law

(b) Kepler's law of planetary motion, giving the relation between a planet's orbital period and the semi-major axis of its elliptical orbit

(c) Equation of pendular motion

(d) Ideal gas law

(e) Fourier's law of heat convection

(f) Law of radioactive decay

(g) Lensmaker's equation in optics

(h) The chemical equilibrium between dissolved carbonate and bicarbonate in water

(i) The law for light passing through an optical prism

(j) Maxwell's laws of electrodynamics

(k) The logistical growth law of a biological species

Problem 3.1: Dimensional Henry coefficient
Often, the concentration of a substance in the gas phase is given by the gas pressure P of that substance. The Henry coefficient of a substance is then defined as: $K_H = \frac{P}{C_{aq}}$. Which dimension and unit does K_H have? How is it linked to the non-dimensional air-water distribution coefficient $K_{a/w}$, if the gas phase of the substance in question can be approximated as an ideal gas?

Problem 3.2: Henry coefficient of methyl bromide
Methyl bromide (CH_3Br) is a gas used in greenhouses to fight insect larvae, for instance in salad cultivation. Using the following data pairs (measured at a temperature of 20 °C), estimate the Henry coefficient K_H for methyl bromide.

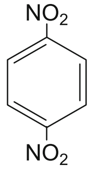
P [atm]	0.2	0.3	0.4	0.6	0.7
C_{aq} [mol L^{-1}]	0.03	0.05	0.06	0.095	0.1

From K_H, calculate the non-dimensional air-water distribution coefficient $K_{a/w}$ through the relation $K_{a/w} = \frac{K_H}{RT}$. Hint: the solution of Problem 3.1 will be of use here.

Problem 3.3: Methyl bromide as ozone killer

Methyl bromide is one of the substances significantly contributing to ozone destruction in the stratosphere. The concentration of methyl bromide in a water sample taken from a water jar in a greenhouse is $C_{aq} = 0.001$ mol L^{-1}. Calculate the total mass of methyl bromide in kg that was present in the greenhouse at the time the sample was taken. The greenhouse is 5 m wide, 20 m long and 2.5 m high. Assume that the system is at equilibrium regarding the water/air distribution.

Problem 3.4: Nonlinear sorption isotherm


1,4-Dinitrobenzene

Nitroaromates are a class of substances that exhibit sorption on mineral surfaces. The following table shows the result of sorption experiments with 1,4-Dinitrobenzene (1,4-DNB) on the clay mineral Kaolinite (data from Haderlein et al. 1996):

C_{aq} [μmol L^{-1}]	0.17	0.51	1.8	3.6	7.6	19.5	26.5
C_{min} [μmol kg$_{min}^{-1}$]	241	633	1,640	2,850	4,240	6,100	7,060

Draw a two-dimensional diagram with the data pairs and try to find a model with a maximum of two free parameters to describe the sorption.

Problem 3.5: Economic theory: supply and demand

A central element of economic theory is the assumption that, for a given good, the price is determined by an equilibrium between supply and demand (see e.g. Samuelson and Nordhaus 2009). The following empirical observations serve as the basis for a graphical solution:

1. Demand for the good increases with decreasing price (Fig. 3.3a).

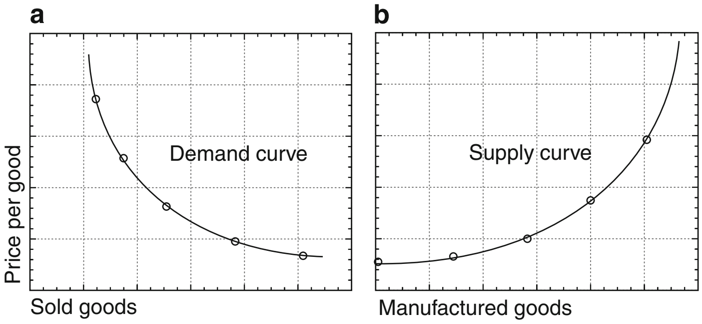


Fig. 3.3: *Economic models: (a) Demand curve. (b) Supply curve*

2. Supply for the good increases with increasing price (Fig. 3.3b)
   - (a) Use the two curves to graphically determine the resulting price.
   - (b) What happens to the price of the good if, for a constant supply curve (Fig. 3.3b), the demand grows, i.e. the demand curve (Fig. 3.3a) moves to the right?
   - (c) What happens to the price and the number of goods sold if the manufacturing costs decrease (for a given price, more goods can be manufactured)?

Chapter 4

Linear Models with One Variable

In the remaining part of the book, we will exclusively deal with dynamic models. As we already noted in the introduction, one of the principal characteristics of natural systems is that they are *not static*.

Dynamic and continuous-time systems are usually described with differential equations. Although natural systems are hardly ever linear in reality, we will first take a close look at linear models (and thus linear differential equations). The field of systems analysis is rooted in physics and the technically-oriented sciences. In those fields, linear models play a particularly important role. They have a key feature: they have analytical solutions which can be linearly combined at will to construct new solutions. These simple solutions are well-suited as building blocks for more complex models.

Nonlinear systems can often be approximated by linear models piece by piece.

Real systems are usually nonlinear. Often, however, they can be approximated by linear models in a piecemeal way, that is, within limited ranges of the system variable. As we will see in Chap. 6, the concepts developed for linear models serve as the point of departure for the analysis of nonlinear models.

First, let us examine continuous-time systems with only *one* system variable. The dynamic models resulting from this describe the change of a *single* variable of the system. We do *not* spatially differentiate the system, we treat it as one box, for instance as a thoroughly mixed volume. The mathematical model for such a system is given by the following first-order differential equation:

$$\frac{\mathrm{d}\mathcal{V}(t)}{\mathrm{d}t} = \mathcal{R} + p\mathcal{V}(t) \tag{4.1}$$

Where:

$\mathcal{V}(t)$	System variable
$\mathcal{R}$	External relation
p	Model parameter

Because such a model contains only a single system variable in a single spatial box we also call it a *one-box model*. Equation (4.1) is an *inhomogeneous, linear, first-order differential equation*. The external relation $\mathcal{R}$

D.M. Imboden and S. Pfenninger, *Introduction to Systems Analysis*,

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constitutes the inhomogeneous term of the differential equation. The equation stays linear even if $\mathcal{R}$ and p are time-dependent.[1] The important condition is that $\mathcal{R}$ and p are not dependent on the system variable $\mathcal{V}$ itself. If $\mathcal{R} = 0$, the equation is called homogeneous.

4.1 The Linear One-Box Model as a Balance Equation

Mathematician's mass balance

Two mathematicians are standing outside a lecture hall, impatiently waiting for all students to leave. The first says: "Now there's only five left". Shortly afterwards eight people leave the room. The two mathematicians stare at each other in astonishment for a moment. Then the second says: "Now if three people go in, the room will finally be empty!"

Whatever the system variable of a one-dimensional system describes, we can always characterize its dynamic behavior with a balance equation of the following form:

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = \{\text{Production processes}\} - \{\text{Loss processes}\} \tag{4.2}$$

By "production" we mean all processes through which the value of the variable $\mathcal{V}$ is increased. Apart from processes taking place within the system, this also includes transport processes from the environment into the system. "Loss" means all reaction and transport processes through which the value of the variable $\mathcal{V}$ decreases.

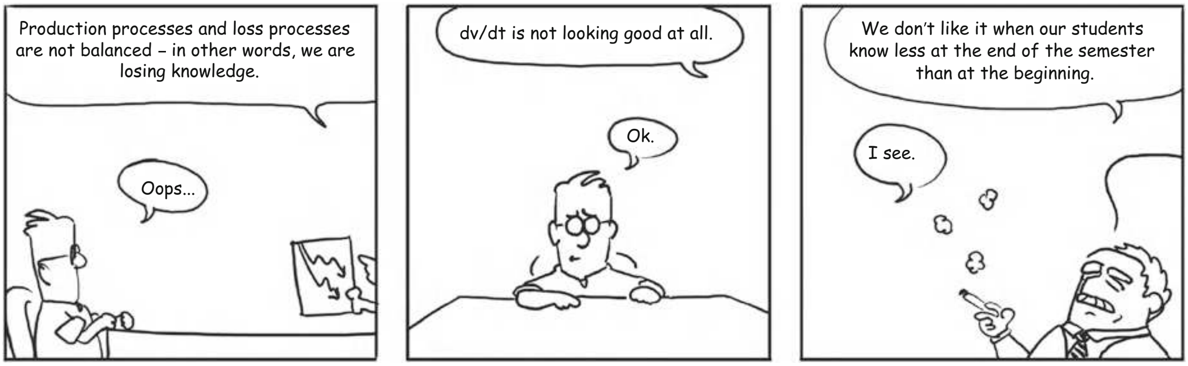
If Eq. (4.2) describes a linear model, both process types consist of a sum of zero-order and first-order processes:

$$\begin{aligned} \{\text{Production processes}\} &= J_p + k_p\mathcal{V} \\ \{\text{Loss processes}\} &= J_l + k_l\mathcal{V} \end{aligned} \tag{4.3}$$

J_p and J_l are the zero-order rates independent of $\mathcal{V}$, while $(k_p\mathcal{V})$ and $(k_l\mathcal{V})$ are the first-order rates that are proportional to $\mathcal{V}$. The parameters k_p and k_l are called first-order specific (conversion) rates. They always have the dimension $[\,\mathrm{T}^{-1}\,]$ independently of $\mathcal{V}$.

---

[1] If p is explicitly time-dependent, the term $p\mathcal{V}$ is a mixture of an internal and external relation (see the explanations on page 45 following Example 4.1).



Balance equation

If we plug Eq. (4.3) into Eq. (4.2), we get[2]:

$$\begin{aligned}\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} &= (J_p + k_p\,\mathcal{V}) - (J_l + k_l\,\mathcal{V}) \\ &= (J_p - J_l) + (k_p - k_l)\,\mathcal{V} \\ &= J^\star + k^\star\,\mathcal{V}\end{aligned} \tag{4.4}$$

The net coefficients $J^\star = J_p - J_l$ and $k^\star = k_p - k_l$ can be positive or negative depending on the value of the individual parameters J_p, J_l, k_p and k_l. What is important is that any one-dimensional linear model can be reduced to the form of the last line of Eq. (4.4), independent of how diverse the individual production and loss processes might be. In the most general case, $J^\star$ and $k^\star$ are arbitrary time-dependent quantities but do not depend on $\mathcal{V}$.

Let's look at an example:

Example 4.1: Fish growth in a pond

In a pond, the total amount of fish M (expressed as the total fish biomass in kg) increases by egg deposition and fish growth after subtracting mortality with the specific rate $k_p = 0.2\,\text{year}^{-1}$. Furthermore, the fish pond is restocked yearly with juvenile fish at $J_p = 500\,\text{kg}\,\text{year}^{-1}$. On average, 40 % of the fish biomass is fished per year (loss rate $k_l = 0.4\,\text{year}^{-1}$). What is the dynamic equation for fish biomass M?

---

[2] From now on, to make things easier to read, we will usually not write the time dependence of the system variables. The notation $\mathcal{V}$ will stand for $\mathcal{V}(t)$.

The model consists of three production and loss terms. One of them is zero-order:

$$J^\star = J_p = 500 \text{ kg year}^{-1}$$

The two others are first-order, they have the specific net rate:

$$k^\star = k_p - k_l = (0.2 - 0.4) \text{ year}^{-1} = -0.2 \text{ year}^{-1}$$

So, overall:

$$\frac{\mathrm{d}M}{\mathrm{d}t} = 500 \text{ kg year}^{-1} - (0.2 \text{ year}^{-1})\, M$$

We will return to this in Example 4.3.

In Sect. 1.2 we differentiated between internal and external relations. Where do we find this distinction in Eq. (4.4) and Example 4.1? We will see that to a certain degree the answer to this question depends on the context of Eq. (4.4) and the underlying mathematical model.

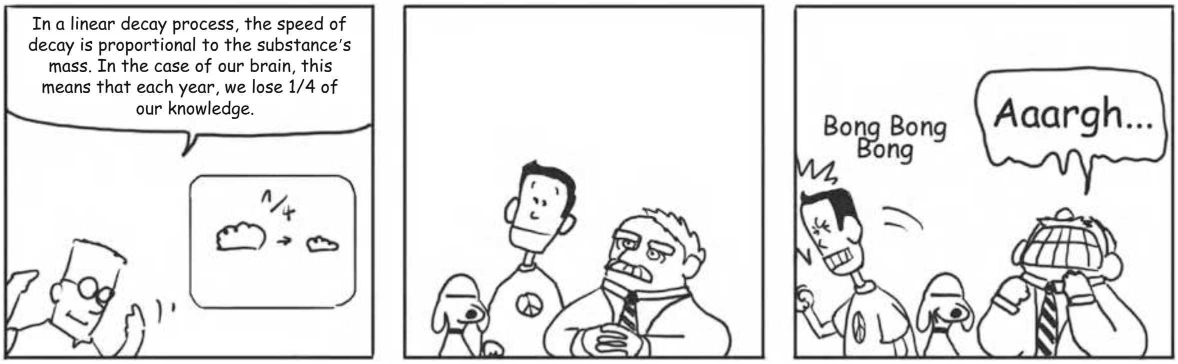
In most cases, the first-order processes belong to the internal relations, as they are controlled by the momentary value of variable $\mathcal{V}(t)$. If the specific rate $k^\star$ is constant in time, the term $(k^\star\mathcal{V})$ indeed only varies as a result of the time-dependent variability of $\mathcal{V}(t)$. This *implicit* time dependence is a typical attribute of internal relations.

Yet, $k^\star$ may be time-dependent as well. This *explicit* time dependence is then not a property of the model itself but an influence from outside. In this case $k^\star(t)$ is an external relation. Thus, the first-order process $k^\star(t)\mathcal{V}(t)$ becomes a combination of internal and external relation. For instance, in Example 4.1, at a given instant the fish breeder may decide to protect the pond from fish-eating birds by laying out a net on its surface, thereby making the parameter k_l smaller. In the model this process would be an external relation.

The zero-order term $J^\star$ can also explicitly depend on time (but not implicitly). If it does, then it certainly represents an external relation. If it is constant, however, there is some room for interpretation: either we interpret $J^\star$ as a fixed (i.e. immutable) system parameter, or we see it as an external relation. For that latter case, we can argue that although the external relation is constant momentarily, it could be changed from "outside the model" at any time.To stick to the fish pond example: the rate of fish addition and the fishing rate could in principle be changed, even if we choose to analyze the model only for the case of fixed values. Summarizing, the important point is that an explicit time dependence of system coefficients always represents external relations.

4.2 Linear Models with Constant Coefficients

Linear decay process



First, we will look at the case of constant (time-independent) coefficients $J^\star$ and $k^\star$. We can interpret this model as free from external relations, in other words, as autonomous. Starting from identical initial states, an autonomous model always develops in the same way.[3]

We will again start from the general equation (4.4):

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = J^\star + k^\star \mathcal{V} \tag{4.5}$$

It has the initial condition $\mathcal{V}(0) = \mathcal{V}^0$ and the following solution (as long as $k^\star$ is not zero):

$$\mathcal{V}(t) = (\mathcal{V}^0 + \frac{J^\star}{k^\star})\,\mathrm{e}^{k^\star t} - \frac{J^\star}{k^\star} \qquad \text{for } k^\star \neq 0 \tag{4.6}$$

For the homogeneous differential equation

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = k^\star \mathcal{V} \tag{4.7}$$

the solution is accordingly:

$$\mathcal{V}(t) = \mathcal{V}^0 \mathrm{e}^{k^\star t} \tag{4.8}$$

By inserting Eq. (4.6) or (4.8) into the original differential equation, you can easily validate the result given above. The initial condition $\mathcal{V}(t = 0) = \mathcal{V}^0$ is correctly expressed, as can be seen by setting $t = 0$ in the solutions.

Let's first discuss the solution of the homogeneous Equation (4.8). As can easily be seen, $\mathcal{V}(t)$ behaves entirely different for $t \longrightarrow \infty$ depending on whether $k^\star$ is negative or positive (we will not discuss the trivial case of $k^\star = 0$). The two cases are shown in Fig. 4.1. They are the exponential

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[3] To be precise, this is only true for deterministic models (see Sect. 2.6).

growth and decay curves. For the case of a negative $k^\star$ we introduce the new specific rate k (which we will use again later):

$$k = -k^\star \quad , \quad k > 0 \tag{4.9}$$

To identify the exponential curve it helps to divide both sides of Eq. (4.8) by $\mathcal{V}^0$ and then to calculate the natural logarithm on both sides:

$$\ln(\frac{\mathcal{V}(t)}{\mathcal{V}^0}) = \ln \mathcal{V}(t) - \ln \mathcal{V}^0 = \ln(\mathrm{e}^{k^\star t}) = k^\star t$$

or:

$$\ln \mathcal{V}(t) = \ln \mathcal{V}^0 + k^\star t \tag{4.10}$$

Thus, if we plot $\ln \mathcal{V}(t)$ against time t, the curve should be a straight line with slope $k^\star$ (see Fig. 4.1).

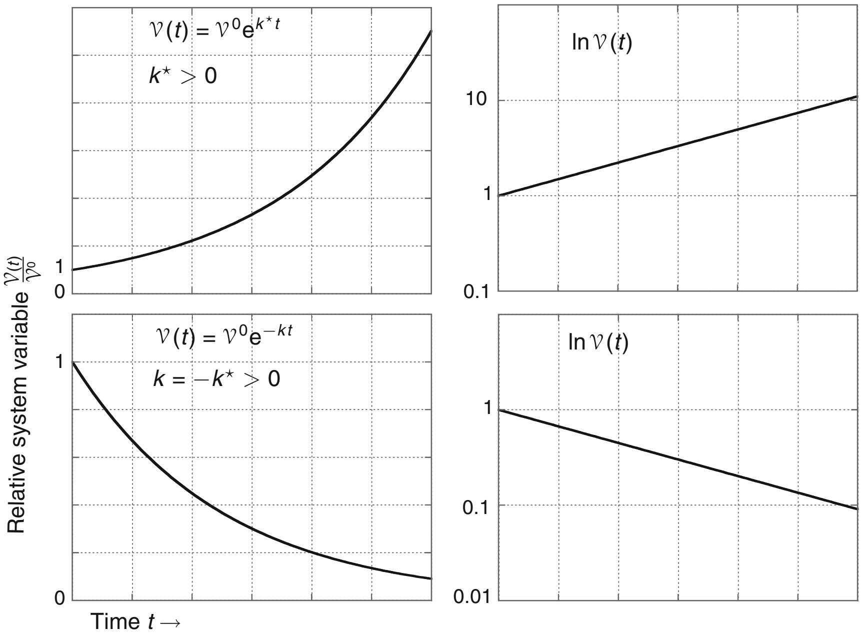


Fig. 4.1: *Solution of the linear homogeneous differential equation for $\mathcal{V}^0 = 1$ with a positive (upper curve) and negative (lower curve) coefficient $k^\star$. The half-logarithmic diagram (on the right-hand side) results in a straight line with slope $k^\star$ (see Eq. 4.10)*

Example 4.2: Exponential population growth

From 1850 to 1975 the world population grew from $N^0 = 1$ billion to $N(t) = 4$ billion people. We assume that specific growth was constant throughout that entire period (which of course is a gross oversimplification). What is the specific growth rate k_p?

The differential equation of the exponential growth model is analogous to Eq. (4.7):

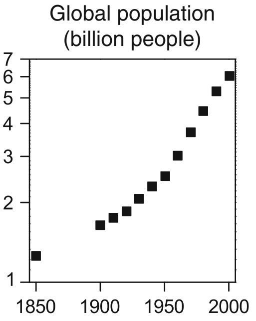
$$\frac{\mathrm{d}N}{\mathrm{d}t} = k_p \cdot N \tag{4.11}$$

We arrive at the solution with Eq. (4.8):

$$N(t) = N^0 \mathrm{e}^{k_p t} \tag{4.12}$$

Solving Eq. (4.12) for k_p and using $t = 125\,\text{year}$, $N(t)/N^0 = 4$, we get:

$$k_p = \frac{1}{t} \ln \frac{N(t)}{N^0} = \frac{1}{125\ \text{year}} \ln 4 \approx 0.01\ \text{year}^{-1} \tag{4.13}$$



In many models, the specific total rate $k^\star$ is negative. With the definition Eq. (4.9) we can write the resulting differential equation in the following form, also replacing $J^\star$ with J to simplify further:

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = J - k\,\mathcal{V} \quad , \quad k > 0 \tag{4.14}$$

This equation has the solution:

$$\mathcal{V}(t) = (\mathcal{V}^0 - \frac{J}{k})\,\mathrm{e}^{-kt} + \frac{J}{k} \quad , \quad k > 0 \tag{4.15}$$

4.2.1 The Steady State

After establishing the system equation for an autonomous linear model and getting to know its solution, we now want to interpret it and use it to draw conclusions about the model. The model is in a special state when $\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = 0$. At that point $\mathcal{V}$ remains constant, and the model is in a so-called steady state. In mathematics, this state of a model is also called fixed point. If the system variable is the average phosphorus concentration in a lake, the concentration stays constant when all input and output processes exactly balance each other. Since the size of some of these processes, e.g. the output, depends on $\mathcal{V}$, this occurs at a specific concentration which is called the steady-state or equilibrium concentration.

Formally, we calculate the steady state value $\mathcal{V}^{\infty}$[4] by setting the left side of Eq. (4.5) equal to zero and solving it for $\mathcal{V} = \mathcal{V}^{\infty}$:

$$\mathcal{V}^{\infty} = -\frac{J^{\star}}{k^{\star}} = \frac{J}{k} \quad , \quad k \neq 0 \text{ and } k^{\star} \neq 0 \tag{4.16}$$

The homogeneous equation (4.7) has the steady state $\mathcal{V}^{\infty} = 0$.

In many cases, the meaning of the variable $\mathcal{V}$ precludes negative values (e.g. when $\mathcal{V}$ represents the amount or concentration of a substance). In that case Eq. (4.16) only makes sense if either $J^{\star}$ or $k^{\star}$ (but not both of them) are negative. In Example 4.1 we encountered a case with $J^{\star} > 0, k^{\star} < 0$. Let us now further analyze the dynamics of the fish pond.

Example 4.3: Steady-state fish biomass in the pond

In Example 4.1 we developed a model for a fish pond that is artificially stocked with new fish while simultaneously being fished. We are now interested in the steady state amount of fish biomass in the pond. According to Eq. (4.16), the following holds:

$$M^{\infty} = -\frac{J^{\star}}{k^{\star}} = -\frac{500 \text{ kg year}^{-1}}{-0.2 \text{ year}^{-1}} = 2{,}500 \text{ kg}$$

Note: Of course, this representation of the fish pond is very simplistic. In nature, growth and death rates are never entirely constant, so that M^{∞} would always fluctuate around an average value.

Each dynamic model implicitly contains a static model.

To summarize: By setting the left side of Eq. (4.5) equal to zero, the differential equation becomes the ordinary algebraic equation (4.16). This equation can also be seen as a *static model* for $\mathcal{V}^{\infty}$ as a function of $J^{\star}$ and $k^{\star}$. In that sense, dynamic models that have steady-state solutions implicitly contain a static model as well.

4.2.2 The Linear Flow Reactor

An application of Eq. (4.14) is the so-called completely mixed linear flow reactor. We can use it to describe a lake as a one-box model:

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[4] The symbol for infinity, which is used here as superscript, indicates that the steady state is formally only reached after an infinite amount of time.

Example 4.4: A lake as linear flow reactor

We consider a lake as a pool of water where a constant amount of water flows through, that is, inflow and outflow are equal and the water volume in the lake remains constant. Starting at time t_0, a constant amount of a substance per time is added through the inflow. The substance is completely mixed in the lake and decays with a first-order reaction. Therefore, the concentration is the same everywhere in the lake, especially also in the water leaving the lake through the outflow. Figure 4.2 shows this model as a box diagram.

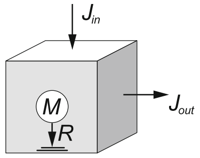


Fig. 4.2: *A lake as a completely mixed flow reactor (one-box model) with a decay reaction*

To model this situation, we first establish a mass balance for the substance with the help of Eq. (4.2):

$$\left\{\begin{array}{c}\text{Change of mass}\\ \text{in the lake per time}\end{array}\right\} = \left\{\begin{array}{c}\text{Supply}\\ \text{per time}\end{array}\right\} - \left\{\begin{array}{c}\text{Removal}\\ \text{per time}\end{array}\right\} - \left\{\begin{array}{c}\text{Reaction}\\ \text{per time}\end{array}\right\}$$

Mathematically, the mass balance can be formulated as a differential equation (M: total mass in the lake $[\mathrm{M}]$, R: reaction per time $[\mathrm{M\ T^{-1}}]$):

$$\frac{\mathrm{d}M}{\mathrm{d}t} = J_{in} - J_{out} - R \tag{4.17}$$

For the mass input J_{in} and the mass removal J_{out} we can write:

$$J_{in} = QC_{in} \tag{4.18}$$

$$J_{out} = QC \tag{4.19}$$

Q	$[\mathrm{L^3\ T^{-1}}]$	Flow through the lake, inflow = outflow
C_{in}	$[\mathrm{M\ L^{-3}}]$	Concentration of the substance in the inflow
C	$[\mathrm{M\ L^{-3}}]$	Concentration of the substance in the lake and outflow

For the first-order reaction R of the substance in the lake we can write:

$$R = k_r M \tag{4.20}$$

where k_r is the first-order reaction rate and has the dimension $[\mathrm{T^{-1}}]$. Thus, we end up with the following mass balance:

$$\frac{\mathrm{d}M}{\mathrm{d}t} = QC_{in} - QC - k_r M . \tag{4.21}$$

If we divide both sides of Eq. (4.21) by the lake's constant volume V, we get the dynamic equation for the substance concentration in the lake ($C = \frac{M}{V}$):

$$\begin{aligned}\frac{\mathrm{d}C}{\mathrm{d}t} &= \frac{Q}{V}C_{in} - \frac{Q}{V}C - k_r C \\ &= k_w C_{in} - (k_w + k_r)C \\ &= k_w C_{in} - k_{tot}C\end{aligned} \tag{4.22}$$

The quotient $\frac{Q}{V}$ is called the specific flow rate k_w. The inverse, $\frac{1}{k_w}$, is the renewal time τ_w of the lake water. The sum $k_w + k_r$ is the total specific rate k_{tot}. The inverse, $\frac{1}{k_{tot}}$, is the mean retention time of the substance in the lake (influenced by both flow and decay).

Equation (4.22) can also be written in terms of the substance input J_{in}:

$$\begin{aligned}\frac{\mathrm{d}C}{\mathrm{d}t} &= \frac{J_{in}}{V} - k_{tot}C \\ &= j_{in} - k_{tot}C\end{aligned} \tag{4.23}$$

The variable j_{in} is the substance input per volume and time with the dimension $[\,\mathrm{ML}^{-3}\mathrm{T}^{-1}\,]$:

$$j_{in} = \frac{J_{in}}{V} = \frac{Q}{V}C_{in} = k_w C_{in} \tag{4.24}$$

Comparing the dynamic equation for the flow reactor (4.23) with Eq. (4.14) yields the following analogy: The system variable in the flow reactor is C. The inhomogeneous term J corresponds to $j_{in} = k_w C_{in}$. The coefficient k is given by the total specific rate $k_{tot} = k_w + k_r$.

We obtain the equilibrium (steady state) concentration in the lake with Eq. (4.16):

$$C^{\infty} = \frac{j_{in}}{k_{tot}} = \frac{k_w}{k_{tot}}C_{in} = \frac{k_w}{k_w + k_r}\,C_{in} \tag{4.25}$$

The concentration C^{∞} is only reached if the substance input J_{in}, or j_{in}, and the specific rate k_{tot} remain constant.

Let us compare this result with the static lake model in Sect. 2.2. According to Eq. (2.2), the equilibrium concentration of phosphorus C_{aq}, which we now call C^{∞}, is:

$$C_{aq} \to C^{\infty} = p \cdot J_{in} \tag{4.26}$$

The equilibrium concentration C^{∞} of the dynamic model can also be expressed, by means of Eqs. (4.18) and (4.25), as a function of substance input J_{in}:

$$C^{\infty} = \frac{k_w}{k_{tot}}C_{in} = \frac{1}{k_{tot}}\frac{Q}{V}C_{in} = \frac{1}{k_{tot} \cdot V}J_{in} \tag{4.27}$$

The parameter p of the static model thus turns out to depend on the total rate constant and the lake volume:

$$p = \frac{1}{k_{tot} \cdot V} \tag{4.28}$$

As noted before, p has the dimension $[\,\mathrm{TL}^{-3}\,]$.

In the following example we utilize the relation between model parameters and steady state:

Example 4.5: Algae growth in a pond with flowing water

In a pond with constant water through-flow and volume $V = 10^4\ \mathrm{m}^3$, favorable conditions let free-floating algae (phytoplankton) grow with a specific growth rate $k_g = 0.5\,\mathrm{d}^{-1}$. Through sedimentation, 20 % of the plankton in the pond is lost daily. How large can the water flow Q be at most, if the algae are not to disappear entirely from the pond?

First, we establish a mass balance for the system:

$$\left\{\begin{matrix}\text{Change of algae}\\ \text{in pond per time}\end{matrix}\right\} = \left\{\begin{matrix}\text{Growth}\\ \text{per time}\end{matrix}\right\} - \left\{\begin{matrix}\text{Outflow}\\ \text{per time}\end{matrix}\right\} - \left\{\begin{matrix}\text{Sedimentation}\\ \text{per time}\end{matrix}\right\}$$

We assume that the conditions for a linear flow reactor (one-box model) are fulfilled. In that case, all three processes of the mass balance can be described as linear functions:

$$\begin{aligned}\frac{\mathrm{d}C}{\mathrm{d}t} &= k_g C - k_w C - k_s C\\ &= (k_g - k_w - k_s)C\end{aligned} \tag{4.29}$$

where:

$k_g = 0.5\,\mathrm{d}^{-1}$	specific growth rate of the algae
$k_w = Q/V$	flow rate through the pond
$k_s = 0.2\,\mathrm{d}^{-1}$	sedimentation rate of the algae in the pond

For the algae concentration not to decrease, the sum of all rates on the right side of Eq. (4.29) must be positive or zero:

$$k_g - k_w - k_s \geq 0 \tag{4.30}$$

Solving for $k_w = Q/V$ results in:

$$k_w = \frac{Q}{V} \leq k_g - k_s \tag{4.31}$$

For the flow Q we then get:

$$Q \leq (k_g - k_s)V = 10^4\ \mathrm{m}^3\ (0.5 - 0.2)\ \mathrm{d}^{-1} = 3{,}000\ \mathrm{m}^3\ \mathrm{d}^{-1} \tag{4.32}$$

4.2.3 Adjustment Behavior and Adjustment Time

Up to this point, the dynamic treatment of a system has not brought us anything beyond what we could have, in principle, derived from the static model. However, the information contained within a dynamic model reaches much beyond the steady state. For example, we are interested in whether the system is indeed moving towards the steady state calculated in Eq. (4.16) and if so, how long it will take to reach it.

Again, let's consider a lake as a linear flow reactor. We now have to solve the differential equation (4.22) by replacing the variables of the general solution (4.15) with the variables of the flow reactor. To keep things simple, we will again call the linear system's total rate k_{tot} simply k. It can, if not explicitly stated otherwise, describe any process such as flow, decay (e.g. radioactive), or sedimentation, but also (for $k < 0$ or $k^\star > 0$, see Eq. 4.9) a linear growth process. We then get:

$$\begin{aligned} C(t) &= (C^0 - \frac{k_w}{k} C_{in})\mathrm{e}^{-kt} + \frac{k_w}{k} C_{in} \\ &= (C^0 - C^\infty)\mathrm{e}^{-kt} + C^\infty \end{aligned} \tag{4.33}$$

In the solution, the steady state concentration $C^\infty = \frac{k_w}{k} C_{in}$ appears. We rewrite the equation in the form:

$$C(t) = C^0 \mathrm{e}^{-kt} + C^\infty (1 - \mathrm{e}^{-kt}) \tag{4.34}$$

and assume that k is positive. The first term on the right-hand side of Eq. (4.34) describes the exponential decay of the initial concentration C^0 in the system. For $t \to \infty$, this term becomes zero. The old system state C^0 is "washed out" of the system; the term describes the so-called washing-out or decay curve. In contrast, the second term describes how—starting from concentration zero—the system develops towards the steady state belonging to the (constant) input $j_{in} = k_w C_{in}$. We will call this term the ingrowth curve. Figure 4.3 shows these two components of the solution as well as their sum. In the language of mathematics one can also say that the general solution of Eq. (4.34) is a linear superposition of two special solutions, the net decay curve and the net ingrowth curve.

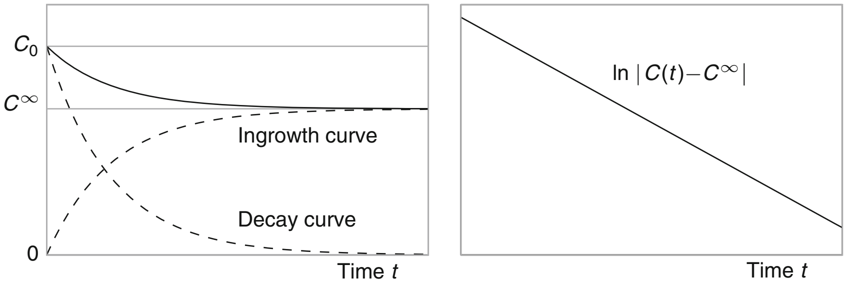


Fig. 4.3: *A linear system's change from its initial state* C^0 *to the steady state* C^∞ *can be interpreted as the sum of two processes, the "decay" of the initial state* C^0 *(*$C^0 \mathrm{e}^{-kt}$*) and the "ingrowth" of the end state* C^∞ *(*$C^\infty(1-\mathrm{e}^{-kt})$*). The continuous curve, the sum of the two dashed curves, shows the course of the system* $C(t)$*. Plotting on a logarithmic scale (on the right) gives a straight line with slope* $-k$

Similar to Eq. (4.10) we can rewrite Eq. (4.33) in the following form:

$$\ln\left(\frac{C(t) - C^\infty}{C^0 - C^\infty}\right) = \ln(C(t) - C^\infty) - \ln(C^0 - C^\infty) = -kt \tag{4.35}$$

Like in Fig. 4.1, if $\ln(C(t) - C^\infty)$ is plotted against t we get a straight line with slope $-k$ (Fig. 4.3).[5]

With that, we have used a dynamic model to calculate the development of the concentration in the lake outside of the steady state. Furthermore, we have shown that independent of the initial value C_0, the system always moves towards the steady state if the rate k is positive.[6]

We now want to turn our attention to the second question: how long does it take for the lake to reach its equilibrium concentration C^∞? In fact, we already know the answer to this question: because the system adjusts exponentially to a new steady state, the equilibrium concentration C^∞ is only reached for $t \to \infty$. It therefore makes more sense to calculate the time after which the concentration falls below a specifically chosen deviation δC from the equilibrium. We will call this the adjustment time.

The adjustment time is the time after which a model has approached its steady state up to a given distance.

A reasonable choice for δC is to define the residual deviation as a fixed fraction κ of the initial difference between steady state and initial state:

$$\delta C = \kappa\,|C^\infty - C^0| = \kappa\,\delta C^0, \qquad \kappa > 0 \tag{4.36}$$

---

[5] The middle part of Eq. (4.35) only makes sense if $(C^0 - C^\infty)$ and thus also $(C^0 - C(t))$ are positive. How to modify Fig. 4.3 for the case where $C^0 < C^\infty$ is left as an exercise to the reader.

[6] As a reminder: In the original formulation of the linear differential equation (4.5) we introduced the first-order term with a positive sign (specific rate $k^\star$). Thus, a finite steady state exists when $k^\star < 0$.

By choosing the absolute value $|C^\infty - C^0|$, δC is always defined as a positive number, independent of whether the initial state is above or below the steady state.

It depends on the user's requirements or preferences what value is chosen for the adjustment criterion κ. If, for example, the concentration C has a measurement error of $\pm 10\,\%$ anyway, it would make little sense to choose κ smaller than 0.1. There are cases where the value of the system variable is known with high precision, however, and adjustment is then understood as a very small deviation from the steady state. In such a case we would choose a small κ.

We define the adjustment time corresponding to κ as τ_κ. The concentration at that time can be written with Eq. (4.34) as:

$$\begin{aligned} C(\tau_\kappa) &= C^0\,\mathrm{e}^{-k\tau_\kappa} + C^\infty(1 - \mathrm{e}^{-k\tau_\kappa}) \\ &= C^\infty + \mathrm{e}^{-k\tau_\kappa}(C^0 - C^\infty) \end{aligned} \tag{4.37}$$

Conversely, the absolute value of the deviation between C^∞ and $C(\tau_\kappa)$ shall have the same value as $\kappa\delta C^0$:

$$|C^\infty - C(\tau_\kappa)| = \kappa\,\delta C^0 = \kappa\,|C^\infty - C^0| \tag{4.38}$$

The combination of these two equations yields:

$$|C^\infty - C^0|\,\mathrm{e}^{-k\tau_\kappa} = \kappa\,|C^\infty - C^0| \tag{4.39}$$

And simplified further:

$$\kappa = \mathrm{e}^{-k\tau_\kappa} \tag{4.40}$$

Taking the natural logarithm on both sides gives the following result for the adjustment time τ_κ:

$$\tau_\kappa = -\frac{\ln\kappa}{k} \tag{4.41}$$

Note: Because κ is a number between 0 and 1, $\ln\kappa$ is negative. Because of the minus sign in Eq. (4.41) the adjustment time τ_κ is therefore positive. If $k < 0$, the steady state would be at infinity and the definition of an adjustment time would not make sense.

In many cases choosing $\kappa = 0.05$ (adjustment to $5\,\%$) appears to be sensible. According to Eq. (4.41) the following holds for the corresponding adjustment time:

$$\tau_{5\,\%} = -\frac{\ln 0.05}{k} = \frac{2.9957}{k} \approx \frac{3}{k} \tag{4.42}$$

Note: Whichever way κ is chosen, the corresponding adjustment time will always be proportional to k^{-1}. Only the factor in the numerator of Eq. (4.41) changes.

Figure 4.4 shows how a linear system approaches the steady state. Due to Eq. (4.39), the initial difference δC^0 disappears exponentially, that is, as e^{-kt}. After time $t = \frac{1}{k}$, δC has sunk to $\delta C_0\,\mathrm{e}^{-1} = 0.37\,\delta C_0$, after time $t = \frac{2}{k}$ to $\delta C_0\,\mathrm{e}^{-2} = 0.14\,\delta C_0$, etc. From Eq. (4.42) we already know that for $t = \frac{3}{k}$ the residual deviation is 0.05 or $5\,\%$.

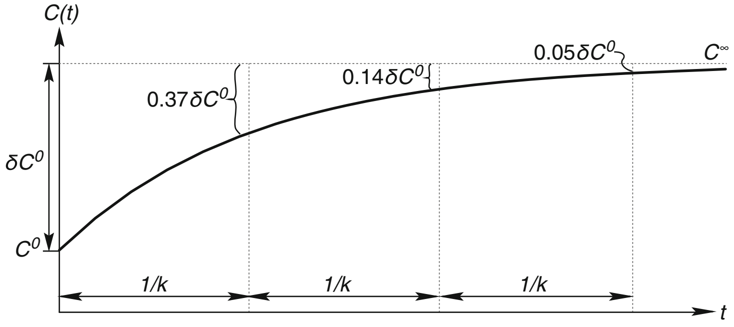


Fig. 4.4: *Adjustment time for a linear system, drawn for the case $C^0 < C^\infty$. After elapsed time $t > \tau_{5\,\%} = \frac{3}{k}$, the deviation from the steady state is less than 5 %*

Let's now look at some examples:

Example 4.6: Adjustment time

For a considerable time, substances have been discharged into a lake with constant inflow and outflow. The lake's water renewal time is $\tau_w = 10$ year. One substance is decomposed in the lake by a first-order reaction with the reaction rate $k_r = 0.9\,\text{year}^{-1}$. The second substance is conservative.[a] The inflow of both substances is suddenly stopped. How long does it take for the respective concentrations in the lake to drop to 5 % of their initial value?

For the conservative substance, the 5 % adjustment time is calculated from just the specific flow rate $k_w = \frac{1}{\tau_w} = 0.1\,\text{year}^{-1}$:

$$\tau_{5\,\%} \approx \frac{3}{k_w} = \frac{3}{0.1}\text{ year} = 30\text{ year}$$

For the reactive substance, the adjustment time is shorter, because in addition to the washing-out process it is also decomposed in the lake:

$$\tau_{5\,\%} \approx \frac{3}{k_w + k_r} = \frac{3}{(0.1 + 0.9)}\text{ year} = 3\text{ year}$$

---

[a] A conservative substance does not react with its environment, i.e. it does not decompose and does not deposit. However, it is removed from the lake via its outflow.

Example 4.7: Half-life

A well-known example of an adjustment time is the half-life $\tau_{1/2}$ of a radioactive isotope. The half-life is defined as the time in which the activity of a radioactive source $A(t)$ decreases by half compared to the initial activity A^0:

$$A(\tau_{1/2}) = 0.5A^0 \qquad (4.43)$$

For the activity of a radioactive isotope with the decay constant k_λ the following holds:

$$A(t) = A^0 \mathrm{e}^{-k_\lambda t} \tag{4.44}$$

With that we can calculate the half-life $\tau_{1/2}$:

$$\begin{aligned} \frac{A(\tau_{1/2})}{A^0} &= 0.5 = \mathrm{e}^{-k_\lambda \tau_{1/2}} \\ \ln 0.5 &= -k_\lambda \tau_{1/2} \\ \tau_{1/2} &= -\frac{\ln 0.5}{k_\lambda} = \frac{\ln 2}{k_\lambda} = \frac{0.693}{k_\lambda} \end{aligned} \tag{4.45}$$

The half-life corresponds to the adjustment criterion $\kappa = 0.5$.

Until now, we calculated the adjustment time from a *relative* criterion (relative adjustment criterion κ): it only depends on the rate k, not on the initial state of the system (see Eq. (4.41)). It can happen, however, that we are interested in an absolute criterion, for instance, the condition that the concentration should approach the steady state up to a deviation of no more than $0.02\,\mathrm{mg\,L^{-1}}$. As the following example shows, the corresponding adjustment time then also depends on the initial concentration.

Example 4.8: Adjustment time to a concentration limit

A toxic substance created as a byproduct in a chemical plant is drained with the effluent into a river. According to environmental regulations, this substance's concentration in the effluent must not exceed $0.1\,\mathrm{\mu g\,L^{-1}}$. However, the values in the effluent fluctuate between 1 and $10\,\mathrm{\mu g\,L^{-1}}$. Therefore it has to be treated in a reactor before being discharged.

The reactor is not operated in through-flow mode. Instead, once filled by the effluent it stays closed until the allowed concentration is reached. The elimination rate for the substance in the reactor is $k_r = 0.1\,\mathrm{h^{-1}}$. How long must the substance stay in the reactor before we are certain that it doesn't exceed the legal concentration limit?

To calculate the adjustment to a concentration limit, we have to take into account the initial concentration $C^0 = 1\,\mathrm{\mu g\,L^{-1}}$ and $C^0 = 10\,\mathrm{\mu g\,L^{-1}}$. The initial concentration must be reduced to 10 % in the first case and to 1 % in the second. This implies that the adjustment criterion κ (see Eq. 4.36) is 0.1 for the first case and 0.01 for the second. From Eq. (4.41) we calculate the corresponding adjustment times:

$$\begin{aligned} \tau_{10\,\%} &= \frac{-\ln 0.1}{k_r} \approx \frac{2.3}{0.1}\,\mathrm{h} = 23\,\mathrm{h} \\ \tau_{1\,\%} &= \frac{-\ln 0.01}{k_r} \approx \frac{4.6}{0.1}\,\mathrm{h} = 46\,\mathrm{h} \end{aligned}$$

In order to meet the discharge concentration limit even for the worst case ($C^0 = 10\,\mu\text{g}\,\text{L}^{-1}$), the effluent must be pretreated in the reactor for at least 46 h, i.e. about 2 days. Note that even in the best case, i.e. with an effluent concentration ten times smaller, we would still need a retention time of about 1 day or just about half the time needed for the worst-case effluent concentration.

4.3 Time-Dependent Coefficients

Until now we assumed that the coefficients $J^\star$ and $k^\star$ in the differential equation (4.5) are constant over time. We have called such a model autonomous. Natural systems, however, are changing all the time. For instance, over the course of a year or even a day the temperature of a lake can change markedly. This in turn may influence the reaction rate k_r of a substance or the growth rate k_g of organisms in the lake. The material input into a natural system is rarely constant. For instance, the concentrations in the effluent of a sewage treatment plant typically vary with a daily rhythm.

Non-autonomous models are explicitly time-dependent.

Thus, natural systems must usually be seen as non-autonomous, which means that the coefficients are time-dependent. Here we will limit our discussion to the case where only the inhomogeneous term J or $J^\star$, but not the rate k or $k^\star$, is time-dependent[7]:

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = J(t) - k \cdot \mathcal{V} \tag{4.46}$$

We continue to treat the specific rate k as constant. The case of a variable k is discussed in Appendix C.1.

For the linear flow reactor with variable input we can write the following dynamic equation:

$$\frac{\mathrm{d}C}{\mathrm{d}t} = j_{in}(t) - kC, \qquad \text{with} \qquad j_{in}(t) = \frac{J_{in}(t)}{V} \tag{4.47}$$

Here, $j_{in}(t)$ is the time-dependent substance input per volume of the system.

As before, we can calculate the steady state by setting the left side of Eq. (4.47) equal to zero. We then get:

$$C^\infty(t) = \frac{j_{in}(t)}{k} \tag{4.48}$$

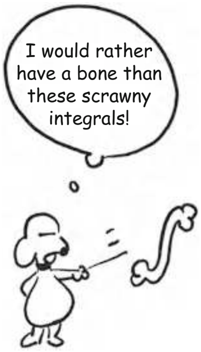
Because $j_{in}(t)$ depends on time, so does the steady state. $C^\infty(t)$ is that concentration which the system would ultimately reach if the input at time t (i.e. $j_{in}(t)$) were to remain fixed at its current value for infinite time.

---

[7] For the following discussion, we use Eq. (4.14) with the minus sign in front of the first-order reaction, since this equation has a finite steady state for $J > 0$. In principle one could also use Eq. (4.5) as the starting point.

The solution of Eq. (4.47) can be constructed with the aid of Eq. (C.8) from Appendix C.1:

$$C(t) = C^0 \mathrm{e}^{-kt} + \int\limits_{t'=0}^{t'=t} \mathrm{e}^{-k(t-t')} j_{in}(t') \mathrm{d}t' \tag{4.49}$$



At first glance, this equation seems very complex. Yet, the first term on the right-hand side should look familiar. In the solution of the case with constant coefficients (Eq. 4.34) it describes the linear decay of the initial state C^0, that is, the decay curve (Fig. 4.3). In essence it describes the behavior of all processes that occurred *before* time $t' = 0$. In contrast, the integral forming the second term of Eq. (4.49) constitutes the "bookkeeping" for the input from time $t' = 0$ up to the present time $t' = t$. This also explains the role of the auxiliary variable t'. Because we characterize the present with the time t and look back from there, we need a second variable t' to keep track of which section of the past we are dealing with at the moment.

In the integral, the input function $j_{in}(t)$ is summed up for the time interval 0 to t. However, because the elimination process $(-kC)$ is active in the system as well, only a fraction of the introduced substance remains at time t. The proportion still remaining in the system is larger the more recent the substance input took place. The factor $\mathrm{e}^{-k(t-t')}$ describes exactly this effect: for the current input $t' = t$, the exponential function is 1. For the input farthest in the past, i.e. for $t' = 0$, the weighting is e^{-kt}. The influence of any input dating back even further is already contained in the initial value C^0.

Formally, we can therefore make the structure of the discussed integral plausible by imagining that the continuous input is divided into many small parts. Because the system is linear, the influence of all these small input events can be summed up to get the overall temporal development of the system. In mathematics this is called the linear superposition principle. Figure 4.5 depicts this principle for two input events. The first input takes place at time t_1 with the magnitude j_1 and duration Δt. Due to the input event, the amount $j_1 \Delta t$ of substance per volume is added to the system. For this first event, we can consider the system as a homogeneous system with the initial condition $C^0 = j_1 \Delta t$. The development of the concentration for $C_1(t)$ is then[8]:

$$C_1(t) = j_1 \Delta t \, \mathrm{e}^{-k(t-t_1)} \tag{4.50}$$

The second input event yields accordingly:

$$C_2(t) = j_2 \Delta t \, \mathrm{e}^{-k(t-t_2)} \tag{4.51}$$

The expression $(t - t_2)$ in the exponential function indicates that the second input took place at time t_2.

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[8] In the following expression, t_1 is the starting time of the integration and $(t - t_1)$ is the elapsed time since t_1.

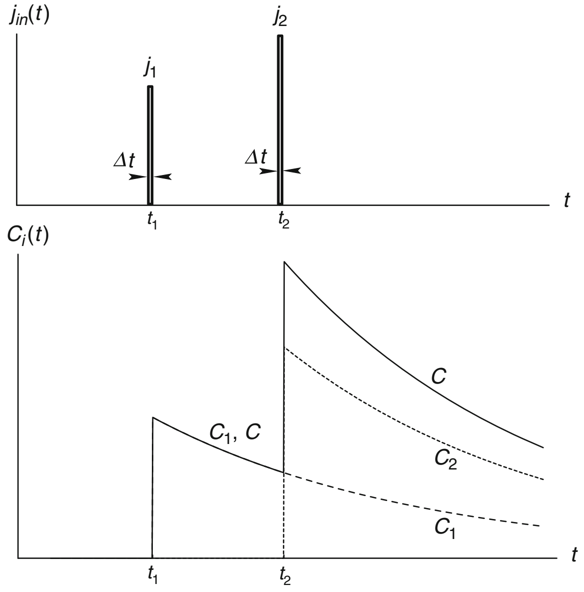

Fig. 4.5: *In a linear system the concentrations of two input events (curves C_1 and C_2) sum up to form the total concentration (curve C)*

The superposition of both solutions results in:

$$C(t) = C_1(t) + C_2(t) = j_1 \Delta t\, \mathrm{e}^{-k(t-t_1)} + j_2 \Delta t\, \mathrm{e}^{-k(t-t_2)} \tag{4.52}$$

If the continuous input is partitioned in ever more and smaller input events, the following sum results:

$$C(t) = \sum_{i=0}^{n} j_i \Delta t\, \mathrm{e}^{-k(t-t_i)} \tag{4.53}$$

Finally, by transforming the sum into an integral ($\Delta t \to 0, n \to \infty$), Eq. (4.53) becomes:

$$C(t) = \int_0^t j_{in}(t')\mathrm{e}^{-k(t-t')}\mathrm{d}t' \tag{4.54}$$

Note that the input function $j_{in}(t')$ can take an arbitrary form. In certain cases, the resulting integral can be solved analytically, whereas in others only a numerical integration is possible.

4.3.1 Exponentially Growing Input

Natural systems are often exposed to an external force which grows at an increasing speed. Such an input can be described by an exponential function (at least for a limited interval of time). We will explore this case with the example of a lake facing increasing eutrophication.

Example 4.9: Increasing eutrophication of a lake

In a lake, the phosphorus load grows about 10 % per year. In the reference year ($t = 0$), the phosphorus input is $j_{in}(0) = 6\,\mathrm{mg\,m^{-3}\,year^{-1}}$ and the average phosphorus concentration in the lake is $C^0 = 50\,\mathrm{mg\,m^{-3}}$. We now want to calculate how large the phosphorus concentration in the lake will be 4 and 8 years later. The total elimination rate of phosphorus in the lake is $k = 0.12\,\mathrm{year^{-1}}$.

We describe the increasing phosphorus input with an exponential function:

$$j_{in}(t) = j_{in}(0)\mathrm{e}^{\beta t} \tag{4.55}$$

β is the rate at which the input grows each year, so for our example[9] $\beta = 0.1\,\mathrm{year^{-1}}$. The average phosphorus concentration in the lake, $C(t)$, can be calculated by inserting Eq. (4.55) into Eq. (4.49):

$$C(t) = C(0)\,\mathrm{e}^{-kt} + \int\limits_0^t \mathrm{e}^{-k(t-t')} j_{in}(0)\,\mathrm{e}^{\beta t'}\,\mathrm{d}t' \tag{4.56}$$

After performing the integrations, we get for $\beta \neq -k$:

$$C(t) = C(0)\mathrm{e}^{-kt} - \frac{j_{in}(0)}{k+\beta}\mathrm{e}^{-kt} + \frac{j_{in}(0)}{k+\beta}\mathrm{e}^{\beta t},\ \beta \neq -k \tag{4.57}$$

With this equation we can calculate the phosphorus concentration in the lake. For $t = 4$ year we get:

$$\begin{aligned} C(t=4) &= 50\ \mathrm{mg\,m^{-3}}\ \mathrm{e}^{-4\times 0.12} - \frac{6\ \mathrm{mg\ m^{-3}\ year^{-1}}}{(0.12+0.10)\ \mathrm{year^{-1}}}\ \mathrm{e}^{-4\times 0.12} \\ &+ \frac{6\ \mathrm{mg\ m^{-3}\ year^{-1}}}{(0.12+0.10)\ \mathrm{year^{-1}}}\ \mathrm{e}^{4\times 0.1} \\ &= (30.9 - 16.9 + 40.7)\ \mathrm{mg\ m^{-3}} \\ &= 54.7\ \mathrm{mg\ m^{-3}} \end{aligned}$$

Correspondingly, for $t = 8$:

$$C(t=8) = (19.1 - 10.4 + 60.7)\ \mathrm{mg\ m^{-3}} = 69.4\ \mathrm{mg\ m^{-3}}$$

Note the increasing speed at which $C(t)$ is growing. In the first 4 years the concentration increases by just under 5 %, while the next 4 years bring an increase of 27 %!

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[9] To be precise, β would have to be slightly smaller than $0.1\,\mathrm{year^{-1}}$, since $\mathrm{e}^{0.1} = 1.105$, which is slightly larger than 1.1. The “precise” β is calculated through the relation $\beta = \ln 1.1 = 0.0953\,\mathrm{year^{-1}}$.

Let us now take a closer look at Eq. (4.57). We observe that $C(t)$ depends on two specific rates. First, the development of the concentration is driven by the already discussed total elimination rate k, which determines how quickly a substance introduced to the system is removed from it. It is therefore a measure for the memory of the system. Second, it is driven by β, which characterizes the speed with which the external relation changes (in our example, the phosphorus input). Furthermore, we see that because of the factor e^{-kt}, the first two terms on the right-hand side of Eq. (4.57) become smaller for increasing time and for very large times can be neglected entirely (more precisely, they can be neglected for $t \gg k^{-1}$). In contrast, the last term grows exponentially (because $\beta > 0$). For very large times we can therefore approximate Eq. (4.57) by:

$$C(t) \approx \frac{j_{in}(0)}{k+\beta}\mathrm{e}^{\beta t} = \frac{j_{in}(t)}{k+\beta}\;, \quad \text{if } t \gg k^{-1} \tag{4.58}$$

$j_{in}(t)$ is the current input (see Eq. 4.55). This result reminds us of the steady state (Eq. 4.48), except that it contains the additional factor β in the denominator. The relative size of k and β therefore determines the extent to which $C(t)$ from Eq. (4.58) and $C^{\infty}(t)$ from Eq. (4.48) differ from each other. Let us now look at the two extreme cases:

Case A: Slowly Changing External Input, i.e. $\beta \ll k$

In the denominator of Eq. (4.58), β can be neglected compared to k. Our approximation is therefore:

$$C(t) \approx \frac{j_{in}(0)}{k}\mathrm{e}^{\beta t} = \frac{j_{in}(t)}{k} = C^{\infty}(t), \quad \text{for } \beta \ll k \quad \text{and} \quad t \gg k^{-1} \tag{4.59}$$

In other words, if the rate of change of the input β is much smaller than the total reaction rate of the system k, the system is almost in the state that is in equilibrium with the current input. In physics, an external change that leaves the system approximately in its steady state is called an adiabatic perturbation.

An adiabatic perturbation is so slow that the system can constantly adjust to the changing steady state.

Case B: Rapidly Changing External Input, i.e. β *not* $\ll k$

In this situation, which we call the non-adiabiatic case, β cannot be neglected in the denominator and we therefore get for $t \gg k^{-1}$:

$$C(t) = \frac{j_{in}(t)}{k+\beta}\;, \quad \text{if } t \gg k^{-1} \tag{4.60}$$

For an exponentially growing perturbation, i.e. for $\beta > 0$, the current system state $C(t)$ is therefore smaller than the steady state belonging to the current input:

$$C(t) = \frac{j_{in}(t)}{k+\beta} < \frac{j_{in}(t)}{k} = C^{\infty}(t)\;, \quad \text{if } \beta > 0 \tag{4.61}$$

As long as the input keeps growing at the same rate, the system is unable to reach the steady state. Instead, it keeps lagging behind a hypothetical steady state.

After all this math, we want to go back to Example 4.9 and see what happens when the input growth is stopped:

Example 4.10: Eutrophication of the lake is stopped

In the lake of the previous example, phosphorus input is stabilized after 20 years of increasing eutrophication. The environmental agency in charge is optimistic but keeps monitoring the phosphorus concentration's further development. Surprisingly, it keeps rising for several years. How can this be explained?

We need to examine the data from the lake more closely: The phosphorus load in the lake grew approximately exponentially with a rate of $\beta = 0.1\,\text{year}^{-1}$ for 20 years. The total specific elimination rate of phosphorus in the lake is $k = 0.12\,\text{year}^{-1}$. Obviously, the external perturbation of the lake corresponds to a non-adiabatic situation.

Twenty years is long enough to apply the approximative solution Eq. (4.58):

$$C(t = 20\,\text{year}) \approx \frac{j_{in}(t = 20\,\text{year})}{k + \beta}$$

Because the two rates β and k have the same order of magnitude, after 20 years the lake is not in the steady state corresponding to its current input. The hypothetical steady-state concentration for the lake would be:

$$C^{\infty}(t = 20\,\text{year}) = \frac{j_{in}(t = 20\,\text{year})}{k}$$

The phosphorus concentration in the lake is smaller than the hypothetical steady state concentration by:

$$\begin{aligned}\frac{C(t = 20\,\text{year})}{C^{\infty}(t = 20\,\text{year})} &= \frac{j_{in}(t = 20\,\text{year})}{k + \beta} \cdot \frac{k}{j_{in}(t = 20\,\text{year})} = \frac{k}{k + \beta} \\ &= \frac{0.12}{0.22} = 54\,\%\end{aligned}$$

If the phosphorus input is stabilized after 20 years, the phosphorus concentration in the lake keeps rising nevertheless—until the steady state concentration $C^{\infty}(t = 20\text{a})$ corresponding to the input $j_{in}(t = 20\text{a})$ is reached. In our lake, the phosphorus concentration will still climb to 1.8 times its size. To find out how long this increase will still take, we can calculate the 5 % adjustment time:

$$\tau_{5\,\%} = \frac{3}{k} = \frac{3}{0.12}\,\text{year} = 25\,\text{year}$$

The phosphorus concentration in the lake will keep rising for another 25 years, even though the phosphorus input is stabilized. Figure 4.6 shows the development of the lake's average phosphorus concentration.

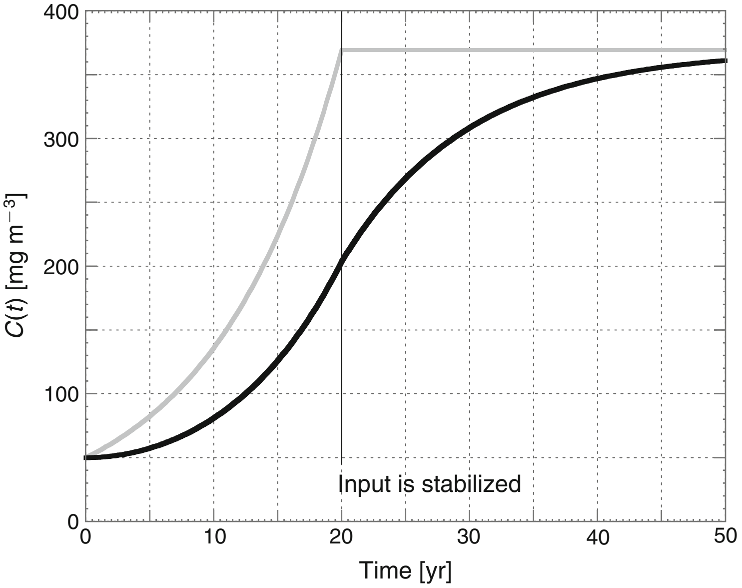


Fig. 4.6: *In a lake, the phosphorus input grows exponentially for 20 years. Then, the input is stabilized. The black curve is the calculated average phosphorus concentration in the lake, the grey curve is the steady state concentration corresponding to the current input. Despite the stabilized input, the average phosphorus concentration keeps rising for years*

4.3.2 Exponentially Falling Input

The input into a natural system can also decrease, for instance, it could fall exponentially. In that case, the rate β in Eq. (4.55) is negative. For a lake this could mean that the phosphorus input decreases exponentially thanks to environmental remediation efforts. The phosphorus concentration in the lake can then be described analogously to Eq. (4.57) by replacing β with $\beta' = -\beta > 0$:

$$C(t) = C(0)\,\mathrm{e}^{-kt} - \frac{j_{in}(0)}{k-\beta'}\,\mathrm{e}^{-kt} + \frac{j_{in}(0)}{k-\beta'}\,\mathrm{e}^{-\beta' t}\,, \qquad k \neq \beta' \tag{4.62}$$

For $k \neq \beta'$ the solution is composed of three terms. Because of the factors e^{-kt} and $\mathrm{e}^{-\beta' t}$ all of them become smaller and smaller with time until they become virtually zero. The relative size of β' and k determines which term survives longer when $t \to \infty$. Once again we look at the two extreme cases for large times t:

Case A: Slowly Falling External Input, i.e. $\beta' \ll k$

In the denominator of Eq. (4.62), β' can be neglected compared with k. The third term becomes speed-determining, i.e. it tends towards zero the slowest. We therefore get:

$$C(t) \approx \frac{j_{in}(0)}{k}\,\mathrm{e}^{-\beta' t} = \frac{j_{in}(t)}{k} = C^{\infty}(t), \qquad \text{for } \beta' \ll k \quad \text{and} \quad t \gg k^{-1} \tag{4.63}$$

Thus, it’s an adiabatic perturbation. The system remains approximatively in equilibrium with the exponentially falling input. Let us look at an example:

Example 4.11: Gradual lake remediation

For many years, a lake exhibits a constant average phosphorus concentration of $C^0 = 350\,\mathrm{mg\,m^{-3}}$. Since this concentration is too high, the phosphorus input, currently at $j_{in}(0) = 42\,\mathrm{mg\,m^{-3}\,year^{-1}}$, is to be reduced through targeted remediation actions. The total elimination rate of phosphorus in the lake is $k = 0.12\,\mathrm{year^{-1}}$. Because the remediation scheme can only gradually be put into place, the phosphorus input is only reduced by $2\,\%$ per year. How does the average phosphorus concentration $C(t)$ in the lake react after remediation begins?

We use Eq. (4.62) and insert $\beta' = 0.02\,\mathrm{year^{-1}}$. Because β' is much smaller than k, the third term of the equation is speed-determining. Figure 4.7 shows the calculated development of the average phosphorus concentration $C(t)$ and the influence of the three terms of Eq. (4.62). Terms 1 and 2 practically neutralize themselves and both tend rapidly towards zero, thus $C(t)$ is determined by the third term.

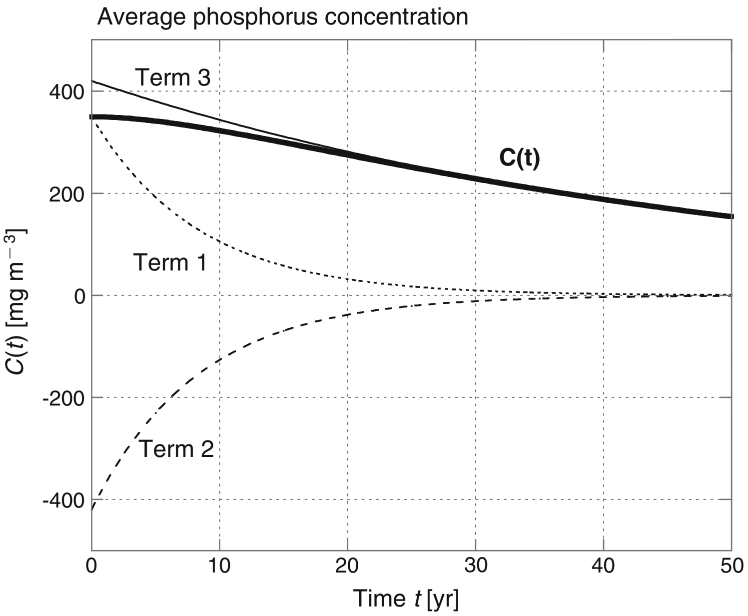


Fig. 4.7: *Development of average phosphorus concentration in a lake with slow reduction of phosphorus input. The system's behavior is determined by the third term of Eq.* (4.62)

Case B: Rapidly Falling External Input, i.e. $\beta' \gg k$

In this case, k can be neglected in the denominator of Eq. (4.62), so the first and second terms are speed-determining. For $t \gg \beta'^{-1}$ we get:

$$C(t) \approx C^0\,\mathrm{e}^{-kt} + \frac{j_{in}(0)}{\beta'}\,\mathrm{e}^{-kt} \tag{4.64}$$

As an example, we look at the same lake again. This time, however, the remediation measures are implemented rapidly:

Example 4.12: Rapid lake remediation

Due to drastic remediation measures the phosphorus input falls exponentially with the rate $\beta' = 1\,\text{year}^{-1}$. How does the phosphorus concentration in the lake change?

Figure 4.8 shows the development calculated from Eq. (4.62) and the influence of the individual terms. As expected, term 3 rapidly tends to zero and can be neglected. Term 2 declines more slowly, but because of the factor $j_{in}(0)/\beta'$ it is much smaller than term 1 and can also be neglected. Thus, the average phosphorus concentration in the lake is determined by term 1. In contrast to Example 4.11, the remediation's success is not determined by the speed of input reduction but by the speed of the lake's *response* to the decreasing contamination. One could argue that an input reduction rate β' much larger than the system's innate elimination rate k does not accelerate the recovery of the lake and is thus economically inefficient.

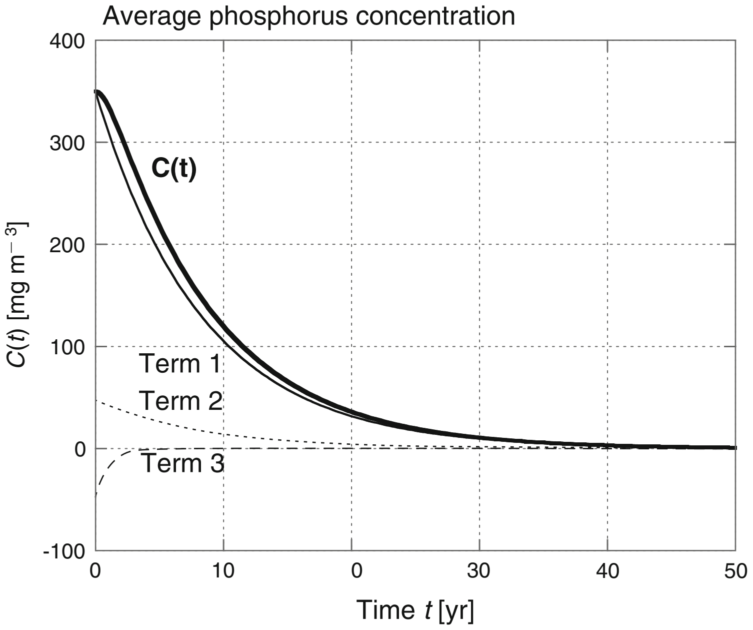


Fig. 4.8: *Development of the average phosphorus concentration in a lake with rapid phosphorus input reduction. The system's behavior is determined by the first term of Eq.* (4.62)

For the sake of completeness, we will briefly look at the special case where $k = \beta' \equiv -\beta$. In this case, the integration of Eq. (4.56) does not lead to Eq. (4.57), but is (with $\beta' = -k$):

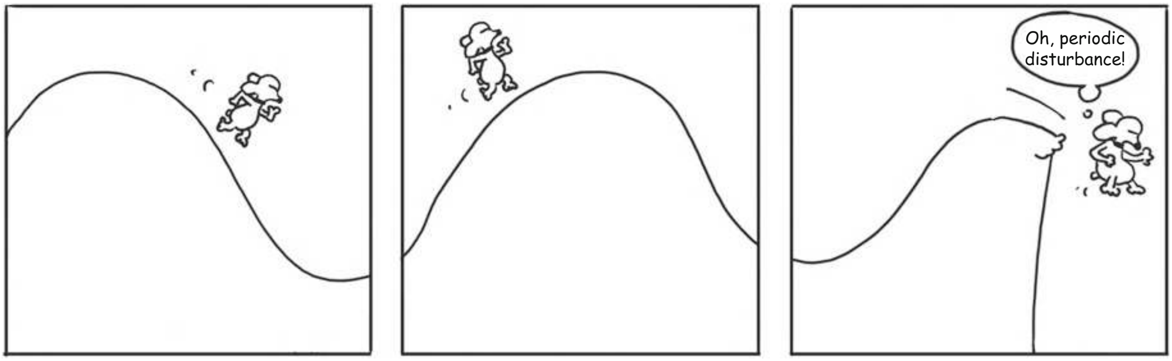
$$\begin{aligned} C(t) &= C(0)\,\mathrm{e}^{-kt} + \int_0^t \mathrm{e}^{-k(t-t')} j_{in}(0)\,\mathrm{e}^{-kt'}\mathrm{d}t' \\ &= C(0)\,\mathrm{e}^{-kt} + \int_0^t \mathrm{e}^{-kt} j_{in}(0)\mathrm{d}t' \end{aligned} \tag{4.65}$$

In fact, the integrand no longer depends on the integration variable t' and Eq. (4.65) becomes:

$$C(t) = C(0)\,\mathrm{e}^{-kt} + t\,\mathrm{e}^{-kt}\,j_{in}(0) \tag{4.66}$$

In this case, the characteristic rates of the system and the external relation are identical.

4.3.3 The Periodic Perturbation of a System



Many natural systems are subject to periodic influences, such as the night/day cycle, the seasons, or the tides. The prototypical periodic fluctuation is the sine function. By superimposing several sine functions with different periods, time shifts and amplitudes, we can construct arbitrary time-varying curves. Thus, if we analyze the behavior of a linear system under the influence of a prototype function as depicted in Fig. 4.9, we have a tool that can also be used to analyze other input functions. We use the function:

$$j_{in}(t) = j_0 + j_1 \sin\omega t \tag{4.67}$$

j_0	e.g. $[\,\mathrm{ML^{-3}T^{-1}}\,]$	Average Input
j_1	e.g. $[\,\mathrm{ML^{-3}T^{-1}}\,]$	Amplitude of the input fluctuation
ω	$[\,\mathrm{T^{-1}}\,]$	Angular frequency of the input fluctuation $\omega = \frac{2\pi}{T}$; T $[\,\mathrm{T}\,]$ Period of the input fluctuation

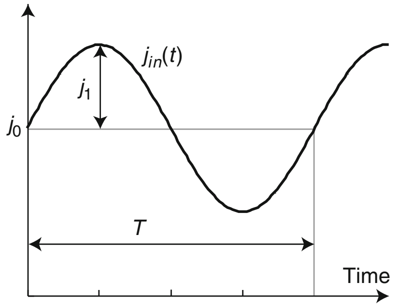


Fig. 4.9: *Periodically fluctuating perturbation with average input j_0, amplitude j_1 and period T*

Again, let's look at the linear flow reactor as an example. The average concentration in the reactor under the influence of a periodically fluctuating input is described by the following differential equation:

$$\frac{\mathrm{d}C}{\mathrm{d}t} = j_{in}(t) - kC = j_0 + j_1 \sin \omega t - kC \tag{4.68}$$

The solution is calculated with Eq. (4.49) by inserting Eq. (4.67) for $j_{in}(t)$ and splitting the integral into two parts:

$$C(t) = C^0 \mathrm{e}^{-kt} + j_0 \int_0^t \mathrm{e}^{-k(t-t')} \mathrm{d}t' + j_1 \int_0^t \sin \omega t' \mathrm{e}^{-k(t-t')} \mathrm{d}t' \tag{4.69}$$

The first integral yields:

$$\frac{j_0}{k}(1 - \mathrm{e}^{-kt}) \tag{4.70}$$

For the second integral we best consult a mathematical reference book where we will find the following solution:

$$\frac{j_1}{\sqrt{k^2+\omega^2}} \sin(\omega t - \eta) + \frac{j_1 \omega}{k^2+\omega^2} \mathrm{e}^{-kt} \qquad \text{with} \quad \eta = \arctan \frac{\omega}{k} \tag{4.71}$$

Thus, the overall concentration in the flow reactor with periodically fluctuating input has the following form:

$$C(t) = \underbrace{\frac{j_0}{k}}_{1} + \underbrace{(C_0 - \frac{j_0}{k})\mathrm{e}^{-kt}}_{2} + \underbrace{\frac{j_1}{\sqrt{\omega^2+k^2}} \sin(\omega t - \eta)}_{3} + \underbrace{\frac{j_1 \omega}{k^2+\omega^2} \mathrm{e}^{-kt}}_{4} \tag{4.72}$$

It consists of four components: Terms 1 and 2 represent the dynamic behavior of a linear system with constant input j_0 (see Eq. 4.15). For large times, i.e. for $kt \gg 1$, only term 1 remains. Terms 3 and 4 describe the influence of the fluctuating component of the input ($j_1 \sin \omega t$) in an analogous way. For $kt \gg 1$, the last term disappears. This means that for $kt \gg 1$, Eq. (4.72) is reduced to the following expression:

$$C(t) \approx \frac{j_0}{k} + \frac{j_1}{\sqrt{k^2+\omega^2}} \sin(\omega t - \eta), \qquad \text{for} \quad kt \gg 1 \tag{4.73}$$

Let's compare this expression with the variable steady state $C^{\infty}(t)$ corresponding to the momentary input $j(t)$:

$$C^{\infty}(t) = \frac{j(t)}{k} = \frac{j_0}{k} + \frac{j_1}{k}\sin\omega t \tag{4.74}$$

By comparing these two equations we notice the following:

1. Compared to the amplitude of Eq. (4.74), the amplitude of the periodic part of Eq. (4.73) is smaller by a factor of $k/\sqrt{k^2+\omega^2}$.
2. The variation of Eq. (4.73) lags behind Eq. (4.74) by the phase η.

Let's now look at the following example:

Example 4.13: Periodically fluctuating substance input with an annual rhythm

In a small mountain lake the nutrient input fluctuates annually due to the early summer snow melt. The angular frequency ω for the periodic substance input therefore amounts to:

$$\omega = \frac{2\pi}{T} = \frac{2\pi}{365\ \mathrm{d}} = 0.0172\ \mathrm{d}^{-1}$$

We use the following equation to describe the variation of substance input into the lake:

$$j_{in}(t) = 6\times 10^{-3}\mu\mathrm{mol\ m}^{-3}\,\mathrm{d}^{-1}(1+\sin\omega t)$$

Thus, $j_0 = j_1 = 0.006\ \mu\mathrm{mol\,m}^{-3}\,\mathrm{d}^{-1}$. The total specific elimination rate of the substance in the lake shall be

$$k = 0.01\ \mathrm{d}^{-1}$$

Figure 4.10 shows the substance input j_{in} (upper diagram) and the average substance concentration $C(t)$ (lower diagram, black curve). The grey curve describes the adiabatic approximation, that is, the concentration that would be in equilibrium with the current input. Because k and ω are of similar magnitudes, the adiabatic approximation does not accurately represent the real concentration in the lake. In fact, the amplitude is smaller by a factor of 0.5 and delayed by $\eta = \arctan(\frac{0.0172}{0.01}) = 1.04$. To convert the delay into a time, we have to compare η with the full period of the sine function ($2\pi = 6.28$) and multiply it with the period of variation $T = 365\,\mathrm{d}$:

$$\Delta T = \frac{\eta}{2\pi}T = \frac{1.04}{6.28}365\ \mathrm{d} = 60\ \mathrm{d}$$

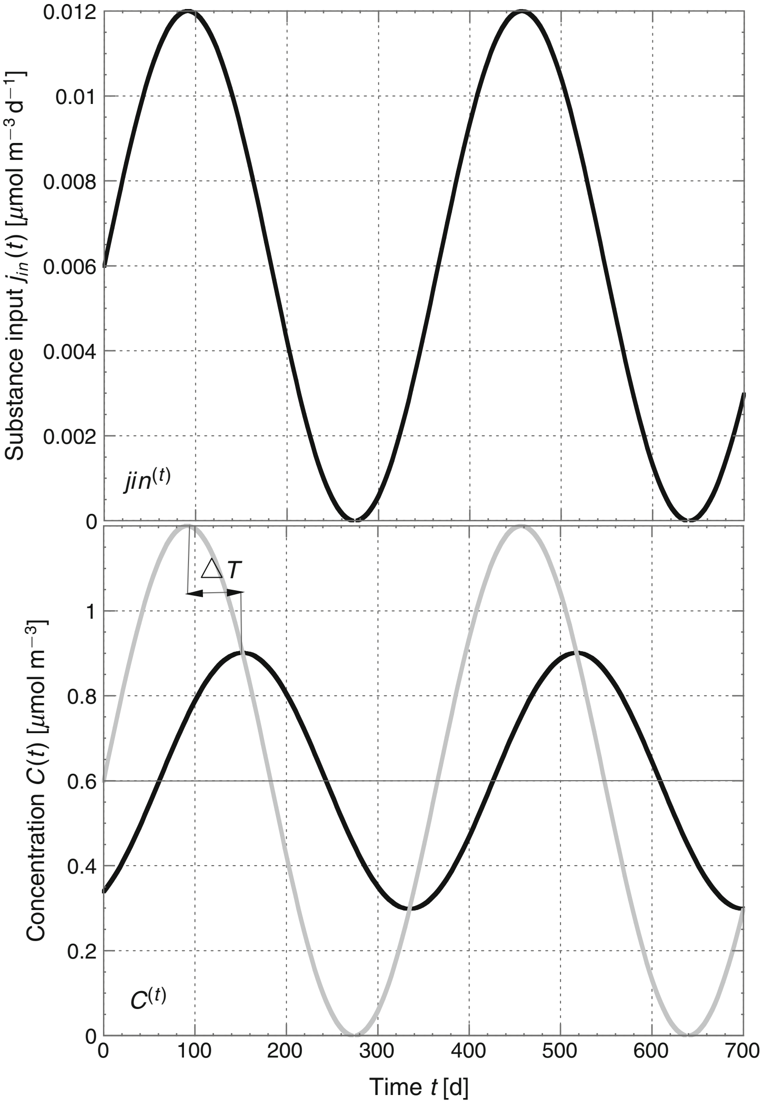


Fig. 4.10: *Development of the average concentration $C(t)$ of a substance in a lake whose substance input j_{in} periodically fluctuates with a period of 1 year (black curve in upper panel). The total elimination rate is $k = 0.01\,\mathrm{d}^{-1}$, the angular frequency of the annual period is $\omega = 0.0172\,\mathrm{d}^{-1}$. Lower panel, black curve: exact solution; grey curve: adiabatic approximation. $\triangle T$ is the delay of $C(t)$ compared to the input variation*

Example 4.13 represents a situation where the two characteristic rate constants, ω and k, are of similar magnitude. Remember that ω describes the pace of the external (periodic) changes while k describes the speed of the system's response to these changes. Once again, we now want to look at the two extreme situations, i.e. when the external perturbation is either much slower or much faster than the system's response.

Case A: Slowly Fluctuating Perturbation $\omega \ll k$

The variation of the perturbation proceeds slowly relative to the average retention time k^{-1} of a substance in the system. The denominator of the second term in Eq. (4.73) can be approximated by $(k^2+\omega^2)^{1/2} \approx (k^2)^{1/2} = k$. The phase difference $\eta = \arctan\frac{\omega}{k}$ becomes very small and can therefore be neglected in the sine function. Thus, from Eqs. (4.73) and (4.74) we get:

$$C(t) \approx \frac{j_0}{k} + \frac{j_1 \sin(\omega t)}{k} = C^{\infty}(t), \qquad \text{for} \quad kt \gg 1 \quad \text{and} \quad \omega \ll k \tag{4.75}$$

In this case, the average concentration in the reactor follows the steady state that corresponds to the current input $j(t) = j_0 + j_1 \sin\omega t$. The slow variation of the external relation thus represents an adiabatic perturbation.

Case B: Rapidly Fluctuating Perturbance $\omega \gg k$

In this case, the variation of the external relation is swift compared to the reaction time of the system. Because $\omega \gg k$, $(k^2+\omega^2)^{1/2}$ in Eq. (4.73) can be approximated by ω. The phase difference $\eta = \arctan\frac{\omega}{k}$ tends to $\frac{\pi}{2}$ for $\frac{\omega}{k} \to \infty$. Thus, we get the following approximate solution for $kt \gg 1$:

$$C(t) \approx \frac{j_0}{k} + \frac{j_1}{\omega}\sin(\omega t - \frac{\pi}{2}), \qquad \text{for} \quad kt \gg 1 \quad \text{and} \quad \omega \gg k \tag{4.76}$$

A linear system filters external fluctuations that are considerably faster than the system's reaction time.

The current system state $C(t)$ lags behind the current perturbation j_{in} by a quarter period $(\frac{\pi}{2})$. The amplitude of the system fluctuation $(\frac{j_1}{\omega})$ is reduced by the factor $\frac{k}{\omega} \ll 1$ relative to the amplitude of the steady state ($\frac{j_1}{k}$, see Eq. 4.74). The system thus remains close to the average steady state $\frac{j_0}{k}$. In effect, a linear system filters external fluctuations out of the system when they are substantially faster then the system's reaction time k^{-1}.

Let us demonstrate these extreme situations with the temperature regime in a small lake.

Example 4.14: Water temperature in a small lake

The average water temperature Θ in a small, vertically well-mixed lake can be approximated by the following linear differential equation:

$$\frac{\mathrm{d}\Theta}{\mathrm{d}t} = k_\Theta(\Theta_{eq} - \Theta) \tag{4.77}$$

The specific thermal exchange rate k_Θ (dimension T^{-1}) is inversely related to the lake's mean depth. It also depends on meteorological parameters such as solar radiation, wind speed and humidity. For medium latitudes and a lake mean depth of 5 m a typical value is $k_\Theta = 0.1\ \mathrm{d}^{-1}$. Θ_{eq} is the equilibrium water temperature, that is, the water temperature which the lake would reach if all meteorological parameters were to remain constant.[a] Θ_{eq} strongly varies with time of day, season and with (irregular) weather events. By looking at Θ_{eq} statistically, we can depict two dominant modes of variation, the annual and the diurnal, and approximate each by a sinusoidal function:

$$\Theta_{eq}(t) = \overline{\Theta}_{eq} + \Theta_{amp} \sin \frac{2\pi}{T} t \tag{4.78}$$

a) **Annual temperature variation**

$$T = 365\ \mathrm{d}, \text{ thus } \omega = \frac{2\pi}{365\ \mathrm{d}} = 0.017\ \mathrm{d}^{-1} \ll k_\Theta = 0.1\ \mathrm{d}^{-1}$$

This case exhibits slow variation with $\eta \backsim 0$. From Eq. (4.75) with $j_0 = k_\Theta \overline{\Theta}_{eq}$, $j_1 = k_\Theta \Theta_{amp}$ we get

$$\Theta(t) \backsim \overline{\Theta}_{eq} + \Theta_{amp} \sin \frac{2\pi}{T} t = \Theta_{eq}(t) \tag{4.79}$$

The exact solution is plotted in the upper panel of Fig. 4.11.

b) **Diurnal temperature variation**

$$T = 1\ \mathrm{d}, \text{ thus } \omega = \frac{2\pi}{1\ \mathrm{d}} = 6.28\ \mathrm{d}^{-1} \gg k_\Theta = 0.1\ \mathrm{d}^{-1}$$

This case shows rapid variation with $\eta \backsim \frac{\pi}{2}$, which corresponds to a delay time of $\Delta T = \frac{365}{4}\ \mathrm{d} = 91\ \mathrm{d}$.

From Eq. (4.76) with j_0 and j_1 as above we get:

$$\Theta(t) \backsim \overline{\Theta}_{eq} + (\frac{k_\Theta}{\omega})\Theta_{amp} \sin(\frac{2\pi}{T} t - \frac{\pi}{2}) \tag{4.80}$$

---

[a] Note that Θ_{eq} is not equal to air temperature since the direct exchange of sensible heat between water and air is just one (minor) process of heat exchange.

Since $\frac{k_\Theta}{\omega} = 0.1/6.28 = 0.016$, the second term of Eq. (4.80) is fairly small whatever the temperature fluctuation Θ_{amp} may be. Thus, water temperature is virtually unaffected by the diurnal variability of the relevant meteorological parameters (including the extreme day/night-variation of short-wave solar radiation). The exact solution is plotted in the lower panel of Fig. 4.11.

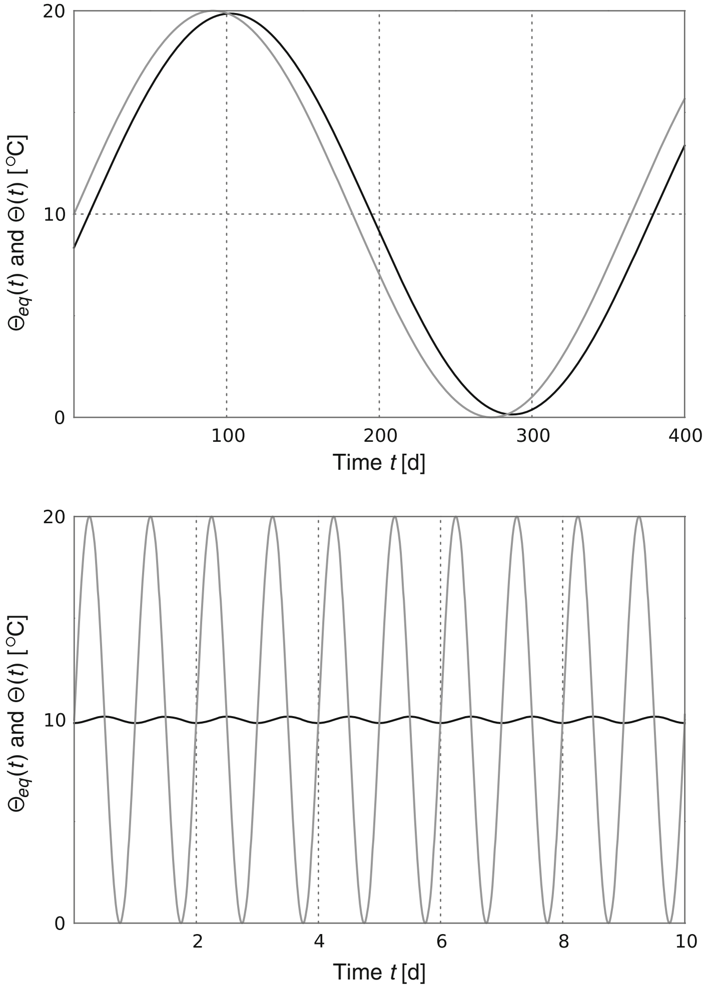


Fig. 4.11: *Average water temperature in a lake with annual variation (above) and diurnal variation (below).* $k_\Theta = 0.1 d^{-1}$, $\Theta_{eq} = 10\,^\circ C$, $\Theta_{amp} = 10\,^\circ C$. *The black plot is the actual temperature* $\Theta(t)$*; the grey plot is the theoretical equilibrium temperature* $\Theta_{eq}(t)$*. In the annual case, the actual temperature slightly lags behind the theoretical equilibrium temperature, while in the diurnal case the fluctuation is so rapid that the actual temperature cannot keep up and hardly deviates from the average*

4.4 Questions and Problems

Question 4.1: What characteristic properties do the solutions of linear differential equations have?

Question 4.2: What is the difference between homogeneous and inhomogeneous linear differential equations?

Question 4.3: Write down the most general form of a linear, first-order inhomogeneous differential equation.

Question 4.4: What requirement must a first-order differential equation fulfill to possess a finite steady state?

Question 4.5: Which dimensions do the variables in Eqs. (4.17) and (4.22) have?

Question 4.6: What is the adjustment time of a linear model? Why is this time not unambiguously defined, but needs the specification of a convention? Name such a convention.

Question 4.7: Try to derive Eq. (4.57) by integration of Eq. (4.56).

Question 4.8: You measure the increase of molecular oxygen concentration in a constantly mixed, open-top glass beaker. The water within has been completely de-gassed beforehand. How can you decide whether the data can be described with a linear model?

Question 4.9: What is meant physically by calling the perturbation of a linear model adiabatic? Give an example.

Question 4.10: The inhomogeneous term of a linear model fluctuates with a period of 1 h around an average value. The system variable remains practically constant. What does this indicate about the system?

Problem 4.1: Adjustment behavior
What does Fig. 4.3 (ingrowth curve, decay curve, $C(t)$) look like for a lake in which, starting from the steady state, the substance input is suddenly cut in half?

Problem 4.2: Radioactive decay
The decay of a radioactive isotope is a first-order reaction often quantified by half-life.

(a) Formulate a model for the radioactive isotope radon-222 (^{222}Rn), a noble gas with a half-life of 3.8 days. Radon-222 is produced by the decay of the radioactive element radium-226 (^{226}Ra, half-life 1,600 years) through an α decay. The initial concentrations of ^{222}Rn and ^{226}Ra are $N_{Ra} = 1 \times 10^8$ atoms/liter and $N_{Rn} = 5 \times 10^4$ atoms/liter, respectively. You can neglect the reduction of ^{226}Ra concentration during the observation period of several weeks. Why is that justifiable?

(b) Often, radioactive isotopes are not characterized by concentration, but by their activity A. A is the number of decays that are registered per time and volume. How do N and A depend on each other? Convert the model developed for N into one for A.

Problem 4.3: Cars in a parking lot

In a downtown car park, 300 cars enter per hour. Fifteen percent of them immediately leave the car park again, having found no free spot. The individual length of stay of parked cars varies. An observer notes that per minute, 1 % of the parked cars leave the car park.

(a) How many parking spots does the car park have?

(b) How long does a car stay in the car park on average (not counting the 15 % unsuccessful visitors)?

(c) We assume that the car park is opened at 6 a.m. and is completely empty at that time. The parking behavior remains exactly as described above: 300 cars enter per hour (of course, initially all of them will find a spot), 1 % of parked cars leave every minute. When is the car park full?

Problem 4.4: Phosphorus in a lake with sedimentation

A lake is loaded with 10 tons of phosphorus annually. On the one hand, phosphorus is continuously added to the sediment at a rate which is proportional to the concentration in the lake water. On the other hand, phosphorus is washed out of the lake through the outflow. Calculate the steady-state phosphorus concentration in the lake, if the annual phosphorus input is reduced to 6 tons a year. How long does it take for the concentration to be within 5 % of the new steady state?

The following is known about the lake:

Volume	$V = 0.2$ km^3
Through-flow of water	$Q = 0.1$ km^3 year^{-1}
Sedimentation	$S = k_s M$ [mg year^{-1}]
Sedimentation rate	$k_s = 0.75$ year^{-1}
Average total phosphorus concentration prior to the input reduction	$C^0 = 40$ mg P m^{-3}

Problem 4.5: Exponential population increase

In a city, new residents continuously arrive from the surrounding rural area. From 1995 to 2010, the total immigration can be approximated by an exponential function (growth rate $\beta = 6.25\,\%$ per year). The birth rate (b) in the city is 2.3 % and the death rate (d) is 0.5 % of the population per year. Effects that are driven by the population's age structure are not taken into account. A census showed that in 1995, 10.9 million people lived in the city, and 0.25 million migrated into it in the same year. How big is the city's population in the year 2020, if growth continues at the same rate?

Problem 4.6: Lake water temperature
In Example 4.14 we introduced a simple linear model to describe the water temperature Θ in a small, vertically well mixed lake. We neglected the possible influence from the inlets and outflow.

(a) Modify Eq. (4.77) to account for the effect of the through-flow of water (inlets, outlet). Assume that the temperature of the inflowing water Θ_{in} is at equilibrium with the momentary meteorological conditions ($\Theta_{in}(t) = \Theta_{eq}(t)$) while the temperature of the outflow is equal to the mean lake temperature ($\Theta_{out}(t) = \Theta(t)$). The water through-flow is expressed by the specific flow rate k_w (Eq. 4.22).

(b) Apply the modified model to Lake A with $k_\Theta = 0.03\ \text{d}^{-1}$, $k_w = 0.02\ \text{d}^{-1}$ (corresponding to a mean water residence time of 50 d). Calculate the lag phase η_A and the lag time ΔT_A of the annual water temperature variation relative to the external forcing $\Theta_{eq}(t)$. Note: If we approximate the year by 360 days and express η_A in angular degrees, then a 1° lag phase corresponds to a lag time of 1 day.

(c) Compare the result obtained in (b) with Lake B, which has the same thermal properties but no through-flow. Calculate η_B and ΔT_B.

(d) Assume that as in Eqs. (4.78) and (4.79), the annual temperature variation in the two lakes can be described by a sinusoidal curve. Calculate the ratio of the temperature amplitudes of the two lakes, $\Theta_{amp,A}/\Theta_{amp,B}$. Explain the result qualitatively.

Problem 4.7: Dye in a well
A joker dumps 1 gram of a fluerescent dye (Fluorescein) into a water fountain. The dye decays photochemically by a first-order reaction with the reaction rate $k_r = 0.1\,\text{h}^{-1}$. The fountain has a volume of $V = 2\,\text{m}^3$, and water continuously flows through it with a rate of $Q = 2\,\text{L/min}$.

(a) Draw a mass balance by using a box diagram and establish the dynamic equation for the dye concentration in the fountain.

(b) The dye remains visible in water down to a concentration of $C_{crit} = 10^{-5}\,\text{g/L}$. How long does it take for the water to appear uncolored again?

(c) Assume that the fountain is operated in a closed loop, i.e., the inflowing water is entirely made up of outflowing water. What is the corresponding dynamic equation? Again, calculate the time t_{crit} for this flow regime until the water appears uncolored.

Problem 4.8: Degradation process in a sewage plant

In the inlet of a sewage plant, the concentration C_{in} of a substance A is measured. If the inlet concentration C_{in} is held constant over a long enough time, one finds the concentration C_{out} in the plant's outlet. The table shows C_{out} for four different inlet concentrations of substance A:

C_{in} (mg/L)	20	50	80	130
C_{out} (mg/L)	1.0	2.5	4.0	6.5

Consider the sewage plant to be a completely mixed reactor with constant flow Q. The average water retention time in the sewage plant is $\tau_w = 2\,\text{d}$.

(a) Draw a box diagram for the mass balance and establish a dynamic equation for the concentration of substance A in the sewage plant.

(b) Give a mathematical relation for the degradation rate R [mg L^{-1} d^{-1}] of substance A as a function of the concentration in the plant C.

(c) Calculate the specific degradation rate k_r [d^{-1}] of substance A in the plant, under the assumption that the process is linear.

(d) Starting from the steady state $C_{in} = 80\,\text{mg/L}$ and $C_{out} = 4.0\,\text{mg/L}$, how long does it take for the concentration C in the plant to fall to 5 % of its initial value, if at time $t = 0$, C_{in} suddenly becomes zero?

(e) What is the answer to question (d) if you start from the steady state with $C_{in} = 20\,\text{mg/L}$ and $C_{aus} = 1.0\,\text{mg/L}$? Explain your answer.

Problem 4.9: Copper accumulation on farm land

By way of atmospheric deposition and the use of fertilizers, 42 mg of copper per square meter and year are added to agricultural land. Through washing-out processes and the crop harvest, the soil loses 0.6 % of its copper content per year.

(a) Establish the differential equation for the change in copper concentration C in the soil.

(b) How large is the copper concentration in the soil at steady state?

(c) How long does it take until the concentration comes to within 5 % of the steady state calculated in (b), if we assume an initial concentration of 0 mg copper per square meter?

(d) In fact, the average copper concentration measured in the soil is $C_{measured} = 6,000\,\mathrm{mg\,m^{-2}}$. How large would the total rate k_{tot} of a linear process that removes copper from the soil be, if $C_{measured}$ represents a steady state and the annual input is $42\,\mathrm{mg\,m^{-2}\,year^{-1}}$?

(e) Does it make sense to interpret the soil's copper content with a steady-state approach, if we know that the copper input grows by 1 % annually and the copper concentration can only be measured with an accuracy of 10 %? Justify your decision with a brief calculation.

Problem 4.10: Tritium in a lake

A lake with the constant volume $V = 3\,\mathrm{km^3}$ has constant in- and outflows with $Q = 300 \times 10^6\,\mathrm{m^3\,year^{-1}}$. For several decades, radioactive tritium (decay constant $k_\lambda = 0.058\,\mathrm{year^{-1}}$) has been added to the inflow with a constant concentration of $C_{in} = 1\,\mathrm{Bq/L}$. The average measured tritium concentration in the lake is $C = 0.44\,\mathrm{Bq/L}$.

(a) Write down the mass balance for tritium in the lake, assuming that the lake can be described as a completely mixed system with the three processes *inflow*, *outflow* and *radioactive decay*.

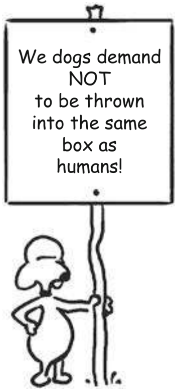
(b) Using the tritium concentration measured in the lake, judge whether there is another process removing tritium from the lake besides radioactive decay. If there is, calculate the reaction rate of this process as a first-order constant k_r.

(c) What happens if starting at time t_0 the tritium input grows annually by 2 %? How large is the tritium concentration in the lake at time $t_0 + 10$ years? (an approximation is sufficient)

(d) Answer question (c) for the case of an input growing by 20 % annually.

Chapter 5

Linear Models with Several Variables



So far we have only dealt with models described by a single system variable. We called these models one-dimensional. To adequately describe a system, however, we often need several variables that interact with each other. This is where multi-dimensional models come into play.

There are two ways to move from a one-dimensional to a multi-dimensional model. First, it could be useful to divide the system variable $\mathcal{V}$ into subcomponents. For instance, we want to split the total phosphorus concentration in a lake into dissolved and particle-bound phosphorus. Or we are interested in two substances A and B that can be converted into each other by a chemical transformation. In both cases we need to add *material differentiation* to our model.

Second, *spatial differentiation* could be necessary in some scenarios, for instance, dividing the overall average phosphorus concentration in a lake into surface and deep water concentration. In this case, we call our model a two-box model, because it contains two spatially separate "boxes". Of course, this expression could also be used for the materially differentiated model: the boxes would be material compartments rather than spatial ones. Mathematically speaking it makes no difference whether we differentiate spatially or materially. Both cases lead us to a system of two or more coupled differential equations.

5.1 Linear Models with Two System Variables

5.1.1 The System of Linear Differential Equations and Its Eigenvalues

In this section, we want to limit our discussion to *two-dimensional* first-order models with constant coefficients.[1] Such models can be described by

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[1] Recall that in Chap. 4, we called models with constant coefficients *autonomous models*.

D.M. Imboden and S. Pfenninger, *Introduction to Systems Analysis*,
DOI 10.1007/978-3-642-30639-6_5,

the following set of differential equations:

$$\begin{aligned} \frac{\mathrm{d}\mathcal{V}_1}{\mathrm{d}t} &= \mathcal{R}_1 + p_{1,1}\mathcal{V}_1 + p_{1,2}\mathcal{V}_2 \\ \frac{\mathrm{d}\mathcal{V}_2}{\mathrm{d}t} &= \mathcal{R}_2 + p_{2,1}\mathcal{V}_1 + p_{2,2}\mathcal{V}_2 \end{aligned} \tag{5.1}$$

The variables have the following meanings:

$\mathcal{V}_i$	i-th system variable
$\mathcal{R}_i$	inhomogeneous term (input) of the i-th system variable, constant
$p_{i,j}$	model parameter, constant

Eq. (5.1) can also be written as a matrix:

$$\begin{pmatrix} \mathrm{d}\mathcal{V}_1/\mathrm{d}t \\ \mathrm{d}\mathcal{V}_2/\mathrm{d}t \end{pmatrix} = \begin{pmatrix} \mathcal{R}_1 \\ \mathcal{R}_2 \end{pmatrix} + \begin{pmatrix} p_{1,1} & p_{1,2} \\ p_{2,1} & p_{2,2} \end{pmatrix} \begin{pmatrix} \mathcal{V}_1 \\ \mathcal{V}_2 \end{pmatrix} \tag{5.2}$$

or

$$\frac{\mathrm{d}\boldsymbol{\mathcal{V}}}{\mathrm{d}t} = \mathbf{R} + \mathbf{P} \cdot \boldsymbol{\mathcal{V}} \tag{5.3}$$

The system then consists of an input vector[2] $\mathbf{R}$, the coefficient matrix $\mathbf{P}$ and the vector of the system variable $\boldsymbol{\mathcal{V}}$.

Example 5.1: Chemical reaction in a reactor (see Fig. 5.1)

We consider a fully mixed reactor with volume V and constant flow rate Q. In the inflow, the substance A is continuously added with the concentration C_{in} ($J_A = QC_{in}$). Inside the reactor, a linear reaction between substances A and B takes place. For example, substance A could be hydrolyzed to substance B $\equiv$ AH$^+$ and back. The specific rates of the forward and return reaction are k_A and k_B. Both substances leave the reactor through the outflow. What are the dynamic equations for C_A and C_B in the reactor?

As in Example 4.4 we begin by establishing the mass balance. This time we need to do this for both substances, A and B, keeping in mind that M_A and M_B are the masses of the substances in the reactor[3]:

$$\begin{aligned} \frac{\mathrm{d}M_A}{\mathrm{d}t} &= QC_{in} - k_A M_A + k_B M_B - QC_A \\ \frac{\mathrm{d}M_B}{\mathrm{d}t} &= k_A M_A - k_B M_B - QC_B \end{aligned} \tag{5.4}$$

---

[2] Variables printed in **bold** indicate vectors or matrices.

[3] Strictly speaking, models that involve chemical conversion processes are atom balance models. The concentrations should therefore be expressed in molar units.

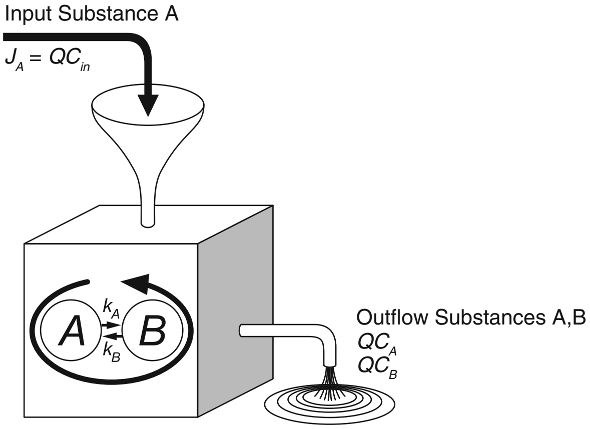


Fig. 5.1: *Linear reaction in a completely mixed reactor with through-flow*

If we divide both equations by the constant reactor volume V, we get analogously to Eq. (4.22):

$$\begin{aligned} \frac{\mathrm{d}C_A}{\mathrm{d}t} &= k_w C_{in} - k_A C_A + k_B C_B - k_w C_A \\ \frac{\mathrm{d}C_B}{\mathrm{d}t} &= k_A C_A - k_B C_B - k_w C_B \end{aligned} \tag{5.5}$$

where $k_w = Q/V$, $C_A = M_A/V$ and $C_B = M_B/V$.

We need to rewrite Eq. (5.5) so that we can compare them to Eq. (5.1) and identify the parameters introduced there:

$$\begin{aligned} \frac{\mathrm{d}C_A}{\mathrm{d}t} &= k_w C_{in} - (k_A + k_w) C_A + k_B C_B \\ \frac{\mathrm{d}C_B}{\mathrm{d}t} &= k_A C_A - (k_B + k_w) C_B \end{aligned} \tag{5.6}$$

Thus:

$$\begin{array}{ll} \mathcal{R}_1 \to k_w C_{in}, & \mathcal{R}_2 \to 0 \\ p_{1,1} \to -(k_A + k_w), & p_{1,2} \to k_B \\ p_{2,1} \to k_A, & p_{2,2} \to -(k_B + k_w) \end{array}$$

As we will see, the coefficient matrix **P** plays a central role in the solution of a system of linear differential equations (even more so in systems with more than 2 dimensions). Therefore, we want to introduce four characteristic quantities of the matrix **P** (see Appendix D):

1. The determinant of **P**:

$$\det(\mathbf{P}) = p_{1,1} p_{2,2} - p_{1,2} p_{2,1} \tag{5.7}$$

2. The trace of **P**:

$$\mathrm{tr}(\mathbf{P}) = p_{1,1} + p_{2,2} \tag{5.8}$$

3. The discriminant of $\mathbf{P}$:

$$\begin{aligned}\Delta(\mathbf{P}) &= \mathrm{tr}(\mathbf{P})^2 - 4\det(\mathbf{P}) \\ &= (p_{1,1}+p_{2,2})^2 - 4p_{1,1}p_{2,2} + 4p_{1,2}p_{2,1} \\ &= (p_{1,1}-p_{2,2})^2 + 4p_{1,2}p_{2,1}\end{aligned} \tag{5.9}$$

4. The two eigenvalues[4] of $\mathbf{P}$:

$$\lambda_i = \frac{1}{2}\left[\mathrm{tr}(\mathbf{P}) \pm \sqrt{\Delta(\mathbf{P})}\right], \qquad i = 1,2 \tag{5.10}$$

The eigenvalues are the solutions of the so-called *characteristic equation*

$$\begin{aligned}\lambda^2 - \lambda(p_{1,1}+p_{2,2}) + p_{1,1}p_{2,2} - p_{1,2}p_{2,1} &= \\ \lambda^2 - \lambda\mathrm{tr}(\mathbf{P}) + \det(\mathbf{P}) &= 0\end{aligned} \tag{5.11}$$

If the coefficient matrix $\mathbf{P}$ has two different eigenvalues λ_i $(i = 1,2)$, that is, if $\Delta(\mathbf{P}) \neq 0$, the two-dimensional system of differential equations (5.1) with constant coefficients $\mathcal{R}_i$ and $p_{i,j}$ has solutions of the form:

$$\begin{aligned}\mathcal{V}_1(t) &= a_{1,0} + a_{1,1}\mathrm{e}^{\lambda_1 t} + a_{1,2}\mathrm{e}^{\lambda_2 t} \\ \mathcal{V}_2(t) &= a_{2,0} + a_{2,1}\mathrm{e}^{\lambda_1 t} + a_{2,2}\mathrm{e}^{\lambda_2 t}\end{aligned} \tag{5.12}$$

The two eigenvalues $\lambda_i (i = 1,2)$ have the dimension of a specific rate, $[\,\mathrm{T}\,]^{-1}$. The six coefficients $a_{i,j} (i = 1,2;\ j = 0,1,2)$ depend on the coefficients $p_{i,j}$ and the initial states $\mathcal{V}_1^0$ and $\mathcal{V}_2^0$. In Appendix D, we discuss in more detail how to get from the differential equation (5.1) to the solution (5.12).

If both eigenvalues are real and negative, all exponential functions in Eq. (5.12) tend to zero for $t \to \infty$. Table 5.1 shows what properties the matrix $\mathbf{P}$ must have for this condition to be fulfilled. Since the exponential functions tend to zero for $t \to \infty$, the coefficients $a_{1,0}$ and $a_{2,0}$ are identical with the system's steady states $\mathcal{V}_1^\infty$ and $\mathcal{V}_2^\infty$. We find the steady states by setting the left sides of Eq. (5.1) to zero, and solving the resulting two coupled equations for the two unknowns $\mathcal{V}_1$ and $\mathcal{V}_2$. We can then call them $\mathcal{V}_1^\infty$ and $\mathcal{V}_2^\infty$:

$$\begin{aligned}a_{1,0} = \mathcal{V}_1^\infty &= \frac{p_{1,2}\mathcal{R}_2 - p_{2,2}\mathcal{R}_1}{p_{1,1}p_{2,2} - p_{1,2}p_{2,1}} = \frac{p_{1,2}\mathcal{R}_2 - p_{2,2}\mathcal{R}_1}{\det(\mathbf{P})} \\ a_{2,0} = \mathcal{V}_2^\infty &= \frac{p_{2,1}\mathcal{R}_1 - p_{1,1}\mathcal{R}_2}{p_{1,1}p_{2,2} - p_{1,2}p_{2,1}} = \frac{p_{2,1}\mathcal{R}_1 - p_{1,1}\mathcal{R}_2}{\det(\mathbf{P})}\end{aligned} \tag{5.13}$$

---

[4] "Eigen" is a German word that means "own", used in the sense of the characteristic (own) values belonging to a particular matrix.

The four other constants $a_{i,j}$ in Eq. (5.12) are better legible if we don't express them by $\mathcal{R}_1$ and $\mathcal{R}_2$, but rather by the constants $a_{1,0}$ and $a_{2,0}$ of Eq. (5.13) (for λ_1, λ_2 real and negative and $\lambda_1 \neq \lambda_2$):

$$\begin{aligned}
a_{1,1} &= q\cdot\left[(p_{1,1}-\lambda_2)(\mathcal{V}_1^0 - a_{1,0}) + p_{1,2}(\mathcal{V}_2^0 - a_{2,0})\right] \\
a_{1,2} &= -q\cdot\left[(p_{1,1}-\lambda_1)(\mathcal{V}_1^0 - a_{1,0}) + p_{1,2}(\mathcal{V}_2^0 - a_{2,0})\right] \\
a_{2,1} &= q\cdot\left[p_{2,1}(\mathcal{V}_1^0 - a_{1,0}) + (p_{2,2}-\lambda_2)(\mathcal{V}_2^0 - a_{2,0})\right] \\
a_{2,2} &= -q\cdot\left[p_{2,1}(\mathcal{V}_1^0 - a_{1,0}) + (p_{2,2}-\lambda_1)(\mathcal{V}_2^0 - a_{2,0})\right] \\
q &= \frac{1}{\lambda_1-\lambda_2} = \frac{1}{\sqrt{\Delta(\mathbf{P})}} = \left[(p_{1,1}-p_{2,2})^2 + 4\,p_{1,2}p_{2,1}\right]^{-\frac{1}{2}}
\end{aligned} \tag{5.14}$$

Only in rare cases would we calculate the solution of Eq. (5.1) manually. It makes more sense to use computer software for that. However, we can get a qualitative view of the system's behavior from the eigenvalues of the coefficient matrix **P**. They are, as Eq. (5.10) shows, relatively easy to find, at least for a two-dimensional system.

Example 5.2: Chemical reaction in a reactor (continued)

In Example 5.1 we analyzed the model of a chemical reactor. We now want to numerically look at its steady state. Assuming we are interested in substance B, we might want at least 90 % of the introduced substance to be in the form B in the outflow. How big can the flow rate Q be at most for this condition to be fulfilled?

We use the following data:

Reactor volume	$V = 10$ m^3
Reaction constants	$k_A = 0.5$ h^{-1}
	$k_B = 0.01$ h^{-1}

If the reactor is run with constant conditions for long enough, the concentrations C_A and C_B in the reactor (and therefore also in the outflow) take on the steady state values C_A^∞ and C_B^∞. The conversion constraint of 90 % can be written as:

$$0.9 \leq \frac{C_B^\infty}{C_A^\infty + C_B^\infty} = \frac{1}{C_A^\infty/C_B^\infty + 1}$$

Solved for C_A^∞/C_B^∞:

$$C_A^\infty/C_B^\infty \leq (1/9) = 0.11$$

Before we use Eq. (5.13) to calculate C_A^∞ and C_B^∞, we have to ensure that the eigenvalues are real and negative and that the determinant is $\det(\mathbf{P}) \neq 0$. According to Example 5.1, we have:

$$\begin{aligned}\det(\mathbf{P}) &= (k_A + k_w)(k_B + k_w) - k_A k_B \\ &= k_w^2 + k_w(k_A + k_B) > 0\end{aligned}$$

This is because all coefficients k_w, k_A, k_B are larger than zero. Furthermore, you can verify that all eigenvalues correspond to case 1 in Table 5.1. Thus we can now calculate the proportion C_A^∞ / C_B^∞ from Eq. (5.13), making use of the fact that $\mathcal{R}_2 = 0$ (see Example 5.1):

$$\frac{C_A^\infty}{C_B^\infty} = \frac{-p_{2,2}\mathcal{R}_1}{p_{2,1}\mathcal{R}_1} = \frac{k_B + k_w}{k_A} \leq 0.11$$

Solving for $k_w = Q/V$ gives:

$$\begin{aligned}k_w = \frac{Q}{V} &\leq 0.11 k_A - k_B \\ &= 0.11 \times 0.5\ \mathrm{h}^{-1} - 0.01\ \mathrm{h}^{-1} \\ &= 0.045\ \mathrm{h}^{-1}\end{aligned}$$

or

$$Q \leq 10\ \mathrm{m}^3 \times 0.045\ \mathrm{h}^{-1} = 0.45\ \mathrm{m}^3\,\mathrm{h}^{-1}$$

So the flow rate Q must not increase beyond $0.45\ \mathrm{m}^3\,\mathrm{h}^{-1}$.

5.1.2 Eigenvalues of a Linear System of Differential Equations: Their Meaning

If the two eigenvalues $\lambda_i (i = 1, 2)$ are distinct, all solutions of a two-dimensional system of linear differential equations look formally very similar (see Eq. 5.12). $\mathcal{V}_i(t)$ consists of three terms at most: a constant and two exponential functions. In special cases some of these terms may be zero. It doesn't come as a surprise that the solutions of a three-dimensional system contain an additional (third) exponential function. Correspondingly, there is a third eigenvalue. An n-dimensional system has n eigenvalues.

The eigenvalues of a linear system determine its temporal behavior.

The properties of the eigenvalues λ_i bring some variety to the solutions in Eq. (5.12). Table 5.1 gives an overview of the possible eigenvalue types and conveys a qualitative impression of the corresponding solutions. Note that the inhomogeneous terms $\mathcal{R}_1$ and $\mathcal{R}_2$ have no influence on the eigenvalues.

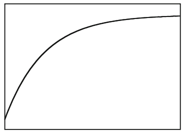
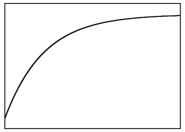
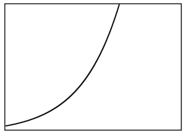
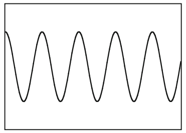
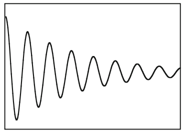
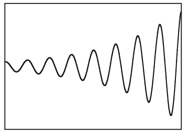
The cases 4–6 in Table 5.1 require an additional explanation: If the discriminant $\Delta(\mathbf{P})$ of the quadratic equation is smaller than zero, the eigenvalues are complex numbers. To interpret the solution Eq. (5.12), we must know the meaning of an exponential function with a complex argument, $\lambda_i = a + \mathrm{i}\, b$[5]:

$$\mathrm{e}^{\lambda_i t} = \mathrm{e}^{(a+\mathrm{i}b)t} = \mathrm{e}^{at}\mathrm{e}^{\mathrm{i}bt} = \mathrm{e}^{at}(\cos bt + \mathrm{i}\sin bt) \qquad (5.15)$$

---

[5] See Appendix C.4.

Table 5.1: *Meaning of the eigenvalues λ_i*

	Eigenvalues[a] $\lambda_i = \frac{1}{2}[\mathrm{tr} \pm (\Delta)^{1/2}]$	Condition	Properties	Solution sketch
(1)	Real, both negative	$\mathrm{tr} < 0, \Delta > 0$ $0 < \Delta^{1/2} < -\mathrm{tr}$	Solution with steady state	
(2)	Real, $\lambda_1 = 0$, $\lambda_2 < 0$	$\mathrm{tr} < 0$, $\Delta > 0$ $\Delta^{1/2} = -\mathrm{tr}$ (corresponds to $\det = 0$)	Solution with steady state	
(3)	Real, at least one positive	$\mathrm{tr} > 0$, $\Delta > 0$	Solution $\rightarrow \infty$ (solution unbounded)[b]	
(4)	Both purely imaginary	$\mathrm{tr} = 0$, $\Delta < 0$	Undamped oscillation	
(5)	Conjugate-complex, with negative real part	$\mathrm{tr} < 0$, $\Delta < 0$	Damped oscillation	
(6)	Conjugate-complex, with positive real part	$\mathrm{tr} > 0$, $\Delta < 0$	Oscillation $\rightarrow \pm\infty$	

[a] To simplify notation, we don't write the argument $(\mathbf{P})$ in Δ, tr und det. In addition, the case $\Delta = 0 (\lambda_1 = \lambda_2)$ is not considered in this list. It is only relevant for special cases.

[b] If only *one* $\lambda_i > 0$, the boundary conditions can still lead to finite solutions if in Eq. (5.12) the coefficient $a_{i,j}$ belonging to the positive λ_i is zero.

A complex eigenvalue thus leads to an oscillating function. If the real part of λ_i, $\mathrm{Re}(\lambda_i) = a$, is negative, the amplitude grows smaller. If however $\mathrm{Re}(\lambda_i) = a$ is positive, the amplitude grows to infinity. For a purely imaginary eigenvalue ($a = 0$) we get a periodic function with constant amplitude, i.e. an undamped oscillation. We will discuss this case in more detail in Sect. 5.1.6.

In the following sections we will consider examples for the different types of eigenvalues. But first we want to introduce an important tool to analyze multi-dimensional models: the phase space.

5.1.3 The Phase Space

One way to illustrate the dynamics of a model with several variables is the phase diagram. In this diagram, the momentary state of the system is a point in the n-dimensional phase space spanned by the n system variables (see Fig. 5.2). The development of the system is then described by a curve, also called trajectory. The system moves along this trajectory; if it reaches a steady state, it stays at that point. Trajectories have two characteristic properties: they do not cross and they have a *direction* that indicates the course of development through time. In Chap. 6 on nonlinear models, the phase diagram will play an important role in analyzing the properties of a system.

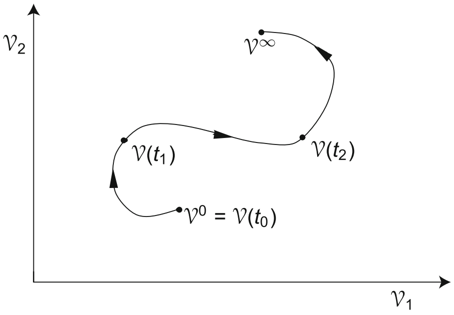
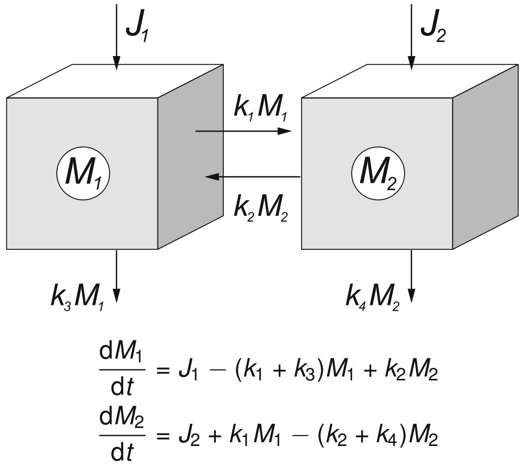


Fig. 5.2: *Phase diagram for a two-dimensional model. The trajectory is the line along which the model moves. It is determined by the initial state* $\mathcal{V}^0$ *and the model equations*

5.1.4 Linear Models with Real, Non-positive Eigenvalues

Real negative eigenvalues (case 1 in Table 5.1) frequently appear in linear models that are based on the mass balance of a system. Figure 5.3 exemplifies the idea of a mass balance. First, we assume that the substance is not produced by a first-order process, but only added from outside of the system (inhomogeneous terms J_1 and J_2). Second, the elimination processes are first order and either lead into the neighboring box ($k_1 M_1$, $k_2 M_2$) or out of the system ($k_3 M_1$, $k_4 M_2$). All k_i are positive.



$$\frac{dM_1}{dt} = J_1 - (k_1 + k_3)M_1 + k_2 M_2$$
$$\frac{dM_2}{dt} = J_2 + k_1 M_1 - (k_2 + k_4)M_2$$

Fig. 5.3: *A linear system in which a substance cannot be created by a first-order process, but only comes from outside the system or a neighboring box. This leads to a system of differential equations with real and non-positive eigenvalues. All k_i are positive*

For the model in Fig. 5.3, the model parameters $p_{i,j}$ from Eq. (5.1) take the following values:

$$\begin{aligned} p_{1,1} &= -(k_1 + k_3); \quad & p_{1,2} &= k_2 \\ p_{2,1} &= k_1; & p_{2,2} &= -(k_2 + k_4) \end{aligned}$$

One can confirm that under these conditions, the coefficients in matrix **P** always have the following properties:

(a) The elements outside of the diagonal $p_{1,2}$ and $p_{2,1}$ are positive. The discriminant Δ of the characteristic equation is therefore larger than zero (Eq. 5.9) and the eigenvalues are real.

(b) The diagonal elements $p_{1,1}$ and $p_{2,2}$ are negative. Furthermore, $-p_{1,1} \geq p_{2,1}$ and $-p_{2,2} \geq p_{1,2}$. The eigenvalues are therefore negative (and real). The model tends to the steady state. Its adjustment time τ is determined by the smaller of the eigenvalues. Analogously to the one-dimensional system, the 5 % adjustment time is:

$$\tau_{5\,\%} \approx \frac{3}{\min|\lambda_i|} = \frac{6}{-\mathrm{tr}(\mathbf{P}) - \sqrt{\Delta(\mathbf{P})}} \qquad (5.16)$$

for $\lambda_i \neq 0, \Delta(\mathbf{P}) > 0$ and $\mathrm{tr}(\mathbf{P}) < 0$. However, Eq. (5.16) cannot be interpreted with the same stringency as its one-dimensional counterpart (Eq. 4.42). Individual variables of a multi-dimensional system of equations can approach their steady state much more quickly if the coefficients $a_{i,j}$ belonging to the smallest eigenvalue are small or even zero for the respective variable. Therefore, Eq. (5.16) should always be used merely as a first, rough estimate. A more detailed examination would require knowing the explicit solution.

(c) If the system is conservative with respect to its mass balance, we have a special case: there are neither internal sources nor sinks. This means that the sum of both variables is constant and one of the two eigenvalues is zero. For the coefficient matrix, $-p_{1,1} = p_{2,1}$ and $-p_{2,2} = p_{1,2}$. The first row of matrix $\mathbf{P}$ is identical with the second row except for the algebraic sign. Such a matrix is called *singular*. Its determinant is zero: $\det(\mathbf{P}) = 0$. Singular matrices have at least one eigenvalue that is zero.

Example 5.3: Chemical reaction in a reactor (continued)

In Examples 5.1 and 5.2 we analyzed a reactor with a chemical reaction between two substances, A and B. We now want to know *how long* it takes for the reactor to reach a steady state.

To perform the calculation, we fix the through-flow Q at 0.4 m^3h^{-1}. Then, $k_w = Q/V = 0.4\ \text{m}^3\text{h}^{-1}/10\ \text{m}^3 = 0.04\ \text{h}^{-1}$. The system and its coefficient matrix have the same structure as the model in Fig. 5.3. The coefficient matrix is:

$$\begin{aligned}
p_{1,1} &= -(k_A + k_w) = -(0.5 + 0.04)\ \text{h}^{-1} = -0.54\ \text{h}^{-1} \\
p_{1,2} &= k_B = 0.01\ \text{h}^{-1} \\
p_{2,1} &= k_A = 0.5\ \text{h}^{-1} \\
p_{2,2} &= -(k_B + k_w) = -(0.01 + 0.04)\ \text{h}^{-1} = -0.05\ \text{h}^{-1}
\end{aligned}$$

We therefore get, according to Eqs. (5.7)–(5.10):

$$\begin{aligned}
\det(\mathbf{P}) &= (0.54 \times 0.05)\ \text{h}^{-2} - (0.01 \times 0.5)\ \text{h}^{-2} = 2.2 \times 10^{-2}\ \text{h}^{-2} \\
\text{tr}(\mathbf{P}) &= -(0.54 + 0.05)\ \text{h}^{-1} = -0.59\ \text{h}^{-1} \\
\Delta(\mathbf{P}) &= \text{tr}(\mathbf{P})^2 - 4\det(\mathbf{P}) = 0.260\ \text{h}^{-2} \\
\lambda_i &= \frac{1}{2}[-0.59\ \text{h}^{-1} \pm (0.260)^{1/2}\ \text{h}^{-1}] \\
\lambda_1 &= -0.040\ \text{h}^{-1}; \qquad \lambda_2 = -0.55\ \text{h}^{-1}
\end{aligned}$$

From any given initial state, the overall 5 % adjustment time according to Eq. (5.16) is:

$$\tau_{5\,\%} = \frac{3}{|\lambda_1|} = \frac{3}{0.04\ \text{h}^{-1}} = 75\ \text{h}$$

This time is about equal to the average retention time of the water in the reactor ($\tau_w = V/Q = 25$ h; $\tau_{5\,\%} \sim 3\tau_w$). It depends only marginally on the time for reaching an equilibrium between phases A and B. As shown in Example 5.4, the latter depends on the sum of the two rates $(k_A + k_B)^{-1} \approx 2$ h.

In the next example, we look at a system with a singular system matrix, i.e. $\det(\mathbf{P}) = 0$. Such systems only have a steady state if they are homogeneous, that is, if $\mathcal{R}_1 = \mathcal{R}_2 = 0$.

Example 5.4: Chemical reaction of two substances

We examine the forward and backward reaction between two chemical substances with the masses M_1 and M_2. This could be the acid-base equilibrium of the acid AH and the corresponding base A^-:

$$\mathrm{AH} + \mathrm{H_2O} \rightleftharpoons \mathrm{H_3O^+} + \mathrm{A^-}$$

or shorter:

$$M_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} M_2$$

We assume that the speed of the forward and backward reactions is proportional to the mass of the corresponding starting substance (i.e., it is a first-order reaction). If k_1 and k_2 are the specific rate constants of the two reactions, the following mass balance results:

$$\begin{aligned} \frac{\mathrm{d}M_1}{\mathrm{d}t} &= -k_1 M_1 + k_2 M_2 \\ \frac{\mathrm{d}M_2}{\mathrm{d}t} &= k_1 M_1 - k_2 M_2 \end{aligned} \tag{5.17}$$

The coefficient matrix for this system is:

$$\mathbf{P} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \tag{5.18}$$

The two Eqs. (5.17) are linearly dependent. The matrix is therefore singular ($\det(\mathbf{P}) = 0$). As per Table 5.1, case 2, one of the eigenvalues is then zero: $\lambda_1 = 0$. What does this mean for the modeled system?

To answer this question, we must look at the system's mass balance. The total mass in the system $M_{tot} = M_1 + M_2$ remains constant, and it is determined by the total mass of the initial state $M_{tot}^0 = M_1^0 + M_2^0$:

$$\frac{\mathrm{d}M_{tot}}{\mathrm{d}t} = \frac{\mathrm{d}M_1}{\mathrm{d}t} + \frac{\mathrm{d}M_2}{\mathrm{d}t} = 0 \tag{5.19}$$

In a linear system, an eigenvalue that is zero always indicates a *conserved quantity*. In our case, the total mass M_{tot} is conserved. As follows from Eq. (5.10), the second eigenvalue has the value (note that $-\mathrm{tr}(\mathbf{P}) = \Delta(\mathbf{P})^{1/2}$):

$$\lambda_2 = \mathrm{tr}(\mathbf{P}) = -(k_1 + k_2) \tag{5.20}$$

The steady state of the model is calculated by setting $\frac{\mathrm{d}M_i}{\mathrm{d}t} = 0$ in Eq. (5.17). Since the equations are linearly dependent they both yield the same result:

$$M_2^\infty = \frac{k_1}{k_2} M_1^\infty = K M_1^\infty \tag{5.21}$$

Instead of one specific steady state or fixed point, we get a whole set of potential steady states which all lie on a straight line, the so-called fixed-point line. It corresponds to the thermodynamic equilibrium of the reaction with the equilibrium constant $K = \frac{k_1}{k_2}$.

We don't need complex calculations to determine which point on the fixed-point line the model is actually moving towards. We only need to remember that the model obeys a mass conservation condition. Figure 5.4 shows the phase diagram of the homogeneous equilibrium reaction (5.17). On the one hand, mass conservation means that the system can only move along the line with slope (-1), which crosses the M_1 or M_2 axis at $M^0_{tot} = M^0_1 + M^0_2$. This is the system's trajectory, labeled A in Fig. 5.4. On the other hand, Eq. (5.21) says that all steady states must lie on a line through the origin with slope $(\frac{k_1}{k_2})$. This is the system's fixed-point line, labeled B in Fig. 5.4. The steady state in accordance to the initial condition (M^0_1, M^0_2) lies at point S, the intersection between the two lines.

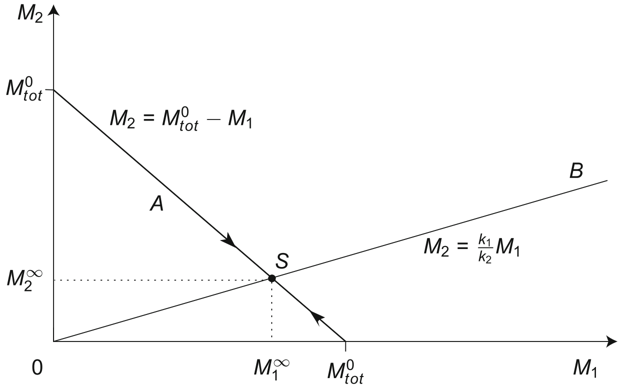


Fig. 5.4: *Phase diagram of the homogeneous chemical equilibrium reaction (Eq. 5.17). The arrows on the trajectory (line A) show the direction in which the system moves in time. Further explanations are in the text*

What remains is the confirmation that the model does indeed move towards the fixed-point line. For this, we solve the system of equations (5.17) by replacing M_2 with $M^0_{tot} - M_1$ in the first equation. We get the following for M_1:

$$\frac{\mathrm{d}M_1}{\mathrm{d}t} = k_2 M^0_{tot} - (k_1 + k_2) M_1 \tag{5.22}$$

Eq. (5.22) is an inhomogeneous linear first-order differential equation with the variable M_1. We already know its solution from Chap. 4 with Eqs. (4.6) and (4.33):

$$M_1(t) = M_1^\infty + (M_1^0 - M_1^\infty)\, \mathrm{e}^{-(k_1+k_2)t} \tag{5.23}$$

The steady state is:

$$M_1^\infty = \frac{k_2}{k_1 + k_2} M^0_{tot} \tag{5.24}$$

Because the total rate $(-[k_1 + k_2])$ is negative, the system does in fact move towards this steady state.

The solution for $M_2(t)$ results either from $M_2 = M_{tot}^0 - M_1$ or analogously to Eq. (5.23):

$$M_2(t) = M_2^\infty + (M_2^0 - M_2^\infty)\,\mathrm{e}^{-(k_1+k_2)t} \tag{5.25}$$

with the steady state

$$M_2^\infty = \frac{k_1}{k_1+k_2} M_{tot}^0 \tag{5.26}$$

As we already noted, *one* eigenvalue of the coefficient matrix is zero. The second eigenvalue is $\lambda_2 = -(k_1 + k_2)$. This explains why, in contrast to Eq. (5.12), the solutions (5.23) and (5.25) only consist of *one* exponential function. Note that the eigenvalue λ_2, and thus the overall response time of the system, only depends on the sum of the two reaction rates k_1 and k_2. It is therefore sufficient if just one of the reaction rates is large for the response time to be small.

Let's look at a second example leading to a homogeneous system of equations. This time, however, the system is not conservative, that is, $\det(\mathbf{P}) \neq 0$:

Example 5.5: Radioactive decay chain

Naturally occurring radioactive isotopes are often used to identify the age of rocks. From the activity ratio[a] between mother and daughter isotope, it is possible to draw conclusions about the rock's age. The amount of mother isotopes N_1 and daughter isotopes N_2 can be described with the following system of differential equations:

$$\begin{aligned} \frac{\mathrm{d}N_1}{\mathrm{d}t} &= -k_{\lambda,1} N_1 \\ \frac{\mathrm{d}N_2}{\mathrm{d}t} &= \ k_{\lambda,1} N_1 - k_{\lambda,2} N_2 \end{aligned} \tag{5.27}$$

$k_{\lambda,i}$ is the decay constant of the isotope i. It is linked to the half-life $\tau_{1/2,i}$ through the following relation: $k_{\lambda,i} = \ln 2/\tau_{1/2,i}$.

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[a] The activity of a radioactive substance is defined as the product of the amount of isotopes and the decay constant k_λ. The activity is measured as the number of decays per time with the unit Bq = 1 Becquerel = 1 decay per second.

We will now examine this system of equations more closely. We notice that N_2 depends on N_1, but N_1 doesn't depend on N_2. Such a system is called hierarchical. The hierarchy of the system is expressed in the so-called triangular form of its coefficient matrix, in which all elements above the diagonal are zero[6]:

$$\mathbf{P} = \begin{pmatrix} -k_{\lambda,1} & 0 \\ k_{\lambda,1} & -k_{\lambda,2} \end{pmatrix} \tag{5.28}$$

This makes determining the eigenvalues and therefore the solution of the system of equations particularly easy. From the characteristic equation (5.11) it follows that the eigenvalues are identical with the diagonal elements:

$$\begin{aligned} \lambda^2 + \lambda(k_{\lambda,1} + k_{\lambda,2}) + k_{\lambda,1}k_{\lambda,2} &= 0 \\ (\lambda + k_{\lambda,1})(\lambda + k_{\lambda,2}) &= 0 \\ \Rightarrow \lambda_1 &= -k_{\lambda,1} \\ \lambda_2 &= -k_{\lambda,2} \end{aligned}$$

A hierarchical system of equations can be solved iteratively, i.e. from top to bottom, by determining $N_1(t)$ from the first equation and inserting the result into the second one. The first differential equation has the solution we already know from Eq. (4.8) in Chap. 4:

$$N_1(t) = N_1^0 \mathrm{e}^{-k_{\lambda,1}t} \tag{5.29}$$

If we now insert the solution for N_1 into the second differential equation, we get:

$$\frac{\mathrm{d}N_2}{\mathrm{d}t} = k_{\lambda,1} N_1^0 \mathrm{e}^{-k_{\lambda,1}t} - k_{\lambda,2} N_2 \tag{5.30}$$

To solve this differential equation we can use the solution for the linear one-box model with exponentially varying input. To do so we can view the first term on the right-hand side of the equation as the input function of the system variable N_2, which exponentially falls with $k_{\lambda,1}$. The initial value of the input function is $j_0 = k_{\lambda,1} N_1^0$. If we now apply Eq. (4.57), and with the initial condition $N_2^0 = 0$, we get:

$$\begin{aligned} N_2(t) &= \frac{k_{\lambda,1}}{k_{\lambda,2} - k_{\lambda,1}} N_1^0 \mathrm{e}^{-k_{\lambda,1}t} - \frac{k_{\lambda,1}}{k_{\lambda,2} - k_{\lambda,1}} N_1^0 \mathrm{e}^{-k_{\lambda,2}t} \\ &= \frac{k_{\lambda,1}}{k_{\lambda,2} - k_{\lambda,1}} N_1^0 \cdot (\mathrm{e}^{-k_{\lambda,1}t} - \mathrm{e}^{-k_{\lambda,2}t}) \end{aligned} \tag{5.31}$$

We see that the solutions for $N_1(t)$ and $N_2(t)$ are sums of exponential functions again. The exponential coefficients are the eigenvalues of the coefficient matrix. Because the system is hierarchical, the second exponential function (with $k_{\lambda,2}$) does not appear in the solution of $N_1(t)$. Only the solution of $N_2(t)$ depends on both decay constants or eigenvalues. Finally, we

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[6] For another configuration of the system variables N_i, the triangular form could also mean that all elements *below* the diagonal are zero.

learn that for the homogeneous system Eq. (5.27) with negative eigenvalues, the steady state is zero.

Let us summarize what we have learned from this example. A hierarchical system can be recognized by the triangular form of the coefficient matrix. Therefore, the eigenvalues are identical with the diagonal elements of this matrix and the system of equations can be solved iteratively. In the next example, we will explore a hierarchical system consisting of two spatially separate boxes:

Example 5.6: Transport of a radioactive isotope through two lakes

A radioactive isotope with the decay constant k_λ is inadvertently introduced into two neighboring lakes. The outflow of one lake leads to the other lake. Both lakes can be seen as completely mixed reactors. Figure 5.5 shows the box diagram of the system. The isotope input J_i takes place via tributaries or directly into the lake. The outflow of the second lake (Q_2) can be larger than the one of the first lake ($Q_{1,2}$), if inflows bring water directly into the second lake. This kind of two-box model was used by Lerman (1972) to describe the concentration of the radioactive isotope strontium-90 in the Great Lakes of North America.

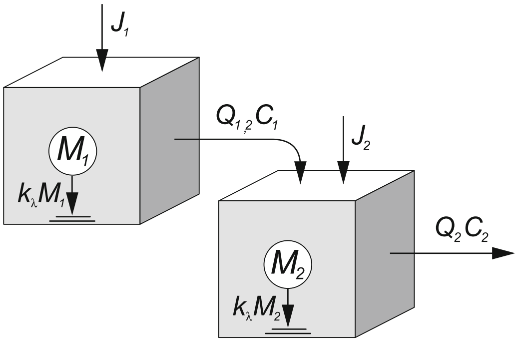


Fig. 5.5: *Transport of a radioactive isotope through a chain of lakes depicted as a box diagram*

First, we establish the mass balance for the two boxes: M_i is the total mass of the isotope in lake i. The external isotope input is given by the input function $J_i\,[\,\mathrm{MT}^{-1}\,]$, and the radioactive decay is described by $-k_\lambda M_i$. The transport processes we take into account are the flow from the first into the second lake and the second lake's outflow. We end up with the following system of differential equations:

$$\begin{aligned}\frac{\mathrm{d}M_1}{\mathrm{d}t} &= \left\{\begin{matrix}\text{Input into}\\ \text{lake 1}\end{matrix}\right\} - \left\{\begin{matrix}\text{Flow into}\\ \text{lake 2}\end{matrix}\right\} - \left\{\begin{matrix}\text{Radioactive}\\ \text{decay}\end{matrix}\right\}\\ &= J_1 - Q_{1,2}C_1 - k_\lambda M_1\end{aligned}$$

$$\begin{aligned}\frac{\mathrm{d}M_2}{\mathrm{d}t} &= \left\{\begin{matrix}\text{Input into}\\ \text{lake 2}\end{matrix}\right\} + \left\{\begin{matrix}\text{Outflow from}\\ \text{lake 1}\end{matrix}\right\}\\ &- \left\{\begin{matrix}\text{Outflow from}\\ \text{lake 2}\end{matrix}\right\} - \left\{\begin{matrix}\text{Radioactive}\\ \text{decay}\end{matrix}\right\}\\ &= J_2 + Q_{1,2}C_1 - Q_2C_2 - k_\lambda M_2\end{aligned} \tag{5.32}$$

Again, $C_i = M_i/V_i$ means the concentration in lake i. For the concentration, the dynamic equations are:

$$\begin{aligned}\frac{\mathrm{d}C_1}{\mathrm{d}t} &= \frac{J_1}{V_1} - \frac{Q_{1,2}}{V_1}C_1 - k_\lambda C_1\\ &= \frac{J_1}{V_1} - (\frac{Q_{1,2}}{V_1} + k_\lambda)C_1\\ \frac{\mathrm{d}C_2}{\mathrm{d}t} &= \frac{J_2}{V_2} + \frac{Q_{1,2}}{V_2}C_1 - \frac{Q_2}{V_2}C_2 - k_\lambda C_2\\ &= \frac{J_2}{V_2} + \frac{Q_{1,2}}{V_2}C_1 - (\frac{Q_2}{V_2} + k_\lambda)C_2\end{aligned} \tag{5.33}$$

The coefficient matrix has the form:

$$\mathbf{P} = \begin{pmatrix} -\left(\frac{Q_{1,2}}{V_1} + k_\lambda\right) & 0\\ \frac{Q_{1,2}}{V_2} & -\left(\frac{Q_2}{V_2} + k_\lambda\right)\end{pmatrix} \tag{5.34}$$

The system is therefore hierarchical and has the following eigenvalues:

$$\lambda_1 = -(\frac{Q_{1,2}}{V_1} + k_\lambda) \qquad \lambda_2 = -(\frac{Q_2}{V_2} + k_\lambda) \tag{5.35}$$

The system of equations can be solved with the same procedure as in Example 5.5; we leave the individual steps as an exercise to the reader. The solution of Eq. (5.33) for $C_1(t)$ is:

$$C_1(t) = C_1^\infty + (C_1^0 - C_1^\infty) \cdot \mathrm{e}^{\lambda_1 t} \tag{5.36}$$

with the steady state

$$C_1^\infty = \frac{J_1}{(-\lambda_1)V_1} = \frac{J_1}{Q_{1,2} + V_1 k_\lambda} \tag{5.37}$$

Because of the system's hierarchy, only the exponential function with the first eigenvalue (λ_1) appears in Eq. (5.36)

Once again, the result (Eq. 5.36) can be inserted in Eq. (5.33). The resulting differential equation with a time-dependent inhomogeneous term can be solved according to the recipe from Eq. (4.57). In the end, the result can be brought into the form consisting of three terms that we already know from Eq. (5.12):

$$\begin{aligned}C_2(t) = C_2^\infty &+ \frac{Q_{1,2}(C_1^0 - C_1^\infty)}{Q_2 - (V_2/V_1)Q_{1,2}}\ \mathrm{e}^{\lambda_1 t}\\ &+ \left[C_2^0 - C_2^\infty - \frac{Q_{1,2}(C_1^0 - C_1^\infty)}{Q_2 - (V_2/V_1)Q_{1,2}}\right]\ \mathrm{e}^{\lambda_2 t}\end{aligned} \tag{5.38}$$

with

$$C_2^\infty = \frac{J_2 + Q_{1,2} C_1^\infty}{Q_2 + V_2 k_\lambda} \tag{5.39}$$

To illustrate this rather complex-looking result, we can look at the concrete case where the outflow of a relatively large lake leads into a much smaller lake. Maybe you can already intuitively guess how a radioactive substance with half-life $\tau_{1/2}$ of about 12 year (this could be tritium, a radioactive isotope of hydrogen denoted ^{3}H) behaves in this system:

Lake 1:	$V_1 =$	100×10^9 m^3
	$Q_{1,2} =$	30×10^8 m^3 year^{-1}
	$J_1 =$	300×10^9 Bq year^{-1}
⇒ Average retention time:	$\tau_1 = V_1/Q_{1,2}$	33 year
Lake 2:	$V_2 =$	5×10^9 m^3
	$Q_2 =$	45×10^8 m^3 year^{-1}
	$J_2 =$	190×10^9 Bq year^{-1}
⇒ Average retention time:	$\tau_2 = V_2/Q_2$	1.1 year
Decay constant of the isotope:	$k_\lambda =$	0.06 year^{-1}
Half-life:	$\tau_{1/2} =$	11.6 year

We can now calculate the steady-state concentrations from Eqs. (5.37) and (5.39):

$$C_1^\infty = 33 \text{ Bq m}^{-3}$$
$$C_2^\infty = 60 \text{ Bq m}^{-3}$$

Let's assume that the isotope influx (J_1 and J_2) is stopped abruptly. Of course, this assumption is unrealistic, because the lakes' catchment area also has a "memory", for instance in the soil, where the isotope is washed out only slowly. Nevertheless, we can hypothetically examine how C_1 and C_2 (the concentration in the two lakes) would develop.

First, we can see that the only change in the system of equations (5.33) concerns the two inhomogeneous terms ($J_1 = J_2 = 0$). The system matrix **P** and therefore also the eigenvalues don't change. They have the following values:

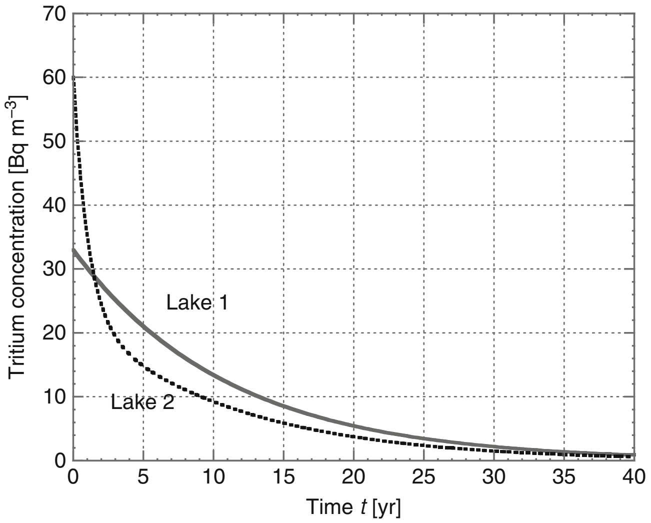
$$\lambda_1 = -0.09 \text{ year}^{-1}; \qquad \lambda_2 = -0.96 \text{ year}^{-1}$$

As per Eq. (5.16), the (absolute) smaller eigenvalue λ_1 determines the lake chain's reaction to the input change:

$$\tau_{5\,\%} = \frac{3}{0.09 \text{ year}^{-1}} = 33 \text{ year}$$

In fact, the two eigenvalues are each composed of the water flow rate and the decay constant. In this example they can therefore explicitly be allocated to the two subsystems. The eigenvalue λ_1 describes the isotope in the first lake, λ_2 the one in the second lake. Figure 5.6 shows the reduction of

Fig. 5.6: *After a quick drop, the tritium concentration in Lake 2 adjusts to the much slower decrease in Lake 1 upstream*



tritium in the two lakes. Starting from the steady-state concentration, the tritium concentration in the second lake declines very rapidly. The first lake, however, reacts more slowly. If the second lake did not lie downstream of another lake, its adjustment time would be $\tau_{5\,\%,\mathrm{Lake2}} = 3/0.96 \approx 3$ year. The memory of the downstream lake is thus located in the water of the upstream lake, much in the same way as the memory of both these lakes lies in the soil of their watersheds. In Problem 5.2 we will return to this example.

5.1.5 Two-Box Model for Stratified Systems

In Chaps. 2 and 4 we explored several aspects of the dynamics of phosphorus in a lake. We now want to further extend our one-box model through the following examples, while introducing an additional element for the construction of models.

Example 5.7: Lake with stratification parameter

An investigation of a lake's phosphorus balance shows that the linear flow reactor model is not always valid, because the phosphorus concentration in the lake's outflow is usually smaller than the average phosphorus concentration in the lake. Instead of being completely mixed, it seems that a lake is sometimes stratified (or layered) in terms of the phosphorus concentration. We could adjust the dynamic equation (4.22) for the concentration of a substance in the lake as follows:

$$\frac{\mathrm{d}C}{\mathrm{d}t} = k_w C_{in} - k_w C_{out} - k_r C \tag{5.40}$$

C_{out}	$[\mathrm{ML}^{-3}]$	Average concentration in the outflow

The price for this extension is the appearance of a new system variable C_{out}. This begs the question how it is related to C. As a first attempt, we set:

$$\frac{C_{out}}{C} = \gamma = \text{const.} \tag{5.41}$$

γ	[-]	Stratification parameter for phosphorus

By doing so we can now eliminate the system variable C_{out} in Eq. (5.40) and again get a one-box model. This model is different from Eq. (4.22):

$$\frac{\mathrm{d}C}{\mathrm{d}t} = k_w C_{in} - (\gamma k_w + k_r) C \tag{5.42}$$

The steady-state concentration in the lake is:

$$C^{\infty} = C_{in} \frac{k_w}{\gamma k_w + k_r} \tag{5.43}$$

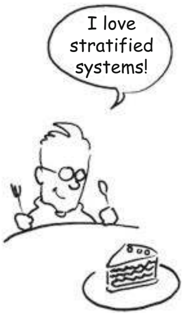
In contrast, the steady-state concentration of the lake as completely mixed flow reactor would be (see Eq. 4.25):

$$C^{\infty} = C_{in} \frac{k_w}{k_w + k_r} \tag{5.44}$$

In summer, the phosphorus concentration at the surface of the water column usually decreases due to algal growth. This renders the stratification parameter smaller than one: $\gamma < 1$. Thus, the average steady-state phosphorus concentration in the stratified lake is higher than in the completely mixed lake. In contrast, the outflow concentration is reduced by the factor γ. All in all, by keeping the water layers with above-average concentrations away from the outlet, the stratification causes the retention time of phosphorus in the lake to increase. This model has an important drawback, however: we don't know how to link the stratification parameter γ to other factors, e.g. to the mean phosphorus concentration in the lake (which may change under the influence of a varying external input). To correct for this deficit of the one-box model, we need to construct a true two-box model.

Many freshwater lakes are thermally stratified in summer. Warm (and thus light) water floats above the heavy and cold deeper water (Fig. 5.7). Due to this temperature distribution, the vertical water circulation is suppressed in the vertical layer with the largest density gradient. This zone is called the thermocline. Above the thermocline lies the so-called (warm) epilimnion, below it the (cold) hypolimnion.

In Chap. 8 we will encounter models that can describe the phosphorus concentration in a stratified lake as a continuous function of depth z and



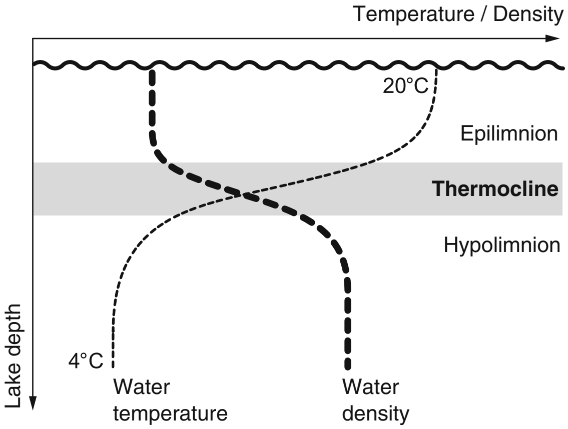


Fig. 5.7: *Vertical temperature and density profile of a lake during summer. The thermocline separates the warm surface water, called epilimnion, from the cold deep water, called hypolimnion. In the thermocline, vertical water and mass transport is reduced in comparison to the layers above and below*

time t, that is, as $C(z, t)$. The resulting equations, however, are usually so complex that they can only be solved numerically by computer.

Multi-box models stand as an intermediate step between one-box models and spatially continuous models.

It is not always justified to jump straight from using a one-box model to a continuous space-time-model. Often, an intermediate solution is most practical. Figure 5.7 suggests such a solution: the partition of the lake into two subsystems, the epilimnion and the hypolimnion, that can each individually be treated as completely mixed. Similarly, in describing the atmosphere, we could divide it into layers such as the troposphere and stratosphere. This approach can deliver acceptable results for many types of systems.

As Fig. 5.8 shows, the spatial segmentation of a system entails the question of how to describe the mass flow between the different subsystems. We will discuss this problem more extensively in Sect. 8.2. For now, and in the following example, we will anticipate and use the outcome of that discussion without further explanation.

Example 5.8: The stratified lake

We want to describe the behavior of a dissolved chemical substance in a lake during the summer months with a two-box model (Fig. 5.8). We choose the average concentrations in the epilimnion and hypolimnion as system variables: $C_E = M_E/V_E$ and $C_H = M_H/V_H$. The direct substance input $J_{in} = QC_{in}$ and outflow $J_{out} = QC_E$ only influence the epilimnion. We describe the water exchange with an exchange flow $Q_{ex}C_E$ and $Q_{ex}C_H$. For this, we assume that the dissolved substance moves passively with the water volume Q_{ex} that is continuously exchanged between epilimnion and hypolimnion. In addition, a linear decay process is taken into account in both boxes. Due to the difference in water temperature and available light, the decay rates $k_{r,E}$ and $k_{r,H}$ in the epilimnion and hypolimnion are not necessarily the same.

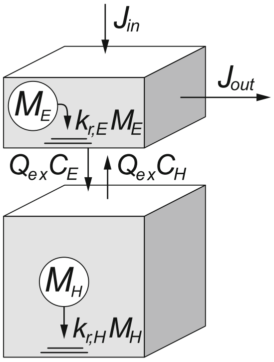


Fig. 5.8: *Two-box model for a substance with decay reaction in a stratified lake*

First, we establish the mass balance for the two boxes. For the epilimnion, it is:

$$\begin{aligned}\frac{\mathrm{d}M_E}{\mathrm{d}t} &= \{\text{Inflow}\} - \{\text{Outflow}\} - \{\text{Decay}\} \pm \{\text{Exchange}\} \\ &= QC_{in} - QC_E - k_{r,E}M_E - Q_{ex}C_E + Q_{ex}C_H\end{aligned} \tag{5.45}$$

For the hypolimnion we get correspondingly:

$$\begin{aligned}\frac{\mathrm{d}M_H}{\mathrm{d}t} &= \pm\{\text{Exchange}\} - \{\text{Decay}\} \\ &= Q_{ex}C_E - Q_{ex}C_H - k_{r,H}M_H\end{aligned} \tag{5.46}$$

After dividing Eq. (5.45) by the epilimnion volume V_E and Eq. (5.46) by the hypolimnion volume V_H we get the dynamic equations for the concentrations:

$$\begin{aligned}\frac{\mathrm{d}C_E}{\mathrm{d}t} &= \frac{Q}{V_E}C_{in} - \frac{Q}{V_E}C_E - k_{r,E}C_E - \frac{Q_{ex}}{V_E}C_E + \frac{Q_{ex}}{V_E}C_H \\ &= k_wC_{in} - k_wC_E - k_{r,E}C_E - k_{ex,E}C_E + k_{ex,E}C_H \\ &= k_wC_{in} - (k_w + k_{r,E} + k_{ex,E})C_E + k_{ex,E}C_H \\ \frac{\mathrm{d}C_H}{\mathrm{d}t} &= \frac{Q_{ex}}{V_H}C_E - \frac{Q_{ex}}{V_H}C_H - k_{r,H}C_H \\ &= k_{ex,H}C_E - k_{ex,H}C_H - k_{r,H}C_H \\ &= k_{ex,H}C_E - (k_{ex,H} + k_{r,H})C_H\end{aligned} \tag{5.47}$$

For Eqs. (5.47) we have defined the following specific rates:

$$k_w = \frac{Q}{V_E}, \quad k_{ex,E} = \frac{Q_{ex}}{V_E}, \quad k_{ex,H} = \frac{Q_{ex}}{V_H} \tag{5.48}$$

We now want to discuss the solutions of this model. First, we note that the equations conform to the general form of Eq. (5.1). Thus, we are dealing with a two-dimensional linear model. The inhomogeneous terms are:

$$\mathcal{R}_1 = k_w C_{in} \qquad \text{and} \qquad \mathcal{R}_2 = 0 \tag{5.49}$$

The coefficient matrix is composed as follows:

$$\mathbf{P} = \begin{pmatrix} -\left(k_w + k_{r,E} + k_{ex,E}\right) & k_{ex,E} \\ k_{ex,H} & -\left(k_{ex,H} + k_{r,H}\right) \end{pmatrix} \tag{5.50}$$

This is no longer a triangular matrix. To determine the eigenvalues, we would have to explicitly solve the characteristic equation. Note that the diagonal elements have a negative sign, whereas the coefficients outside of the diagonal are positive. Furthermore, $-p_{1,1} > p_{2,1}$ and $-p_{2,2} > p_{1,2}$. The eigenvalues of such a matrix are, as we have seen in Sect. 5.1.4 (Case b), always real and negative. This means that the steady states of the system exist and will be reached. We can now use Eq. (5.13) to calculate the steady state:

$$\begin{aligned} C_E^{\infty} &= \frac{(k_{ex,H} + k_{r,H}) k_w \, C_{in}}{\left(k_w + k_{r,E} + k_{ex,E}\right)\left(k_{ex,H} + k_{r,H}\right) - k_{ex,E} k_{ex,H}} \\ C_H^{\infty} &= \frac{k_{ex,H} k_w \, C_{in}}{\left(k_w + k_{r,E} + k_{ex,E}\right)\left(k_{ex,H} + k_{r,H}\right) - k_{ex,E} k_{ex,H}} \end{aligned} \tag{5.51}$$

An example with concrete numbers is shown in Table 5.2.

Note that at steady state the concentration in the epilimnion is larger than in the hypolimnion. This seems to contradict our earlier discussion about the stratification parameter and the vertical distribution of phosphorus during lake stratification. If such inconsistencies between model results and real-world experience or data appear, it is always useful to check the consistency of the model results. In other words, we want to verify quantitatively whether the solution of the system of differential equations (5.47) is formally correct.

Let's look at the mass balance of the hypolimnion: At steady state, the loss through decay at rate $k_{r,H}$ has to be compensated for by a net transport through the thermocline. The net transport $k_{ex,H}(C_E - C_H)$ is only directed from the epilimnion into the hypolimnion if $C_E > C_H$. Thus, the model result is formally correct.

The apparent discrepancy between model and reality must therefore have another reason. In fact, many substances (including phosphorus) are influenced by another transport process: the (directed) transport by sedimenting (sinking) particles from the epilimnion into the hypolimnion. We have failed to take this process into account in our model so far. In Problem 5.5 we will analyze its effects (for further information on this process, also see Chap. 23 in Schwarzenbach et al. 2003).

Table 5.2: *Numeric example for the mass balance of a stratified lake*

Volume: $V_{tot} = 150 \times 10^6\ \text{m}^3$
$V_E = 50 \times 10^6\ \text{m}^3$
$V_H = 100 \times 10^6\ \text{m}^3$

Water flow: $Q = 0.34 \times 10^6\ \text{m}^3\text{d}^{-1}$

Total substance input: $J_{in} = 40\ \text{t}\,\text{year}^{-1}$

Specific decay rates: $k_{r,E} = 0.02\ \text{d}^{-1}$
$k_{r,H} = 0.002\ \text{d}^{-1}$

Water exchange: $Q_{ex} = 0.5 \times 10^6\ \text{m}^3\text{d}^{-1}$

Calculation of parameters:

$$\begin{aligned} C_{in} &= \frac{J_{in}}{Q} = \frac{1.1 \times 10^8\,\text{mg}\,\text{d}^{-1}}{0.34 \times 10^6\ \text{m}^3\,\text{d}^{-1}} = 320\ \text{mg}\,\text{m}^{-3} \\ k_w &= \frac{Q}{V_E} = 6.8 \times 10^{-3}\ \text{d}^{-1} \\ k_{ex,E} &= \frac{Q_{ex}}{V_E} = 1 \times 10^{-2}\ \text{d}^{-1} \\ k_{ex,H} &= \frac{Q_{ex}}{V_H} = 5 \times 10^{-3}\ \text{d}^{-1} \end{aligned}$$

Calculation of matrix elements $p_{i,j}$ and $\mathcal{R}_i$

$$\begin{aligned} p_{1,1} &= -(0.68 \times 10^{-2} + 0.02 + 0.01)\ \text{d}^{-1} = -0.0368\ \text{d}^{-1} \\ p_{1,2} &= 0.01\ \text{d}^{-1} \\ p_{2,1} &= 0.005\ \text{d}^{-1} \\ p_{2,2} &= -(0.005\ \text{d}^{-1} + 0.002\ \text{d}^{-1}) = -0.007\ \text{d}^{-1} \\ \mathcal{R}_1 &= k_w C_{in} = 2.18\ \text{mg}\,\text{m}^{-3}\text{d}^{-1} \\ \mathcal{R}_2 &= 0 \end{aligned}$$

Steady states:

$$C_E^\infty = 73\ \text{mg}\,\text{m}^{-3} \qquad \text{and} \qquad C_H^\infty = 52\ \text{mg}\,\text{m}^{-3}$$

Average value across the whole lake:

$$C^\infty = \frac{1}{V_{tot}}(V_E C_E^\infty + V_H C_H^\infty) = \frac{1}{3}C_E^\infty + \frac{2}{3}C_H^\infty = 59\ \text{mg}\,\text{m}^{-3}$$

Stratification parameter in the steady state according to Example 5.7:

$$\gamma = \frac{C_{out}^\infty}{C^\infty} \approx \frac{C_E^\infty}{C^\infty} = \frac{73}{59} = 1.24$$

We also have to think about another problem: how realistic is it to assume that the lake is at steady state? We've mentioned before that lakes in a temperate climate exhibit stratification primarily during summer. In autumn, this stratification is broken up by two processes: the cooling of the surface water and the influence of strong autumn winds. It is possible, therefore, that during winter the lake is completely mixed and behaves like a one-box model. We now want to calculate the adjustment time for the two-box model and compare this with the duration of the lake's stratification period.
To estimate the adjustment time we need the eigenvalues of the coefficient matrix **P**. We calculate them with the help of Eq. (5.10):

$$\begin{aligned}\lambda_1 &= \frac{1}{2}(\mathrm{tr}(\mathbf{P}) + \sqrt{\Delta(\mathbf{P})}) \\ &= \frac{1}{2}(-0.0438 + \sqrt{0.00109})\ \mathrm{d}^{-1} \approx -0.0054\ \mathrm{d}^{-1} \\ \lambda_2 &= \frac{1}{2}(\mathrm{tr}(\mathbf{P}) - \sqrt{\Delta(\mathbf{P})}) \\ &= \frac{1}{2}(-0.0438 - \sqrt{0.00109})\ \mathrm{d}^{-1} \approx -0.038\ \mathrm{d}^{-1}\end{aligned}$$

The absolute smallest eigenvalue generally determines the adjustment time of a linear system.

The adjustment time can be estimated with the (absolute) smallest eigenvalue (Eq. 5.16):

$$\tau_{5\,\%} \approx \frac{3}{|\lambda_1|} = \frac{3}{0.0054\ \mathrm{d}^{-1}} = 555\ \mathrm{d}$$

The lake would therefore have to remain stratified for more than a year for the calculated equilibrium concentrations to be reached. As we have seen, this is not what happens in reality.

Let us try to capture the complex mixing cycle of a lake in a temperate European climate with a model. To do so, we assume that the lake is completely mixed from the beginning of January until the end of April, that is, for 120 days. Then, a stagnation period of 8 months begins, during which the lake is stratified. The model of the lake thus changes back and forth from a one-box model in winter to a two-box model in summer. The initial concentrations at the beginning of the two-box phase are identical ($C_E^0 = C_H^0$), and correspond to the final concentration of the preceding one-box phase. At the transition from the two-box to the one-box phase, the initial concentration is calculated from the volume-weighted final state of the two-box phase:

$$C^0 = \frac{C_E(t)\,V_E + C_H(t)\,V_H}{V_E + V_H} \tag{5.52}$$

Figure 5.9 shows the temporal variation of the dissolved substance described in Example 5.8 in a lake undergoing an annual cycle of stratification and destratification. For the stratification period, the numbers from

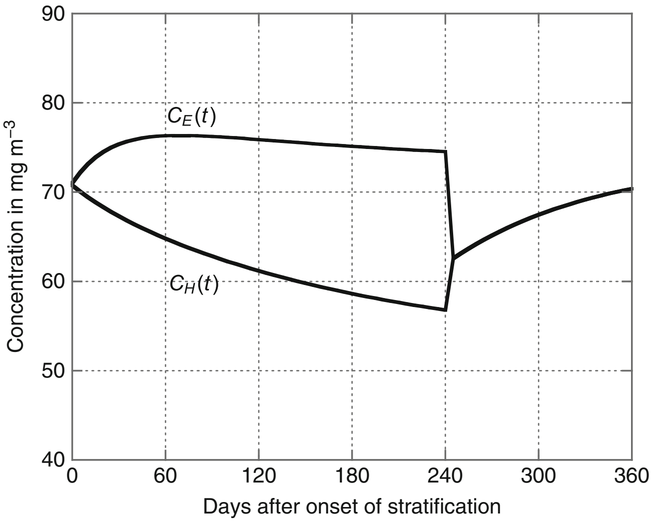


Fig. 5.9: *The mixing cycle of a lake can be simulated with a periodic change between a one-box and a two-box model. The example shows the balance for a dissolved substance with the coefficients from Table 5.2. The coefficients for the one-box model are calculated with Eqs. (5.52), (5.53) and (5.54). The subscripts E and H stand for epilimnion (upper layer) and hypolimnion (lower layer), respectively*

Table 5.2 were used. For the mixing period, the elimination rate k_r and the flow rate k_w were adjusted as follows:

$$k_r = \frac{k_{r,E}V_E + k_{r,H}V_H}{V_E + V_H} \tag{5.53}$$

$$k_w = \frac{Q}{V_E + V_H} \tag{5.54}$$

The computation starts at time $t = 0$ with the onset of stratification. Concentrations in the epilimnion and the hypolimnion develop differently. In the epilimnion, the concentration increases, while it decreases in the hypolimnion, yet the steady state is not reached. After 8 months (245 days), the lake is instantaneously and completely mixed, resulting in an average concentration in the entire lake which lies below the steady-state concentration of the mixing period. Thus, the concentration increases further over the next 120 days but is still well below the steady-state value when the cycle starts over at the onset of stratification.

In reality, the transition between complete mixing in winter and complete stratification in summer is not sudden, but gradual. Nevertheless, the basic outcome of the mixing cycle is reproduced quite well with this two-phase model.

5.1.6 Linear Models with Non-real Eigenvalues

The examples so far were all based on the principle of mass balance in systems with linear transformation and transport processes. We have seen that the coefficient matrix of such systems always leads to real, non-positive eigenvalues and that the steady state can in fact be reached.

As already suggested in Sect. 5.1.2, linear two-dimensional systems can also have non-real eigenvalues. Let's look at the following linear homogeneous system of differential equations, with the two functions $y_1(t)$ and $y_2(t)$. For now, we will not think about what these variables could stand for.

Example 5.9: Systems with purely imaginary eigenvalues

$$\begin{aligned} \frac{\mathrm{d}y_1}{\mathrm{d}t} &= k_1 y_2 \\ \frac{\mathrm{d}y_2}{\mathrm{d}t} &= -k_2 y_1 \qquad \text{with} \quad k_1, k_2 > 0 \end{aligned} \tag{5.55}$$

Note that the derivative of y_1 with respect to time is proportional to y_2, the derivative of y_2 proportional to y_1. This reciprocal dependence already lets us suspect that the solutions must be trigonometric functions. But first let's look at the system's coefficient matrix:

$$\mathbf{P} = \begin{pmatrix} 0 & k_1 \\ -k_2 & 0 \end{pmatrix} \tag{5.56}$$

Its characteristic equation (see Eq. 5.11) is:

$$\begin{aligned} \lambda^2 + k_1 k_2 &= 0 \\ \lambda^2 &= -k_1 k_2 \end{aligned} \tag{5.57}$$

Because k_1 and k_2 are positive, we get two purely imaginary eigenvalues:

$$\lambda = \pm \mathrm{i}\sqrt{k_1 k_2} = \pm \mathrm{i}\omega \qquad \text{with} \quad \omega = \sqrt{k_1 k_2} \tag{5.58}$$

The general solution of Eq. (5.12) applies to this model, too. Because the system is homogeneous ($\mathcal{R}_i = 0$), the steady state is $y_i^\infty = 0$ according to Eq. (5.13). The solutions are therefore of the following form:

$$\begin{aligned} y_1(t) &= a_{1,1}\mathrm{e}^{\mathrm{i}\omega t} + a_{1,2}\mathrm{e}^{-\mathrm{i}\omega t} \\ y_2(t) &= a_{2,1}\mathrm{e}^{\mathrm{i}\omega t} + a_{2,2}\mathrm{e}^{-\mathrm{i}\omega t} \end{aligned} \tag{5.59}$$

In other words, they can be expressed by a sum of two trigonometric functions[7]:

$$\begin{aligned} y_1(t) &= b_{1,1}\cos\omega t + b_{1,2}\sin\omega t \\ y_2(t) &= b_{2,1}\cos\omega t + b_{2,2}\sin\omega t \end{aligned} \tag{5.60}$$

The constants $b_{i,j}$ are determined by the initial condition (y_1^0, y_2^0). For example, we can choose for $t = 0$:

$$y_1^0 = 0 \qquad , \qquad y_2^0 = 1 \tag{5.61}$$

---

[7] The relation between the descriptions in Eqs. (5.59) and (5.60) can be calculated from Euler's formula, $\mathrm{e}^{\mathrm{i}\omega t} = \cos\omega t + \mathrm{i}\sin\omega t$. If the variables $y_i(t)$ are real functions, this also holds for the coefficients $b_{i,j}$. The $a_{i,j}$ from Eq. (5.59) however are generally complex numbers. For details see Appendix C.4.

Then, with $b_{1,1} = 0$ and $b_{2,1} = 1$, we get from Eq. (5.60):

$$\begin{aligned} y_1(t) &= b_{1,2} \sin \omega t \\ y_2(t) &= \cos \omega t + b_{2,2} \sin \omega t \ . \end{aligned}$$

To determine the two other constants $b_{i,j}$, we insert Eq. (5.60) into the differential equations (5.55) and get the identities:

$$\begin{aligned} \frac{\mathrm{d}y_1}{\mathrm{d}t} &= \omega b_{1,2} \cos \omega t = k_1 \left(\cos \omega t + b_{2,2} \sin \omega t\right) \\ \frac{\mathrm{d}y_2}{\mathrm{d}t} &= -\omega \sin \omega t + \omega b_{2,2} \cos \omega t = -k_2 b_{1,2} \sin \omega t \end{aligned}$$

which can only be fulfilled if $b_{2,2} = 0$ and $b_{1,2} = \omega / k_2 = (k_1/k_2)^{1/2}$.

We thus get this solution for our chosen initial condition:

$$\begin{aligned} y_1(t) &= \sqrt{\frac{k_1}{k_2}} \sin \omega t \\ y_2(t) &= \cos \omega t \end{aligned} \qquad (5.62)$$

In Fig. 5.10, the two functions are depicted as a time and a phase diagram for the case $\frac{k_1}{k_2} = 4$. The time diagram shows two undamped harmonic oscillations that are shifted by a fourth of a period. The phase diagram shows a closed elliptic trajectory. The system circulates the steady state without ever reaching it.

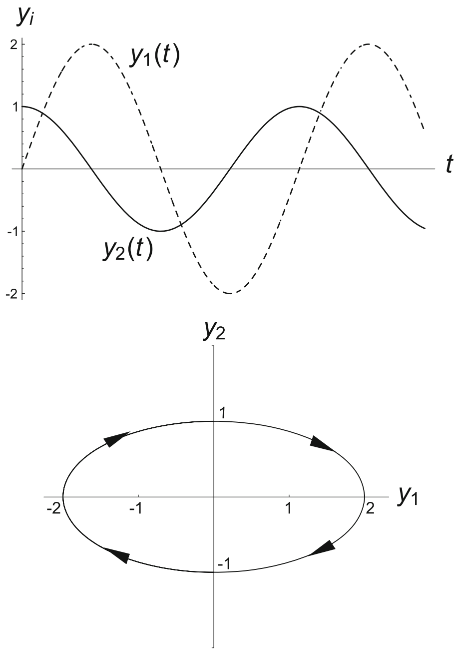
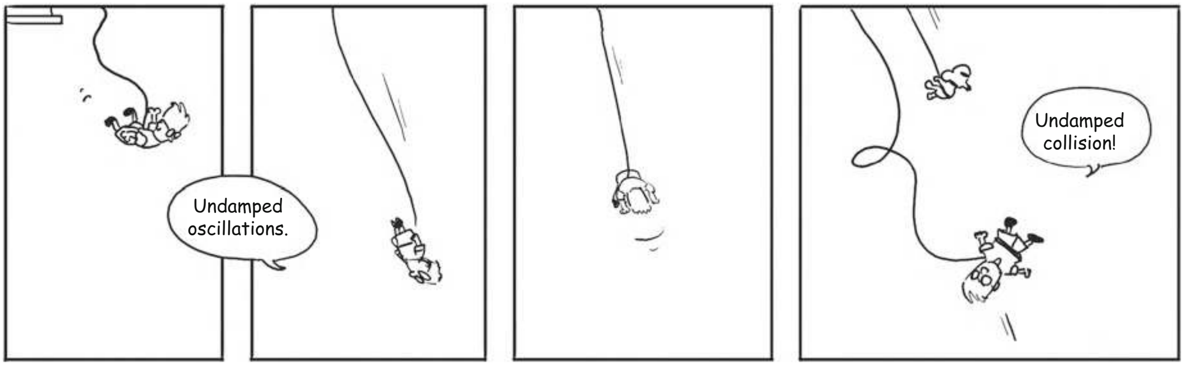


Fig. 5.10: *The solution Eq.* (5.60) *with the initial condition* $y_1^0 = 0$ *and* $y_2^0 = 1$, *above as a time diagram, below as a phase diagram.* $(k_1/k_2) = 4$

Undamped oscillations



We know from experience that undamped oscillations represent unusual situations which do not really occur in natural systems. In fact, undamped systems are unstable in a certain sense, since an arbitrarily small term in one of the two equations radically changes the long-term behavior of the system. As an illustration we modify Example 5.9 by introducing an additional term into the second equation, the meaning of which will become clear later.

Example 5.10: Oscillation with damping term

In the second equation of the model, Eq. (5.55), we introduce the additional term $-\varepsilon y_2$. For now, ε is an arbitrary positive parameter. The modified model equations are:

$$\begin{aligned} \frac{\mathrm{d}y_1}{\mathrm{d}t} &= k_1 y_2 \\ \frac{\mathrm{d}y_2}{\mathrm{d}t} &= -k_2 y_1 - \varepsilon y_2, \qquad \varepsilon > 0 \end{aligned} \tag{5.63}$$

Note that mathematicians like to use the parameter ε whenever they want to point out that this term can be arbitrarily small. As our analysis will show, it is the mere existence of this additional term—and not its size—which is responsible for a fundamental difference between Examples 5.9 and 5.10. The model has the coefficient matrix:

$$\mathbf{P} = \begin{pmatrix} 0 & k_1 \\ -k_2 & -\varepsilon \end{pmatrix} \tag{5.64}$$

Its characteristic equation is slightly modified compared to Eq. (5.57):

$$\lambda^2 + \lambda\varepsilon + k_1 k_2 = 0 \tag{5.65}$$

with the eigenvalues

$$\lambda_i = \frac{1}{2}\left(-\varepsilon \pm \sqrt{\varepsilon^2 - 4k_1 k_2}\right) = -\frac{\varepsilon}{2} \pm \sqrt{\frac{\varepsilon^2}{4} - k_1 k_2} \tag{5.66}$$

This result encompasses the entire behavior spectrum of a simple linear oscillatory system as described by Eqs. (5.63). First, we note that Eq. (5.55) is contained within Eq. (5.63) as a special case ($\varepsilon = 0$). That system has undamped oscillations as its solutions. If we now let ε grow by an arbitrarily small amount larger than zero, so that $\varepsilon^2 \ll 4k_1k_2$ remains valid, the expression below the root of Eq. (5.66) remains negative and the eigenvalues can be approximated as follows:

$$\begin{aligned}\lambda_i &= -\frac{\varepsilon}{2} \pm \mathrm{i}\sqrt{k_1k_2 - \frac{\varepsilon^2}{4}} \\ &\approx -\frac{\varepsilon}{2} \pm \mathrm{i}\sqrt{k_1k_2} \\ &= -\frac{\varepsilon}{2} \pm \mathrm{i}\omega, \qquad \omega = \sqrt{k_1k_2}\end{aligned} \tag{5.67}$$

ω is identical with the definition in Eq. (5.58). Also note that ε can be neglected in the root, but not outside of it, because the term outside transforms the purely imaginary eigenvalues into complex numbers with a negative real part. From Table 5.1 (Case 5), we already know that the solution of the corresponding differential equation is a damped equation.

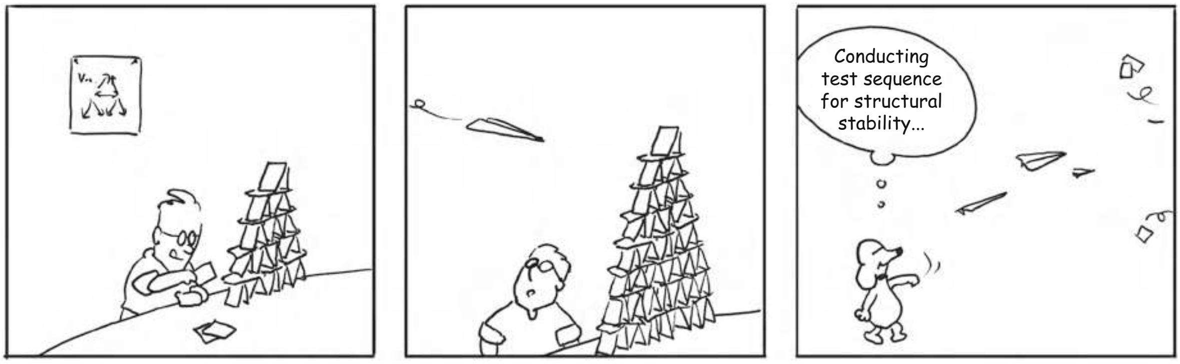
Let's take a closer look at these solutions. Analogously to Eq. (5.60), they have the form:

$$\begin{aligned}y_1(t) &= a_{1,1}\mathrm{e}^{(-\frac{\varepsilon}{2}+\mathrm{i}\omega)t} + a_{1,2}\mathrm{e}^{(-\frac{\varepsilon}{2}-\mathrm{i}\omega)t} \\ &= \mathrm{e}^{-\frac{\varepsilon}{2}t}\left[a_{1,1}\mathrm{e}^{\mathrm{i}\omega t} + a_{1,2}\mathrm{e}^{-\mathrm{i}\omega t}\right] \\ y_2(t) &= \mathrm{e}^{-\frac{\varepsilon}{2}t}\left[a_{2,1}\mathrm{e}^{\mathrm{i}\omega t} + a_{2,2}\mathrm{e}^{-\mathrm{i}\omega t}\right]\end{aligned} \tag{5.68}$$

If these equations are expressed by sine and cosine functions, we get a modified form of Eq. (5.60) where the factor $\mathrm{e}^{-\frac{\varepsilon}{2}t}$ appears in front of the right side of the equations. This additional term has a damping effect on the oscillation and ensures that the model reaches the steady state zero for $t \to \infty$ (see Fig. 5.11a). The seemingly unimportant small term $-\varepsilon y_2$ in Eq. (5.63) thus radically changes the long-term behavior of the model. We call this kind of behavior a *structural instability*.

Linear models with purely imaginary eigenvalues are structurally unstable.

Structural instability



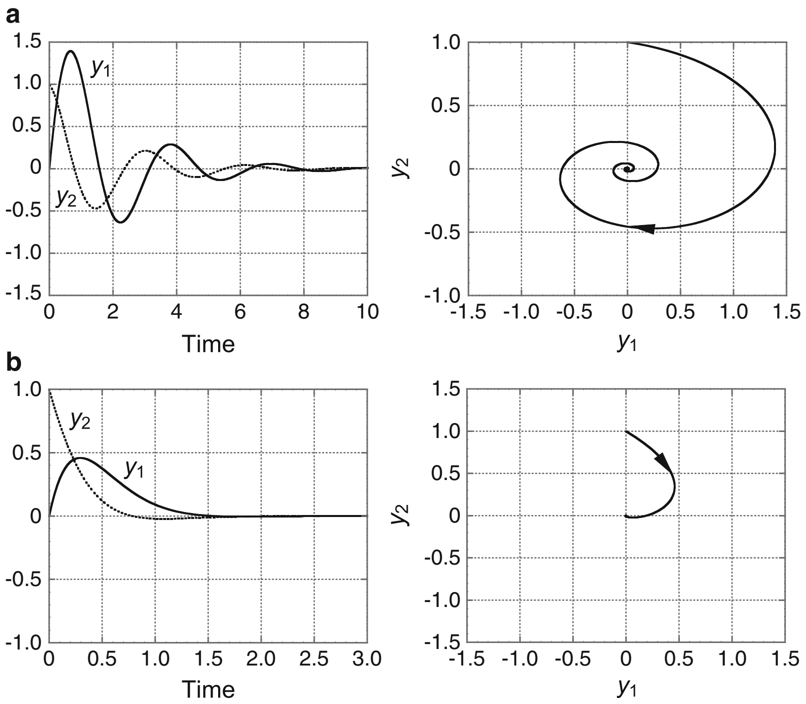


Fig. 5.11: *(**a**) Weakly damped oscillation, to the left as time diagram, to the right as phase diagram for* ($k_1 = 4, \; k_2 = 1$) *and* $\varepsilon = 1$. *(**b**) Strongly damped oscillation (creeping pendulum) with* $\varepsilon = 6$ *and an unchanged* k_i

If ε increases, but the condition $\varepsilon < 4k_1k_2$ still holds, the expression under the root in Eq. (5.67) remains negative, i.e. the eigenvalues remain non-real. However, the angular frequency ω (which, for weak damping, remains practically the same as in the undamped case) now drops to lower values:

$$\omega \to \omega^\star = \sqrt{k_1k_2 - \frac{\varepsilon^2}{4}} \tag{5.69}$$

A radical change of behavior takes place for

$$\frac{\varepsilon^2}{4} \geq k_1k_2 \tag{5.70}$$

According to Eq. (5.66), both eigenvalues are now real and negative and the system "creeps" without oscillation towards the steady state $y_1 = y_2 = 0$ (see Fig. 5.11b). As we will see in Example 5.11, the equations introduced in Examples 5.9 and 5.10 can be used to describe an oscillator or a pendulum, among other things. Therefore, a system with strong damping is also called a *creeping oscillation* or a *creeping pendulum*.

As a concrete example for a model with a structural instability, we use a classic example from physics: the harmonic oscillator. In Chap. 6, we will encounter another application from an entirely different field.

Example 5.11: The harmonic oscillator

We consider the mass M, which is held at rest by a spring with constant spring constant f. The spring constant describes the linear relation between the spring force K and the spring displacement x from its equilibrium position at $x = 0$:

$$K = -fx \tag{5.71}$$

If M is displaced from its equilibrium position, the mass is subjected to an acceleration according to Newton's laws of motion:

$$M\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = K = -fx \tag{5.72}$$

x	[L]	Displacement from equilibrium position
f	[MT^{-2}]	Spring constant (force per displacement)
M	[M]	Mass
K	[MLT^{-2}]	Spring force

As we might remember from school, the solutions of Eq. (5.72) are harmonic oscillations. To demonstrate the connection to the previous model (Eq. 5.55), we choose the following new variables to describe the harmonic oscillator:

$$\begin{aligned} y_1 &\equiv x \\ y_2 &\equiv \frac{\mathrm{d}x}{\mathrm{d}t} \end{aligned} \tag{5.73}$$

If we differentiate y_1 with respect to time t, it follows that:

$$\frac{\mathrm{d}y_1}{\mathrm{d}t} = \frac{\mathrm{d}x}{\mathrm{d}t} = y_2 \tag{5.74}$$

On the other hand, if we convert Eq. (5.72) with the relation

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = \frac{\mathrm{d}y_2}{\mathrm{d}t} \tag{5.75}$$

then it follows that:

$$M\frac{\mathrm{d}y_2}{\mathrm{d}t} = -fy_1 \tag{5.76}$$

or:

$$\frac{\mathrm{d}y_2}{\mathrm{d}t} = -\omega^2 y_1 \qquad \text{with} \qquad \omega = \sqrt{\frac{f}{M}} \tag{5.77}$$

The dynamic equation (5.72) for the harmonic oscillator is a second-order differential equation. With the conversions above, we have transformed it into a system of two first-order differential equations: (5.74) and (5.77). This system has the following coefficient matrix:

$$\mathbf{P} = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix} \tag{5.78}$$

This matrix has the same type of eigenvalues as Eq. (5.55). Therefore, the model of the harmonic oscillator must be structurally unstable as well. If we introduce a very small damping term (γ: damping constant) that is proportional to the speed of the moving mass M, $\frac{\mathrm{d}x}{\mathrm{d}t}$, we get:

$$M\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -fx - \gamma\frac{\mathrm{d}x}{\mathrm{d}t} \tag{5.79}$$

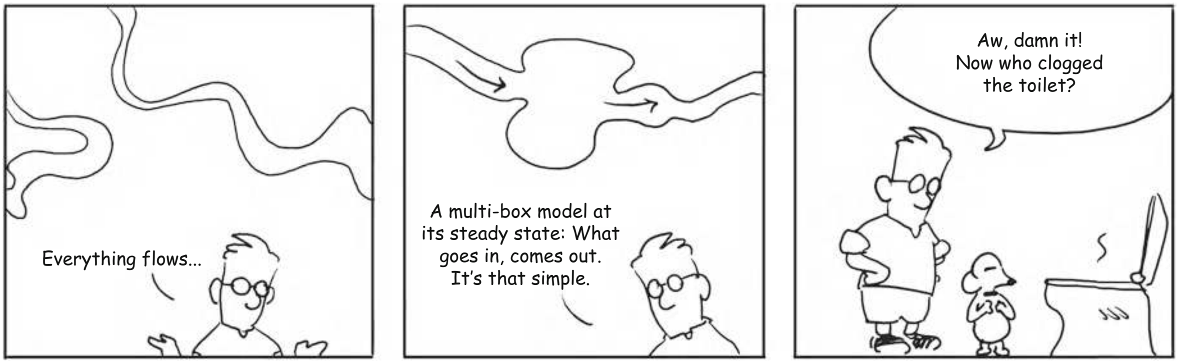
Or, transformed to a first-order system of differential equations:

$$\begin{aligned} \frac{\mathrm{d}y_1}{\mathrm{d}t} &= y_2 \\ \frac{\mathrm{d}y_2}{\mathrm{d}t} &= -\omega^2 y_1 - \frac{\gamma}{M}y_2 = -\omega^2 y_1 - \varepsilon y_2 \end{aligned} \tag{5.80}$$

The damping constant per mass, γ/M, takes over the role of ε in Eq. (5.63). The amplitude of the oscillation becomes smaller and smaller with time t, until the oscillator eventually remains still at its equilibrium position ($x = 0$). If the damping exceeds a certain value, the oscillator “creeps” into this position. We will return to this type of differential equations when we look at two-dimensional nonlinear systems in Chap. 6.

Let us now summarize our insight so far. To examine the behavior of a model and its steady state, we need to calculate the eigenvalues λ_i of the coefficient matrix. If both of them are real and negative or zero, the model reaches a steady state. If non-real eigenvalues occur, the model still reaches a steady state as long as their real parts are negative or zero. If purely imaginary eigenvalues occur, the model undergoes an undamped oscillation. Eigenvalues with positive real parts lead to solutions that diverge towards infinity.

Multi-box model



5.2 Linear Models with Several System Variables

Only a small step remains to move from linear models with two variables to linear models with more variables. The coefficient matrix $\mathbf{P}$ now becomes a $(n \times n)$ matrix, according to the number n of system variables:

$$\mathbf{P} = \begin{pmatrix} p_{1,1} & p_{1,2} & \cdots & p_{1,n} \\ p_{2,1} & p_{2,2} & \cdots & p_{2,n} \\ \vdots & & & \\ p_{n,1} & p_{n,2} & \cdots & p_{n,n} \end{pmatrix} \tag{5.81}$$

The solution of the resulting n-dimensional systems of differential equations in turn consists of sums of exponential terms of the form $\mathrm{e}^{\lambda_i t}$, where λ_i are the eigenvalues of the coefficient matrix.[8] For a model with n system variables we therefore get the following solution:

$$\begin{aligned} \mathcal{V}_1(t) &= a_{1,0} + a_{1,1}\mathrm{e}^{\lambda_1 t} + a_{1,2}\mathrm{e}^{\lambda_2 t} + \ldots + a_{1,n}\mathrm{e}^{\lambda_n t} \\ \mathcal{V}_2(t) &= a_{2,0} + a_{2,1}\mathrm{e}^{\lambda_1 t} + a_{2,2}\mathrm{e}^{\lambda_2 t} + \ldots + a_{2,n}\mathrm{e}^{\lambda_n t} \\ &\vdots \\ \mathcal{V}_n(t) &= a_{n,0} + a_{n,1}\mathrm{e}^{\lambda_1 t} + a_{n,2}\mathrm{e}^{\lambda_2 t} + \ldots + a_{n,n}\mathrm{e}^{\lambda_n t} \end{aligned} \tag{5.82}$$

Or, shorter:

$$\mathcal{V}_i(t) = a_{i,0} + \sum_{j=1}^{n} a_{i,j}\mathrm{e}^{\lambda_j t} \quad , \qquad i = 1, \ldots n \tag{5.83}$$

As in the case of two-dimensional models, the eigenvalues of the coefficient matrix are calculated with the characteristic equation. For larger matrices this is easiest with an appropriate computer program. The behavior of multi-dimensional models can then be analyzed by looking at the eigenvalues, just as we did for two-dimensional systems. If all eigenvalues are real and negative, the coefficients $a_{i,0}$ are identical with the corresponding steady states $\mathcal{V}_i^{\infty}$ of the system.

Only in few cases does it make sense to construct very large linear models. If circumstances require a complex model, it will often contain nonlinear components as well.[9] For this reason we will make do with a single example here (a further one can be found in Problem 5.3).

The carbon cycle is one of the most important geochemical cycles in our environment. We will try to describe it with a simplified linear multi-dimensional model.

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[8] For simplification, we assume that the system does not have multiple eigenvalues.

[9] Certain optimization problems can be described by very large linear systems of equations that are then solved with methods called *linear programming*.

Example 5.12: The global carbon cycle

Figure 5.12 shows the global carbon cycle in highly simplified form as a box diagram. Carbon is stored in three geochemical reservoirs: the atmosphere, the ocean surface and the deep sea. It is stored predominantly in the form of carbon dioxide (CO_2) as well as carbonate ($CO_3^=$ or HCO_3^-). Of course, carbon is continuously exchanged between these reservoirs. The fourth important reservoir is terrestrial biomass. Ocean biomass is so small that we can neglect it. The size of the four boxes and the width of the arrows roughly represent the system's pre-industrial steady state. By far the largest reservoir is the deep sea, while the atmosphere is the smallest. The fact that carbon exchange between the deep sea and the other reservoirs is small will be important for the model.

With the onset of rapid industrialization in the mid-nineteenth century, the combustion of fossil fuels (initially mostly coal, then also oil and gas) led to an increase of atmospheric CO_2 concentration. The pre-industrial CO_2 concentration was around 280 ppmv.[a] The value in the atmosphere box in Fig. 5.12 represents this concentration. Figure 5.13 shows the rapid increase of atmospheric CO_2 concentration during the past 150 years. By now, of course, the CO_2 concentration has surpassed 390 ppmv and the carbon cycle is no longer in an equilibrium.

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[a] The unit ppmv is a non-dimensional concentration measure. It means *parts per million per volume*, that is, 1 ppmv means that a 10^{-6} volume portion of the air consists of CO_2.

We want to construct a dynamic model from the pre-industrial steady state (Fig. 5.12). Then, we will treat the disturbance of the system through fossil fuel combustion as a singularity in time, i.e., we will introduce the total amount of 300×10^{15} g C into the atmosphere at time $t = 0$ in one fell swoop. This represents roughly the amount of carbon introduced to the atmosphere by the burning of fossil fuels between 1,850 and 2,000, not taking into account additional sources of carbon such as emissions from land-use change and deforestation.

We want to answer three questions with our model:

1. How does the carbon inventory $M_i(t)$ develop over time in the four boxes?
2. Where will the additional carbon be stored in the long term?
3. How long will it take for the system to reach an equilibrium again, if no further (anthropogenic or natural) disturbances occur?

How do we get from the static image in Fig. 5.12 to a dynamic model? At this point we have to make an assumption about how the fluxes $F_{i,j}$

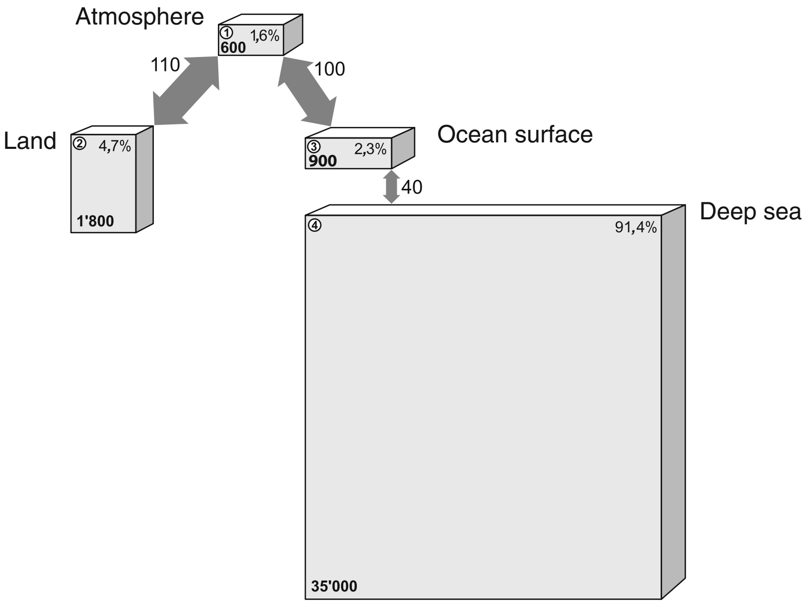

Fig. 5.12: *Simplified global carbon model with the most important exchange fluxes. The numbers in the boxes give the yearly carbon stock (unit is* $10^{15}\,g\,C$*), the numbers next to the arrows give the fluxes (unit* $10^{15}\,g\,C\,a^{-1}$*), the percent values give the relative proportion of the entire carbon stock that the box holds. The situation represents roughly the pre-industrial steady state (numbers are simplified from Moore et al. 1994)*

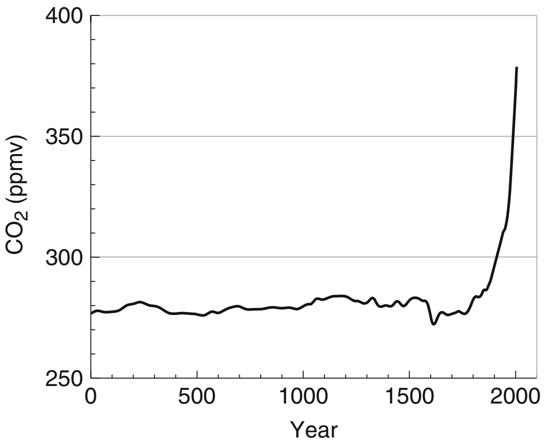

Fig. 5.13: *Atmospheric concentrations of* CO_2 *over the last 2,000 years (Source: Forster et al. (2007))*

between the boxes react to changes of substance mass in the reservoirs. We define them such that the first index (i) denominates the receiving box and the second index (j) the originating box (see Table 5.3). Since we want to construct a linear model, the simplest way is to describe the fluxes $F_{i,j}$ as linear functions of the content M_j of the originating box. To do so, we will first look at the two boxes *atmosphere* and *land* (Fig. 5.14).

Table 5.3: *Exchange rates and dynamic equations of the global linear carbon model. Labeling of fluxes and rates: first index = number of the destination box, second index = number of the originating box*

M_i	$[10^{15}\,\mathrm{g\,C}]$	Reservoir size of the box i
$F_{i,j}$	$[10^{15}\,\mathrm{g\,C\,year^{-1}}]$	Flux from box j into box i
$k_{i,j}$	$[\mathrm{year}^{-1}]$	linear flux rate for the transport from box j into box i

Calculation of the rates:

Because we assume $F_{i,j}$ to be proportional to the originating reservoir j, we get:

$$F_{i,j} = k_{i,j} M_j \qquad \text{thus} \qquad k_{i,j} = \frac{F_{i,j}}{M_j}$$

Values of the specific transfer rates $k_{i,j}$:

$k_{1,2} = 0.061\ \mathrm{a}^{-1}$	(Land → atmosphere)
$k_{2,1} = 0.183\ \mathrm{a}^{-1}$	(Atmosphere → land)
$k_{1,3} = 0.111\ \mathrm{a}^{-1}$	(Ocean surface → atmosphere)
$k_{3,1} = 0.167\ \mathrm{a}^{-1}$	(Atmosphere → ocean surface)
$k_{3,4} = 1.14 \times 10^{-3}\ \mathrm{a}^{-1}$	(Deep sea → ocean surface)
$k_{4,3} = 0.044\ \mathrm{a}^{-1}$	(Ocean surface → deep sea)

The dynamic mass balance equations for the reservoirs are:

$$\begin{aligned}
\frac{\mathrm{d}M_1}{\mathrm{d}t} &= -(k_{2,1} + k_{3,1})M_1 + k_{1,2}M_2 + k_{1,3}M_3 \\
\frac{\mathrm{d}M_2}{\mathrm{d}t} &= k_{2,1}M_1 - k_{1,2}M_2 \\
\frac{\mathrm{d}M_3}{\mathrm{d}t} &= k_{3,1}M_1 - (k_{1,3} + k_{4,3})M_3 + k_{3,4}M_4 \\
\frac{\mathrm{d}M_4}{\mathrm{d}t} &= k_{4,3}M_3 - k_{3,4}M_4
\end{aligned}$$

We calculate the specific exchange rates $k_{i,j}$ between land and atmosphere as follows:

$$\begin{aligned}
k_{1,2} &= \frac{F_{1,2}}{M_2} = \frac{110 \times 10^{15}\ \mathrm{g\ a^{-1}}}{1,800 \times 10^{15}\ \mathrm{g}} = 0.061\ \mathrm{a}^{-1} \\
k_{2,1} &= \frac{F_{2,1}}{M_1} = \frac{110 \times 10^{15}\ \mathrm{g\ a^{-1}}}{600 \times 10^{15}\ \mathrm{g}} = 0.183\ \mathrm{a}^{-1}
\end{aligned}$$

Table 5.3 shows the calculations for the transfer rates and the transport equations of the entire model. The smallest rates are, as we already noted, the ones between the ocean surface and the deep sea.

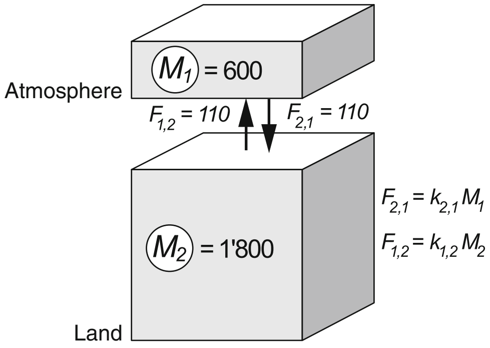

Fig. 5.14: *From the description of the steady state we can calculate exchange rates for a linear dynamic model by assuming that the flux between two boxes is a linear function of mass in the originating box (Excerpt from Fig. 5.12)*

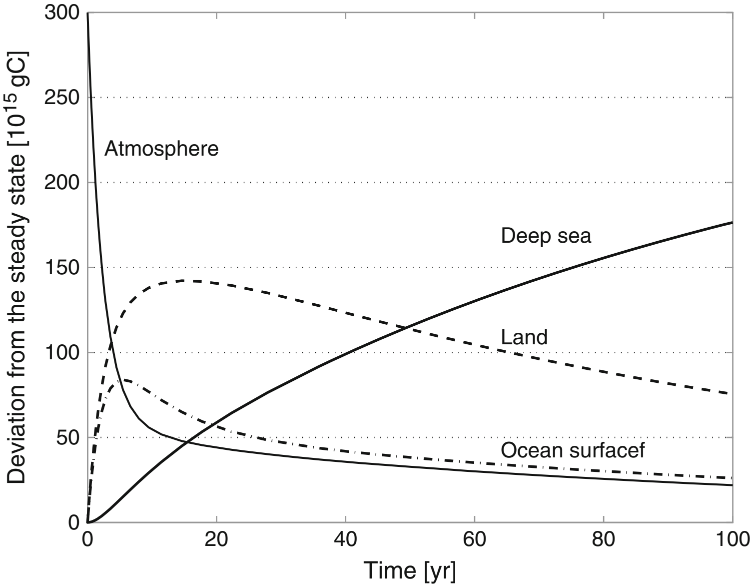

Fig. 5.15: *Numerical solution of the linear carbon model. Starting from the sudden addition of* 300×10^{15} *g C to the atmosphere, the figure shows the deviation of the four carbon reservoirs from their pre-industrial steady state as a function of elapsed time. Note that after 50 years, the system is still far from a new steady state. For any point in time the sum of all curves is equal to the added mass of* 300×10^{15} *g C*

How can this simple model be used to answer the three questions posed above? The dynamic development of the four carbon reservoirs $M_i(t)$ can be calculated analytically or with the aid of a computer program. In the first case, each variable $M_i(t)$ is described by a constant and four time-dependent exponential functions (see Eq. 5.83). The initial values of $M_i (i = 2, 3, 4)$ are those in Fig. 5.12, while the atmospheric reservoir (M_1) is increased by the anthropogenic input of 300×10^{15} to 900×10^{15} g C.

Figure 5.15 shows the result of a numerical simulation of the model's development through time. As expected, the biggest reservoir, M_4 (the deep sea), reacts most slowly. That is because it's only coupled to the other reservoirs by a fairly small (relative to the reservoir size) mass flux.

The second question, regarding the new steady state, can easily be answered from Table 5.3 without solving the system of equations. Because we are dealing with a linear homogeneous model, the relative sizes of the M_i at steady state remain unchanged, i.e. as given by the pre-industrial values of Fig. 5.12. In other words: Each box absorbs an amount of the additional carbon ($300 \times 10^{15}\,\mathrm{g\,C}$) in proportion to its original size. Even though the deep sea reacts slowly, it will—always according to our simple model—eventually contain 91.4 % of the additional carbon. Overall, the $300 \times 10^{15}\,\mathrm{g\,C}$ only make up 0.8 % of the sum of all reservoirs ($38'300 \times 10^{15}\,\mathrm{g\,C}$). In the new steady state, the reservoirs will therefore have grown by less than 1 % of their original size. In fact, the carbon drama of modern society is not primarily one of total mass but results from the unfavorable fact that by burning fossil fuels we load a fairly small carbon reservoir which is dynamically "far away" from the largest reservoir, the deep sea.[10]

Finally, to predict how long it will take for the new equilibrium to be reached (thereby answering our last question), we need to calculate the eigenvalues of the coefficient matrix **P**:

$$\mathbf{P} = \begin{pmatrix} -0.35 & 0.061 & 0.111 & 0 \\ 0.183 & -0.061 & 0 & 0 \\ 0.167 & 0 & -0.155 & 0.00114 \\ 0 & 0 & 0.044 & -0.00114 \end{pmatrix} \tag{5.84}$$

Because **P** is constructed from the steady-state solution of a *homogeneous* system of equations, the matrix must be singular with one eigenvalue of zero. The result of a numerical eigenvalue calculation confirms this prediction.
We get:

$$\begin{aligned} \lambda_1 &= -0.443\,\mathrm{year}^{-1} \\ \lambda_2 &= -0.114\,\mathrm{year}^{-1} \\ \lambda_3 &= -0.00971\,\mathrm{year}^{-1} \\ \lambda_4 &= 0 \end{aligned}$$

Thus, we can estimate the adjustment time with Eq. (5.16):

$$\tau_{5\,\%} \approx \frac{3}{\min\left(|\lambda_i| \neq 0\right)} = \frac{3}{0.00971\,\mathrm{year}^{-1}} \approx 310\,\mathrm{year} \tag{5.85}$$

Of course, this carbon model is not very realistic. First, we treated the anthropogenic disturbance as a single input event. Figure 5.13 however shows that an exponentially growing input function comes much closer to reality. A second simplification is the assumption that all fluxes are linear functions of the reservoir sizes.

Nevertheless, the model illustrates important properties of the carbon cycle that are confirmed by more complex models. As mentioned above, the anthropogenic disturbance, although relatively small compared to the natural fluxes, has a large impact on the atmosphere for two reasons: the

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[10] Of course, this leaves aside the increasing acidity of our oceans as a result of their atmospheric carbon uptake, a process which has severe effects of its own.

disturbance is directed at the smallest reservoir, and that reservoir is positioned “far” from the main reservoir—the deep sea. Experienced systems thinkers will be able to make qualitative statements like this just from looking at Fig. 5.12 and the sizes of the different mass transfer rates $k_{i,j}$.

5.3 Questions and Problems

Question 5.1: In many cases, one-dimensional models are insufficient to describe important properties of a system. Name different possibilities to further develop a one-dimensional model into a two-dimensional or multi-dimensional model.

Question 5.2: To at least how many model parameters can a two-dimensional linear homogeneous model be reduced?

Question 5.3: Which properties/characteristic quantities of the coefficient matrix of a multi-dimensional model are important for the temporal behavior of the system variable?

Question 5.4: What is the characteristic equation of a matrix?

Question 5.5: Homogeneous linear systems of differential equations with real eigenvalues only have a steady state if the coefficient matrix has a certain property. Which one?

Question 5.6: What is meant by the structural instability of a model?

Question 5.7: What is a hierarchical linear model? Give a systemic and a mathematical explanation/definition.

Question 5.8: Which property of a linear system is indicated by the occurrence of an eigenvalue of zero?

Question 5.9: For a car, the parts that behave like a creeping pendulum play an important role. If they lose this property, they urgently need replacement. Which parts are they?

Question 5.10: How can the overall reaction rate of a linear model be determined? Are there special cases where some system variables move towards a steady state much more rapidly than the overall rate would indicate? Give a mathematical explanation and a concrete example.

Question 5.11: CO_2 sequestration is the idea of capturing and pumping anthropogenic CO_2 into the deep sea. Why would this idea make sense from a systems point of view, leaving aside the negative ecological consequences and the technical difficulties? How would Fig. 5.15 look qualitatively, if the entire anthropogenic carbon output were deposited in the deep sea right from the outset?

Question 5.12: The net flux between two neighboring spatial boxes can be described as a linear function of the concentration difference between them. In Example 5.8 we applied this principle. What idea is it based on?

Problem 5.1: Reactor with two substances

In Examples 5.1–5.3 we analyzed a reactor with through-flow in which a chemical conversion between the substances A and B takes place. Calculate the development of the concentrations $C_A(t)$ and $C_B(t)$ for the parameters given in Example 5.2, an input concentration of $C_A^{in} = 1$ mol m^{-3}, and the initial concentrations $C_A^0 = C_B^0 = 0$.

Problem 5.2: Chain of lakes

Let's take another look at Example 5.6 with the radioactive isotopes in the chain of lakes:

(a) The model equations for the total isotope mass in the two lakes (Eq. 5.32) cannot be solved, because apart from M_i, they also contain the "extrinsic" concentrations C_i. Transform the system of equations so that a solvable two-dimensional linear system of differential equations for M_i results. Show that the eigenvalues are identical with those of Eq. (5.33) for C_i.

(b) Combine the two lakes into a "super system" and formulate the differential equation for the sum of the isotope mass in both lakes, $M = M_1 + M_2$. Why does this not result in a one-dimensional model? Which additional assumption is needed for it to become one?

(c) Why doesn't it make sense to apply the same procedure to the sum of *concentrations*?

Problem 5.3: Radioactive decay chain with three isotopes

Consider the decay chain of three radioactive isotopes:

$$^{222}\mathrm{Rn} \rightarrow \ldots\ ^{214}\mathrm{Pb} \rightarrow\ ^{214}\mathrm{Bi} \rightarrow \ldots\ ^{210}\mathrm{Pb}\,(\rightarrow)$$

The dots indicate that we are neglecting certain intermediate products with a very short half-life. Although ^{210}Pb is not stable either, it has a much larger half-life than the other isotopes shown in the chain. Its decay plays no role in the following problem.

To simplify, we choose the following notation (half-life in parentheses):

$$X \equiv\ ^{222}\mathrm{Rn}\ (3.8\ \mathrm{d}), \quad Y \equiv\ ^{214}\mathrm{Pb}\ (26.8\ \mathrm{min}), \quad Z \equiv\ ^{214}\mathrm{Bi}\ (19.8\ \mathrm{min})$$

Establish the system of differential equations for the activities A_i and calculate the coefficient matrix. Then, calculate the activity of ^{214}Bi as a function of time, $A_Z(t)$, and from that, derive a an approximate formula for $t > 10$ h. The initial activities A_i^0 are: $A_X^0 = 1{,}000$ Bq, $A_Y^0, A_Z^0 = 0$ Bq. (1 Bq = 1 decay per second).

Problem 5.4: Tritium in a sewage treatment plant

A simplified description of a sewage treatment plant is given in the box diagram below (Fig. 5.16). At time $t = 0$, an accident causes a substantial amount of the radioactive isotope tritium to enter the combined sedimentation and aeration tank. In the tank, a tritium activity of $A_1(0) = 10^6\,\mathrm{Bq/m^3}$ (1 Bq = 1 Bequerel = 1 decay per second) is measured. After this isolated input event, the tritium activity in the inflow is once again zero.

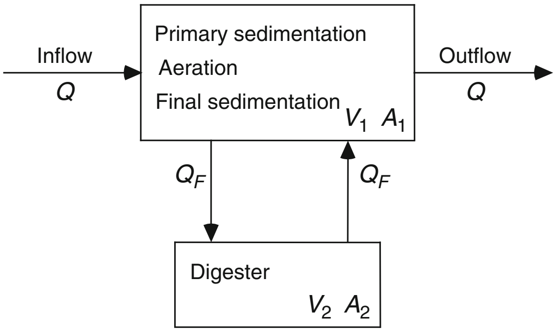


Fig. 5.16: *Box diagram of a sewage treatment plant*

$$V_1 = 10^4\,\mathrm{m}^3 \qquad Q = 10^4\,\mathrm{m^3 d^{-1}}$$
$$V_2 = 3{,}000\,\mathrm{m}^3 \qquad Q_F = 60\,\mathrm{m^3 d^{-1}}$$

(a) Establish the dynamic equations for the tritium activities in the combined sedimentation/aeration tank ($A_1(t)$) and in the anaerobic digestion tank ($A_2(t)$) for the time after the accident ($t > 0$).

(b) The half-life of tritium is $t_{1/2} = 12$ year. Compare the decay constant of tritium with the different water transport rates of the system. How large is the influence of radioactive decay on the tritium activity in the plant's outflow?

(c) Estimate the eigenvalues of the system. Hint: set the absolutely smallest matrix element and the radioactive decay constant of tritium equal to zero.

(d) With what rate does the activity in the outflow decline after a few months?

Problem 5.5: Stratified lake with sedimentation

We consider a stratified lake with a total volume of $V_{tot} = V_1 + V_2 = 3 \times 10^8\,\mathrm{m}^3$. The volume of the surface layer V_1 is $1 \times 10^8\,\mathrm{m}^3$. Inflow and outflow (rate $Q = 1 \times 10^6\,\mathrm{m^3\,d^{-1}}$) only occur via the surface layer. The vertical exchange rate between the two layers is $Q_{ex} = 5 \times 10^6\,\mathrm{m^3\,d^{-1}}$.

(a) How large is the average water retention time

- In the volume V_1 with respect to inflow, outflow and exchange rate?
- In the volume V_2 with respect to the exchange rate?

(b) A conservative substance (inflow concentration $C_{in} = 100\,\mathrm{mg\,m^{-3}}$) flows into the lake at time $t = 0$. For $t < 0$, $C_1(t) = C_2(t) = 0$. Calculate the steady state concentrations C_1^{∞} and C_2^{∞}. How long does it take for the system to approach these values up to 5 %?

(c) How do the answers to question (b) change if the substance is radioactive with a decay constant of $k_\lambda = 1 \times 10^{-2}\,\mathrm{d^{-1}}$?

(d) Answer question (b) for a non-radioactive (that is, conservative) substance which adsorbs on particles and then gets transported with them from the surface into the deep water and finally to the sediment. The relevant flows are linear functions of the masses $M_1 = C_1\,V_1$ and $M_2 = C_2\,V_2$:

Transport $V_1 \rightarrow V_2 : k_{s1}\,M_1$
Transport $V_2 \rightarrow \text{sediment} : k_{s2}\,M_2$
Use $k_{s1} = 0.02\,\mathrm{d^{-1}}, k_{s2} = 0.005\,\mathrm{d^{-1}}$.

Also, neglect the fact that the lake's cross section decreases with depth, i.e., assume that the entire sediment flux from V_1 ends up in the volume V_2. Remember that at the transition from equations for M_i to those for C_i the volumes are different: not the same amount of mass leaves V_1 per volume as arrives in V_2 per volume (Eqs. 5.45–5.48 may be helpful here).

(e) Compare the results from (b) to those from (d) and attempt to explain qualitatively the respective ratios between C_1^{∞} and C_2^{∞}.

Problem 5.6: Conservative substance in a chain of lakes
We consider two successive, completely mixed lakes (volumes V_1 and V_2), with a constant through-flow Q_0.

$V_1 = 1 \times 10^5\,\mathrm{m^3} \quad , \quad V_2 = 2 \times 10^6\,\mathrm{m^3}$
$Q_0 = 1 \times 10^5\,\mathrm{m^3\,d^{-1}}$

(a) Due to an accident, $M = 200\,\mathrm{kg}$ of a conservative pollutant enters the upper lake (Lake 1) at $t = 0$. Describe the concentration development in both lakes, $C_1(t)$ und $C_2(t)$. How long does it take until $C_1(t)$ and $C_2(t)$ have decreased to 10 µg/L?

(b) What is the maximum concentration reached in Lake 2, and when is it reached?

(c) After 5 days, measurements show that the concentration in Lake 2's outflow is decreasing exponentially ($e^{-\alpha t}$). How large is α?

(d) How would $C_1(t)$ and $C_2(t)$ change if, for storing electric energy, water would be pumped at an average rate of $Q_p = 4 \times 10^5\,\mathrm{m^3\,d^{-1}}$ from Lake 2 to Lake 1, and the flow from Lake 1 to Lake 2 would increase correspondingly by Q_p? When do C_1 and C_2 decrease below 10 µg/L?

(e) Explain the differences between the results from (a) and (d) qualitatively.

Problem 5.7: Temperature control by a thermostat

The heating system of a building is controlled by a thermostat. The thermostat opens and closes the valve of the system which feeds warm water into the radiators mounted throughout the building. The system works as follows:

1. Without heating, the building temperature y would decrease due to heat loss through the walls and windows by the constant rate L:

$$\frac{\mathrm{d}y}{\mathrm{d}t} = -L$$

2. The temperature increase per unit of time due to heating is proportional to the position of the valve, x, where $x = 0$ means that the valve is closed. For simplicity, it is assumed that x has no upper limit. The proportionality factor is k_1.
3. The valve opens and closes with a speed which is linearly related to the difference between the actual room temperature y and the target room temperature y_0. The proportionality factor is k_2.

Answer the following questions:

(a) Formulate the set of differential equations for x and y and discuss the properties of the solutions. Is a steady state reached?

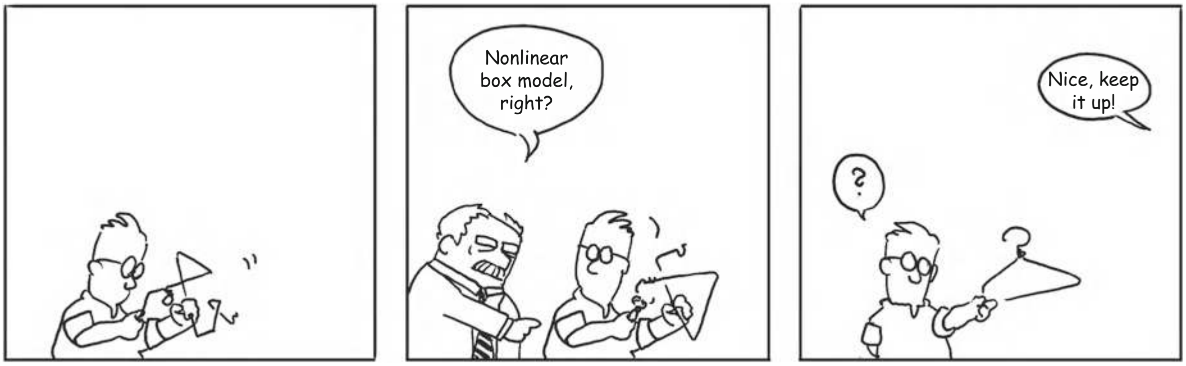
(b) Discuss the limits of the model. Hint: in some cases the position of the valve may become negative. What happens qualitatively to the solution if the dynamic equations are modified such that $\mathrm{d}x/\mathrm{d}t$ becomes 0 as soon as x drops below 0?

(c) How should the coefficients k_1 and k_2 be chosen to make the oscillations of y small?

(d) Are there other means to dampen the temperature fluctuations in the building?

Chapter 6

Nonlinear Models



Natural systems are rarely linear. Even if they are, that linearity often exists only within a limited range of the system variables $\mathcal{V}_i$. Indeed, the surprising diversity in the behavior of natural systems is mostly a result *nonlinear* processes. Despite ever more powerful computers, the behavior of many nonlinear systems can only be predicted over small periods: the weather forecast is a prime example of this.

Continuous nonlinear systems (in time) are described by nonlinear differential equations. If the system variables are continuous in time *and* space, we are dealing with nonlinear partial differential equations, such as those occurring in fluid dynamics. The field of fluid dynamics describes the dynamics of gaseous and fluid systems and forms the basis of atmospheric science and oceanography. It can be used to model such phenomena as the Gulf stream or a tropical cyclone. In this chapter, we will start with spatially discrete models, i.e. our usual box model approach. In Chap. 8 we will introduce spatially continuous models and get a first glimpse at the colorful world of these types of models.

Nonlinear differential equations can only be solved analytically in special cases. We usually have to apply numerical methods, which is not the topic of this book. In some cases, however, nonlinear models can be approximated by linear equations so that their behavior near the steady state

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can be analyzed. But in this chapter we will also go beyond such approximations and discuss some behavioral traits of nonlinear models that have no resemblance with the behavior of their linear siblings anymore.

6.1 Nonlinear Models with One System Variable

6.1.1 Autonomous Nonlinear Models

Let's look at a first-order nonlinear system[1] with *one* system variable $\mathcal{V}$. In the most general case, it can be described by the following differential equation:

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = g(\mathcal{V}(t), t) \tag{6.1}$$

With this seemingly cumbersome notation we want to point out that the general function g can depend on time both explicitly and implicitly via $\mathcal{V}$ (see Sect. 4.1). The explicit time dependence arises from the external and the implicit time dependence from the internal relations.

In many cases (but not in all) we can functionally separate the influence of external and internal relations, so that we can rewrite Eq. (6.1) in the following form:

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = \mathcal{R}(t) + f(\mathcal{V}) \tag{6.2}$$

Some points to note: we want the function of the external relation $\mathcal{R}$ to be independent of $\mathcal{V}$. If it is constant in time, it can be integrated into the function f. In that case the system is *autonomous*. We also don't want f to explicitly depend on time. Finally, $f(\mathcal{V})$ determines whether the model is linear: if $f(\mathcal{V})$ is *not* of the form $a + b\mathcal{V}$, the model is nonlinear.

Let's examine an *autonomous* (i.e. $\mathcal{R} = 0$) nonlinear model more closely. A classic example is the logistic growth model. It was introduced by Verhulst (1838) to describe population growth. Pearl and Reed (1920) used it to model population dynamics in the United States from 1790 on. The logistic growth model was the basis on which many later models in population ecology were based (see e.g. Krebs 2001, May and McLean 2007).

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[1] As a reminder: *First-order* means that only the first derivative of $\mathcal{V}$ with respect to time appears. Systems with higher derivatives, which are often found in physics, can be transformed into multi-dimensional first-order systems (see Example 5.11).

Example 6.1: Logistic growth model

In Example 4.2 we discussed the exponential growth model. Exponential growth cannot go on forever, because the population would grow to infinity. The logistic growth model "fixes" this behavior: for small population sizes N, growth is exponential, but it levels off as population increases, eventually becoming zero. In a similar fashion as in Eq. (4.11), we can describe logistic growth with a specific growth rate k_p, which now itself depends on N:

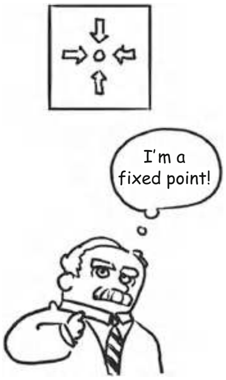
$$\frac{\mathrm{d}N}{\mathrm{d}t} = k_p(N) \cdot N \tag{6.3}$$

For $k_p(N)$ we choose a function that decreases linearly from a maximum value k_p° at $N = 0$, reaching zero at $N = N_{max}$: $k_p = k_p^\circ(1 - \frac{N}{N_{max}})$. Inserting this in Eq. (6.3) yields:

$$\frac{\mathrm{d}N}{\mathrm{d}t} = k_p^\circ(1 - \frac{N}{N_{max}})N \equiv f(N) \tag{6.4}$$

The growth rate k_p° has the dimension $[\mathrm{T}]^{-1}$, N_{max} has the same dimension as N, e.g. a population number, or a population number per surface area.

For the following considerations it will be helpful to plot the change function $f(N)$. In our example, $f(N)$ is a parabola with a downward facing opening that intersects the N-axis at $N = 0$ and $N = N_{max}$ (Fig. 6.1a). These two N-intersects of $f(N)$ show where the function $N(t)$ "stands still", that is, where $\frac{\mathrm{d}N}{\mathrm{d}t} = 0$. Thus, they are called *fixed points*. The linear models we dealt with so far had at most *one* fixed point, which we called the steady state.[2] Now, however, we have two. This begs the question whether the system is moving towards one of the fixed points, and if so, towards which one.



In the next section we will discuss a general recipe to answer that question. For our current example, it is easy to see that the population $N(t)$ develops towards the value N_{max} except in the case where the initial value N^0 is zero, since from nothing, nothing can grow! In fact, the differential equation (6.4) can be analytically integrated, which gives the following result[3]:

$$N(t) = N_{max}\frac{N^0}{(N_{max} - N^0)\,\mathrm{e}^{-k_p^\circ t} + N^0} \tag{6.5}$$

---

[2] From now on we will only speak of fixed points, since the concept of a steady state makes less sense as we move towards higher-dimensional and more abstract models.

[3] Since discussing fundamental mathematical principles is not the aim of this book, we will not go through the integration of Eq. (6.4) in detail. Just one note: the solution can be derived by using the variable separation method.

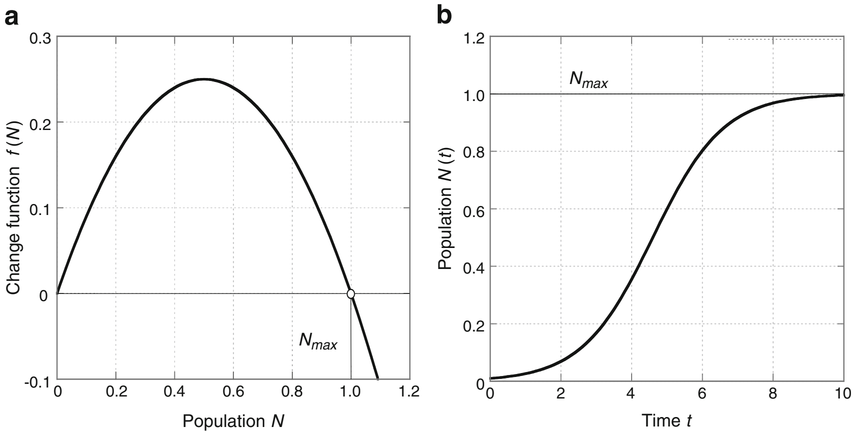


Fig. 6.1: *The logistic growth model: (**a**) change function* $\frac{\mathrm{d}N}{\mathrm{d}t} = f(N)$ *for* $k_p^\circ = 1$ *and* $N_{max} = 1$*; (**b**) behavior of the population size* $N(t)$ *(see Eq. 6.5) for* $k_p^\circ = 1$, $N_{max} = 1$ *and* $N^0 = 0.01$

Equation (6.5) is shown in Fig. 6.1b. If the initial state is $N^0 \ll N_{max}$, $N(t)$ initially (if $t \ll (k_p^\circ)^{-1}$) grows exponentially ($N(t) = N^0 \mathrm{e}^{k_p^\circ t}$) and, for $t \gg (k_p^\circ)^{-1}$, reaches the constant value N_{max}.

6.1.2 Fixed Points of Nonlinear Models with One Variable

In Sect. 4.2.1 we saw that a linear one-dimensional differential equation has at most *one* fixed point. If the inhomogeneous term is constant, the system approaches this fixed point irrespective of its initial state. In contrast, as Example 6.1 shows, a nonlinear model can have several fixed points. This leads to the question whether there are any general rules describing the system's behavior around these fixed points. In this section, we will first formulate an answer for one-dimensional models. The more complex situation of multi-dimensional nonlinear models will follow in Sect. 6.2.

The following discussion assumes that the external relation $\mathcal{R}$ is constant in time, since otherwise the system would not have any constant fixed points. We therefore write Eq. (6.1) in the following form:

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = g(\mathcal{V}), \tag{6.6}$$

We also allow for a possible constant external relation, incorporating it into the change function $g(\mathcal{V})$, and treat the system as autonomous. We assume that $g(\mathcal{V})$ has k roots $\mathcal{V}_i^\infty (i = 1, \ldots, k)$, that is, the following holds for all $\mathcal{V}_i^\infty$:

$$g(\mathcal{V}_i^\infty) = 0 \qquad \text{for} \quad i = 1, \ldots, k \tag{6.7}$$

The $\mathcal{V}_i^\infty$ are then fixed points of the differential equation (6.6). If the system variable $\mathcal{V}$ reaches a fixed point, the model stays put at that position, because:

$$\left.\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t}\right|_{\mathcal{V}_i^\infty} = 0 \tag{6.8}$$

$\mathcal{V}$ cannot move away from this point, except if the external relation $\mathcal{R}$ (and with it, $g(\mathcal{V})$) were to change.

The fixed points of a one-dimensional systems are therefore the roots of $g(\mathcal{V})$. If $g(\mathcal{V})$ is an n-degree polynomial, there is a maximum of n real roots. These, together with the virtual fixed points $\mathcal{V} = \infty$ und $\mathcal{V} = -\infty$, divide the $\mathcal{V}$-axis into $(n + 1)$ intervals (Fig. 6.2a). Because a one-dimensional system can only move along one variable axis, each fixed point represents a barrier that the system cannot overcome. Sections between two neighboring fixed points are called *invariant areas*. They are a characteristic feature of one-dimensional models. In two- and n-dimensional models, the system can move in a two or n-dimensional space (see Fig. 5.2). Therefore, fixed points can usually be "bypassed".

Intervals between fixed points of a one-dimensional nonlinear model are called invariant areas.

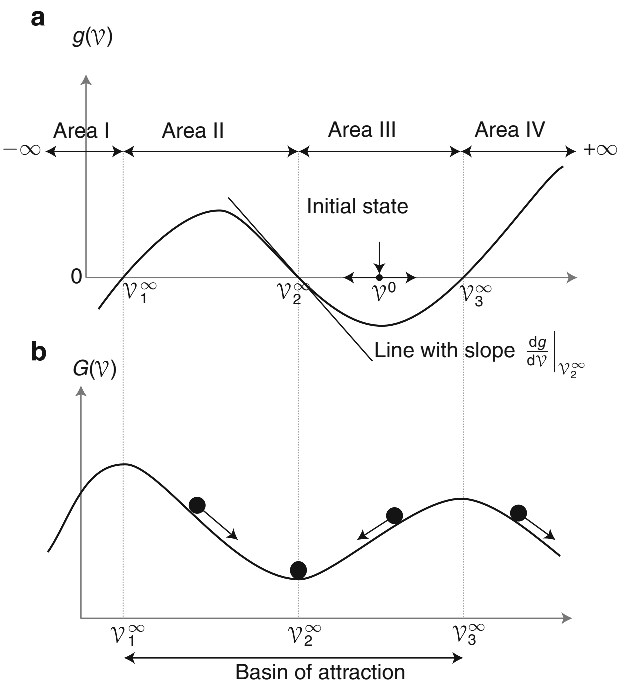


Fig. 6.2: *(**a**) A one-dimensional system with three fixed points partitions the variable axis into four so-called invariant areas (I–IV). From the initial state* $\mathcal{V}^0$*, the system can only move to the fixed points* $\mathcal{V}_2^\infty$ *and* $\mathcal{V}_3^\infty$*. It cannot leave the invariant area III, however. (**b**) Topographic illustration of the same stability conditions as in (**a**), as what we call a stability landscape. The ball (which is infinitely damped, i.e., does not behave like a ball in reality) stays still at* $\mathcal{V}_2^\infty$*.* $\mathcal{V}_1^\infty$ *and* $\mathcal{V}_3^\infty$ *are unstable positions, at which a small nudge in either direction will set the ball in motion. Relation between* $g(\mathcal{V})$ *and* $G(\mathcal{V})$*:* $g(\mathcal{V}) = -\frac{dG(\mathcal{V})}{d\mathcal{V}}$

Let's imagine a model with an initial state $\mathcal{V}^0$ lying inside area III of Fig. 6.2a. So far, we don't know towards which of the neighboring fixed points this model will move. But we can attempt to answer the question intuitively: in area III, as we can see in Fig. 6.2a, $g(\mathcal{V})$ is negative. According to Eq. (6.6), $\mathrm{d}\mathcal{V}/\mathrm{d}t < 0$, that is, $\mathcal{V}$ decreases and the model moves leftwards on the $\mathcal{V}$ axis. This movement keeps up until the model reaches the fixed point $\mathcal{V}_2^\infty$, where it stops and remains.

To make these thoughts more formal, we can look at the change function $g(\mathcal{V})$ in the immediate vicinity of the fixed point $\mathcal{V}_i^\infty$, e.g. at $\mathcal{V}_i^\infty + \varepsilon$ with a small ε. We can then describe $g(\mathcal{V})$ at the point $\mathcal{V}_i^\infty$ as a Taylor series[4] and abort after the linear term:

$$g(\mathcal{V}_i^\infty + \varepsilon) \approx g(\mathcal{V}_i^\infty) + \varepsilon \frac{\mathrm{d}g(\mathcal{V})}{\mathrm{d}\mathcal{V}}\bigg|_{\mathcal{V}_i^\infty} \tag{6.9}$$

However, since $\mathcal{V}_i^\infty$ is a fixed point, $g(\mathcal{V}_i^\infty) = 0$. Thus, it follows from Eqs. (6.6) and (6.9):

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t}\bigg|_{\mathcal{V}_i^\infty + \varepsilon} = g(\mathcal{V}_i^\infty + \varepsilon) \approx \varepsilon \frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\bigg|_{\mathcal{V}_i^\infty} \tag{6.10}$$

Because the derivative $\frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}|_{\mathcal{V}_i^\infty}$ is independent of ε, our approximation in Eq. (6.10) replaces the function $g(\mathcal{V})$ with a straight line in the vicinity of $\mathcal{V}_i^\infty$. In other words, we have created a linear model out of a nonlinear one. Figure 6.2a shows the linearized velocity function in the proximity of $\mathcal{V}_2^\infty$. If we define $k \equiv \frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\Big|_{\mathcal{V}_2^\infty}$[5] and describe ε as the deviation of the momentary state from the fixed point $\mathcal{V}_2^\infty, \varepsilon = \mathcal{V} - \mathcal{V}_2^\infty$ then Eq. (6.10) becomes:

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = k(\mathcal{V} - \mathcal{V}_2^\infty) = -k\mathcal{V}_2^\infty + k\mathcal{V} \tag{6.11}$$

This is nothing else than the linear inhomogeneous differential equation (4.5) with constant coefficients. If $k < 0$, the solution tends to the fixed point $\mathcal{V}_2^\infty$. For $k > 0$ the model moves away from it.[6] For $k = 0$ the system is indifferent: it just stands still where it is. These statements are valid whether the initial state is to the left or right of the fixed point in question, as long as the absolute value of the deviation $|\varepsilon|$ is not too large. The fixed point $\mathcal{V}_2^\infty$ in Eq. (6.2) "attracts" the system inside area II as well. We thus call $\mathcal{V}_2^\infty$ a stable fixed point or an attractor. Areas II and III together form its basin of attraction.

In contrast, the model moves away from the fixed point $\mathcal{V}_3^\infty$ in both directions as soon as it deviates to the left or right by the small value ε.

---

[4] A function $g(x)$ that is n times differentiable can be described as a power series (Taylor series) in the vicinity of location x_0:
$g(x) = g(x_0) + (x - x_0)\frac{g'(x_0)}{1!} + (x - x_0)^2 \frac{g''(x_0)}{2!} + \ldots + (x - x_0)^n \frac{g^{(n)}(x_0)}{n!} + \ldots$

[5] You can verify that k has the dimension $[\mathrm{T}]^{-1}$.

[6] If the system were indeed linear, $\mathcal{V}$ would tend to ∞. Since Eq. (6.11) is only valid for the vicinity of $\mathcal{V}_2^\infty$, this is of course not generally true for a nonlinear model.

Formally, this can also be seen from Eq. (6.11) since here, $k > 0$. This is called an unstable fixed point. It is like a needle standing on its tip: theoretically, there is a point where it can stand still, but in reality even just the disturbance caused by thermal movements prevents the needle from remaining upright.

Figure 6.2b shows the stability relations by using a topographic function $G(\mathcal{V})$, where $g(\mathcal{V}) = -\frac{\mathrm{d}G}{\mathrm{d}\mathcal{V}}$. Stable fixed points correspond to a minimum, unstable ones to a maximum of the topographic function $G(\mathcal{V})$.

The stable and unstable fixed point are shown in Fig. 6.3 (cases 1 and 2). The figure further shows four functions (cases 3 through 6) whose slope $k \equiv \frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\Big|_{\mathcal{V}_i^\infty}$ is zero at the fixed point. Cases 3 and 4 are one-sided attractors; we call these fixed points one-sided stable. In case 5, within a finite area around the fixed point, the model does not move. This fixed point is called indifferent. Finally, case 6 shows a velocity function whose first nonzero term of the Taylor series is the third differentiation. An example of such a curve would be $g(\mathcal{V}_6^\infty + \varepsilon) = \alpha\varepsilon^3$. If $\alpha < 0$ (corresponding to case 6 in the figure), the fixed point is stable, for $\alpha > 0$ it is unstable.

Let's summarize: the slope of the change function $g(\mathcal{V})$ determines the character of the fixed point, according to the following rules:

$$
\begin{array}{ll}
\left.\dfrac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\right|_{\mathcal{V}_i^\infty} < 0 & \text{Stable fixed point } \mathcal{V}_i^\infty \\
\left.\dfrac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\right|_{\mathcal{V}_i^\infty} > 0 & \text{Unstable fixed point } \mathcal{V}_i^\infty \\
\left.\dfrac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\right|_{\mathcal{V}_i^\infty} = 0 & \begin{array}{l}\text{Higher-order differentiations of} \\ g(\mathcal{V}) \text{ need to be considered}\end{array}
\end{array}
\tag{6.12}
$$

If a model only has *one* attractor towards which all systems initiated in finite space move, that attractor is called asymptotically stable, or global. Since the change function of a linear model is a straight line, a linear model has one root at most, and thus a single fixed point. This can be stable or

Linear models have one attractor at most. It is asymptotically stable (or global).

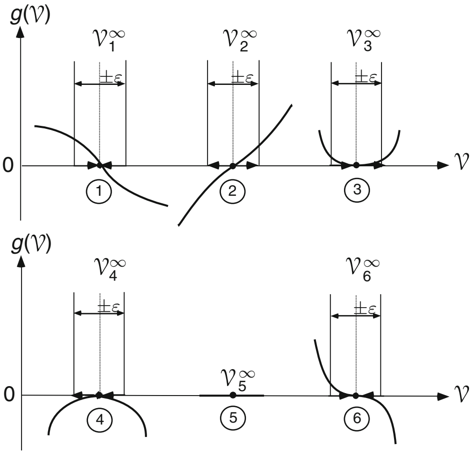


Fig. 6.3: *The various fixed points of a one-dimensional model* $\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = g(\mathcal{V})$*. The fixed points are the roots of* $g(\mathcal{V})$*. The slope of* g *at the fixed point* ($k \equiv \frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\big|_{fixedpoint}$) *determines the fixed point's character: (1)* $k < 0$*: stable, (2)* $k > 0$*: unstable, (3) and (4)* $k = 0$*: one-sided stable, (5)* $k = 0$*: indifferent, (6) first and second differentiation at* $\mathcal{V}_6^\infty$ *are zero (see text). The arrows give the model's direction of movement*

unstable, depending on whether the specific rate k is positive or negative. If $k < 0$, the only fixed point is stable and therefore an asymptotically stable attractor. This is the reason why linear models behave so monotonously.

6.1.3 Non-autonomous Nonlinear Models

Let us now look at non-autonomous nonlinear models and assume that we can explicitly separate the external relation from the internal relation, as is the case in Eq. 6.2. The fixed points of the system thus fulfill the relation

$$f(\mathcal{V}_i^\infty) = -\mathcal{R}(t) \text{ for } i = 1, \dots, k \tag{6.13}$$

Of course, it only makes sense to analyze the system's behavior in the vicinity of the fixed points $\mathcal{V}_i^\infty$ if $\mathcal{R}(t)$ has, at least for a certain time, a constant value $\mathcal{R}(t) = \mathcal{R}_o$. The $\mathcal{V}_i^\infty$ are thus—in the sense of a static model—functions of $\mathcal{R}_o$. That is, a set of fixed points belongs to each $\mathcal{R}_o$. This set can also be empty (meaning that there are no finite fixed points). Let's look at an example:

Example 6.2: Fish pond with logistic growth

In a fish pond, the fish grow according to the logistic growth function Eq. (6.4) (see Example 6.1). Furthermore, a certain amount of fish J_r

is removed per unit of time by fishing. Therefore we can describe the pond's fish population with the following nonlinear differential equation:

$$\frac{\mathrm{d}N}{\mathrm{d}t} = k_p^\circ N(1 - \frac{N}{N_{max}}) - J_r = f(N) - J_r \equiv g(N) \qquad (6.14)$$

where $f(N)$ is the logistic growth curve (Eq. 6.4).

We now want to graphically determine the stability properties of this model. We find the fixed points by setting the change function $g(\mathcal{V})$ equal to zero, which is equivalent to $f(N) = J_r$. Graphically, we find the fixed points by moving the logistic growth curve from Fig. 6.1 downwards by the amount J_r (Fig. 6.4a). From that, and with the help of Eq. (6.12), we immediately see that N_1^∞ is an unstable and N_2^∞ a stable fixed point.

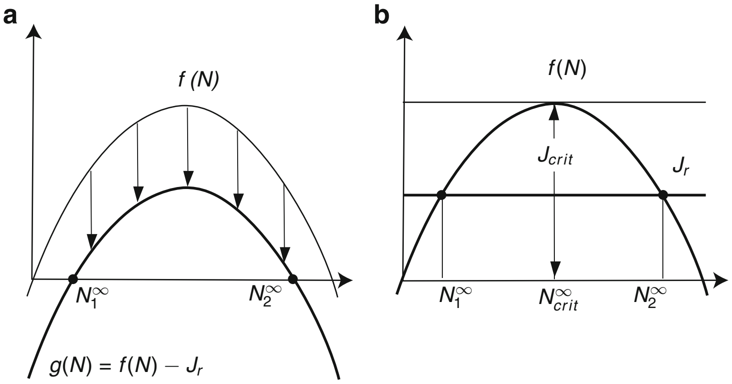


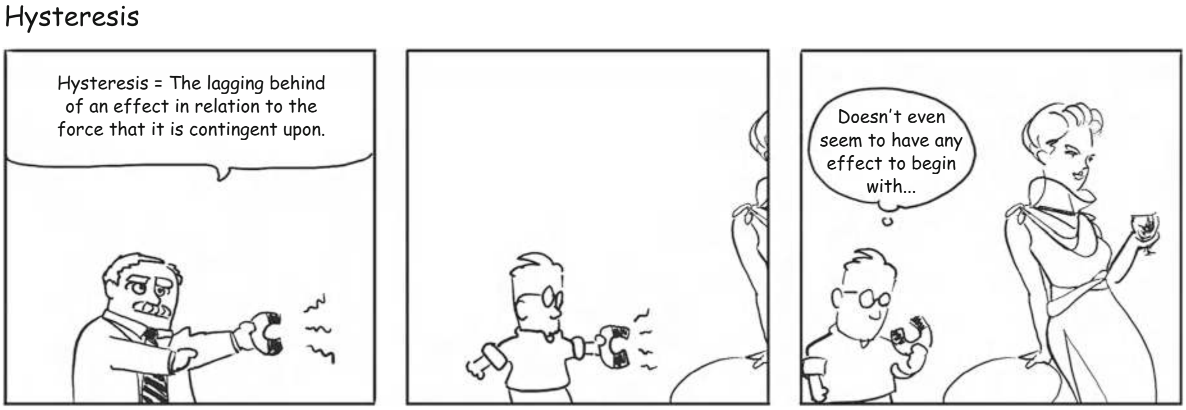
Fig. 6.4: *Logistic growth and fishing in a fish pond (Example 6.2). We can either determine the fixed points from the total velocity function $g(N)$ (right-hand figure) or by intersecting the logistic growth function $f(N)$ with J_r (left-hand figure). If $J_r > J_{crit}$, there are no finite fixed points any more and the fish in the pond eventually become extinct*

For the following considerations another graphical representation can be useful: in Fig. 6.4b we intersect the logistic growth curve $f(N)$ with the fishing rate J_r and in so doing find the same fixed points whose stability behavior we already know.

What happens to the system if we treat the fishing rate J_r as an external relation? It seems that, if the initial state is $N^0 < N_1^\infty$, the fish population grows less rapidly than it is being fished, so the fish die out. If $N^0 > N_1^\infty$ however, an equilibrium between growth and fishing sets in. Furthermore, we see that with increasing fishing rate J_r the fixed point N_1^∞ grows while N_2^∞ decreases. Ultimately, the two fixed points meet at $N_{crit}^\infty = N_{max}/2$, which is when the fishing rate reaches $J_{crit} = k_p^\circ(N_{max}/4)$. For $J_r > J_{crit}$ the fish always become extinct.

There is one final comment to be made: Eq. (6.14) has the drawback that $N(t)$ can become < 0, because the fishing rate J_r is constant whether or not there are sufficient fish left in the pond. This problem could be formally solved by setting $\mathrm{d}N/\mathrm{d}t = 0$ as soon as $N = 0$. In Problem 6.2 we will discuss a form of Eq. (6.14) that eliminates this problem another way.

6.1.4 Hysteresis in Nonlinear Models



The dependence of a system on its history is called hysteresis.

We have seen that for a constant external relation $\mathcal{R}_o$, nonlinear models can have several possible fixed points $\mathcal{V}_i^\infty$. If $\mathcal{R}_o$ is changed adiabatically (that is, slow enough), the $\mathcal{V}_i^\infty$ change along with it, too. In the process, a phenomenon called *hysteresis* can occur.[7]

We now want to show that hysteresis always occurs when the system has several fixed points for a given constant value of the external relation $\mathcal{R}$. As a starting point, we choose Eq. (6.2) and replace $\mathcal{R}(t)$ by the constant value J. According to Eq. (6.13) the fixed points are defined by the following relation:

$$f(\mathcal{V}_i^\infty) = -J \tag{6.15}$$

If $f(\mathcal{V})$ is a continuous function and intersects the line $-J$ at least twice, then it must alternately intersect $-J$ from above and below. In the first case, the slope of $f(\mathcal{V})$ is negative and, according to Eq. (6.12), the fixed point is stable. In the second case, the fixed point is unstable. Thus, stable and unstable fixed points alternate.[8] Figure 6.5 shows a function $f(\mathcal{V})$ that has three roots, the first one at zero. One could describe $f(\mathcal{V})$ by the third-order polynomial

$$f(\mathcal{V}) = -\mathcal{V}(\mathcal{V}-a)(\mathcal{V}-b); \qquad a, b > 0 \tag{6.16}$$

The polynomial has a local minimum at $\mathcal{V}_A$ (value $f_A < 0$) as well as a local maximum at $\mathcal{V}_B$ (value $f_B > 0$).[9]

---

[7] One of the most well-known hysteresis phenomena is the magnetization of a ferromagnet.

[8] As a simplification, we leave cases with $\frac{\mathrm{d}f}{\mathrm{d}\mathcal{V}} = 0$ at the fixed point aside.

[9] We leave it to the reader to express these values explicitly as a function of the two roots a and b.

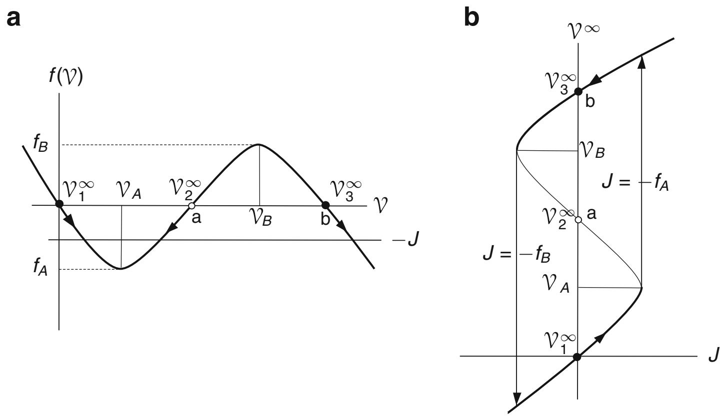


Fig. 6.5: *(**a**) Velocity function of the dynamic model* $\frac{d\mathcal{V}}{dt} = J + f(\mathcal{V})$*. For a constant* J*, the fixed points are found where* $f(\mathcal{V})$ *intersects the horizontal line* $-J$*.* ● = *stable fixed point,* ○ = *unstable fixed point. (**b**) The three fixed point branches as a function of* J*: thick curve = stable fixed point, thin curve = unstable fixed point. For a growing* J *the model jumps at* $J = -f_A > 0$ *from* $\mathcal{V}_1^\infty$ *to* $\mathcal{V}_3^\infty$*. For declining* J*, the jump takes place at* $J = -f_B < 0$

First, let's look at the case $J = 0$. The three fixed points $\mathcal{V}_i^\infty (i = 1, 2, 3)$ are then obviously identical with the roots of $f(\mathcal{V})$. According to Eq. (6.12), the fixed points at 0 and b are stable, and at a, unstable. If we now let J grow, we will find the fixed points from the intercept points of $f(\mathcal{V})$ with the horizontal line $-J$. In the case of Fig. 6.5a, $\mathcal{V}_1^\infty$ and $\mathcal{V}_3^\infty$ wander to the right towards larger values of $\mathcal{V}$, whereas $\mathcal{V}_2^\infty$ moves left. If $-J$ reaches the value f_A, the two fixed points $\mathcal{V}_1^\infty$ and $\mathcal{V}_2^\infty$ fuse, and only the (stable) fixed point $\mathcal{V}_3^\infty$ remains.

Figure 6.5b plots the position of the fixed points as a function of the external relation J. The thick curves represent stable fixed points, the thin one the unstable fixed point. The figure shows that for J between $-f_B$ and $-f_A$, three "fixed point branches" exist. If J grows beyond $-f_A$, the system jumps from the $\mathcal{V}_1^\infty$ branch directly to the $\mathcal{V}_3^\infty$ branch. In contrast, if J declines from large values, the system jumps at $J = -f_B$ from the $\mathcal{V}_3^\infty$ branch to the $\mathcal{V}_1^\infty$ branch. These abrupt jumps take place at different places depending on whether J is increasing or decreasing; this is what we call hysteresis.

We can concretise the situation shown in Fig. 6.5 by looking at the following model[10]:

$$\frac{d\mathcal{V}}{dt} = J - k\mathcal{V} + \varphi(\mathcal{V}) = J + f(\mathcal{V}) \qquad (6.17)$$

---

[10] See Scheffer et al. (2002). The authors give several examples of systems whose behavior can be described by Eq. (6.17). One of them forms the basis for Example 6.3, see below.

where $\varphi(\mathcal{V})$ is a function that, at a critical value $\mathcal{V}_{crit}$, jumps relatively steeply from a very small value (≈ 0) to the value $\varphi_\circ$ (see Fig. 6.6a below). Such behavior can be described by the function

$$\varphi(\mathcal{V}) = \varphi_\circ \frac{\mathcal{V}^p}{\mathcal{V}^p + \mathcal{V}_{crit}^p} \tag{6.18}$$

where the exponent p determines the steepness of the jump in the vicinity of $\mathcal{V}_{crit}$. The bigger p is, the more abrupt the function $\varphi(\mathcal{V})$ changes from 0 to $\varphi_\circ$.

The compound function $f(\mathcal{V}) = -k\mathcal{V} + \varphi(\mathcal{V})$ is shown in Fig. 6.6a on the right. The structure of this function's roots is the same as in the case shown in Fig. 6.5a. Again, we can intersect the curve with the line $(-J)$ and observe the change of the three fixed points as a function of J (Fig. 6.6b). Because the middle (increasing) branch of $f(\mathcal{V})$ rises approximately vertically, the corresponding fixed point $\mathcal{V}_2^\infty \approx \mathcal{V}_{crit}$ (as far as it still exists) is practically independent of J. The (catastrophic) jumps between the stable fixed point branches happen at approximately $J = k\mathcal{V}_{crit}$ and $J = k\mathcal{V}_{crit} - \varphi_\circ$.

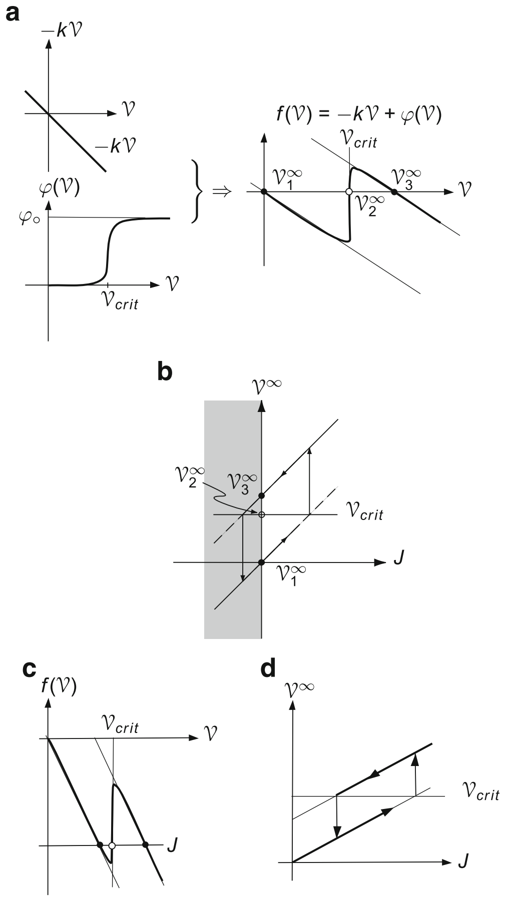


Fig. 6.6: *Analysis of the behavior of Eq. (6.17) as a function of the external relation J.*
*(**a**) Velocity function $f(\mathcal{V}) = -k\mathcal{V} + \varphi(V)$.*
*(**b**) Fixed points as a function of J and hysteresis of the system.*
*(**c**) and (**d**) like (**a**) and (**b**) but with a higher specific rate k, so that hysteresis takes place in the positive range of J.*
● *= stable fixed point,*
○ *= unstable fixed point*

In many cases, Eq. (6.17) describes a system for which only positive values of J and k make sense (see Example 6.3 below). As Fig. 6.6b demonstrates, this can imply that the jump to the upper fixed point branch is an irreversible process, because the corresponding jump back would have to occur under a negative value of J (area marked grey in Fig. 6.6b). If, however, $k\mathcal{V}_{crit} > \varphi_\circ$ (Fig. 6.6c, d), both transitions occur at positive values of J. In this case, for $J = 0$ the system only has one fixed point $\mathcal{V} = 0$.

Example 6.3: Water transparency in a lake[a]

In shallow lakes there is a fragile interaction between nutrient concentration and water transparency. High nutrient concentrations favor the growth of phytoplankton and therefore increase the particle concentration and turbidity (muddiness) of the water column: the higher the turbidity, the lower the water transparency. Low transparency leads to the sudden disappearance of plants growing underneath the water surface (so-called macrophytes) because they no longer get enough sunlight.

Up to a certain nutrient concentration, the macrophytes manage to control the plankton concentration and thus improve their growth conditions. Numerous mechanisms are involved in this process. The nutrient concentration in the water is reduced by the macrophytes themselves. Their growth improves conditions for zooplankton (e.g. *Daphnia*—small crustaceans), which for their part reduce suspended phytoplankton by feeding on them. Furthermore, the presence of macrophytes reduces the re-suspension of sediment.

If the nutrient concentration exceeds a certain critical value, these mechanisms no longer suffice to keep turbidity low, and the macrophytes start to die off. The result is that the elimination of phytoplankton ceases. To return the system to its original state, the nutrient concentration must (at least temporarily) be reduced to below the value at which the water plants disappeared. Some sort of ecological intervention may be necessary, such as the removal of certain fish that decimate the algae-eating *Daphnia*.

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[a] Adapted from Scheffer et al. (2002).

We can use the following simple model to describe the situation described above. We choose the concentration of suspended phytoplankton B as our system variable. B is simultaneously a measurement for the turbidity of the water column:

$$\frac{\mathrm{d}B}{\mathrm{d}t} = J_N + f(B) \tag{6.19}$$

with

$$f(B) = \begin{cases} -f_s(B) & \text{for} \quad B \le B_{crit} \\ -\alpha f_s(B) & \text{for} \quad B > B_{crit} \end{cases} \tag{6.20}$$

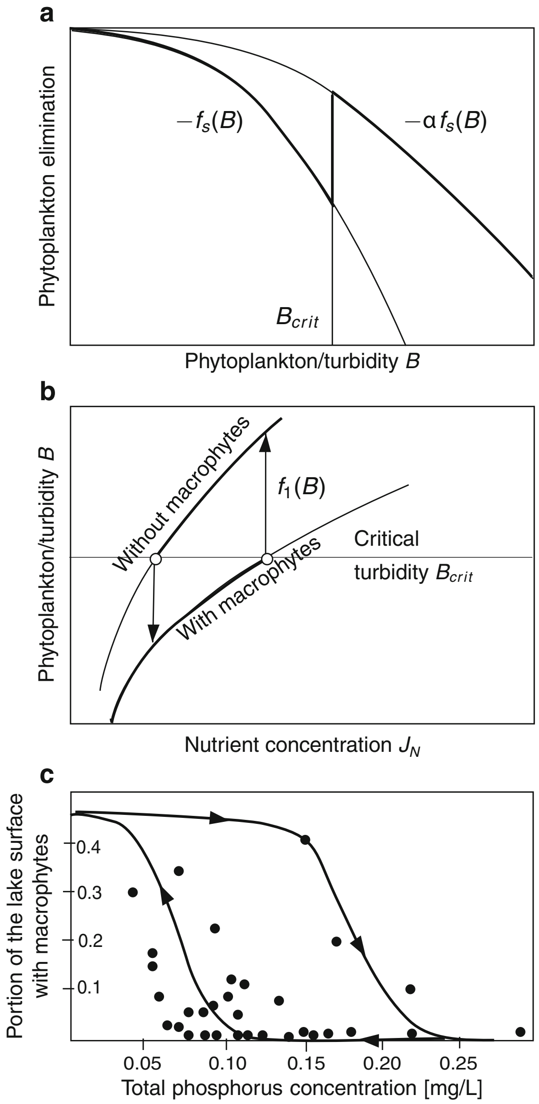

Fig. 6.7: *(**a**) Elimination function of the turbidity with and without macrophytes. Note that qualitatively, the function resembles the one in Fig. 6.6c. (**b**) Steady-state turbidity as a function of nutrient concentration. (**c**) Measurements in Dutch lakes show that hysteresis in the system is indeed related to the distribution of macrophytes. The macrophytes disappear at a higher phosphorus concentration than the one where they reappear as the concentration decreases (From Scheffer et al. (2002), data in (**c**) from Meijer (2000))*

The inhomogeneous term J_N describes the nutrient input. In lakes, the critical nutrient is usually phosphorus. The function $f_s(B)$ describes the elimination of phytoplankton, with $f_s(B)$ monotonously increasing with B (Fig. 6.7a). The constant α is the "reduction coefficient"; it describes by which factor the function $f_s(B)$ is reduced if the critical nutrient concentration B_{crit} is overshot and the macrophytes die off.

Figure 6.7b shows the fixed-point phytoplankton concentration (and accordingly the turbidity) B^∞ as a function of nutrient input J_N. We get B^∞ from Eq. (6.19) by setting $\mathrm{d}B/\mathrm{d}t = 0$:

$$f(B^\infty) = -J_N \tag{6.21}$$

The model shows hysteresis. Measurements in Dutch lakes show that the phosphorus concentration at which macrophytes disappear is ins fact higher than the one at which they reappear as the nutrient concentration decreases (Fig. 6.7c).

Let's now take another look at hysteresis from a somewhat different angle:

Example 6.4: Nonlinear phosphorus model

A weak point of the lake models we've discussed so far (Examples 2.2, 4.9, 4.10–4.12) is the inadequate description of phosphorus deposition into the sediment. So far, we described it as a linear function of the average phosphorus concentration ($k_s C$). Yet observations show that in most lakes, the specific phosphorus sedimentation rate k_s decreases with growing concentration and can even become negative. Such a negative rate would indicate re-dissolution of phosphorus from the sediment into the water.

Once again, we describe the lake as a linear flow reactor (see Example 4.4), but introduce a concentration-dependent specific phosphorus sedimentation rate $k_s(C)$. Compared to Eq. (4.22), the dynamic equation for the average phosphorus concentration is slightly changed:

$$\frac{\mathrm{d}C}{\mathrm{d}t} = k_w C_{in} - k_w C - k_s(C)C \tag{6.22}$$

This equation is no longer linear, because k_s is a function of C. To model the behavior of $k_s(C)$ as simply as possible, we choose the following function:

$$k_s(C) = \begin{cases} k_s & \text{for} \quad C < C_{crit} \\ 0 & \text{for} \quad C \geq C_{crit} \end{cases} \tag{6.23}$$

The function $k_s(C)$ is plotted in Fig. 6.8. In reality, $k_s(C)$ would decrease continuously, rather than abruptly as in our model. Eq. (6.23) has the advantage that the model can be analyzed relatively easily while retaining all important properties of a realistic model.

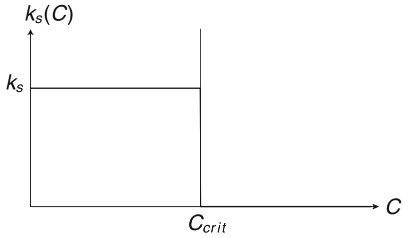

Fig. 6.8: *Specific sedimentation rate k_s as a function of the average phosphorus concentration C in the lake: if the phosphorus concentration is higher than C_{crit}, k_s becomes zero and no more phosphorus is added to the sediment*

If we insert Eq. (6.23) into Eq. (6.22), the following model equation results:

$$\frac{\mathrm{d}C}{\mathrm{d}t} = k_w C_{in} - k_w C - \begin{cases} k_s C & \text{for} \quad C < C_{crit} \\ 0 & \text{for} \quad C \geq C_{crit} \end{cases} \tag{6.24}$$

This is actually a superposition of two linear models. The current value of C determines which of the two linear equations is valid. If, in a given case, the concentration C never were to exceed the critical value C_{crit}, the model would not "know" about its double life, and only behave according to Eq. (4.22).[11]

Remember that Eq. (6.24) is non-autonomous due to its input term $(k_w C_{in})$. In general, that is, if C_{in} is not constant in time, the model will not reach a fixed point. Yet, as in previous examples, it is useful to analyze the hypothetical fixed point as a function of an assumed constant input concentration C_{in}. In other words, we are looking for the static model, $C^{\infty} = f(C_{in})$, which the dynamic model (Eq. 6.24) implicitly contains. Much like the dynamic model is a superposition of two linear models, the static model is a superposition of two fixed-point lines:

$$C^{\infty}(C_{in}) = \begin{cases} C_{in} \frac{k_w}{k_w + k_s} \equiv C_A^{\infty} & \text{for} \quad C^{\infty} < C_{crit} \\ \\ C_{in} \equiv C_B^{\infty} & \text{for} \quad C^{\infty} \geq C_{crit} \end{cases} \tag{6.25}$$

The fixed-point lines are plotted in Fig. 6.9. Line **A** ($C^{\infty} < C_{crit}$) has a slope of $\frac{k_w}{k_w + k_s}$, line **B** a slope of 1. The horizontal line at C_{crit} delimits the scope of the two fixed-point lines. We note that for an input concentration C_{in} between C_{crit} and $C^{\star} = \frac{k_w + k_s}{k_w} C_{crit} > C_{crit}$, both fixed-point lines are technically valid. How does the model really behave?

Let's imagine that initially, C_{in} is so small that the corresponding fixed-point concentration is $C_A^{\infty} < C_{crit}$. If C_{in} now grows so slowly that the

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[11] We brought up the phenomenon of linearity within a limited area in the introduction to Chap. 6.

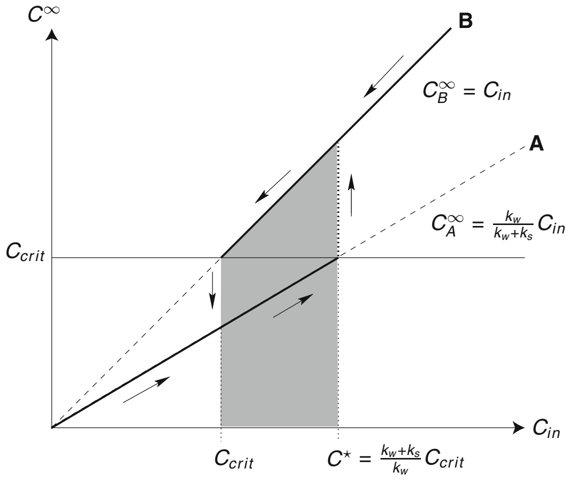

Fig. 6.9: *Relation between the input concentration C_{in} and the two fixed-point lines (Eq. 6.25). If C_{in} lies between C_{crit} and $C^\star$ (shaded area in the graph), two fixed points exist. The model's previous history then decides which fixed point is actually reached: again, we see hysteresis*

model adiabatically moves along in its fixed point,[12] then, at an input concentration of $C^\star$, C_A^∞ reaches the critical value C_{crit}:

$$C_A^\infty(C^\star) = \frac{k_w}{k_w + k_s} C^\star = \frac{k_w}{k_w + k_s} \frac{k_w + k_s}{k_w} C_{crit} = C_{crit} \tag{6.26}$$

At C_{crit}, the model now jumps to the upper fixed-point line **B**. If, on the other hand, the model moves downwards on **B** coming from large values of C_{in}, it won't jump back to **A** at $C_{in} = C^\star$ but only at $C_{in} = C_{crit}$.

To summarize: despite its simplicity, the model (6.24) has allowed us to see two phenomena that are typical for nonlinear models (and do *not* occur in linear models):

1. The model has critical states in which even the smallest of changes in the input (external relation) lead to large changes in the behavior of the system variable.

2. There is an interval of the input variable C_{in} in which the behavior of the system depends on its prior history (hysteresis).

6.1.5 Synergism in Nonlinear Models

Apart from the occurrence of hysteresis, nonlinear models have another property which fundamentally differentiates them from linear models: *synergistic effects*. They are the phenomena by which several forces influencing a system from the outside can influence each other either by reinforcement or compensation.

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[12] Question to the reader: How should we specify the attribute *slow* here?

Synergism

Synergism: interaction between different external forces, so that the overall influence is smaller or larger than the sum of the individual influences.

To understand more clearly what we mean by "influence each other" we remember those systems where a mutual influence doesn't exist: linear systems. In Sect. 4.3 we looked at a linear model with time-dependent input and saw that the input can be divided into many individual input chunks—the system "processes" each input as if the others didn't exist (see Fig. 4.5). The combination of all input events is obtained from the sum (superposition) of all individual events. In general, this method cannot be applied to nonlinear models.

To illustrate this, we can think of the following question: what is the influence of water polluted with zinc and mercury on the growth of a specific algae species? We can assume that each of the two heavy metal concentrations on its own would reduce the algae growth rate by 10 %. If the effects on algae growth of the two heavy metals were independent of each other, the overall effect would be a growth rate reduction of 20 %. This is the case without synergism. In reality, however, we will often observe that the effects of two pollutants mutually reinforce each other, so the reduction of growth rate might be more than 20 %. Some substances may also compensate each other's effects (think poison and antidote). In both cases we speak of synergism.

Example 6.5: Synergism in the nonlinear phosphorus model

In Fig. 6.10, we look at the influence of two input events on the behavior of phosphorus concentration in a lake with nonlinear sedimentation (Eq. 6.24). If the sum of the two events leads to a phosphorus concentration greater than the critical value C_{crit}, the phosphorus concentration's behavior is no longer identical with the sum of the individual events.

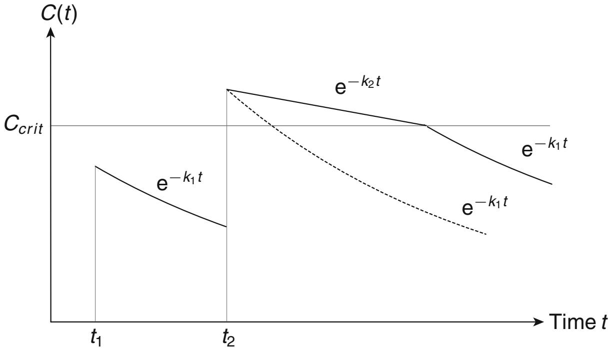

Fig. 6.10: *In the phosphorus model from Eq.* (6.24)*, the actual concentration development (black continuous line) is not identical with the sum of all individual events (dashed line)*

Remember: synergistic effects can only be described by nonlinear models. We thus begin to see how in many ways, the possibilities of linear models are too limited to adequately describe real-world phenomena.

6.2 Nonlinear Box Models with Several System Variables

6.2.1 The Jacobian Matrix

Multi-dimensional nonlinear models greatly increase the potential of mathematical modeling. The diversity gained, however, comes at the cost of only being able to analytically solve the systems of differential equations for a limited number of special cases. Most nonlinear models have to be solved numerically. In contrast to analytical solutions, computer simulations have the drawback that certain characteristic properties of the model cannot be analyzed (or only with a large number of simulations). One of these properties is a system's behavior in the vicinity of a fixed point.

We will now look at that behavior, and in the process learn some tricks that let us, to an extent, skirt around numerical solutions. Let's consider an n-dimensional model that is described by the following system of n first-order differential equations:

$$\frac{\mathrm{d}\mathcal{V}_i}{\mathrm{d}t} = g_i(\mathcal{V}_1, \dots, \mathcal{V}_n), \qquad i = \{1, \dots, n\} \tag{6.27}$$

As in the one-dimensional case (see Eq. 6.6), we assume that all existing external relations are constant in time and thus integrated into the functions g_i.

The fixed points of the system of differential equations (6.27) are the q solutions of the n-dimensional system of regular but nonlinear equations[13]:

$$0 = g_i\left(\mathcal{V}_1^k, \mathcal{V}_2^k, \dots, \mathcal{V}_n^k\right), \quad k = \{1, 2, \dots, q\}, \qquad i = \{1, 2, \dots, n\} \tag{6.28}$$

---

[13] Note that here we slightly modify the notation introduced in Eq. (6.7). We leave out the symbol ∞, the numbering of the fixed point k becomes the upper index, and the lower index indicates the variable.

If the system were linear, it would have at most $q = n$ solutions. For systems of nonlinear equations, the number of fixed points q can be arbitrarily large.

To examine the system's behavior around a fixed point k, we can build on the method that we used for one-dimensional models in Sect. 6.1.2. Because it is difficult to imagine surfaces in more than three dimensions, we first look at a two-dimensional system with the variables $\mathcal{V}_1$ and $\mathcal{V}_2$. We can represent each of the two velocity functions g_i $(i = 1, 2)$ as a surface in three-dimensional space. Two of the dimensions are spanned by the two variables themselves. This is the phase space as we have already encountered it, or more precisely, the phase plane. Along the third axis, standing perpendicular to this plane, we plot the value of g_1 or g_2. This way we get two topographical maps with mountains and valleys. Where both of these topographies intersect the phase plane there is a fixed point. Around this fixed point, we can approximate the development of g_1 and g_2 with tangents in the direction of $\mathcal{V}_1$ or $\mathcal{V}_2$, just as we did in Eq. (6.9) (or Fig. 6.2). In total we get four tangents, with the slopes $\frac{\partial g_1}{\partial \mathcal{V}_1}$, $\frac{\partial g_1}{\partial \mathcal{V}_2}$, $\frac{\partial g_2}{\partial \mathcal{V}_1}$ and $\frac{\partial g_2}{\partial \mathcal{V}_2}$. The symbol for the partial derivative (∂) indicates that the slope is being determined along the chosen direction ($\mathcal{V}_1$ or $\mathcal{V}_2$) and that the other coordinate is held constant. Applying this principle to more than two dimensions, we get n^2 such slopes. Below, we will explicitly plot these velocity surfaces for Example 6.6 (Fig. 6.13).

Somewhat more formally, we assume that the system is arbitrarily close to the fixed point k, so:

$$\mathcal{V}_i = \mathcal{V}_i^k + \varepsilon_i \ , \quad i = \{1, \ldots, n\} \tag{6.29}$$

or, written as vectors:

$$\boldsymbol{\mathcal{V}} = \boldsymbol{\mathcal{V}}^k + \boldsymbol{\varepsilon} \tag{6.30}$$

Because by definition, at the fixed point itself all change functions g_i are zero, we can approximate them in the vicinity of $\boldsymbol{\mathcal{V}}^k$ with the following Taylor series, aborting after the first-order derivatives:

$$g_i(\boldsymbol{\mathcal{V}}) = g_i(\boldsymbol{\mathcal{V}}^k + \boldsymbol{\varepsilon}) = \sum_{j=1}^{n} \left(\frac{\partial g_i}{\partial \mathcal{V}_j} \right) \Bigg|_{\boldsymbol{\mathcal{V}}^k} \cdot \varepsilon_j \qquad i = \{1, \ldots, n\} \tag{6.31}$$

The vertical line with the argument $\boldsymbol{\mathcal{V}}^k$ tells us to calculate the partial derivatives at the fixed point $\boldsymbol{\mathcal{V}}^k$. Because $\boldsymbol{\mathcal{V}}^k$ is constant in time, $\mathrm{d}\mathcal{V}_i/\mathrm{d}t = \mathrm{d}\varepsilon_i/\mathrm{d}t$. Thus, as an approximation, Eq. (6.27) becomes an n-dimensional *linear* system of the deviation variables ε_i:

$$\frac{\mathrm{d}\varepsilon_i}{\mathrm{d}t} = \sum_{j=1}^{n} B_{i,j}(\boldsymbol{\mathcal{V}}^k)\varepsilon_j \qquad i = \{1, \ldots, n\} \tag{6.32}$$

with

$$B_{i,j}(\boldsymbol{\mathcal{V}}^k) = \left(\frac{\partial g_i}{\partial \mathcal{V}_j}\right)\Bigg|_{\boldsymbol{\mathcal{V}}^k} \tag{6.33}$$

The $B_{i,j}(\boldsymbol{\mathcal{V}}^k)$ can be written as a matrix:

$$\mathbf{B}(\boldsymbol{\mathcal{V}}^k) = \left(\begin{array}{ccc} \frac{\partial g_1}{\partial \mathcal{V}_1} & \frac{\partial g_1}{\partial \mathcal{V}_2} & \cdots \\ \frac{\partial g_2}{\partial \mathcal{V}_1} & \frac{\partial g_2}{\partial \mathcal{V}_2} & \cdots \\ \vdots & \vdots & \ddots \end{array}\right)\Bigg|_{\boldsymbol{\mathcal{V}}^k} \tag{6.34}$$

where the argument $\boldsymbol{\mathcal{V}}^k$ indicates that the derivatives of the velocity functions g_i in the matrix are to be calculated at the selected fixed point k. $\mathbf{B}$ is the so-called Jacobian matrix. It describes the system of nonlinear equations in an approximated linearized manner in the vicinity of the fixed points. Written in matrix form, Eq. 6.32 is:

$$\frac{\mathrm{d}\boldsymbol{\varepsilon}}{\mathrm{d}t} = \mathbf{B}(\boldsymbol{\mathcal{V}}^k)\boldsymbol{\varepsilon} \tag{6.35}$$

The expressions (6.32) and (6.35) are thus linear approximations of the nonlinear system (6.27). By way of the eigenvalues of the Jacobian matrix we can now analyze the behavior of the model around the fixed point. We must keep in mind however that under some circumstances such a stability analysis may only be valid in very small ε surroundings of $\boldsymbol{\mathcal{V}}^k$. Furthermore, there are nonlinear models whose velocity functions g_i are not differentiable, so that no Jacobian matrix can be calculated. Finally, there are cases where the linearized model cannot make any statement about the real model (see Sect. 6.2.4).

6.2.2 Characterizing the Fixed Points of Multi-dimensional Systems

Again, for simplification, we consider a two-dimensional model. In contrast to the one-dimensional case the fixed points $\boldsymbol{\mathcal{V}}^k$ *don't* divide the phase space into invariant areas. It is also possible that the model does not even reach a fixed point, but rather oscillates around it, as we have already seen in the example of the harmonic oscillator (Example 5.11).

In Sect. 5.1.1 we analyzed the properties of the eigenvalues of a two-dimensional linear model and summarized the results (Table 5.1). In the vicinity of their fixed points, nonlinear two-dimensional models can be approximated by linear models. The Jacobian matrix thereby takes over the role of the coefficient matrix $\mathbf{P}$ which we introduced in Eq. (5.3). At this point we want to summarize the classification of the fixed points (as detailed in Table 5.1) once again; at the same time, in Fig. 6.11, we want to visualize the trajectories in the two-dimensional phase space near a fixed point. Each pattern has a specific pair of eigenvalues λ_1 and λ_2 of the Jacobian matrix $\mathbf{B}$ associated with it.

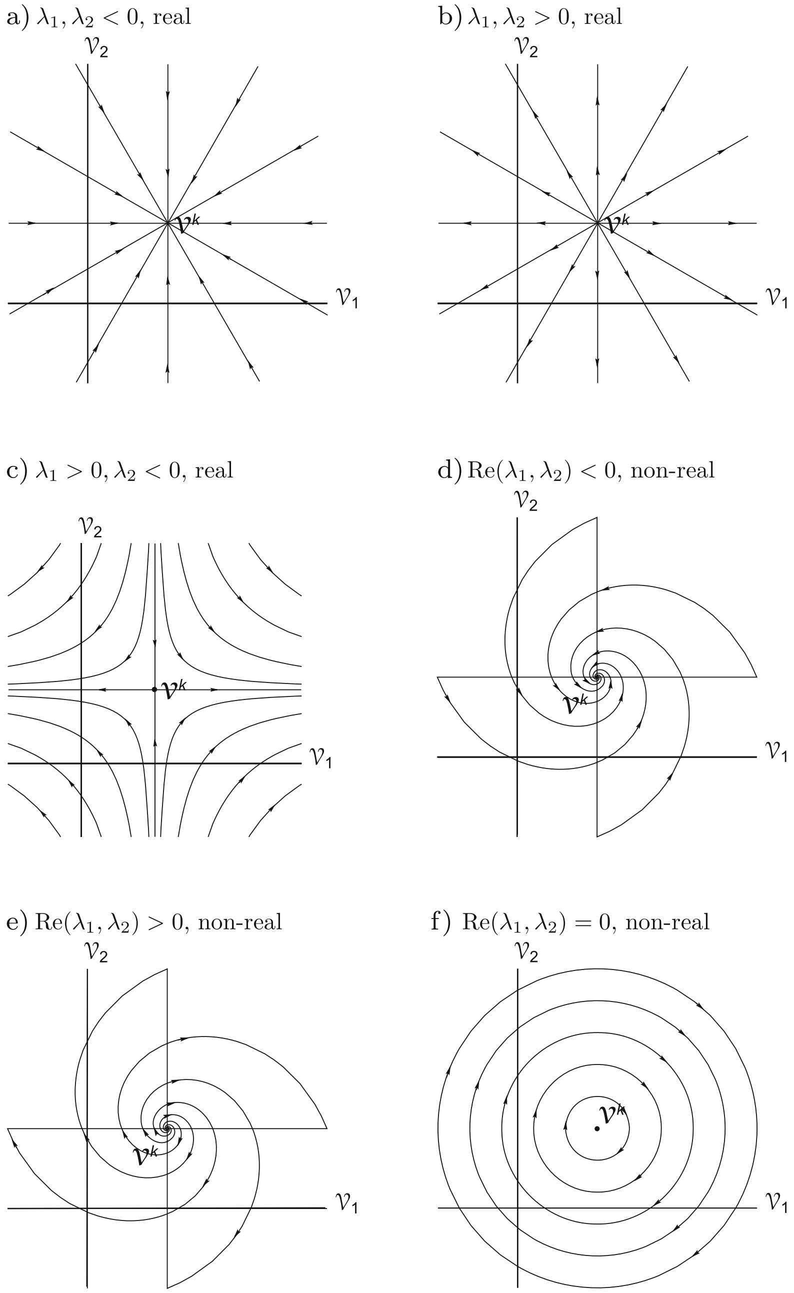

Fig. 6.11: *Characterization of the behavior of two-dimensional models in their phase space near a fixed point* $\boldsymbol{\mathcal{V}^k}$. $\mathcal{V}_1$ *und* $\mathcal{V}_2$ *are the system variables. (**a**) Stable star, (**b**) unstable star, (**c**) saddle point (unstable), (**d**) stable fixed point with oscillation, (**e**) unstable fixed point with oscillation, (**f**) undamped oscillation: center. See text for further explanations*

Real eigenvalues

(a) Both eigenvalues are real and negative ($\lambda_1, \lambda_2 < 0$): stable fixed point, also called *stable star* (Fig. 6.11a).

(b) Both eigenvalues are real and positive ($\lambda_1, \lambda_2 > 0$): unstable fixed point, also called *unstable star* (Fig. 6.11b).

(c) Eigenvalues are real and have different signs, e.g. ($\lambda_1 > 0, \lambda_2 < 0$): Unstable fixed point, also called *saddle point* (Fig. 6.11c).

It is easily possible to extend the definitions above to one-sided stable and indifferent situations, that is, to include cases with an eigenvalue of zero.

Non-real eigenvalues

If the eigenvalues are non-real, λ_1 and λ_2 only differ in the sign of their imaginary parts.[14] The system variables oscillate around the fixed point in three possible ways:

(d) $\mathrm{Re}(\lambda_1, \lambda_2) < 0$: The model moves on a spiral towards the fixed point (Fig. 6.11d); the fixed point is stable.

(e) $\mathrm{Re}(\lambda_1, \lambda_2) > 0$: The model moves away from the fixed point on a spiral (Fig. 6.11e); the fixed point is unstable.

(f) $\mathrm{Re}(\lambda_1, \lambda_2) = 0$, i.e. purely imaginary eigenvalues. The model moves on a closed curve around the fixed point without ever reaching it (Fig. 6.11f). The fixed point is called a center.

It can be shown that, except for case f (center), examining the fixed points by linearization does indeed yield an accurate description of the nonlinear system.[15] This holds at least in a (possibly very small) area around the fixed point. In the case of a center (case f), we *cannot* decide whether the behavior of the real (nonlinear) model follows categories d, e or f. We will illustrate this with Example 6.9. Furthermore, there is still another possibility: the convergence of the trajectory towards a closed curve around the fixed point. This case is called a *limit cycle* and we will illustrate it in Example 6.8 below.

If the fixed point is a center, the system's behavior in its vicinity cannot be determined by linearization.

For nonlinear models with more than two dimensions, the eigenvalues of the Jacobian matrix are still useful to analyze the behavior near the fixed point. If $n = 4$, for example, the eigenvalues can be calculated from the solution of a fourth-order equation. The more dimensions a model has, the more diverse the possible combinations of real and non-real parts of the eigenvalues become. Thus the diversity of the behavior of fixed points also rises. In certain cases, e.g. if all solutions are real, we can still

---

[14] Because they are the solutions of a system of quadratic equations, non-real eigenvalues only occur as conjugate-complex pairs (see Eq. 5.10).

[15] As a reminder: the calculation of the Jacobian matrix presupposes that the velocity functions g_i are differentiable at the fixed point.

make qualitative statements relatively easily. A more general discussion of n-dimensional models goes beyond the scope of this book, however.

In the following, we will concentrate on two-dimensional nonlinear models and, to conclude the chapter, introduce a special three-dimensional model.

6.2.3 Predator-Prey Model

Wisdom of the hare

An old hare is lecturing a young one. “It’s time you learnt about the predator-prey model.” — “Why is that important?” — “It’s an ancient wisdom that gives hope to us hares. It foretells that there are lynxes; they eat hares. But as more and more hares are eaten, the lynxes start starving and their numbers dwindle. Thus the population of hares increases again, and the circle of life begins anew... it means that we hares can never die out completely!” — “But... I thought that there have been no lynxes here for a long time. The humans eradicated them all!” — “Well, yes, but one day there *could* be lynxes again. So mark my words!” The little hare thinks for a while and then smiles: “Ok, I think I understand. The people hunt us, so there are less of us, and in turn, less people too, so then there are more of us again...” — “Each model has its limits...” the old hare wants to continue his lecture, but the young one has already run off to spread the news to his friends.

We begin our discussion of two-dimensional models with the predator-prey model by Lotka and Volterra.

Example 6.6: Predator-prey model by Lotka and Volterra

One of the most well-known models from mathematical ecology is the predator-prey model, developed almost simultaneously by Albert Lotka (1924) and Vito Volterra (1926). In its original form, it describes a theory of competition between two species. Applied to an interaction between a predator and its prey, we can reduce the model to the following assumptions:

1. A population of prey animals X increases with the specific net rate k_1.
2. A population of predators Y dies with the specific net rate k_2.

3. The prey is eaten by the predators, which results in an increase of predators and a corresponding decrease of prey by k_3XY.[a]

Figure 6.12 graphically shows the model. Mathematically, it is described by two coupled differential equations:

$$\begin{aligned}\frac{\mathrm{d}X}{\mathrm{d}t} &= k_1X - k_3XY \\ \frac{\mathrm{d}Y}{\mathrm{d}t} &= -k_2Y + k_3XY\end{aligned} \tag{6.36}$$

---

[a] Of course, the assumption that one eaten prey animal results in the "creation" of one additional predator, as suggested by Eq. (6.36), is not particularly realistic. The model could be improved by replacing k_3 with $k_3^* = \alpha k_3$ ($\alpha < 1$) in the second Eq. (6.36). Although this changes Eqs. (6.37), (6.40) and (6.41), it does not change the eigenvalues of the linearized system or the fundamental structure of the system of equations (6.36).

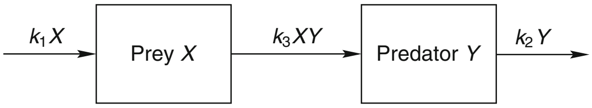

Fig. 6.12: *Model by Lotka and Volterra for the interaction between predator Y and prey X*

Because of the two terms $\pm k_3XY$, the model is nonlinear. It has two fixed points, first, the trivial fixed point $X_1^\infty = 0, Y_1^\infty = 0$, and second:

$$X_2^\infty = \frac{k_2}{k_3}, \qquad Y_2^\infty = \frac{k_1}{k_3} \tag{6.37}$$

We get this result by setting the left sides of Eqs. (6.36) equal to zero. To determine the stability of the fixed points, we will analyze the model's behavior in the vicinity of the second fixed point by introducing new variables. This is somewhat more laborious than the method with the Jacobian matrix, but also easier to understand. We define δ_X and δ_Y as the deviation of the population sizes from the fixed point:

$$\delta_X = X - X_2^\infty, \qquad \delta_Y = Y - Y_2^\infty \tag{6.38}$$

Since X_2^∞, Y_2^∞ are constant, it follows that:

$$\frac{\mathrm{d}\delta_X}{\mathrm{d}t} = \frac{\mathrm{d}X}{\mathrm{d}t} \quad \text{and} \quad \frac{\mathrm{d}\delta_Y}{\mathrm{d}t} = \frac{\mathrm{d}Y}{\mathrm{d}t} \tag{6.39}$$

In Eqs. (6.36), X and Y can be replaced by the new variables δ_X and δ_Y. After some algebraic conversions, we get:

$$\begin{aligned}\frac{\mathrm{d}\delta_X}{\mathrm{d}t} &= -k_2\delta_Y - k_3\delta_Y\delta_X \\ \frac{\mathrm{d}\delta_Y}{\mathrm{d}t} &= k_1\delta_X + k_3\delta_Y\delta_X\end{aligned} \tag{6.40}$$

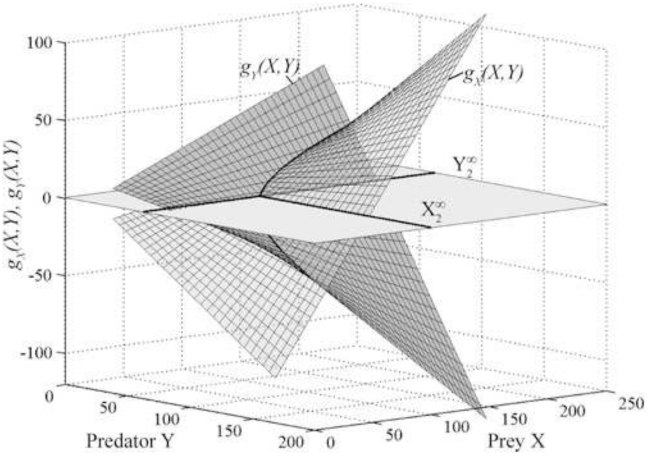

Fig. 6.13: *Velocity functions $g_X(X,Y)$ and $g_Y(X,Y)$ of the Lotka-Volterra model (6.36). The nontrivial fixed point (X_2^∞, Y_2^∞) is located where the two plains intersect the zero plain. The slopes of the plains at this point along the X and Y axes correspond to the elements of the Jacobian matrix (Eq. 6.34). The model parameters are as in Fig. 6.14*

The method of linearization implies that we allow only small deviations from the fixed point and disregard products of small quantities, $\delta_X \delta_Y$. This results in:

$$\frac{\mathrm{d}\delta_X}{\mathrm{d}t} = -k_2 \delta_Y, \qquad \frac{\mathrm{d}\delta_Y}{\mathrm{d}t} = k_1 \delta_X \tag{6.41}$$

Of course, the resulting system of linear differential equations (6.41) could also have been produced by the method of the Jacobian matrix (see Problem 6.3). Figure 6.13 shows the two velocity functions $g_X(X,Y)$ and $g_Y(X,Y)$. The fixed point is located where the two planes intersect the zero plain.

Maybe you noticed that we are already acquainted with Eq. 6.41 from Example 5.9: we only have to replace δ_Y with y_1 and δ_X with y_2. This way we know without further calculations that the eigenvalues are purely imaginary ($\lambda_1 = \pm \mathrm{i}(k_1 k_2)^{1/2}$, see Eq. 5.58). The nonlinear fixed point (6.37) is therefore a center. In Chap. 5 we showed that the undamped harmonic oscillator (Example 5.11) can also be described by this type of equation. The solutions are undamped harmonic oscillations of the pendulum's displacement and speed, with the speed lagging behind the displacement by a quarter period. Likewise, Fig. 5.10 could be carried over to the predator-prey model: y_1 could be interpreted as the number of predators and y_2 as the number of prey.

Before we reach any premature conclusions, we need to remember that in the case of the harmonic oscillator the system of equations itself had the form of Eq. (5.55) (or 6.41), whereas in the case of the Lotka-Volterra model, we got Eq. (6.41) only as a linearized approximation of the original system Eq. (6.36). Furthermore, the fixed point is a center. In Sect. 6.2.2 we noted that for a center, the method of linearizing (the Jacobian matrix method) says nothing about how the nonlinear model actually behaves at the fixed point. In Example 6.8 we will show that for a center, the real (i.e. nonlinear) model can behave according to one of three behavioral patterns: it either moves towards the fixed point (the fixed point is an attractor),

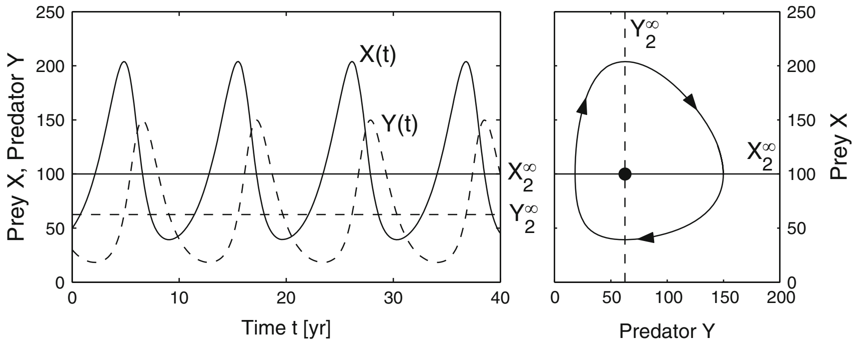

Fig. 6.14: *Numerical solutions of the Lotka-Volterra predator-prey model. On the left, temporal behavior of the two system variables* X, Y*. On the right, the phase space with fixed point at* (X_2^∞, Y_2^∞)*. Parameters used:* $k_1 = 0.5\,year^{-1}$, $k_2 = 0.8\,year^{-1}$, $k_3 = 0.008\,year^{-1}$*. Initial condition:* $X^0 = 50, Y^0 = 30$*. Nontrivial fixed point at* $X_2^\infty = 100, Y_2^\infty = 62.5$

moves away from it, or it circles it on a closed trajectory like the undamped harmonic oscillator (see Fig. 5.10).

It can be shown that the Lotka-Volterra model belongs to the third category (see e.g. Arrowsmith and Place 1992). In Fig. 6.14, X and Y are shown both as functions of time and in the two-dimensional phase space. The plot shows that the trajectory describes a closed curve, but not an ellipse as in Fig. 5.10. Correspondingly, $X(t)$ and $Y(t)$ are also not pure sine or cosine functions. This non-harmonic (yet undamped) behavior reminds us that the real system of Eqs. (6.36) is nonlinear and that Eq. (6.41) is merely a linear approximation.

The kinship between the Lotka-Volterra model and the model of the harmonic oscillator suggests that they also share the feature of structural instability. The following example demonstrates that this is indeed the case.

Example 6.7: Predator-prey model with self-interaction

We will now make a minor change to the predator-prey model from Example 6.6 by assuming that for large prey populations, the prey animals themselves impede and potentially even kill or eat one another. We can describe the resulting negative effect on the prey population dynamics in Eq. (6.36) with an additional term of the form $(-k_4X^2)$. k_4 is an arbitrarily small coefficient of self-interaction. Note that because the variable X appears squared, the new term is only relevant for large values of X. The modified system equations are:

$$\begin{aligned} \frac{\mathrm{d}X}{\mathrm{d}t} &= k_1X - k_3XY - k_4X^2 \\ \frac{\mathrm{d}Y}{\mathrm{d}t} &= -k_2Y + k_3XY \end{aligned} \tag{6.42}$$

The system still has two fixed points. The trivial fixed point ($X_1^\infty = Y_1^\infty = 0$) remains unchanged. The nontrivial fixed point however is slightly changed compared to Eq. (6.37):

$$X_2^\infty = \frac{k_2}{k_3}, \qquad Y_2^\infty = \frac{k_1}{k_3} - \frac{\epsilon}{k_3}; \quad \text{with} \quad \epsilon = k_4 \frac{k_2}{k_3} \tag{6.43}$$

Problem 6.4 asks you to calculate the Jacobian matrix of Eq. (6.42) and determine the eigenvalues at the nontrivial fixed point. From the results of that calculation, the deviation of X and Y from the nontrivial fixed point is described by the following approximative system of linear equations:

$$\begin{aligned} \frac{\mathrm{d}\delta_X}{\mathrm{d}t} &= -k_2\delta_Y - \epsilon\delta_X \\ \frac{\mathrm{d}\delta_Y}{\mathrm{d}t} &= (k_1 - \epsilon)\delta_X \end{aligned} \tag{6.44}$$

We assume that the prey's self-interaction is arbitrarily small but nonzero. In particular, $\epsilon \ll k_1$ holds. The system (6.44) thus essentially differs from the original equations (6.41) only by the additional term $-\epsilon\delta_X$ in the first equation (just like the damped pendulum, Eq. 5.63). We already know what this means for the eigenvalues (see Eq. 5.67)—they receive a (very small) negative real part:

$$\lambda_i \approx -\frac{\epsilon}{2} \pm \mathrm{i}\omega, \quad \omega = \sqrt{k_1 k_2} \tag{6.45}$$

With that, the fixed point (X_2^∞, Y_2^∞) becomes stable, that is, an attractor (Fig. 6.11d). The oscillation of the predator and prey populations is damped around the fixed point. The system eventually assumes the constant values X_2^∞ and Y_2^∞. Furthermore, because the fixed point is no longer a center (as it was in our first predator-prey model), we know now that the nonlinear system qualitatively behaves like its linearized counterpart. Figure 6.15 shows the dynamic behavior of the modified predator-prey model.

The Lotka-Volterra model profoundly influenced the beginning of ecological systems modeling.

The Lotka-Volterra model profoundly influenced the thinking of the first ecological modelers. The Hudson Bay Company's 100-year catch statistics of the Canada lynx and its prey, the snowshoe hare, were often cited as a textbook example of the periodic oscillations of a predator-prey pair as predicted by the model (Fig. 6.16). The catch statistics show the population density of both species. It exhibits a regular fluctuation with a period of about 10 years. With some goodwill, we can see that the maximum hare population does indeed occur just before the maximum of the lynx—as predicted by the Lotka-Volterra model.

This apparent confirmation of the Lotka-Volterra model does not stand up to critical examination, however. First, we know from our mathematical considerations that the model is structurally unstable. Thus there are many reasons why the fluctuations should disappear. Second, the snowshoe hare population also fluctuates in areas where there are no lynxes. And finally, the lynx does not subsist exclusively on a snowshoe hare diet.

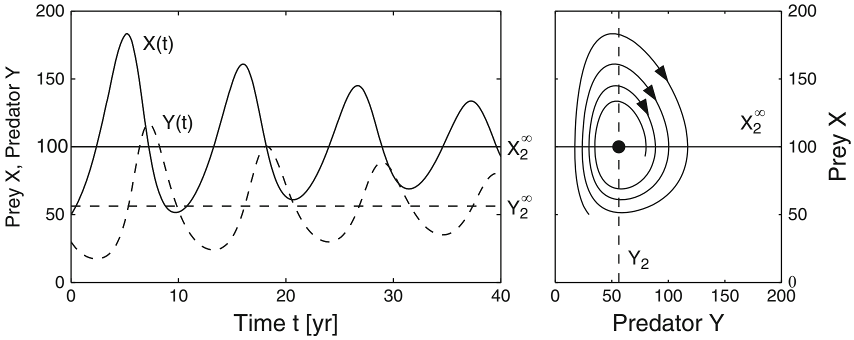

Fig. 6.15: *Modified predator-prey model: compared to Fig. 6.14, the dynamic prey equation has an additional prey-prey self-interaction term (Eq. 6.42). Therefore the oscillations of the predator and prey populations Y and X are damped and the system moves towards the nontrivial fixed point. The position of the fixed point itself and the period of the oscillations change only very slightly for a small self-interaction. Parameters and initial condition are like in Fig. 6.14, and* $k_4 = 5 \times 10^{-4}\ a^{-1}$

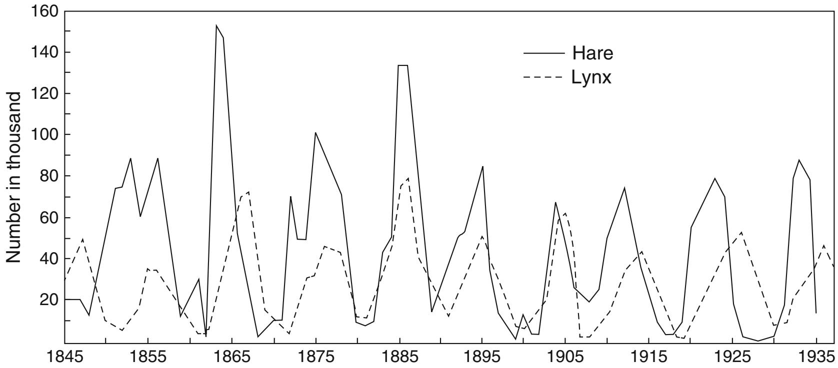

Fig. 6.16: *Population fluctuations of snowshoe hare and lynx, from the catch statistics of the Hudson Bay Company. This is a classic example of cyclical oscillation of population densities (Source: MacLulich 1937 cited in Odum 1971)*

In short, this example demonstrates that building a model for measured data can stimulate the development of an interesting new theory even if it turns out not to be that relevant for the original data. Indeed, the Lotka-Volterra model could be credited as the origin of mathematical ecology. Thus it doesn't surprise that many further models emerged based on it, attempting to remedy the deficiencies of their predecessor. One of these is the Holling-Tanner model (May 1974, p. 84).

Example 6.8: Holling-Tanner predator-prey model

In the Holling-Tanner model, the interaction between prey X and predator Y is expressed by the following system of nonlinear differential equations:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = r(1-\frac{X}{X_k})X - w\frac{XY}{X+K_X} \tag{6.46}$$

$$\frac{\mathrm{d}Y}{\mathrm{d}t} = s(1-J\frac{Y}{X})Y \tag{6.47}$$

$$\text{with} \quad r, s, w, J, X_k, K_X > 0$$

In Eq. (6.46), the first term describes the logistic growth of the prey (see Example 6.1). X_k is the hypothetical equilibrium population of X if there were no predators. The second term of Eq. (6.46) simulates the decimation of prey by the predators. In contrast to the Lotka-Volterra model, the predators have a limited appetite: for $X \gg K_X$, it reaches the value $-wY$ which is independent of X. Eq. (6.47) describes the growth of the predator population. It is only positive if $JY/X < 1$, i.e. if $Y < X/J$. In other words: the predator population can only grow if at least J prey animals are available per predator.

For a detailed discussion of the properties of this model, we refer to Arrowsmith and Place (1992). For us, the important point is that the solutions of the Holling-Tanner model also show periodic oscillations of X and Y around an equilibrium value. However, in contrast to the Lotka-Volterra model, it is structurally stable. Apart from the trivial ($Y = X = 0$) and semi-trivial fixed point ($Y = 0, X = X_k$), the model has the nontrivial fixed point (X^∞, Y^∞) that results from the intersection of a parabola and a line (Fig. 6.18).[16] The parabola results from Eq. (6.46) with $\mathrm{d}X/\mathrm{d}t = 0$:

$$Y^\infty = \frac{r}{w}(1-\frac{X^\infty}{X_k})(X^\infty + K_X) \tag{6.48}$$

The line results from Eq. (6.47) with $\mathrm{d}Y/\mathrm{d}t = 0$:

$$Y^\infty = \frac{X^\infty}{J} \tag{6.49}$$

In the phase space, the system's trajectory eventually moves to a closed curve around the fixed point (X^∞, Y^∞). In contrast to the Lotka-Volterra model, this closed cycle is not fixed by the initial state once and for all. Rather, the trajectories move towards an "attraction curve" and then follow it (Fig. 6.17). Such a curve is called a limit cycle. A limit cycle is thus a "curve attractor" to which the system is attracted. Figure 6.18 shows the tuning of the periodic oscillations of $X(t)$ and $Y(t)$ to the limit cycle.

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[16] The stability properties of the semi-trivial fixed point will be discussed in Problem 6.5.

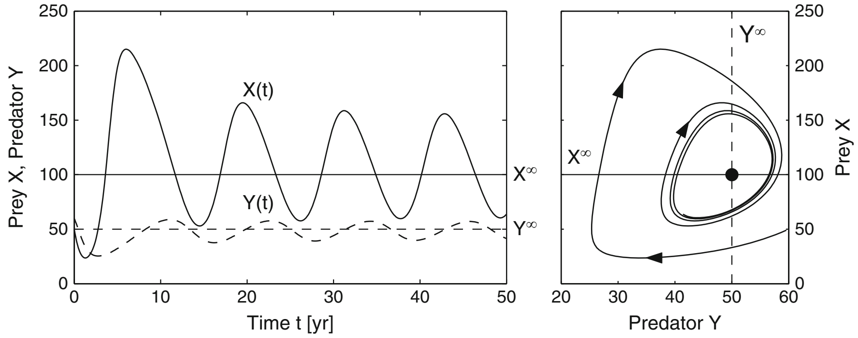


Fig. 6.17: *Numerical solution of the Holling-Tanner model. The system moves towards the limit cycle. Parameters used:* $r = 2.5\,year^{-1}$, $s = 0.225\,year^{-1}$, $w = 5\,year^{-1}$, $X_k = 300$, $K_X = 50$, *J=2. Initial conditions:* $X^0 = 50$, $Y^0 = 60$

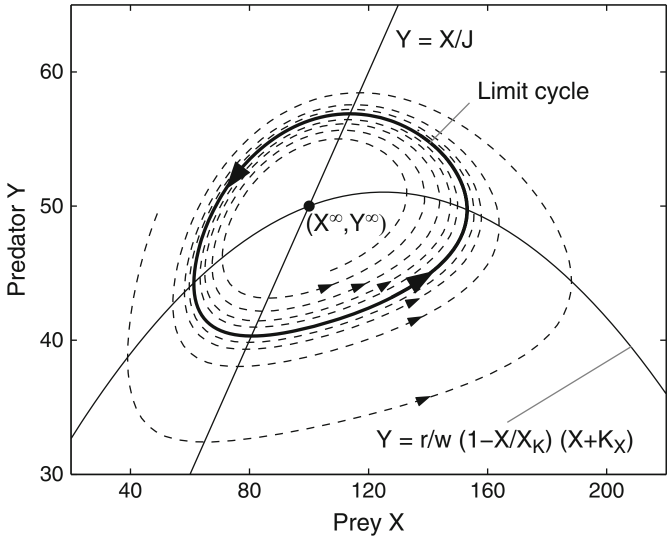


Fig. 6.18: *Determination of the nontrivial fixed point* (X^{∞}, T^{∞}) *from two curves (Eqs. 6.48 and 6.49) and calculation of two trajectories. The first* $(X^0 = 50, Y^0 = 50)$ *approaches the limit cycle from its outside, the second* $(X^0 = 105, Y^0 = 45)$ *from the inside. Model parameters are as in Fig. 6.17*

6.2.4 The Behavior of Models in the Vicinity of Centers

As we already mentioned earlier, in the vicinity of a center, the behavior of a nonlinear system *cannot* be determined with the linearization method. The following example (from Arrowsmith and Place 1992) demonstrates this.

Example 6.9: Two nonlinear models with center

We examine the following two linear models (x, y are the system variables).

Model 1:

$$\begin{aligned}\frac{\mathrm{d}x}{\mathrm{d}t} &= -y + x(x^2 + y^2)\\ \frac{\mathrm{d}y}{\mathrm{d}t} &= x + y(x^2 + y^2)\end{aligned} \tag{6.50}$$

Model 2:

$$\begin{aligned}\frac{\mathrm{d}x}{\mathrm{d}t} &= -y - x(x^2 + y^2)\\ \frac{\mathrm{d}y}{\mathrm{d}t} &= x - y(x^2 + y^2)\end{aligned} \tag{6.51}$$

The only difference between the two models is the sign of the second term on the right-hand side of the equations. Both models have the fixed point $x = y = 0$. The Jacobian matrices at the fixed point are identical:

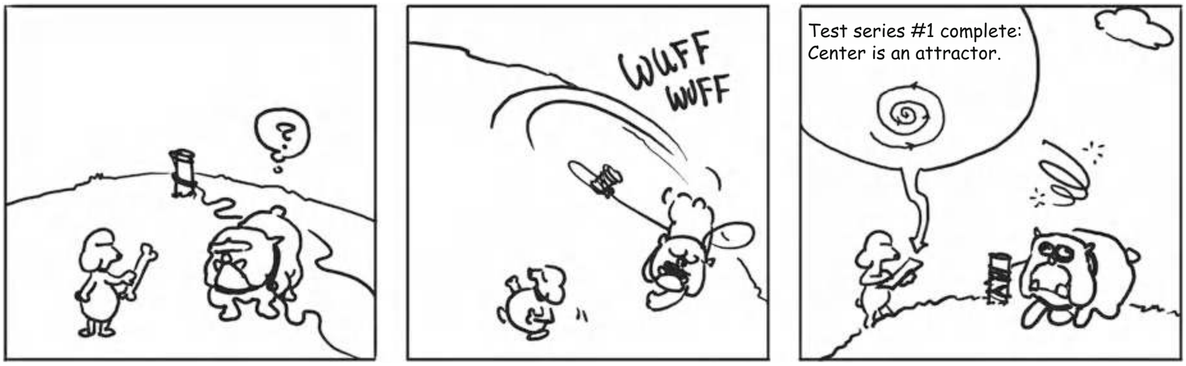
$$\mathbf{B} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{6.52}$$

We already know that the eigenvalues are purely imaginary ($\lambda_i = \pm \mathrm{i}$). The fixed points of the linearized systems are centers. But how do the nonlinearized systems really behave in the proximity of the fixed point? To answer this question, we introduce two new variables r and θ to replace x and y:

$$r = \sqrt{x^2 + y^2}, \qquad \theta = \arctan \frac{y}{x} \tag{6.53}$$

Of course, we didn't choose these particular notations for r and θ by accident: they are the polar coordinates in the original phase space (x, y). Now we have to formulate the new dynamic equations, which requires

Center



some effort, but nothing more than the chain rule of differentiation. We demonstrate the procedure with model 1[17]:

$$\begin{aligned}\frac{\mathrm{d}r}{\mathrm{d}t} &= \frac{\mathrm{d}r}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\mathrm{d}r}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}t}\\ &= \frac{x}{\sqrt{x^2+y^2}}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{y}{\sqrt{x^2+y^2}}\frac{\mathrm{d}y}{\mathrm{d}t}\\ &= \frac{-xy}{\sqrt{x^2+y^2}} + x^2\sqrt{x^2+y^2} + \frac{xy}{\sqrt{x^2+y^2}} + y^2\sqrt{x^2+y^2}\\ &= (x^2+y^2)^{\frac{3}{2}} = r^3\end{aligned} \tag{6.54}$$

$$\begin{aligned}\frac{\mathrm{d}\theta}{\mathrm{d}t} &= \frac{\mathrm{d}\theta}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\mathrm{d}\theta}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}t}\\ &= \frac{-y/x^2}{1+(x/y)^2}[-y+x(x^2+y^2] + \frac{1/x}{1+(x/y)^2}[x+y(x^2+y^2]\\ &= \frac{y^2}{x^2+y^2} - xy + \frac{x^2}{x^2+y^2} + xy = 1\end{aligned}$$

For model 2, the result is almost identical, except that $\mathrm{d}r/\mathrm{d}t$ has an inverted sign:

$$\frac{\mathrm{d}r}{\mathrm{d}t} = -r^3; \qquad \frac{\mathrm{d}\theta}{\mathrm{d}t} = 1 \tag{6.55}$$

The new variables r and θ have decoupled the two systems of differential equations (6.50) and (6.51). The arc function $\theta(t)$ has the trivial form:

$$\theta(t) = \theta_0 + t \tag{6.56}$$

This means that in both cases, the trajectory turns with constant angular velocity in a (mathematically) positive direction of rotation (which is counter-clockwise) around the coordinate origin. The difference between the two models is that in the case of Eq. (6.50) (model 1) the radius grows with time (outward spiral), whereas in the second case, the radius decreases (inward spiral) until the system comes to a rest in the fixed point $x = y = 0$. The two solutions are shown in Fig. 6.19 together with the trajectory of the undamped linear oscillator ($r = \text{const}$). Note that the third graph, the linear approximation of both nonlinear models, is not capable of making a distinction between them.

6.2.5 Nonlinear Models with Three and More Variables

In nonlinear systems of differential equations with more than two variables, a new phenomenon can occur: deterministic chaos. A system becomes

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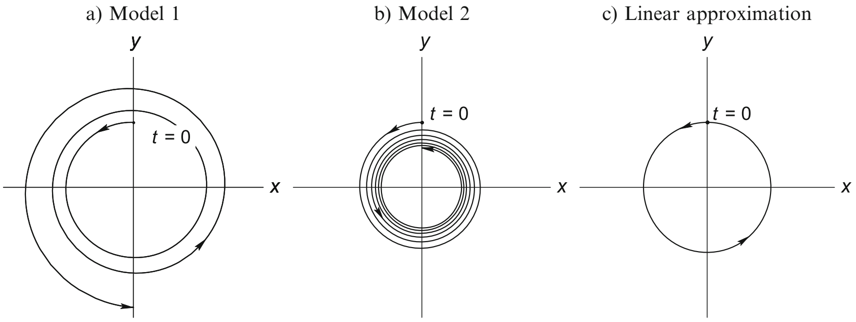
[17] Remember that $\frac{\mathrm{d}}{\mathrm{d}z}(\arctan z) = \frac{1}{1+z^2}$.



a) Model 1 b) Model 2 c) Linear approximation

Fig. 6.19: *The behavior of a system near a center cannot be predicted from the Jacobian matrix. Model 1 (Eq. 6.50) moves away from the center at $x = y = 0$, model 2 (Eq. 6.51) moves towards it. The linear approximation is a circular trajectory around the center*

chaotic if two trajectories starting from arbitrarily close initial points suddenly develop completely differently. Often, chaotic systems remain close to an attractor for a certain timespan, only to suddenly jump into a completely different course that unfolds around another attractor. Such attractors are called *strange attractors*. The chaos is called deterministic (as opposed to stochastic) because the underlying equations are entirely deterministic, i.e., they contain no random quantities. Because in reality, a system's state can never be measured to perfect precision (no measurement is without measurement error), there are always tiny differences between apparently identical states. These differences can be responsible for the diverging development from two seemingly equivalent initial states.

A well-founded discussion of deterministically chaotic systems would go beyond the scope of this book. We merely want to discuss one example: the Lorenz system. In order for deterministic chaos to occur, the system of differential equations has to be at least three-dimensional.[18]

Example 6.10: Lorenz model and deterministic chaos

In 1963, the atmospheric physicist Lorenz established a simple model to describe the coupling between heat convection and heat transport in a fluid (water, air, etc). He used three variables (x, y, z) with the following meaning:

x	Circulation speed of the convection source
y	Temperature difference between the upwards and downwards flowing fluid
z	Deviation of the vertical temperature gradient from the equilibrium

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[18] For difference models, *one* dimension is sufficient (see Chap. 7).

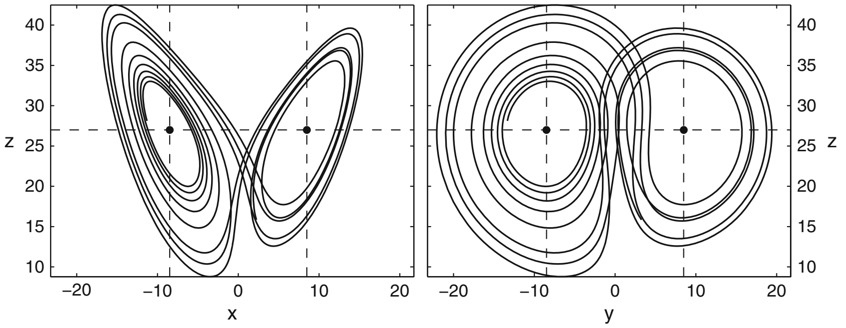

Fig. 6.20: *Solution of the Lorenz model (Example 6.10) with the parameters* $a = 10$, $b = 28$ *and* $c = 8/3$. *Initial conditions* $(x^0, y^0, z^0) = (-11.3, -13.3, 28.0)$. *Attractor at* $(\pm 8.4853,\ \pm 8.4853,\ 27.0000)$. *On the left, trajectories in three-dimensional phase space are projected onto the* (x, z) *plane, on the right, onto the* (y, z) *plane*

The system of differential equations has the following form:

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= a(y - x) \\ \frac{\mathrm{d}y}{\mathrm{d}t} &= bx - y - xz \\ \frac{\mathrm{d}z}{\mathrm{d}t} &= xy - cz \end{aligned} \tag{6.57}$$

a, b, c are positive constants with $b > 1$. The system has three fixed points:

(1) $x = y = z = 0$
(2) $x = y = \sqrt{(b-1)c}, \quad z = b - 1$
(3) $x = y = -\sqrt{(b-1)c}, \quad z = b - 1$

For certain parameter values a, b, c, the system seems to jump randomly between trajectories around the second and third fixed point. The resulting form has been called the “Lorenz butterfly” (Fig. 6.20). More about the Lorenz equations and chaos more generally can be found in Strogatz (1994).

6.3 Questions and Problems

Question 6.1: Explain the difference between implicit and explicit time dependence of a model.

Question 6.2: Define the term *autonomous system*.

Question 6.3: Give examples of systems where the implicit and explicit time dependence cannot be broken up as we did in Eq. (6.2). You can modify systems we introduced previously to get such examples.

Question 6.4: Give some properties that distinguish nonlinear from linear systems.

Question 6.5: What do we mean by the *area of attraction* of a fixed point?

Question 6.6: Characterize a linear system by its fixed points.

Question 6.7: What is an asymptotically stable fixed point?

Question 6.8: What do we mean with the term *hysteresis* in a model? Under which circumstances does it occur in a model with one variable?

Question 6.9: Why don't linear models exhibit hysteresis?

Question 6.10: Nonlinear models can describe synergistic effects. What do we mean by that?

Question 6.11: Which properties of a linear model are we speaking about if we say that linear models show no synergism?

Question 6.12: Which mathematical idea is behind the Jacobian matrix? What can we use this matrix for?

Question 6.13: What is the Jacobian matrix of a one-dimensional model?

Question 6.14: What do we mean by a *center*? What is special about it?

Question 6.15: What advantage does the Holling-Tanner predator-prey model have over the Lotka-Volterra model?

Question 6.16: What do we mean by *deterministic chaos*? When can it occur in systems of differential equations?

Problem 6.1: Mountain lake with time-dependent elimination rate
In Example 4.13 we analyzed a mountain lake with a yearly fluctuating nutrient input as a linear model. The total substance elimination rate of the lake was given as $k = 0.01\,\mathrm{d}^{-1}$. In fact, this rate also fluctuates over the year, because the substance-specific rate k_r depends on the season, as does the outflow rate k_w. To keep things simple, we assume that the total elim-

ination rate is $k = 0.005\,\mathrm{d}^{-1}$ for the first 6 months of the year, while for the rest of the year it is $k = 0.015\,\mathrm{d}^{-1}$. Analyze the resulting model, in particular by answering the following questions:

(a) Does this change make the model nonlinear?

(b) Can the model be described in the form of Eq. (6.2)?

(c) Identify the external relations.

(d) Sketch out a way to solve the model.

Problem 6.2: Fish in a pond
In Example 6.2 we discussed the model of a fish pond. We assumed that the fish grow logistically and that the fishing rate is constant. The model has the disadvantage that it can formally lead to negative fish populations. Modify the model so that the fishing rate is a linear function of the fish population N. The specific fishing rate is k_f.

(a) Establish the model equation and determine the fixed point(s) and its/their stability.

(b) Draw the model space graphically with the aid of the individual components of the change function (as we did in Fig. 6.4).

(c) How must we choose k_f so that the fixed-point fishing yield is maximized?

(d) Calculate the maximum allowable specific rate k_f so that the fish population does not go extinct.

Problem 6.3: Jacobian matrix of the Lotka-Volterra model
Calculate the Jacobian matrix of the Lotka-Volterra model (Eq. 6.36) as a function of the two system variables X and Y. Evaluate the matrix at the two fixed points of the model, determine the corresponding eigenvalue pairs and characterize the two fixed points according to their stability.

Problem 6.4: Predator-prey model with self-interaction
Calculate the Jacobian matrix for the predator-prey model with self-interaction (Eq. 6.42). Use it to determine the eigenvalues at the fixed point and characterize the fixed point's stability.

Problem 6.5: Semi-trivial fixed point of the Holling-Tanner model
One of the fixed points of the Holling-Tanner model (Example 6.8) is $X = X_k$, $Y = 0$. Examine the stability of the system at this fixed point with the Jacobian matrix and draw a qualitative sketch of the trajectories in the area surrounding the fixed point.

Problem 6.6: Nonlinear biomass growth in a pond

In a completely mixed pond with an average water retention time of $\tau_w = V/Q$ (V: pond volume, Q: flow rate), the growth of biomass concentration B depends on the concentration N of a limiting nutrient. Biomass B and nutrient N are expressed with the same units, e.g. $N =$ phosphorus per volume as dissolved nutrient and $B=$ phosphorus per volume incorporated into the biomass. The growth function G (transfer of phosphorus per volume and time into the biomass) has the following form ($N_0 > 0, k_w > 0$):

$$G(N,B) = \begin{cases} f_w N(N_0 - N)\,B & \text{for} \quad 0 \leq N \leq N_0 \\ 0 & \text{for} \quad N > N_0 \end{cases}$$

The decay function (recirculation of biomass phosphorus into dissolved nutrient phosphorus) has the form:

$$R(N,B) = k_A B, \qquad k_A > 0$$

The system has a constant nutrient input J_N (mass per time), the biomass input is zero.

(a) Draw a box diagram for the N/B system (don't forget the throughflow!).

(b) Graphically discuss the development of the growth function through time.

(c) Determine the fixed points and their stability.

(d) What is the condition (expressed by the coefficients) for a finite biomass to establish itself in the lake?

Problem 6.7: Lotka-Volterra with two prey animals

We consider a Lotka-Volterra model consisting of three species (two prey animals X_1, X_2, one predator Y). The following processes are taken into account:
Linear growth of the prey X_1, $k_1 X_1$
Linear growth of the prey X_2, $k_2 X_2$
Linear death rate of the predator, $k_3 Y$
Feeding rate of the predator for prey $X_1 : k_4 X_1 Y$
Feeding rate of the predator for prey $X_2 : k_5 X_2 Y$

(a) Draw a box diagram and formulate the dynamic equations.

(b) Identify the fixed points and their stability.

(c) Which species survive in the long run?

Numerical values:
$k_1 = 0.05\,\text{year}^{-1}$
$k_2 = 0.03\,\text{year}^{-1}$
$k_3 = 0.02\,\text{year}^{-1}$
$k_4 = 0.002\,\text{year}^{-1}$
$k_5 = 0.001\,\text{year}^{-1}$

(The variables X_1, X_2, Y are non-dimensional.)

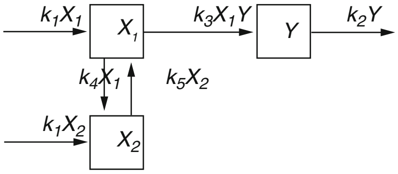

Fig. 6.21: *Lotka-Volterra model with a prey niche. X_1: prey in unprotected habitat, X_2: prey in niche (protected from predators), Y: predator*

Problem 6.8: Lotka-Volterra with prey niche

In the following modified Lotka-Volterra model, the prey animal can retreat into a protected niche (Fig. 6.21).

(a) Establish the dynamic equations.

(b) What are the conditions for the coefficients k_i so that a nontrivial[19] fixed point exists?

(c) What does the condition found in (b) mean biologically? How could we meaningfully modify the model (i.e. by introducing an improvement which makes sense from a biological point of view) so that a nontrivial fixed point always exists?

Problem 6.9: Competition for living space

Two species A and B are in direct competition for the same living space. The dynamics of the two populations, whose size are denoted by A and B, are influenced by the following processes:

1. Without the competing species, population A grows linearly with the constant rate k_1.
2. Similarly, without competition population B grows according to the following logistic model:

$$\frac{\mathrm{d}B}{\mathrm{d}t} = (k_3 - k_4 B)B \qquad \text{if} \qquad A = 0$$

3. The competition between populations A and B leads to a reduction of growth in both populations. The reduction is proportional to the product AB, where for A the proportionality factor is k_2 while for B it is k_5.

(a) Write down the dynamic equations for both populations.

(b) Determine all fixed points A_i^∞, B_i^∞ (the subscript i refers to the different fixed points).

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[19] The trivial fixed point is $X_1 = X_2 = Y = 0$.

(c) Determine the stability properties of those fixed points where both populations are different from zero. Hint: use the Jacobian matrix.

Use the following values for question (c) and assume that A and B are non-dimensional:

$k_1 = 4\ \mathrm{a}^{-1}; \quad k_2 = 1\ \mathrm{a}^{-1}; \quad k_3 = 6\ \mathrm{a}^{-1}; \quad k_4 = 1\ \mathrm{a}^{-1}; \quad k_5 = 1\ \mathrm{a}^{-1}$

Chapter 7

Time-Discrete Models

7.1 Time-Discrete Models with One Variable

In Sect. 2.4 we briefly introduced systems that change stepwise at certain times rather than continuously. Such systems and the corresponding models are called discrete in time or simply *time-discrete*. Starting from the initial time t_0 with $n = 0$, the times at which the stepwise changes take place are numbered sequentially: $t_1, t_2, t_3, \ldots$. The system variable $\mathcal{V}$ is only defined for these discrete times. We indicate them with the superscript[1] (n): $\mathcal{V}^{(n)}$.

A time-discrete model is like a recipe that tells us how, using the variable at a previous time, we can calculate its value at the next discrete time step $(n + 1)$. It is not even that important whether the index (n) actually describes consecutive time steps, or simply a sequence of events. In the stochastic bed of nails (Fig. 2.7), we let a ball roll down an inclined plane along a random path. Although we interpreted the left vertical axis in Fig. 2.7 as time axis, we could just as well have seen it as a series of impacts. At each impact ("time step"), the ball hits a nail and, according to a given probability distribution, rolls down to the next ("later in time") level.

As an illustration of how discrete models function, we choose a simple example from number theory. It states that the series of all quadratic numbers $Q^{(n)} \equiv n^2$ can be obtained with the following recipe:

$$Q^{(n+1)} = Q^{(n)} + 2\sqrt{Q^{(n)}} + 1 \tag{7.1}$$

As a starting point we choose $Q^{(0)} = 0$. The relation in Eq. (7.1) can either be proven mathematically or simply checked for its validity by explicit calculation of $Q^{(1)}, Q^{(2)}$ and so on. We thus have a recipe to determine $Q^{(n+1)}$ from $Q^{(n)}$, that is, how to calculate $(26)^2$ if we already know that $(25)^2 = 625$: $(26)^2 = 625 + 2 \times 25 + 1 = 676$. If we interpret $Q^{(n)}$ as a time

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[1] The index is put into brackets to distinguish it from a power exponent.

D.M. Imboden and S. Pfenninger, *Introduction to Systems Analysis*,
DOI 10.1007/978-3-642-30639-6_7,

series, this simple recipe describes how a discrete-time system develops. The instructions in Eq. (7.1) are then similar to a differential equation in time.

7.1.1 Difference Equations and the Numerical Solution of Differential Equations

At first sight, we could expect that analyzing and solving an iterative equation such as Eq. (7.1) is much easier than solving a differential equation such as Eq. (4.7):

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = k^\star \cdot \mathcal{V} \tag{4.7}$$

The algebraic solution of Eq. (4.7) cannot be found with a simple computer program,[2] whereas Eq. (7.1) seems an obvious candidate to be tackled with a simple iterative program. In fact, the most primitive integration algorithm for ordinary differential equations is based on the idea of approximating the continuous progression of time with finite intervals of size Δt. We define:

$$\mathcal{V}(t_n) \equiv \mathcal{V}^{(n)} \qquad \text{with} \qquad t_n = t_0 + n \cdot \Delta t \tag{7.2}$$

In discrete models, difference equations take the place of differential equations.

We then write Eq. (4.7) for a finite time step with a so-called *difference equation*:

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} \longrightarrow \frac{\Delta\mathcal{V}}{\Delta t} = \frac{\mathcal{V}^{(n+1)} - \mathcal{V}^{(n)}}{\Delta t} = k^\star \cdot \mathcal{V}^{(n)} \tag{7.3}$$

Solving for $\mathcal{V}^{(n+1)}$ gives us:

$$\mathcal{V}^{(n+1)} = (1 + \Delta t \cdot k^\star)\mathcal{V}^{(n)} \tag{7.4}$$

If we begin with the initial state $\mathcal{V}^{(0)}$ and apply the equation m consecutive times, we get:

$$\mathcal{V}^{(m)} = (1 + \Delta t \cdot k^\star)^m \mathcal{V}^{(0)} \tag{7.5}$$

This expression does not seem to have much in common with the exact solution of the differential equation (4.7), which, as we learned in Eq. (4.8), is an exponential function. Of course, the numerical approximation of the solution of (4.7) should eventually transform into the exact solution if only we choose the time step Δt small enough. If the integration should take place over the entire time period T, a given time step results in $m = T/\Delta t$ iterations. In the limit case, we have $\Delta t \longrightarrow 0$ and $m \longrightarrow \infty$. Inserted in Eq. (7.5), $\mathcal{V}^{(m)} \equiv \mathcal{V}(T)$ thus becomes a limit of the form:

$$\mathcal{V}(T) = \lim_{m\to\infty}[(1 + \frac{k^\star T}{m})^m]\mathcal{V}^{(0)} \tag{7.6}$$

---

[2] By "simple" we exclude advanced software such as Mathematica with which we could algebraically integrate.

As can be learnt from mathematical handbooks, $\lim_{m\to\infty}(1+\frac{A}{m})^m = e^A$, so with $A \equiv k^\star T$:

$$\mathcal{V}(T) = e^{k^\star T}\mathcal{V}^0 \tag{7.7}$$

This result is in full accordance with Eq. (4.8).

Let us exemplify the relation between discrete and continuous temporal change with an example which is familiar to all of us: the calculation of interest on a bank account.

Example 7.1: Bank interest

At the start of the year, you deposit 1,000€ in your bank account. The bank offers a generous yearly interest rate of 5 %. Calculate the account balance at the end of the year, if

(a) The interest is added to the account once per year;

(b) The interest is added quarterly;

(b) The interest is added monthly;

(d) The interest is added *continuously*.

We choose the variables $N_0 = 1{,}000$€ and $p = 0.05$. For the different scenarios, our account balance is then:

(a) $N(t=1) = N_0(1+p) = 1.05\times\ 1{,}000$€ $=1{,}050$€

(b) $N(t=\frac{1}{4}) = N_0(1+\frac{p}{4})$, thus
$N(t=\frac{2}{4}) = N(t=\frac{1}{4})(1+\frac{p}{4}) = N_0(1+\frac{p}{4})^2$
$\ldots$
$\Rightarrow N(t=1) = N_0(1+\frac{p}{4})^4 = (1+\frac{0.05}{4})^4\ N_0 = 1050.95$€

(c) Analogously to (b) we get
$N(t=1) = N_0(1+\frac{p}{12})^{12} = 1051.16$€

(d) To calculate the continuous interest payment, we use Eq. (7.7):
$N(t=1) = N_0 e^p = N_0 e^{0.05} = 1051.27$€

Fortunately for us depositors, the fact that interest is only payed once a year does not make such a big difference for small interest rates. For larger rates, it *would* make a difference however. For instance, for a rate of 20 % per year the balance would grow by 22.14 % over a year for continuous interest payment, compared to the "mere" 20 % if the interest is added once per year.

In many (but not in all) cases, the numerical solution of a differential equation approaches the exact solution if the time step is chosen small enough.[3] One could think, therefore, that a time-discrete difference equation is nothing more than a course-grained variant of a differential equation. One would then further assume that no fundamentally new system behavior is to be expected. These premature conclusions would be wrong, however. Let's take it step by step and look at how these models really behave.

7.1.2 First-Order Linear Models

We first examine the following inhomogeneous, linear, discrete, first-order equation with constant coefficients a_0 and I:

$$\mathcal{V}^{(n+1)} = I + a_0\mathcal{V}^{(n)} \tag{7.8}$$

Eq. (7.8) is of first order because $\mathcal{V}^{(n+1)}$ only depends on the immediate predecessor value $\mathcal{V}^{(n)}$. We already encountered the case $I = 0$ with Eq. (7.4) and in Example 7.1. As we will see, terms of the form $a_1\mathcal{V}^{(n-1)}$, $a_2\mathcal{V}^{(n-2)}$ etc. can occur on the right-hand side of Eq. (7.8). In such a case, the equation would become second, third or higher order.

Let's think of the linear differential equation that is related to the time-discrete linear Eq. (7.8). What does it look like? In other words: for which differential equation does Eq. (7.8) form a numerical approximation?

To answer this question, we need to bring Eq. (7.8) into the difference form (Eq. 7.3) by subtracting $\mathcal{V}^{(n)}$ on both sides:

$$\begin{aligned}\mathcal{V}^{(n+1)} - \mathcal{V}^{(n)} &= I + (a_0 - 1)\mathcal{V}^{(n)}\\ \text{or}\quad \frac{\mathcal{V}^{(n+1)} - \mathcal{V}^{(n)}}{\Delta t} &= J + k^\star\mathcal{V}^{(n)}\\ \text{with } J = \frac{I}{\Delta t}, \qquad k^\star &= \frac{a_0 - 1}{\Delta t}\end{aligned} \tag{7.9}$$

As we already know, the differential equation corresponding to Eq. (7.9), $\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = J + k^\star\mathcal{V}$, has the fixed point $\mathcal{V}^\infty = -\frac{J}{k^\star}$ for $k^\star < 0$. If our analogy between differential and difference equation is correct, with an infinite number of iterations and if $(a_0 - 1) < 0$ or $a_0 < 1$, Eq. (7.9) would have to tend to:

$$\mathcal{V}^\infty = -\frac{I/\Delta t}{(a_0 - 1)/\Delta t} = -\frac{I}{a_0 - 1} \tag{7.10}$$

We can check whether our conjecture is true by applying Eq. (7.8) several times in a row, starting with $\mathcal{V}^{(0)} \equiv \mathcal{V}_0$:

$$\begin{aligned}\mathcal{V}^{(1)} &= I + a_0\mathcal{V}_0\\ \mathcal{V}^{(2)} &= I + a_0\mathcal{V}^{(1)} = I + a_0(I + a_0\mathcal{V}_0) = I(1 + a_0) + a_0^2\mathcal{V}_0\\ \mathcal{V}^{(3)} &= I + a_0\mathcal{V}^{(2)} = \ldots = I(1 + a_0 + a_0^2) + a_0^3\mathcal{V}_0\end{aligned}$$

---

[3] We don't want to suggest that the "forward integration" we used in Eq. (7.3) is a particularly good strategy for numerical integration. There are in fact more efficient and reliable methods.

From this we can already see the general rule:

$$\mathcal{V}^{(n)} = I \cdot \sum_{i=0}^{n-1} (a_0)^i + a_0^n \mathcal{V}_0 \tag{7.11}$$

With the formula for the calculation of geometric sums,

$$\sum_{i=0}^{n-1} (a_0)^i = \frac{a_0^n - 1}{a_0 - 1} \qquad (a_0 \neq 1) \tag{7.12}$$

we finally get (for $a_0 \neq 1$)[4]:

$$\mathcal{V}^{(n)} = I \frac{a_0^n - 1}{a_0 - 1} + a_0^n \mathcal{V}_0 = -\frac{I}{a_0 - 1} + a_0^n \left(\frac{I}{a_0 - 1} + \mathcal{V}_0\right) \tag{7.13}$$

If $|a_0| < 1$, that is if $-1 < a_0 < 1$, the second term in Eq. (7.13) disappears for $n \to \infty$, so that:

$$\mathcal{V}^{\infty} = \lim_{n\to\infty} \mathcal{V}^{(n)} = -\frac{I}{a_0 - 1}, \quad -1 < a_0 < 1 \tag{7.14}$$

The assumption formulated in Eq. (7.10) is therefore only partially correct, because there is not only an *upper* bound ($a_0 < 1$). Equation (7.14) shows a lower bound, too: a_0 must also not become too negative (in fact, not more negative than -1). Otherwise the system oscillates back and forth between increasing positive and negative values. Figure 7.1 summarizes the different cases. Finally, we would like to note that similar to the case of an inhomogeneous linear differential equation, Eq. (7.8) could have been transformed into a homogeneous difference equation by introducing a new variable. It could then have been solved according to Eq. (7.5) (see Problem 7.1).

Example 7.2: Fish population in a pond

In a fish pond, fishing and natural mortality mean that only about 40 % of the individuals of a given fish species survive each year. Each spring, 1,200 individuals are set free in the pond. At the beginning of the year 2000, there were 1,000 fish in the pond.

(a) Calculate the fish population $N^{(n)}$ at the beginning of 2001 and 2002.

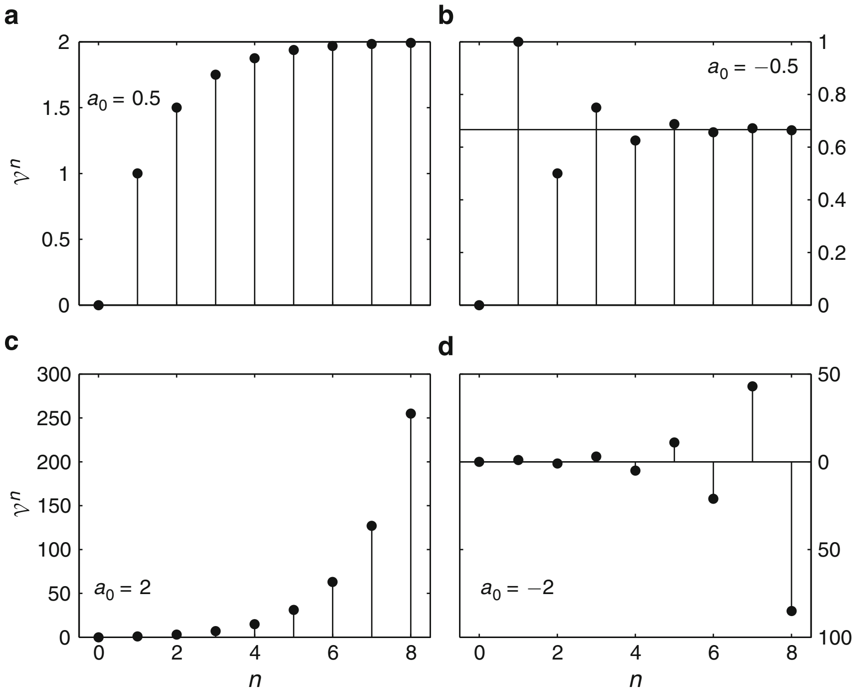
(b) In the long term, what is the fish population at the beginning of the year?

(c) If, at the beginning of 2000, there had been no fish in the pond, how long would it take for the difference to the first case (N^0 =1,000 in the year 2000) to be less than ten fish?

---

[4] For $a_0 = 1$, the result follows directly from Eq. (7.11): $\mathcal{V}^{(n)} = nI + \mathcal{V}_0$

Fig. 7.1: *Different solutions of the discrete linear first-order model (Eq. 7.8) with $I = 1$. (**a**) $0 < a_0 < 1$: direct convergence, (**b**) $-1 < a_0 < 0$: oscillating convergence, (**c**) $a_0 > 1$: direct divergence, (**d**) $a_0 < -1$: oscillating divergence*



(a) We begin our analysis in the year 2000 (N^0 =1,000) and apply Eq. (7.8) with $a_0 = 0.4$, I =1,200:
In the year 2001: $N^{(1)}$ =1,200+0.4×1,000 = 1,600
In the year 2002: $N^{(2)}$ =1,200+0.4×1,600 = 1,840

(b) Because $|a_0| < 1$, in the long run, at the end of each winter (i.e. just before the new fish are set free) the fish population reaches the following value (Eq. 7.14):

$$N^{\infty} = -\frac{1,200}{0.4 - 1} = 2,000$$

(c) If we apply Eq. (7.13) to our example,

$$N^{(n)} = \frac{I}{(1 - a_0)}(1 - a_0^n) + a_0^n N^0,$$

we can see that the influence of the initial state N^0 is limited to the last term. In the first case, this term is $(0.4)^n\times$ 1,000, in the second case it is zero. Thus we must ask ourselves for which n the following relation is valid:

$$(0.4)^n \times 1,000 = 10$$

If we transform the expression and take the logarithm on both sides, it follows that[5]:

$$n = \frac{\log(10/1,000)}{\log(0.4)} = \frac{\log(0.01)}{\log(0.4)} = \frac{-2}{-0.40} = 5$$

After 5 years at most, it no longer matters whether initially there were 1,000 or no fish in the pond.

7.1.3 Higher-Order Linear Models

Time-discrete models of higher (e.g. q) order are expressed by an iterative equation in which $q+1$ consecutive parameter values ($V^{(n)}, V^{(n+1)}, \ldots, V^{(n+q)}$) are put in a relation to each other. If the system is linear, the equation can be brought into the following form:

$$I + a_0 \mathcal{V}^{(n+q)} + a_1 \mathcal{V}^{(n+q-1)} + \ldots + a_q \mathcal{V}^{(n)} = 0 \tag{7.15}$$

In fact, the inhomogeneous Eq. (7.15) can be transformed into a homogeneous one by choosing a new variable which lacks the term I. More precisely, we choose the variable:

$$\hat{\mathcal{V}}^{(j)} = \mathcal{V}^{(j)} + b, \quad j = 1, 2, \ldots \tag{7.16}$$

If $\sum\limits_{i=0}^{q} a_i \neq 0$, and if we choose

$$b = \frac{I}{\sum\limits_{i=0}^{q} a_i} \tag{7.17}$$

then an iterative equation for $\hat{\mathcal{V}}^{(n)}$ emerges which, apart from the missing term I, has exactly the form of Eq. (7.15). Note that the solution of Eq. (7.15) requires the specification of q initial conditions (e.g. $\mathcal{V}^{(0)}$, $\mathcal{V}^{(1)}$, …, $\mathcal{V}^{(q-1)}$).

Example 7.3: Bottle recycling

A beverage manufacturer launches a new product in a special returnable bottle. Due to capacity limitations, the company can produce a maximum of 10,000 bottles per month. Experience shows that 70 % of

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[5] Either the natural logarithm or the common (base-10) logarithm work. The following numbers correspond to the common logarithm.

bottles are returned in the following month, and another 10 % a month later. The rest of the bottles is lost. The beverage company would like to know:

(a) How the monthly available number of bottles develops through time, and

(b) How many bottles it can refill per month in the long run.

The sale of the product begins in month 1 with the first 10, 000 bottles.

The iterative equation for the problem has the form

$$N^{(n+2)} = 0.7N^{(n+1)} + 0.1N^{(n)} + 10,000 \tag{7.18}$$

where $N^{(n)}$ is the number of available bottles in month n after launching the product. The initial conditions are:

$$\begin{aligned} N^{(0)} &= 0 \\ N^{(1)} &= 10,000 \end{aligned}$$

Without having to calculate much, we can easily answer the question about the long-term availability of bottles (that is, the fixed point N^{∞}). Twenty percent of the bottles never come back, which means they need to be replaced by new bottles (10,000 per month). This implies that, at the fixed point, 50, 000 bottles are filled each month, since 20 % of that are the 10,000 new ones. The bottle inventory develops as follows:

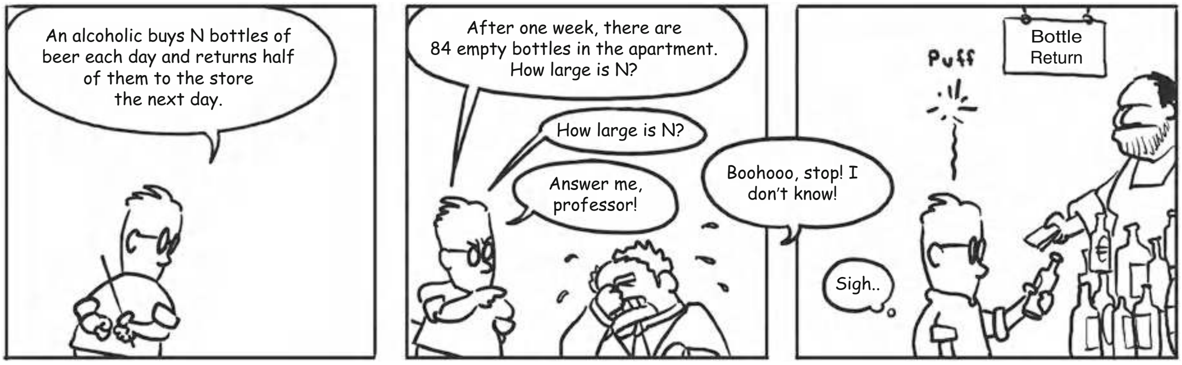
$$\begin{aligned} \text{2nd month: } N^{(2)} &= 0.7N^{(1)} + 0.1N^{(0)} + 10,000 \\ &= 7,000 + 0 + 10,000 = 17,000 \\ \text{3rd month: } N^{(3)} &= 0.7N^{(2)} + 0.1N^{(1)} + 10,000 \\ &= 11,900 + 1,000 + 10,000 = 22,900 \end{aligned}$$

At the fixed point, the following must hold: $N^{(n+2)} = N^{(n+1)} = N^{(n)} = N^{\infty}$. Therefore:

$$\begin{aligned} N^{\infty} &= 0.7N^{\infty} + 0.1N^{\infty} + 10,000 \\ \rightarrow N^{\infty} &= \frac{10,000}{0.2} = 50,000 \end{aligned}$$

Calculating the monthly values $N^{(n)}$ with the “recipe” in Eq. (7.18) is easily done on a computer; this would show that the value indeed asymptotically approaches $N^{\infty} = 50,000$.

Recycling bottles



In Sect. 7.1.2 we saw that a time-discrete model can also lead to divergent solutions (see Fig. 7.1). It would therefore be useful to have a mathematical tool to analyze equations of the form (7.15) more generally.
To that end, we look at the homogeneous form of Eq. (7.15), which we get via the transformation in Eq. (7.16):

$$a_0 \hat{\mathcal{V}}^{(n+q)} + a_1 \hat{\mathcal{V}}^{(n+q-1)} + \ldots + a_q \hat{\mathcal{V}}^{(n)} = 0 \tag{7.19}$$

We now claim that the following function[6] is a solution of Eq. (7.19):

$$\hat{\mathcal{V}}^{(n)} = \lambda^n \tag{7.20}$$

Inserting into Eq. (7.19) yields:

$$a_0 \lambda^{n+q} + a_1 \lambda^{n+q-1} + \ldots + a_q \lambda^n = 0$$

After dividing by λ^n we get an equation that is independent of the iteration step n:

$$a_0 \lambda^q + a_1 \lambda^{q-1} + \ldots + a_q = 0 \tag{7.21}$$

This is the characteristic equation of Eq. (7.19). In general, it has q (real or complex) solutions λ_j $(j = 1, \ldots, q)$. The general solution of Eq. (7.19) therefore results from a linear combination of all λ_j:

$$\hat{\mathcal{V}}^{(n)} = \sum_{j=1}^{q} A_j (\lambda_j)^n \tag{7.22}$$

The A_j are determined by the initial conditions. We want to limit our discussion of Eq. (7.22) to those situations in which the roots of the characteristic Eq. (7.21), λ_j, are real, and differentiate between two cases:

1. The absolute value of all λ_j is smaller than 1: $|\lambda_j| < 1$. Then, $\hat{\mathcal{V}}^{(n)}$ converges to zero for $n \to \infty$.

---

[6] Equation (7.20) makes it clear why we prudently write $\mathcal{V}^{(n)}$: The n in parentheses gives us the n-th iteration step, whereas λ^n actually means the n-th power.

2. At least one root is ≥ 1 in absolute value. Then, it follows that $\hat{\mathcal{V}}^{(n)} \to \pm\infty$ (excluding special initial conditions).

As a reminder: If Eq. (7.19) indeed developed from an inhomogeneous equation, then, because of Eq. (7.16), the following holds for the first case ($\hat{\mathcal{V}}^{(n)} \to 0$):

$$\lim_{n\to\infty} \mathcal{V}^{(n)} = \lim_{n\to\infty} \hat{\mathcal{V}}^{(n)} - b = -b = -\frac{I}{\sum\limits_{i=0}^{q} a_i} \tag{7.23}$$

Let's go back to Example 7.3 and analyze it again with the general theory. To do so, we write Eq. (7.18) in the form of Eq. (7.15):

$$10,000 - N^{(n+2)} + 0.7N^{(n+1)} + 0.1N^{(n)} = 0 \tag{7.24}$$

The characteristic equation is:

$$\begin{aligned} -\lambda^2 + 0.7\lambda + 0.1 &= 0 \\ \rightarrow \quad \lambda &= -\frac{1}{2}[-0.7 \pm \{(0.7)^2 + 0.4\}^{1/2}] \\ &= -\frac{1}{2}[-0.7 \pm 0.943] \\ \rightarrow \quad \lambda_1 = +0.822; \quad \lambda_2 &= -0.122 \end{aligned}$$

We are dealing with case 1 (convergence), therefore, as per Eq. (7.23):

$$N^{\infty} = -b = -\frac{10,000}{(-1 + 0.7 + 0.1)} = \frac{10,000}{0.2} = 50,000$$

This conforms to our earlier result. Finally, the general solution of Eq. (7.24) with the initial values of $N^{(0)} = 0$, $N^{(1)} = 10,000$ is (also see Problem 7.4):

$$N^{(n)} = 50,000 - 48,850\ (0.822)^n - 1,150\ (-0.122)^n \tag{7.25}$$

7.1.4 Nonlinear Models

Even though the question of whether linear difference models tend to a fixed point is not as easily answered as for the case of linear differential equations, simple recipes (as in Fig. 7.1) to analyze their long-term behavior do exist. In the case of nonlinear systems, however, the matter becomes quite a bit more complex. In this section we will only look at first-order nonlinear models and merely give one example of the multifaceted world of such models.

We consider a (time-discrete) difference model of the form:

$$\mathcal{V}^{(n+1)} - \mathcal{V}^{(n)} = g(\mathcal{V}^{(n)}) \tag{7.26}$$

$g(\mathcal{V}^{(n)})$ is an arbitrary function of $\mathcal{V}^{(n)}$, for instance the logistic growth function (see Eq. 6.4):

$$g(\mathcal{V}^{(n)}) = k(b - \mathcal{V}^{(n)})\mathcal{V}^{(n)}\ , \quad k, b > 0 \tag{7.27}$$

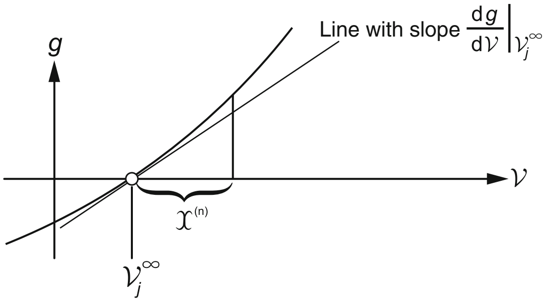


Fig. 7.2: *As in the case of one-dimensional nonlinear differential equations, the behavior of a nonlinear difference model near a fixed point can be analyzed with local linearization. To do so, the function* $g(\mathcal{V})$ *is replaced by a straight line at the fixed point* $\mathcal{V}_j^\infty$*. The line has the slope* $\frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}|_{\mathcal{V}_j^\infty}$. $\mathcal{X}^{(n)}$ *indicates the deviation of* $\mathcal{V}^{(n)}$ *from the fixed point.*

Obviously, the roots of the function $g(\mathcal{V}^{(n)})$ are the fixed points of the model, since there, according to (7.26), $\mathcal{V}^{(n+1)} = \mathcal{V}^{(n)}$. As in the case of nonlinear differential equations we analyze the behavior of the system at the fixed point $\mathcal{V}_j^\infty$ by introducing a new discrete variable:

$$\mathcal{X}^{(n)} = \mathcal{V}^{(n)} - \mathcal{V}_j^\infty \tag{7.28}$$

It then follows from Eq. (7.26):

$$\mathcal{X}^{(n+1)} - \mathcal{X}^{(n)} = g(\mathcal{V}^{(n)}) = g(\mathcal{V}_j^\infty + \mathcal{X}^{(n)}) \tag{7.29}$$

If the deviation from the fixed point ($\mathcal{X}^{(n)}$) is small, g can be developed into a Taylor series and broken off after the linear term (see Fig. 7.2):

$$g(\mathcal{V}_j^\infty + \mathcal{X}^{(n)}) = g(\mathcal{V}_j^\infty) + \frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\bigg|_{\mathcal{V}_j^\infty} \mathcal{X}^{(n)} + \dots \tag{7.30}$$

Since $\mathcal{V}_j^\infty$ is a fixed point, by definition, $g(\mathcal{V}_j^\infty) = 0$. We get a linear difference equation for $\mathcal{X}^{(n)}$[7]:

$$\mathcal{X}^{(n+1)} - \mathcal{X}^{(n)} = \frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\bigg|_{\mathcal{V}_j^\infty} \mathcal{X}^{(n)} \tag{7.31}$$

A simple transformation results in:

$$\mathcal{X}^{(n+1)} = \left(1 + \frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\bigg|_{\mathcal{V}_j^\infty}\right) \mathcal{X}^{(n)} = A\,\mathcal{X}^{(n)} \tag{7.32}$$

---

[7] Obviously, the procedure is completely analogous to the one we used for nonlinear differential equations in Chap. 6.

From our earlier discussion (e.g. in Fig. 7.1), we already know that Eq. (7.32) tends to the fixed point if the following holds:

$$|A| = \left| 1 + \left.\frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\right|_{\mathcal{V}_j^\infty} \right| < 1 \tag{7.33}$$

Expressed by $\left.\frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\right|_{\mathcal{V}_j^\infty}$ this means, in accordance with the continuous case (Eq. 6.12), that the fixed point $\mathcal{V}_j^\infty$ is unstable if the following holds:

$$\left.\frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\right|_{\mathcal{V}_j^\infty} \geq 0 \quad \Leftrightarrow \quad \mathcal{V}_j^\infty \;\; \text{unstable} \tag{7.34}$$

The inverse is not true however: in fact, because of Eq. (7.33) the fixed point can also be unstable due to a strongly *negative* slope of the function g. Altogether, the conditions for stability are:

$$0 > \left.\frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\right|_{\mathcal{V}_j^\infty} > -2 \quad \Leftrightarrow \quad \mathcal{V}_j^\infty \;\; \text{stable} \tag{7.35}$$

Example 7.4: Discrete logistic growth

The time-discrete logistic growth model is well-suited to have a brief exemplary look at the surprising world of nonlinear difference models. Eq. (7.27) describes discrete logistic growth. The model has two fixed points: $\mathcal{V}_1^\infty = 0$ and $\mathcal{V}_2^\infty = b$. Combining the logistic growth equation with the model function (7.26) yields the following model equation:

$$\mathcal{V}^{(n+1)} - \mathcal{V}^{(n)} = k(b - \mathcal{V}^{(n)})\mathcal{V}^{(n)} \equiv g(\mathcal{V}) \;, \quad k, b > 0$$

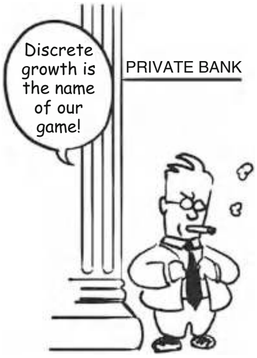
$g(\mathcal{V})$ has the derivative:

$$\frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}} = -2k\mathcal{V}^{(n)} + kb \;, \tag{7.36}$$

For the two fixed points this results in:

$$\left.\frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\right|_{\mathcal{V}_1^\infty} = +kb \;, \quad \left.\frac{\mathrm{d}g}{\mathrm{d}\mathcal{V}}\right|_{\mathcal{V}_2^\infty} = -kb \;, \quad k, b > 0 \tag{7.37}$$

As long as $kb < 2$, the second fixed point $\mathcal{V}_2^\infty$ is stable. The first fixed point, $\mathcal{V}_1^\infty = 0$, is always unstable.



For the following analysis of the logistic growth model we closely follow Arrowsmith and Place (1992). With the new variable $x^{(n)} = \frac{k}{1+kb}\mathcal{V}^{(n)}$ the model equation takes the form

$$x^{(n+1)} = \mu(1 - x^{(n)})x^{(n)} \equiv F_\mu(x^{(n)}) \;, \quad \mu \equiv 1 + kb \tag{7.38}$$

The function $F_\mu(x)$ is a downward-facing parabola with its apex at $x = \frac{1}{2}$, intersecting the x-axis at $x = 0$ and $x = 1$ (Fig. 7.3a). Note that $F_\mu(x)$ only depends on the parameter μ: we add it as an index to the function F because it will play an important role.

The model has reached an equilibrium x^∞ if the following holds:

$$x^\infty = F_\mu(x^\infty) = \mu x^\infty(1 - x^\infty) \tag{7.39}$$

Solving for x^∞ gives (next to the trivial solution $x^\infty = 0$):

$$x^\infty = \frac{\mu - 1}{\mu} \tag{7.40}$$

Graphically speaking, we get x^∞ as the intersection of the parabola $y = F_\mu(x)$ with the line $y = x$ (Fig. 7.3a). The evolution of the system from an initial point $x^{(0)}$ to the fixed point x^∞ can also be shown graphically (Fig. 7.3b).

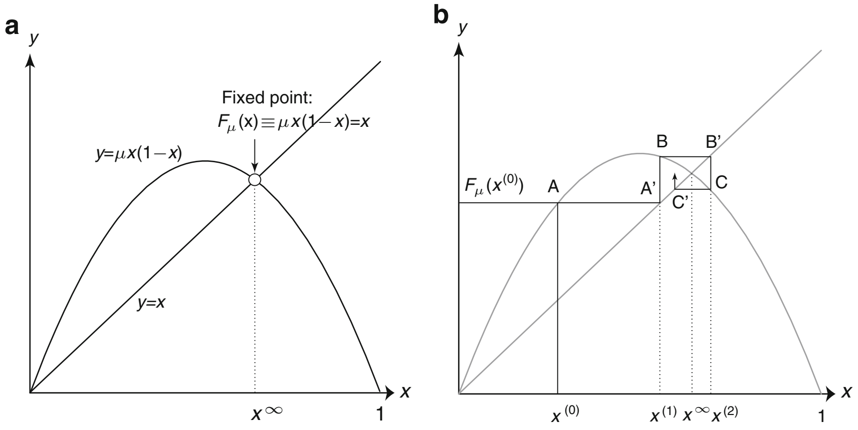


Fig. 7.3: *(**a**) Graphical determination of the fixed point of the discrete model* $x^{(n+1)} = \mu x^{(n)}(1 - x^{(n)}) \equiv F_\mu(x^{(n)})$*. See text for further explanations. (**b**) The movement of the model from the initial state* $x^{(0)}$ *to the fixed point* x^∞ *can be determined graphically: After the first iteration,* $F_\mu(x^{(0)})$ *takes on the new* x *value* $x^{(1)}$*, at point A. That* x *value can be found by mirroring* $x^{(1)} = F_\mu(x^{(0)})$ *on the line* $x = y$ *(point A'). The value* $F_\mu(x^{(1)})$*, belonging to* $x^{(1)}$*, lies at point B. By mirroring B on the line* $x = y$ *(point B') we get* $x^{(2)}$ *or point C, and so forth, all the way to the fixed point* x^∞ *(From Arrowsmith and Place (1992))*

As shown above, the nontrivial fixed point is stable for $0 < kb < 2$ which translates into the stability condition $1 < \mu < 3$. Yet, for $\mu \geq 3$ there are fixed points as well, although of a different kind. For instance, for $\mu = 3.2$, the system ends on a closed path that oscillates between the two

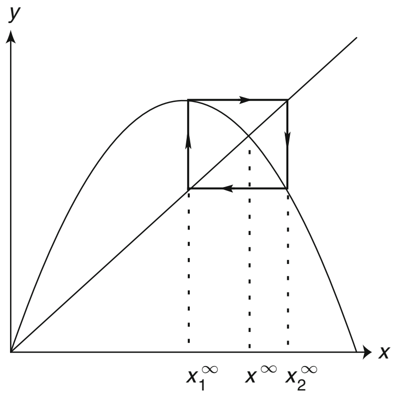


Fig. 7.4: *Behavior of the discrete model* $x^{(n+1)} = \mu x^{(n)}(1 - x^{(n)})$ *for* $\mu = 3.2$. *In contrast to Fig. 7.3b, the trajectory is not moving towards the fixed point* $x^\infty = \frac{\mu-1}{\mu} = 0.6875$, *but rather oscillates between the two points* x_1^∞ *and* x_2^∞. *More about this case is found in Fig. 7.5c*

values x_1^∞ and x_2^∞ lying on either side of x^∞ (Fig. 7.4).[8] In other words: if we only consider every other value $x^{(n)}$, i.e. only either the even or odd n, these sequences again reach a fixed point. We thus have to formulate a new specification from the iterative equation Eq. (7.38) that directly takes us from $x^{(n)}$ to $x^{(n+2)}$, skipping the intermediate step $x^{(n+1)}$. We name this "double-jump function" $F_\mu^{(2)}$. To get $F_\mu^{(2)}$ out of F_μ, we insert $y = \mu x(1-x)$ in the function $F_\mu(y) = \mu x(1 - y)$:

$$F_\mu^{(2)}(x) = \mu^2 x(1 - x)[1 - \mu x(1 - x)] \tag{7.41}$$

$F_\mu^{(2)}$ is a fourth-order polynomial and must not be confused with the square of F_μ. Its fixed points can be calculated—as in the case of F_μ—from the following equation:

$$x^\infty = F_\mu^{(2)}(x^\infty) \tag{7.42}$$

Graphically, they can be found from the intersection of $y = F_\mu^{(2)}(x)$ with the line $y = x$.

In Fig. 7.5 we plotted $F_\mu^{(2)}(x)$ for three different values of μ. We are interested in the nontrivial ($x \neq 0$) intersections of the curve with the line $x = y$. For $\mu = 2.8$ (Fig. 7.5a) there is a single intersection point x^∞. Of course, it is identical with the fixed point of the "single-jump function" F_μ (as per Eq. 7.40, $x_\infty = \frac{1.8}{2.8} = 0.643$), since if the system doesn't move anymore after a single jump, it will also remain motionless after two, three, or q jumps.

For $\mu = 3$, the curve $y = F_\mu^{(2)}(x)$ has a slope of exactly 1 at the intersection—as does the function $y = x$ (Fig. 7.5b). For even larger values of μ (e.g. for $\mu = 3.2$, see Fig. 7.5c), the original intersection point x^∞ is divided into two new intersection points x_1^∞ and x_2^∞. These two drift apart

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[8] Strictly speaking this is only true if the initial point does not lie at $x^\infty = \frac{\mu-1}{\mu} = \frac{(3.2-1)}{3.2} = 0.6875$.

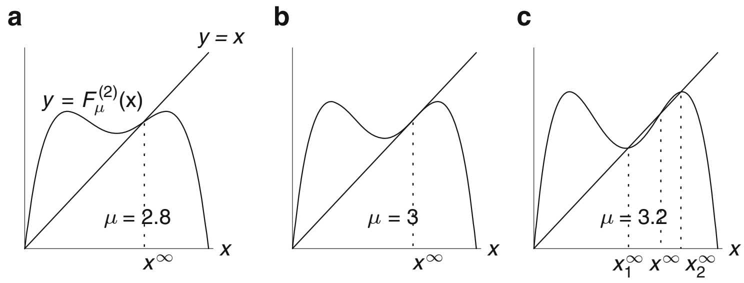

Fig. 7.5: *(**a**) The fixed points of the "double-jump function" (Eq. 7.32) result from the intersection of the curves* $y = F_\mu^{(2)}(x)$ *and* $y = x$*. (**b**) For* $\mu = 3$*, the system shows a bifurcation: The intersect* x^∞ *splits into the two points* x_1^∞ *and* x_2^∞ *(period doubling). (**c**) "Two-jumps function" for the situation shown in Fig. 7.4 (From Arrowsmith and Place (1992))*

further for an increasing μ. The "double-jump system" then has three fixed points in total (the middle one, x^∞, being unstable). The "single-jump system" in contrast jumps back and forth between x_1^∞ and x_2^∞. In fact, Fig. 7.5c represents the case shown as "single-jump system" in Fig. 7.4.

The behavior of the system at $\mu = 3$ is called *phase doubling*. The points at which this doubling occurs are called *bifurcation points*. In order to get further bifurcation points, we have to examine the "four-jumps function" $F_\mu^{(4)}$, or $F_\mu^{(8)}$, $F_\mu^{(16)}$ and so forth. In fact, the model experiences further phase doublings with growing μ. Yet the story does not end here: Above the critical value $\mu^\star = 3.8284\ldots$, completely new situations for which no periodic cycles exist appear on the scene. For $\mu > 4$ these aperiodic fluctuations play the predominant role if the system did not start on a periodic solution by chance. This strange behavior is another example of *deterministic chaos*, which we already encountered in Sect. 6.2.5.

The emergence of deterministic, but unpredictable (that is, apparently chaotic) behavior is not actually that surprising—we know it very well from our own experience. We can take the 104 cards from a Solitaire card game as an example. They can be mixed in 104! ways (factorial of 104, a number

Even one-dimensional non-linear difference models can exhibit chaotic (not easily predictable) behavior.

Bifurcation

with more than 160 digits). If we now deal a certain set of cards from our deck, and make our decisions strictly according to certain rules, we will be able to win the game for certain sets of cards but not for others. Switching two cards could be enough to turn a set without a solution into one with a solution. Even though all steps are completely determined, we will be unable to deduce any regularity that could let us predict whether the game will work out or not.

7.2 Time-Discrete Models with Several Variables

7.2.1 Linear Models

After this short glance at the complex world of chaos, we'll try to get to firmer ground again and to conclude this chapter by having a look at multi-dimensional discrete models. In essence, we will concentrate on the discussion of first-order multi-dimensional linear models and only explicitly solve the two-dimensional case.

A first-order q-dimensional linear difference model can be expressed by the following algebraic system of equations:

$$\mathcal{V}_i^{(n+1)} = I_i + \sum_{j=1}^{q} p_{ij} \mathcal{V}_j^{(n)} \quad , \quad i = 1 \dots q \tag{7.43}$$

The p_{ij} are the elements of the coefficient matrix $\mathbf{P} = (p_{ij})$ which we already introduced for multi-dimensional linear differential equations (see Eq. 5.81). So we can also write Eq. (7.43) in matrix form:

$$\boldsymbol{\mathcal{V}}^{(n+1)} = \mathbf{I} + \mathbf{P}\boldsymbol{\mathcal{V}}^{(n)} \tag{7.44}$$

$\mathbf{P}$ is a $(q \times q)$ matrix; $\boldsymbol{\mathcal{V}}^{(n+1)}$,$\boldsymbol{\mathcal{V}}^{(n)}$ and $\mathbf{I}$ are q-dimensional vectors.

Outwardly, the difference equation (7.44) now looks like Eq. (7.8), except that the coefficient a_0 from there has become the matrix $\mathbf{P}$ while $\boldsymbol{\mathcal{V}}^{(n)}$ and $\mathbf{I}$ have become vectors. Indeed, formally we can write the solution for Eq. (7.44) in the same way as Eq. (7.11):

$$\boldsymbol{\mathcal{V}}^{(n)} = (\mathbf{P})^n \cdot \boldsymbol{\mathcal{V}}^0 + \sum_{i=0}^{n-1} (\mathbf{P})^i \ \mathbf{I} \tag{7.45}$$

Calculating the power of matrices is quite complicated in general, so the formal solution Eq. (7.45) is of little use for concrete calculations. There is one important exception, however: if the matrix $\mathbf{P}$ were to have a diagonal form by chance, its powers would be diagonal too, so that we could simply take the power of the diagonal elements of the original matrix. If $\mathbf{P}$ is diagonal, this also means that the original algebraic system of equations (7.43) can be broken down into q disjoint equations which can all be solved independently of each other.

And with that, we are (as in Sect. 5.2), once again faced with eigenvalues. If we should succeed to diagonalize the coefficient matrix through the introduction of new variables, we could use all the tools we learnt for one-dimensional systems in Sect. 7.1.2 to solve Eq. (7.43).

Instead of more theoretical considerations and the risk of loosing track of the essential issues, we now want to turn to the concrete example of a two-dimensional system and use it to illustrate the important concepts step by step.

7.2.2 Linear Models with Two Variables

Example 7.5: Who wins against the bank?

Two gamblers (X and Y) agree on the following rules of a game with money, to be applied successively through each round of the game:

1. Player X receives from or pays to the bank 2/3 of the amount which she currently posesses, minus 1/3 of the amount that player Y has.
2. At the same time player Y receives from or pays to the bank 1/3 of the amount that he currently has, minus 2/3 of the amount that player X holds.

When we write "receives from or pays to", that is because the balances $X^{(k)}$ and $Y^{(k)}$ can also become negative, in which case the term that described money received from the bank now represents money lost to it.
The initial balance is $X^0 = 600$ and $Y^0 = 900$. How do the players' balances develop? Determine a general formula for the balance after k rounds, $X^{(k)}$ and $Y^{(k)}$. Does the bank lose money by performing these transactions?

First, we establish the iterative equation by translating the rules into mathematical expressions step by step. The change of balance in the k-th step is:

$$\begin{aligned} X^{(k)} - X^{(k-1)} &= \frac{2}{3}X^{(k-1)} - \frac{1}{3}Y^{(k-1)} \\ Y^{(k)} - Y^{(k-1)} &= -\frac{2}{3}X^{(k-1)} + \frac{1}{3}Y^{(k-1)} \end{aligned} \tag{7.46}$$

Eq. (7.46) can be transformed to:

$$\begin{aligned} X^{(k)} &= \frac{5}{3}X^{(k-1)} - \frac{1}{3}Y^{(k-1)} \\ Y^{(k)} &= -\frac{2}{3}X^{(k-1)} + \frac{4}{3}Y^{(k-1)} \end{aligned} \tag{7.47}$$

Or, in matrix form (and calling the (2×2) matrix $\mathbf{P}$):

$$\begin{pmatrix} X^{(k)} \\ Y^{(k)} \end{pmatrix} = \begin{pmatrix} 5/3 & -1/3 \\ -2/3 & 4/3 \end{pmatrix} \begin{pmatrix} X^{(k-1)} \\ Y^{(k-1)} \end{pmatrix} = \mathbf{P} \begin{pmatrix} X^{(k-1)} \\ Y^{(k-1)} \end{pmatrix} \tag{7.48}$$

Whether the bank goes bust or not can be decided by looking at the development of the sum $S^{(k)} = X^{(k)} + Y^{(k)}$ throughout the game. If we add up the two equations from Eq. (7.47), we get:

$$S^{(k)} \equiv X^{(k)} + Y^{(k)} = X^{(k-1)} + Y^{(k-1)} \equiv S^{(k-1)} \tag{7.49}$$

So there is no danger for the bank; the sum of balances stays constant at $S^0 = X^0 + Y^0 =$1,500. On the other hand, however, the bank also doesn't make any profit. But what about the distribution of the total amount amongst the two players?

Table 7.1: Example 7.5: State of the game after the first four rounds

k	$X^{(k)}$	$Y^{(k)}$	$S^{(k)}$
0	600	900	1,500
1	700	800	1,500
2	900	600	1,500
3	1,300	200	1,500
4	2,100	−600	1,500

Table 7.1 shows the state of the game after the first four rounds, calculated by applying Eq. (7.47) successively. Not a good game for Y! Even though he began with a head start, after only four rounds he's already in debt. How does the game go on?

It would be elegant if we could formulate the solution of the system of equations similarly as the one for the one-dimensional system (Eq. 7.8). Let's recall Eq. (7.49): the difference equation of the sum $S^{(k)} \equiv X^{(k)} + Y^{(k)}$ is solvable by itself, without calculating the individual solutions of $X^{(k)}$ and $Y^{(k)}$. We will apply a trick (the benefit of which will become apparent soon): we'll look for a second linear combination[9] of $X^{(k)}$ and $Y^{(k)}$ whose iterative equation is solvable by itself. Indeed, such a form exists:

$$T^{(k)} = 2X^{(k)} - Y^{(k)} \tag{7.50}$$

---

[9] A linear combination of two variables X and Y is an arbitrary linear expression of the form $aX + bY$. Of course the sum of X and Y is a linear combination with $a = b = 1$.

If, with the aid of the original iterative equations (7.47), we replace the variables $X^{(k)}$ and $Y^{(k)}$ in Eq. (7.50) with their "predecessors" $X^{(k-1)}$ and $Y^{(k-1)}$, it follows that:

$$\begin{aligned}
T^{(k)} &= 2\,\left[\frac{5}{3}X^{(k-1)} - \frac{1}{3}Y^{(k-1)}\right] - \left[-\frac{2}{3}X^{(k-1)} + \frac{4}{3}Y^{(k-1)}\right] \\
&= \left[\frac{10}{3} + \frac{2}{3}\right]\,X^{(k-1)} - \left[\frac{2}{3} + \frac{4}{3}\right]\,Y^{(k-1)} \\
&= 4X^{(k-1)} - 2Y^{(k-1)} = 2\,(2X^{(k-1)} - Y^{(k-1)})
\end{aligned}$$

So:

$$T^{(k)} = 2T^{(k-1)} \tag{7.51}$$

The solution of the iterative equation now becomes very simple:

$$T^{(k)} = 2^k T^0 = 2^k\,(2X^0 - Y^0) = 2^k \times 300 \tag{7.52}$$

What remains is to replace the original variables $X^{(k)}$ and $Y^{(k)}$ with the new variables $S^{(k)}$ and $T^{(k)}$, whose solutions we know (see Eqs. 7.49 and 7.52). After a bit of algebra we find:

$$\begin{aligned}
X^{(k)} &= \frac{1}{3}\,(S^{(k)} + T^{(k)}) \\
Y^{(k)} &= \frac{1}{3}\,(2S^{(k)} - T^{(k)})
\end{aligned} \tag{7.53}$$

By using the solutions for $S^{(k)}$ and $T^{(k)}$ we can thus also reconstruct those for $X^{(k)}$ und $Y^{(k)}$:

$$\begin{aligned}
X^{(k)} &= \frac{1}{3}\,(S^{(0)} + 2^k T^{(0)}) \\
&= \frac{1}{3}\,(1,500 + 2^k \times 300) \\
Y^{(k)} &= \frac{1}{3}\,(2S^{(0)} - 2^k T^{(0)}) \\
&= \frac{1}{3}\,(3,000 - 2^k \times 300)
\end{aligned} \tag{7.54}$$

It now immediately becomes clear that player Y must loose. In Problem 7.6 we ask how large the initial sums $X^{(0)}$ and $Y^{(0)}$ have to be so that (with the same rules) player Y wins or the amounts of the two players remain constant. Of course, the latter situation represents a fixed point.

How could one have guessed the trick we applied to solve Eq. (7.46)? In the following section, we will discuss the deeper meaning of the solution and the method we used to get to it.

7.2.3 The Role of Eigenvalues and Eigenfunctions

As elegant as the solution of Example 7.5 may be, it does not explain which intuition we followed when we introduced the new variables $S^{(k)}$ and $T^{(k)}$

(Eqs. 7.49 and 7.50). Although it was possible, with some experience, to see from the system of equations (7.46) or (7.47) that the sum of the two variables $X^{(k)}$ and $Y^{(k)}$ remains constant, the choice of Eq. (7.50) appears quite random.

Of course, behind this method lurks a mathematical concept that we frequently mentioned: the determination of the eigenvalues (and associated eigenfunctions) of a linear system. In Appendix D we explain the procedure for a n-dimensional system. Without using computational methods, only two-dimensional systems can be solved by hand with reasonable effort. Table 7.2 on the next page summarizes the approach for Example 7.5.

There would be a lot more to say about time-discrete models and their difference equations (we haven't even mentioned multi-dimensional non-linear models in passing!). Nevertheless, we want to close the discussion here. There is other literature available to delve deeper into the topic (e.g. Luenberger 1979).

Table 7.2: The solution of two-dimensional difference models with eigenfunctions, explained with Example 7.5. Appendix D gives an overview of all equations used here

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The matrix **P** of the system (7.47) is:

$$\mathbf{P} = \begin{pmatrix} 5/3 & -1/3 \\ -2/3 & 4/3 \end{pmatrix} \tag{7.55}$$

with

$$\mathrm{tr}(\mathbf{P}) = \frac{5}{3} + \frac{4}{3} = 3$$

$$\det(\mathbf{P}) = \frac{1}{9}(20 - 2) = 2$$

Eigenvalues (D.13):

$$\lambda_i = \frac{1}{2}[3 \pm \sqrt{3^2 - 4 \times 2}] = \frac{1}{2}[3 \pm 1]$$

$$\lambda_1 = 2, \quad \lambda_2 = 1$$

Eigenfunctions (D.17):

$$\begin{aligned} z_1 &= -\frac{2}{3}X + (2 - 5/3)Y = -\frac{2}{3}X + \frac{1}{3}Y \\ &= -\frac{1}{3}(2X - Y) \\ z_2 &= (1 - 4/3)X - \frac{1}{3}Y = -\frac{1}{3}(X + Y) \end{aligned}$$

Note: Except for the constant factors, z_1 and z_2 are consistent with the variables S und T, that is, $z_1 = -\frac{T}{3}$ and $z_2 = -\frac{S}{3}$. The eigenfunctions are only determined to a constant factor.
Determinant (D.21):

$$D = -2 \times 2 + 2 \times \frac{4}{3} + 1 \times \frac{5}{3} = \frac{1}{3}[-12 + 8 + 5] = \frac{1}{3}$$

So, according to (D.20) the reverse transformation is:

$$\begin{aligned} X &= 3\left[-\frac{1}{3}z_1 - (2 - \frac{5}{3})z_2\right] = -(z_1 + z_2) \\ Y &= 3\left[-(1 - \frac{4}{3})z_1 - \frac{2}{3}z_2\right] = z_1 - 2z_2 \end{aligned}$$

The result conforms with Eq. (7.53), if—as mentioned before—we take into account that $z_1 = -T/3$ and $z_2 = -S/3$.

7.3 Questions and Problems

Question 7.1: Explain the difference between a time-discrete model and a model that is continuous in time.

Question 7.2: Explain the relationship between the terms *difference model* and *time-discrete model*.

Question 7.3: Why is it important whether the interest is paid out yearly or quarterly for interest rates above 10 % per annum, but much less so for 2 %?

Question 7.4: Explain the difference between *order* and *dimension* of a difference model.

Question 7.5: Give examples of algebraic formulas for:

(a) A one-dimensional, linear first-order difference model.
(b) Like (a), but nonlinear.
(c) Like (a), but second-order.
(d) Like (a), but two-dimensional.
(e) Like (d), but non-linear.

Question 7.6: What is the difference between one-dimensional nonlinear difference models from the corresponding differential models, in terms of the stability of a fixed point?

Question 7.7: Explain the difference between $(F_\mu)^2$ (Eq. 7.38) and $F_\mu^{(2)}$ (Eq. 7.41).

Question 7.8: What do we mean by *deterministic chaos* in difference models?

Question 7.9:

(a) Which dimension must a nonlinear first-order difference model have at least, so that in principle, deterministic chaotic behavior could occur?

(b) What is the answer to that question for nonlinear systems of differential equations?

Question 7.10: What is the characteristic equation of a qth-order linear difference model? Is there a characteristic equation for nonlinear models?

Problem 7.1: Elimination of the inhomogeneous term
Calculate the fixed point $\mathcal{V}^\infty$ of the time-discrete model $\mathcal{V}^{(n+1)} = I + a_0\mathcal{V}^{(n)}$ by introducing a new variable $\hat{\mathcal{V}}^{(n)}$ which converts the model equation into the homogeneous relation $\hat{\mathcal{V}}^{(n+1)} = b\hat{\mathcal{V}}^{(n)}$. Derive a corresponding recipe for a linear qth-order iteration model.

Problem 7.2: Consumer loan

A credit institute charges its credit card holders a monthly interest of 2.5 % on the amount they owe. What yearly interest rate does this equate to?

Problem 7.3: Reactor with chloride

In a chemical reactor, 10 kg of chloride are added weekly. All chloride is completely mixed with the water in the reactor. Once per week, 20 % of the solution in the tank is emptied.

(a) How much chloride is there in the tank immediately before the weekly discharge, if the reactor has already been in operation for a very long time?

(b) If the reactor contains no chloride at time $t = 0$, how many weeks does it take until the amount of chloride in the tank has reached the value calculated in (a) to within a 5 % deviation?

Note: chloride is conservative in the reactor, i.e. it does not react. The reactor is completely mixed before the weekly discharge.

Problem 7.4: Returnable bottles

Let's take another look at the beverage manufacturer from Example 7.3.

(a) Prove Eq. (7.25).

(b) Deduce a corresponding relation, if in the first month initially only 5,000 bottles are produced, but 10,000 in every following month.

Problem 7.5: Fibonacci numbers

The Fibonacci numbers are a sequence of numbers that can be defined by the iterative equation $y^{(n+2)} = y^{(n+1)} + y^{(n)}$. With $y^{(1)} = y^{(2)} = 1$, they are therefore $1, 1, 2, 3, 5, 8, \ldots$. With the characteristic equation, develop a relation of the following form that describes the Fibonacci numbers:

$$y^{(n)} = A_1\lambda_1^n + A_2\lambda_2^n \ldots$$

Note: the result will deliver irrational expressions for both the λ values and the coefficients A_i (they contain $\sqrt{5}$). Nevertheless, the resulting $y^{(n)}$ will be rational, even integer numbers!

Problem 7.6: Gambling

In Example 7.5, for unchanged rules, how do we have to choose the initial balances for the two players (X^0 and Y^0), so that

(a) player Y wins?

(b) both players keep a constant balance?

Problem 7.7: Students in a study program

In a given subject, 120 students start studying per year. On average, five students per year drop out prematurely. The study duration is 5 years. How many students are enrolled in the program in total (i.e. in all years combined) once the system has reached a fixed point?

Problem 7.8: Fish in a pond

In a pond, each winter $J = 10,000$ fish are introduced. In summer, together with the offspring from natural reproduction, these fish form age cohort 1, $N_1^{(i)}$, of the i-th year. A fraction of $a = 0.1$ of this age group survives the winter (the rest is either caught by fishermen or dies), it becomes next year's age cohort 2, $N_2^{(i+1)}$. Higher-order age cohorts are not taken into account because due to the high death rate, they are very small. The contribution of natural reproduction in $N_1^{(i)}$ is calculated as follows: each fish of age cohort 1 of the previous year produces $b_1 = 0.5$ offspring (that is, $b_1 N_1^{(i-1)}$), each fish of age cohort 2 of the previous year produces $b_2 = 2$ (i.e. $b_2 N_2^{(i-1)}$).

(a) Draw a box diagram to describe $N_1^{(i)}$ and $N_2^{(i)}$.

(b) Establish the iterative equations for $N_1^{(i)}$ and $N_2^{(i)}$.

(c) Convert the two coupled first-order difference equations into a single second-order difference equation for $N_1^{(i)}$.

(d) Calculate $N_1^{(i)}$ and $N_2^{(i)}$ by iterating through the first years. Use the initial values $N_1^{(0)} = 0,\ N_2^{(0)} = 0$.

(e) To solve this equation, convert the inhomogeneous into a homogeneous equation by using a new variable (see Eq. 7.16). Look for a general solution for $N_1^{(i)}$ (and subsequently also for $N_2^{(i)}$) by using the characteristic equation.

(f) How large is the fish population at the fixed point (if there is one)? In other words, calculate $N_1^{(\infty)} + N_2^{(\infty)}$.

Chapter 8

Models in Time and Space

Transport and transformation

8.1 Mixing and Transformation

Natural systems have a spatial structure, but until now, we either completely ignored it (as in the case of the one-box model) or we described it in a highly simplified manner (as in the two-box model of a stratified lake, Example 5.8).

In this chapter, we will discuss situations where continuity in time as well as in space is important. In the most general case, this implies mathematically describing the system variable $\mathcal{V}_i$ as a continuous function of the spatial coordinates (x, y, z)[1] and of time t:

$$\mathcal{V}_i \to \mathcal{V}_i(x, y, z, t) \tag{8.1}$$

$\mathcal{V}_i$ can represent any scalar quantity, for instance the three-dimensional temperature distribution in the Atlantic Ocean as a function of time, or the

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[1] x, y, z are the three axes of a Cartesian coordinate system. Of course we could also use different coordinates, such as the spherical coordinates r, θ, φ.

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north/south component of wind velocity in the troposphere. In the latter case, the variable could be combined with the wind velocities along the other two Cartesian coordinate axes (east/west and upwards/downwards) to form the three-dimensional vector field of wind speed, which plays an important role in weather and climate models.

In our examples, we will primarily deal with scalar fields (temperature, concentrations, etc) rather than vector fields. In addition, we will concentrate on one-dimensional spatial models. For instance, we want to model the dynamics of the vertical oxygen distribution in a lake $C(z,t)$ (as shown in Chap. 2, Fig. 2.6). Before we start building our model, however, we have to make sure that it is justified to consider the concentration variations along the vertical axis only (i.e. to neglect the concentration changes along the horizontal axes x and y).

Usually, measurements show relatively similar O_2 concentrations across a lake at a given depth, even in lakes spanning several kilometers, whereas the vertical changes vary significantly over depths as little as a few meters. This suggests that it is justified to approximate the three-dimensional O_2 distribution $C(x,y,z,t)$ with a single[2] vertical profile $C(z,t)$, just as in Fig. 2.6. Limnologists would explain the one-dimensional behavior of lakes as follows. O_2 production by photosynthesizing plankton and O_2 consumption due to respiration and decay of organic matter primarily depend on the available light intensity, i.e. vary primarily with depth. Physics adds another observation that completes the explanation: in lakes (as in the sea), mixing processes along the horizontal axes are much quicker and more intensive than in the vertical. Potential concentration differences along the horizontal dimension are therefore evened out quickly, whereas they can remain for a long time along the vertical dimension.

What makes sense for the lake example can be used as the basis for a more general theory of the spatial structure of scalar fields. At each location in a natural system, transport and transformation processes occur simultaneously.[3] The relative speed of the two processes determines whether spatial structures can form and remain, or whether transport processes constantly counterbalance them and keep the system in a state of homogeneous mixing. In Fig. 8.1 we compare typical mixing times τ_{mix} with transformation times τ_r. The former indicate, for instance, how long it takes for a substance introduced to the atmosphere to vertically propagate in the troposphere (vertical tropospherical mixing time). One could also look at horizontal tropospherical mixing in the southern or northern hemisphere, global tropospherical mixing, or the mixing between troposphere and stratosphere. These mixing processes (ordered above by increasing duration) are system-specific, i.e. they depend on the properties of the system in which the mixing processes occur. In the examples above, they depend on the mixing dynamics of the atmosphere.

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[2] Most appropriately an average profile, or one measured at the lake's center.

[3] Transport processes occur not only in fluid systems (atmosphere and hydrosphere), but also in solid materials, only much slower and therefore much less obvious (e.g. molecular diffusion in solid matter).

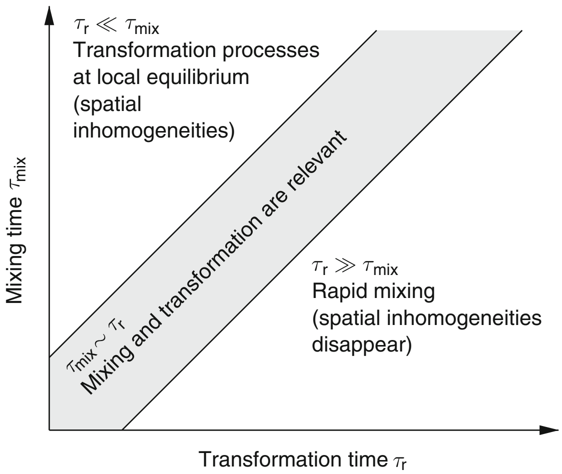

Fig. 8.1: *Schematic display of the relative magnitude of transformation time τ_r and mixing time τ_{mix}. For $\tau_r \gg \tau_{mix}$, the system is spatially completely mixed (homogeneous). For $\tau_r \ll \tau_{mix}$, all system components are locally at equilibrium but spatial inhomogeneities prevail. At the transition area ($\tau_r \sim \tau_{mix}$) both mixing and transformation determine the system's spatial structure*

While the mixing time is system-specific, the transformation time[4] τ_r is a substance-specific quantity. For instance, τ_r could be defined by the half-life $\tau_{1/2}$ of a radioactive isotope (as in Example 4.7) or the adjustment time of a reactive chemical substance (as in Example 4.8). In a system characterized by a given mixing time τ_{mix}, there can be substances with a transformation time of τ_r either much larger, much smaller or of a similar magnitude as τ_{mix}. In Fig. 8.1, these substances would be, respectively, in the area of *rapid mixing*, the area of *transformation processes at local equilibrium*, or in the transition area (shaded diagonal). Examples for the diverse relations between transformation and transport are qualitatively shown in Fig. 8.2.

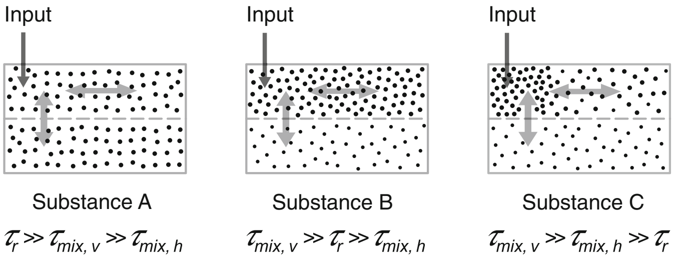

Fig. 8.2: *Spatial distribution of three substances A, B and C in a system with rapid horizontal (h) and slow vertical (v) mixing ($\tau_{mix,h} \ll \tau_{mix,v}$). The transformation time of substance A is largest (low reactivity), that of substance C smallest (high reactivity). Substance A is distributed almost equally across the system, substance C very unequally. Substance B exhibits vertical inhomogeneity, but is horizontally well mixed*

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[4] The time needed to reach locally complete (or almost complete) reactive equilibrium.

8.2 Advection, Diffusion and Exchange

In the following subsections, we will discuss the processes responsible for transport and mixing and show how the mixing times (τ_{mix}) introduced above can be quantified.

8.2.1 Advection (Directed Transport)

Transport processes can be directed or the result of many small random movements.

There are essentially two types of transport processes: directed and undirected (random) ones. The directed process is called advection. In a fluid medium (e.g. water, air), advection results from flow. Flow can be quantified with the flow vector $\mathrm{v} = (v_x, v_y, v_z)$. All substances that are contained in a fluid element moved by flow are transported in the same direction, that of the flow vector $\boldsymbol{v}$ (Fig. 8.3a). Therefore, we call advective transport directed.

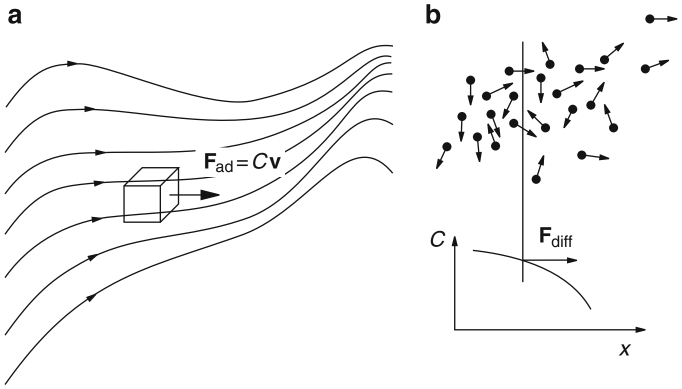


Fig. 8.3: *(**a**) The transport in a flow field ($\mathbf{F}_{\mathrm{ad}}$, advective transport) is directed, i.e. it has the same direction for all substances contained in a given volume of fluid, and an absolute value that is proportional to the various substance concentrations C. (**b**) Diffusive transport results from a large number of random individual movements. The net flux, $\mathbf{F}_{\mathrm{diff}}$, is directed from the higher to the lower concentration (Fick's first law)*

The advective mass flow F_{ad} (transported mass per time and per area perpendicular to the flow) is:

$$\mathrm{F}_{ad} = C\ \mathrm{v} \quad [ML^{-2}T^{-1}] \tag{8.2}$$

where C $[\mathrm{M\ L^{-3}}]$ is the concentration of the substance. This vector equation can also be written component-wise:

$$F_{ad,x} = Cv_x \ ; \quad F_{ad,y} = Cv_y \ ; \quad F_{ad,z} = Cv_z \tag{8.3}$$

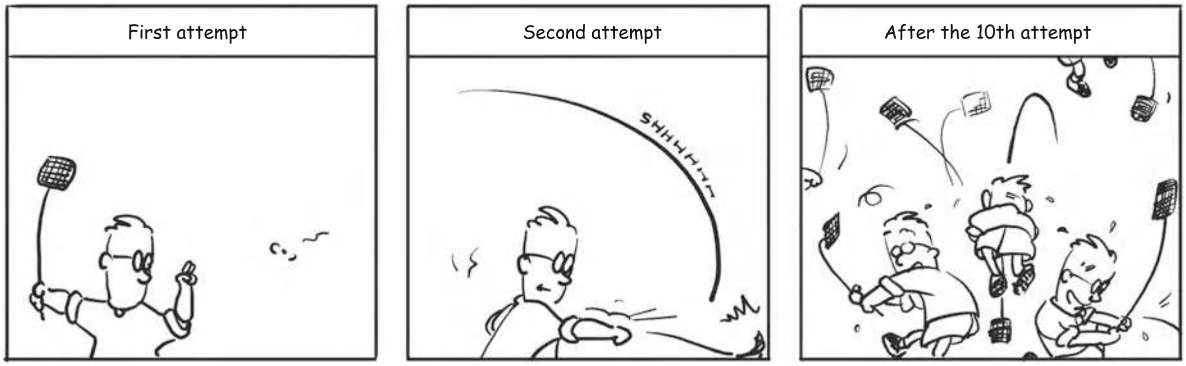
x, y, z are the Cartesian coordinates and $F_{ad,x}, v_x, \ldots$ the respective components of the vectors $\mathrm{F}_{ad,x}$ and $\boldsymbol{v}$.

The distance covered in time t by a fluid element and the substances it contains is $x_{ad} = v_x t$ (analogous for the other coordinates). Strictly speaking, however, this is only true if t is chosen small enough so that the flow can be considered to be straight during this time. The mixing time by advection in a system with the extent L can be written as:

$$\tau_{mix,ad} = \frac{L}{v} \tag{8.4}$$

where for simplicity we have omitted the coordinate subscripts x, y or z.

Directed and undirected movement



8.2.2 Diffusion: Undirected Transport

Diffusive transport is a result of individual random movement. The best illustration is the thermal movement of gas molecules. As an example, let's look at the behavior of benzene molecules which are inhomogeneously (i.e. irregularly) distributed in a volume of air (Fig. 8.3b). Even though the velocity vectors of the individual benzene molecules don't point in the same direction, for this particular situation they nonetheless cause a net benzene transport from the left to the right side. This is simply because the benzene concentration on the left side is higher, and therefore, the probability that a molecule crosses the "virtual boundary" from left to right is higher than the other way around.

Mathematically, this behavior is described by *Fick's first law*. Written for one spatial dimension (x-axis), it reads[5]:

$$F_{diff,\ x} = -D_x \frac{\partial C}{\partial x} \quad [ML^{-2}T^{-1}] \tag{8.5}$$

D_x	$[\mathrm{L^2T^{-1}}]$	Diffusion coefficient in x direction
$\frac{\partial C}{\partial x}$	$[\mathrm{M\,L^{-4}}]$	Partial derivative of substance concentration in x direction

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[5] Because C depends on several coordinates $(t, x, \ldots)$, we use the symbol for the partial derivative (∂) in the following discussion, to remind you that when calculating the derivative the other coordinates are held constant.

Analogous equations are valid for y and z directions. If the cause of the transport process is thermal movement of the molecules, D_x is called the molecular diffusion coefficient. Usually, it is the same for all three dimensions ($D_x = D_y = D_z \equiv D$). Thus the three components of Eq. (8.5) can be summarized in one vector equation:

$$\mathrm{F}_{diff} = -D\ \boldsymbol{\nabla} C \tag{8.6}$$

$\boldsymbol{\nabla}$ is the gradient operator:

$$\boldsymbol{\nabla} C = \begin{pmatrix} \partial C/\partial x \\ \partial C/\partial y \\ \partial C/\partial z \end{pmatrix} \tag{8.7}$$

Eq. (8.5) is called a *flux-gradient model* (as is Eq. 8.6, of course). The minus sign shows that transport is always directed against the gradient, i.e. from the higher to the lower concentration. Wherever undirected random processes are involved, flux-gradient models appear, as for instance in heat conduction (Fourier's law).

Determining the mixing time $\tau_{mix,diff}$ for diffusion is somewhat more difficult than for advection. We could ask ourselves, for instance, how a concentration jump (a front) in a fluid behaves under the influence of diffusion, or how quickly a substance initially concentrated in one spot spreads through space (in one, two, or three dimensions). In all these cases we can express the diffusive mixing distance with the following equation:

$$L_{diff} = a(Dt)^{1/2} \tag{8.8}$$

where the numerical factor depends on whether diffusion occurs along one, two or three spatial dimensions. In the case of one-dimensional diffusion, $a = \sqrt{2}$. This yields the famous Einstein-Smoluchowski relation[6]:

$$L_{diff} = (2Dt)^{1/2} \tag{8.9}$$

Note that in contrast to advection, in which the distance L grows linearly with time t, diffusion only advances proportionally to $\sqrt{t}$ since it is undirected and not "goal-oriented". Solving Eq. (8.8) for t yields the diffusive mixing time $\tau_{mix,diff}$:

$$\tau_{mix,diff} = \frac{1}{a^2}\,\frac{L^2}{D} = \frac{L^2}{2D} \tag{8.10}$$

where the expression on the far right corresponds to the Einstein-Smoluchowski relation for one dimension.

8.2.3 Exchange at Boundary Layers

In Fig. 8.3b, we imply that mass flow takes place through an *imaginary* boundary layer. In many situations, however, the boundary is physically

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[6] In Chap. 8.4.1 we will derive this relation for a special case (see Eq. 8.54)

real, for instance between a liquid and a gas. Transport across this boundary is called *gas exchange*. At the interface between the gaseous and liquid phase, the concentration (expressed as mass per volume) exhibits a sudden jump, i.e. a mathematical discontinuity, so that the concentration gradient needed for the application of Eq. (8.5) becomes infinitely large.

We thus need a different approach. In Sect. 3.1 we showed that the equilibrium between two chemical phases A and B can be described by a static equilibrium relation of the following form (eq = equilibrium):

$$K_{A/B} = \left(\frac{C_A}{C_B}\right)_{eq} \tag{8.11}$$

Thus, for a given C_B there is a value $C_A^{eq} = K_{A/B} C_B$ which is in equilibrium with C_B. If A signifies air ($A = a$) and B water ($B = w$), then $K_{A/B}$ is the non-dimensional Henry coefficient $K_{a/w}$ (Eq. 3.2).

The mass flow across a real boundary (such as the water surface) is described by the following expression:

$$F_{A/B} = v_{A/B}(C_A - C_A^{eq}) \quad [ML^{-2}T^{-1}] \tag{8.12}$$

$F_{A/B}$:	Mass flux per area and time between A and B ($F_{A/B} > 0$, if net transport from A to B)
$v_{A/B}$ [L T^{-1}]:	Exchange velocity at the boundary layer
$C_A^{eq} = C_B K_{A/B}$ [M L^{-3}]:	Concentration in A that is at equilibrium with the concentration in B, C_B (Eq. 8.11).

Equation (8.12) is the result of undirected transport as well. The molecules (or other objects) cross the boundary layer in both directions. At equilibrium ($C_A = C_A^{eq}$), the two fluxes compensate each other ($F_{A/B} = 0$).

The exchange model Eq. (8.12) can also be applied to the flux between two identical phases. In Example 5.8 we described the mass exchange between the epilimnion and the hypolimnion of a stratified lake, with Q_{ex} describing the water volume exchanged per time. If Q_{ex} is normalized by the area A through which the exchange takes place, we get a quantity with the dimension of a velocity which we call the *exchange velocity*: $v_{ex} = Q_{ex}/A$ [L T^{-1}]. In the following example, we will encounter yet another application of the exchange model Eq. (8.12).

Example 8.1: Museum with a Roman gold treasure

In a museum, a separate room A showcases a famous Roman treasure of gold coins. The room is only reachable from the neighboring room B (see Fig. 8.4). On weekends, when visitor numbers peak, room A is often hopelessly overcrowded. The museum's director therefore decides to analyze visitor behavior so that museum staff in room B can foresee precarious conditions and take measures in time. The study shows the following result:

(1) Each minute, 30 % of visitors in room B decide to enter the treasure chamber A.

(2) Each minute, 10 % of visitors inside the treasure chamber (A) decide to leave.

The goal is to prevent visitor numbers in A from exceeding the critical value of $N_A^{crit} = 30$.

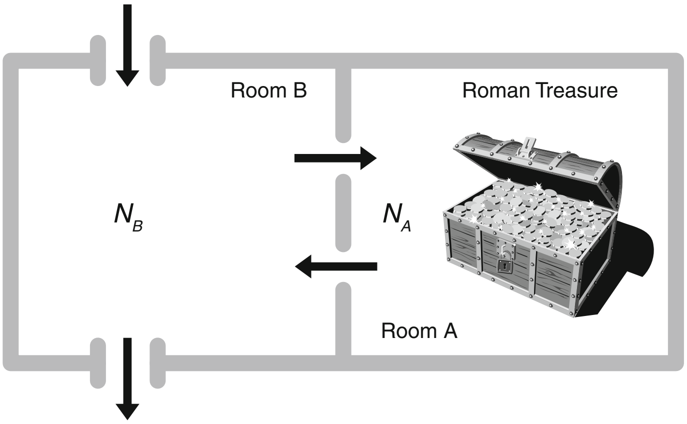


Fig. 8.4: *The flow of visitors between exhibition room A containing the roman treasure, and room B through which visitors must pass, can be described by an exchange model.* N_A, N_B *= number of visitors in the rooms A and B*

We use $k_B N_B$ to denote the transition rate of visitors from B to A, and $k_A N_A$ for A to B. N_A and N_B are the number of visitors in the respective rooms. From observations (1) and (2) it follows that $k_B = 0.3\ \text{min}^{-1}$ and $k_A = 0.1\ \text{min}^{-1}$. The *net flow* of visitors from B to A is:

$$F_{B\to A} = k_B N_B - k_A N_A \tag{8.13}$$

Room A is in equilibrium with room B if $F_{B\to A} = 0$, that is, for:

$$N_A^{eq} = \frac{k_B}{k_A}\, N_B \tag{8.14}$$

We can replace N_B in Eq. (8.13) with N_A^{eq}. It then follows that:

$$F_{B\to A} = k_B \left(\frac{k_A}{k_B}\, N_A^{eq}\right) - k_A N_A = k_A (N_A^{eq} - N_A) \tag{8.15}$$

This relation has the same form as the exchange flow in Eq. (8.12). For $N_A \leq N_A^{crit}$ to remain true, $N_A^{eq} < N_A^{crit}$ must hold, therefore:

$$N_A^{eq} = \frac{k_B}{k_A}\, N_B \leq N_A^{crit} \tag{8.16}$$

This condition is fulfilled as long as the following is true:

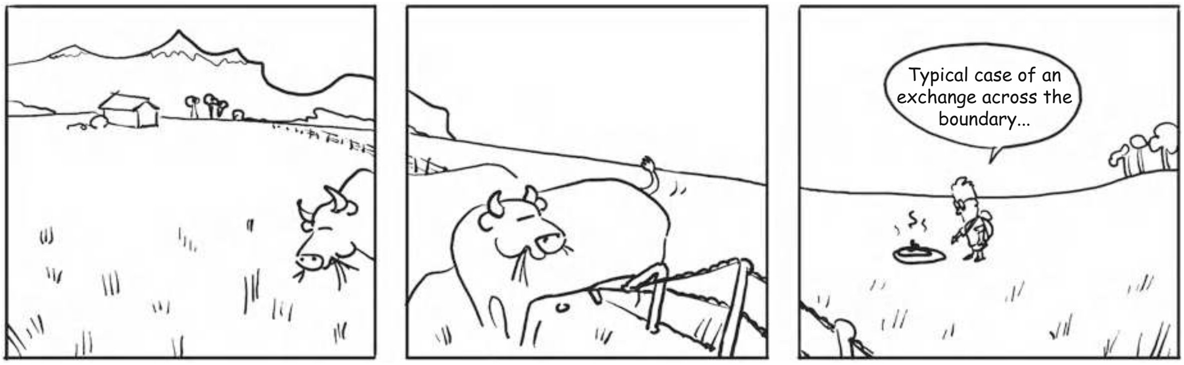
$$N_B \leq \frac{k_A}{k_B}\, N_A^{crit} = \frac{0.1}{0.3}\, 30 = 10 \tag{8.17}$$

If N_B suddenly exceeds this value, the museum staff has time of about $\tau \sim 1/k_A = 10$ min to bar entry to room A.

It's important to note that the formalism developed in Eqs. (8.13)–(8.17) implies a precision and controllability which in reality does not exist. The visitor behavior which we used to determine the model parameters k_A and k_B is only meaningful in a *statistical* sense. The real values fluctuate around their mean. We could describe this fluctuation by the standard deviations σ_A and σ_B. When dealing with statistical fluctuations, *absolute* requirements such as "N_A must not exceed N_A^{crit}" often cannot be fulfilled except through absolute conditions (such as simply keeping room A or B locked).

For real (statistical) systems it is often more appropriate to work with probabilistic requirements such as "N_A shall not exceed N_A^{crit} with a probability larger than p (e.g. $p = 5\,\%$ or 0.05)". The situation then becomes a typical problem of probability theory. And finally, in order to ease the demand on museum staff to manage visitor flows, we could of course also install light barriers at the treasure chamber's entrance and exit. This would allow us to constantly monitor N_A and trigger a signal as soon as N_A^{crit} is exceeded.

Boundary layers



8.2.4 Gas Exchange

Fick's first law (Eq. 8.5) and the exchange model (Eq. 8.12) are two different mathematical approaches to the same physical phenomenon. In both cases, the net flux results from the summation of many random individual

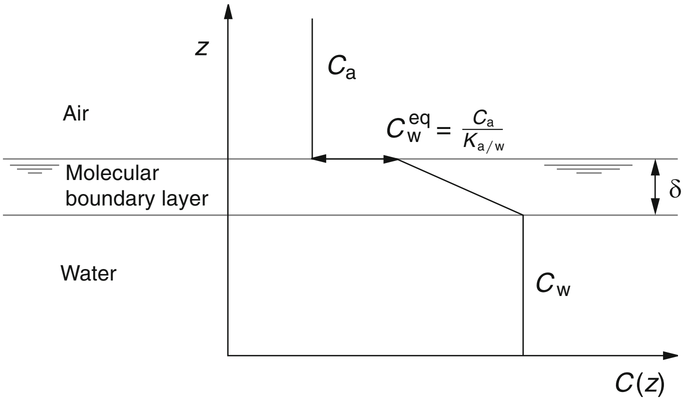


Fig. 8.5: *Film model to describe gas exchange of a volatile substance. See text for explanations*

processes. With the example of gas exchange we will now show that the two models are not just physically but also mathematically related.

The so-called film model for the exchange of a volatile substance (substance with a large Henry coefficient) assumes that on the water side of the water surface, a thin film exists (the molecular boundary layer with thickness δ) through which dissolved substances can only travel by molecular diffusion (Fig. 8.5). In the air and in the water beneath the boundary layer, mixing is so rapid that we can assume the concentrations C_a and C_w as spatially constant. At the very boundary between air and water, the two phases are at equilibrium ($C_w^{eq} = C_a/K_{a/w}$, $K_{a/w}$ = non-dimensional Henry coefficient). Inside the boundary layer we observe a linear concentration profile from C_w^{eq} to C_w. The mass flow, according to Fick's first law, is then as follows (see Eq. 8.5):

$$\begin{aligned} F_{w\to a} &= -D\frac{\partial C}{\partial x} = -D\frac{C_w^{eq} - C_w}{\delta} \\ &= v_{w/a}(C_w - C_w^{eq}), \quad v_{w/a} = \frac{D}{\delta} \end{aligned} \tag{8.18}$$

Thus, the exchange velocity $v_{w/a}$ can also be interpreted by the Fickian diffusion model. A similar case will be discussed in Example 8.2. More about modeling the exchange at boundary layers can be found in Schwarzenbach et al. (2003).

8.2.5 Turbulent Diffusion

In fact, making the distinction between advective and diffusive transport is not as easy as suggested so far. Flow processes in natural systems (such as the atmosphere or hydrosphere) are almost always turbulent. Turbulent flow—as opposed to laminar flow—consists of a superposition of flow patterns with a range of different spatial and temporal structures. If, for instance, wind velocity along a certain direction is continuously measured

Table 8.1: *Typical diffusion coefficients in the environment (From Schwarzenbach et al. 2003)*

System	Diffusion coefficient ($\mathrm{cm^2 s^{-1}}$)[a]
Molecular	
In water	10^{-6}–10^{-5}
In air	10^{-1}
Turbulent, in the ocean	
Vertical, surface layer[b]	10^{-1}–10^{4}
Vertical, deep layer	1–10
Horizontal	10^{2}–10^{8}
Turbulent, in lakes	
Vertical, epilimnion[b]	10^{-1}–10^{4}
Vertical, hypolimnion	10^{-3}–10^{-1}
Horizontal[c]	10^{1}–10^{7}
Turbulent, in the atmosphere	
Vertical[d]	10^{4}–10^{5}
In running water	
Turbulent, vertical	1–10
Turbulent, lateral	10^{1}–10^{3}
Longitudinal dispersion	10^{-5}–10^{6}

[a] $1\,\mathrm{cm^2 s^{-1}} = 8.64\,\mathrm{m^2 d^{-1}}$
[b] Maximal values
[c] Horizontal diffusion depends on the considered spatial extent
[d] In the atmosphere, horizontal transport primarily occurs by advection (wind)

at steady state as a function of time, the average wind velocity $\bar{v}$ can be determined for different averaging intervals (e.g., 1 min, 5 min, 1 h, etc.). At a given point in time, the actual wind velocity $v(t)$ deviates by $v'(t)$ from $\bar{v}$: $v(t) = \bar{v} + v'(t)$.[7] The turbulent velocity component $v'(t)$ fluctuates in an apparently random manner around an average value of 0. Note that the separation between average velocity and fluctuation depends on the duration of the averaging interval and is therefore to a certain extent arbitrary.

Due to the stochastic (that is, unpredictable) nature of v', the advective transport equation (8.2) can only be evaluated if we limit ourselves to the

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[7] $\bar{v}$ is, of course, time-dependent too, but due the averaging, its variation is smoother than that of v'.

average flow. It can be shown that the effect of the fluctuation v' on the mass flow results in an additional undirected transport. Therefore it often makes sense to describe this so-called *turbulent mass flow* in the same form as Eq. (8.5):

$$F_{turb,x} = -K_x \frac{\partial C}{\partial x} \tag{8.19}$$

The molecular diffusion coefficient is replaced by the much larger *turbulent diffusion coefficient* K. Because the effect of turbulence is usually more pronounced along the horizontal than the vertical axes (see Sect. 8.1), it makes sense to add a subscript to K to indicate along which axis turbulent transport is being considered (i.e. K_x, K_y or K_z).

The molecular diffusion coefficient is a property of the diffusing substance and the fluid in which diffusion takes place. It's usually listed in physical or chemical manuals. In contrast, the turbulent diffusion coefficient depends on the medium (lake, ocean, atmosphere, etc.) and on time. For instance, it makes a significant difference whether we look at turbulent diffusion in the atmosphere during a calm or windy period, a thunderstorm or a tornado. Because of the arbitrary distinction between average flow and turbulence resulting from the averaging interval, the horizontal diffusion in ocean and atmosphere depends on the spatial extent of the diffusion process considered. The figures given in Table 8.1 are typical values; the actual quantitative determination of turbulent diffusion coefficients can be a very time-consuming procedure. More about this can be found in Schwarzenbach et al. (2003), as well as a detailed explanation of the related phenomenon of *dispersion*, which appears along the direction of advective flow (for instance in flowing waters).

Example 8.2: Turbulent exchange through the thermocline

Figure 8.6 shows the vertical concentration profile of dissolved molecular oxygen (O_2) measured in June in a small lake with a depth of 25 m. Because of measured biomass sedimentation, we estimate that below 10 m the O_2 consumption rate per area and time is $R = 1.5\,\mathrm{g\ m^{-2}d^{-1}}$.

From temperature measurements, scientists studying the lake have determined a vertical turbulent diffusion coefficient of $K_z = 0.6\,\mathrm{m^2d^{-1}}$ for the thermocline (the layer between 5 and 10 m depth). In greater depths, K_z is about ten times as large, in the layer above 5 m even a hundredfold larger.

Estimate whether the vertical O_2 transport can compensate the O_2 loss and if not, how long it will take for the deep water to become completely anoxic (O_2-free). The current stock of O_2 in the deep water is $M^\star = 30\,\mathrm{g\ m^{-2}}$.

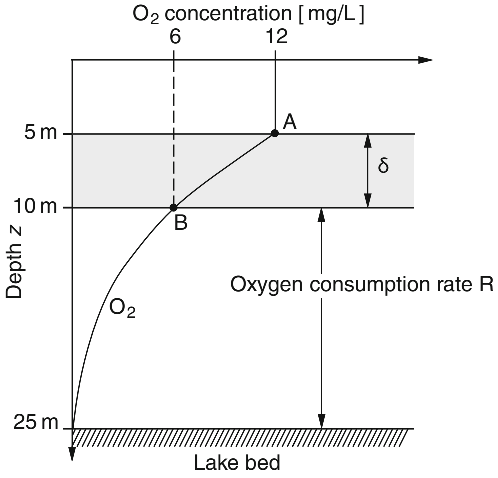

Fig. 8.6: *Vertical profile of dissolved molecular oxygen (O_2) concentration in a lake (see Example 8.2 and Problem 8.2)*

The bottleneck for vertical O_2 transport is the thermocline; transport is significantly faster above and below. The flux of O_2 across the thermocline per area and time can be calculated from Eq. (8.18):

$$F_{thermocline} = \frac{K_z}{\delta}(C_A - C_B) = v_{ex}(C_A - C_B)$$

With:
$K_z = 0.6\,\mathrm{m^2 d^{-1}}$
$\delta = 5\,\mathrm{m}$
$v_{ex} = K_z/\delta_S = 0.12\,\mathrm{m\ d^{-1}}$
$C_A = 12\,\mathrm{mg/L} = 12\,\mathrm{g\ m^{-3}}$
$C_B = 6\,\mathrm{g\ m^{-3}}$
(C_A, C_B: O_2 concentration at A and B)
Thus: $F_{thermocline} = 0.12\,\mathrm{m\ d^{-1}} \times 6\,\mathrm{g\ m^{-3}} = 0.72\,\mathrm{g\ m^{-2}d^{-1}}$

In the deep water, a net O_2 loss of $(R - F_{thermocline}) \sim 0.8\,\mathrm{g\ m^{-2}d^{-1}}$ occurs. The O_2 stock $M^\star = 30\,\mathrm{g\ m^{-2}}$ only lasts for about another 5 weeks.

Note that if the O_2 reserves in the deep water decline, the concentration at the lower boundary of the thermocline changes too, and with it, the flow through the thermocline. If C_A remains constant, $F_{thermocline}$ takes on the maximum value (for $C_B = 0$) of:

$$F_{thermocline}(\text{max.}) = v_{ex} C_A = 0.12\ \mathrm{m\ d^{-1}} \times 12\,\mathrm{g\ m^{-3}} = 1.44\,\mathrm{g\ m^{-2}d^{-1}}$$

Only after all oxygen in the deep water has completely disappeared will $F_{thermocline}$ be of similar magnitude as the loss rate R. In Problem 8.2 we will deal with the question whether C_A does indeed remain constant.

8.3 Steady-State Transport/Transformation Models

So far, we looked at transport with equations describing mass flow and mixing time. In this section, we want to combine transport processes with transformation processes in order to construct integrated transport and transformation models.

8.3.1 The Divergence Theorem: From Flux to Local Change

To get from mass fluxes to the local change of a system property (such as concentration or temperature), we consider the test volume shown in Fig. 8.7. It has a length of Δx along the x-axis; its frontal area A is perpendicular to the x-axis. We assume that mass transport in y and z direction is zero. Furthermore, the property under consideration in the test volume is conservative, i.e. its transformation rate is zero. Then, the balance equation for the test volume $V = A\Delta x$ is:

$$\frac{\partial M}{\partial t} = AF_x(x) - AF_x(x + \Delta x) \tag{8.20}$$

Where:

M: Total value of the property (*e.g., mass, energy, etc.*) in V
$F_x(x), F_x(x + \Delta x)$: Property flux (*e.g., mass or energy flux*)
per area and time in x direction at location x and $x + \Delta x$, respectively.

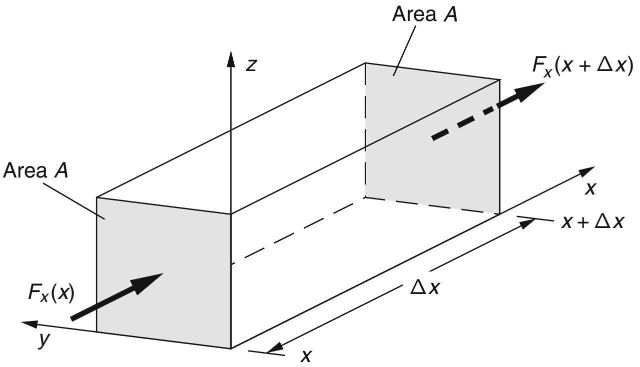

Fig. 8.7: *The divergence theorem establishes a link between flux and local change. See text for further explanations*

The average property density (*e.g., concentration*) in V is $C = M/V$. For a constant V, the following holds:

$$V\frac{\partial C}{\partial t} = A\Delta x\frac{\partial C}{\partial t} = A(F_x(x) - F_x(x + \Delta x))$$

After dividing by $A\Delta x$:

$$\frac{\partial C}{\partial t} = \frac{F_x(x) - F_x(x + \Delta x)}{\Delta x} = -\frac{F_x(x + \Delta x) - F_x(x)}{\Delta x}$$

If we now take the limit $\Delta x \to 0$, the right-hand side will be the negative derivative of F_x with respect to x:

$$\frac{\partial C}{\partial t} = -\frac{\partial F_x}{\partial x} \tag{8.21}$$

In the same way we can calculate the effect on C of the other flow components (F_y, F_z). This ultimately gives us the following result:

$$\frac{\partial C}{\partial t} = -\left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right) = -\boldsymbol{\nabla}\mathrm{F} \tag{8.22}$$

On the right-hand side is the so-called divergence of the transport vector $\boldsymbol{F}$.[8] Equation (8.22) is the *divergence theorem*. It states that the change of a scalar quantity (concentration C) inside an infinitely small test volume is equal to the divergence of the vector $\boldsymbol{F}$ describing the flux of this quantity. In other words: if we know all the fluxes at the surface of a volume, we know what happens inside that volume (of course assuming that the volume contains no sources or sinks).

It is remarkable that, to derive the divergence theorem in Eq. (8.22), we didn't need any information about how the flux came to be and how it is mathematically formulated. The theorem holds for any conservative vector field. We now want to apply it to the advective and diffusive flow equation[9]:

For advection (Eq. 8.3):

$$\begin{aligned}\left(\frac{\partial C}{\partial t}\right)_{ad} &= -\frac{\partial}{\partial x}(Cv_x) - \frac{\partial}{\partial y}(Cv_y) - \frac{\partial}{\partial z}(Cv_z) \\ &= -C\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right) - v_x\frac{\partial C}{\partial x} - v_y\frac{\partial C}{\partial y} - v_z\frac{\partial C}{\partial z}\end{aligned} \tag{8.23}$$

It can be shown that for a non-compressible fluid, the divergence of the flow field is zero, so the expression in parentheses in Eq. (8.23) disappears. What remains is:

$$\left(\frac{\partial C}{\partial t}\right)_{ad} = -v_x\frac{\partial C}{\partial x} - v_y\frac{\partial C}{\partial y} - v_z\frac{\partial C}{\partial z} \tag{8.24}$$

For diffusion (Eq. 8.6):

$$\begin{aligned}\left(\frac{\partial C}{\partial t}\right)_{diff} &= -\frac{\partial}{\partial x}\left(-D_x\frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial y}\left(-D_y\frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial z}\left(-D_z\frac{\partial C}{\partial z}\right) \\ &= D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} \\ &\quad + \frac{\partial D_x}{\partial x}\frac{\partial C}{\partial x} + \frac{\partial D_y}{\partial y}\frac{\partial C}{\partial y} + \frac{\partial D_z}{\partial z}\frac{\partial C}{\partial z}\end{aligned} \tag{8.25}$$

---

[8] Note the different meaning of the symbol $\boldsymbol{\nabla}$ in Eqs. (8.22) and (8.6). In the latter case, $\boldsymbol{\nabla}$ creates a vector (the gradient vector) from a scalar (C), in the former case, a scalar (the divergence) from a vector($\boldsymbol{F}$).

[9] To do so, we need the differentiation rule for a product of two functions.

Fick's second law describes the diffusion-induced change of concentration over time.

If the diffusion coefficients are spatially constant, the last three terms of Eq. (8.25) disappear. The first three terms then form *Fick's second law of diffusion*. Let's look at the case of isotropic diffusion ($D_x = D_y = D_z \equiv D$, i.e. diffusion that is equal in all three spatial directions, which is usually the case for molecular but not turbulent diffusion). In this case, Fick's second law takes on the following form, in which it usually appears in the literature:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \tag{8.26}$$

Table 8.2 gives an overview of the effects of diffusion and advection on the flow and local change of a scalar (such as concentration or temperature).

Table 8.2: *The effect of diffusion and advection on the flow or the local change of a property. The equations are formulated for the case of a concentration, C. Note that when moving through the table each step to the right or downwards results in a change of sign and an increase of the derivative by one order*

	Flow F [M $L^{-2}T^{-1}$]	Local concentration change $\frac{\partial C}{\partial t}$ [$ML^{-3}T^{-1}$][a]
Advection	$+v_x\ C$	$-v_x \frac{\partial C}{\partial x}$
Diffusion	$-D_x \frac{\partial C}{\partial x}$	$+D_x \frac{\partial^2 C}{\partial x^2}$

[a] For $v_x,\ D_x =$ constant. Analogous equations exist for the other spatial coordinates y and z

8.3.2 Transport and Transformation: Steady State

We consider a one-dimensional system with diffusion, advection and transformation. The local concentration change is (if $D_x, v_x =$ constant):

$$\begin{aligned}\frac{\partial C}{\partial t} &= \left(\frac{\partial C}{\partial t}\right)_{diff} + \left(\frac{\partial C}{\partial t}\right)_{ad} + \left(\frac{\partial C}{\partial t}\right)_{transformation} \\ &= D_x\frac{\partial^2 C}{\partial x^2} - v_x\frac{\partial C}{\partial x} + \left(\frac{\partial C}{\partial t}\right)_{transformation}\end{aligned} \tag{8.27}$$

If we limit ourselves to transformations of zero and first order we get[10]:

$$\frac{\partial C}{\partial t} = D_x\frac{\partial^2 C}{\partial x^2} - v_x\frac{\partial C}{\partial x} - k_r C + J \tag{8.28}$$

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[10] It makes sense to write the zero-order reaction as a positive and the first-order reaction as a negative function.

This is a linear partial second-order differential equation. Its solutions depend on the initial and boundary conditions. We will discuss examples in Sect. 8.4 and in Appendix E. For the moment, we want to look at the steady state. We determine it by setting the left side of Eq. (8.28) equal to zero. Because only the derivatives with respect to the spatial coordinate x remain, the equation becomes a regular differential equation (except that we are now looking at derivatives with respect to space rather than time).

The steady-state solution of Eq. (8.28) is described by:

$$D_x \frac{d^2C}{dx^2} - v_x \frac{dC}{dx} - k_r C + J = 0 \tag{8.29}$$

Note that we replaced the partial with the regular derivative.

Equation (8.29) is a (regular) linear, inhomogeneous second-order differential equation. We can transform it into a system of coupled linear first-order differential equations. In Sect. 5.1.1, we learned that, if the coefficients (D_x, v_x, k_r, J) are constant, the solutions generally consist of two exponential functions and a constant term. You can find the result in Appendix C.3. Applied to Eq. (8.29), we get:

$$C(x) = A_1 \mathrm{e}^{\lambda_1 x} + A_2 \mathrm{e}^{\lambda_2 x} + \frac{J}{k_r} \tag{8.30}$$

The λ_i $(i = 1, 2)$ are again the eigenvalues of the system. As in Chaps. 5 and 7 (Eqs. 5.11 and 7.21), we determine them from the characteristic equation. In the case of a *second-order* linear system, the characteristic equation is a *second-order* equation, in other words a quadratic one:

$$D_x \lambda_i^2 - v_x \lambda_i - k_r = 0 \tag{8.31}$$

Its solutions are:

$$\begin{aligned} \lambda_i &= \frac{1}{2D_x}\left[v_x \pm (v_x^2 + 4D_x k_r)^{1/2}\right] \\ &= \frac{v_x}{2D_x}\left[1 \pm \left(1 + \frac{4D_x k_r}{v_x^2}\right)^{1/2}\right] \qquad [\,\mathrm{L}^{-1}\,] \end{aligned} \tag{8.32}$$

The eigenvalues λ_i determine the spatial structure of the solution, for instance the behavior of $C(x)$ for $x \to \pm\,\infty$. Their dimension is $[\,\mathrm{L}^{-1}\,]$. Note that the eigenvalues *don't* depend on the inhomogeneous term J.

The coefficients A_i depend on the boundary conditions of the system. A second-order equation needs two boundary conditions for its solution to be unique. If we are looking for the solution of Eq. (8.29) for a finite interval, e.g. on the x-axis between $x = 0$ and $x = x_L$, we have six possibilities to specify the boundary conditions. We can either directly specify the two boundary values:

$$C_0 \equiv C(x=0) \quad ; \quad C_L \equiv C(x=x_L) \tag{8.33}$$

Or we can specify the first derivatives at the boundaries:

$$C_0' \equiv \left.\frac{dC}{dx}\right|_{x=0} \quad ; \quad C_L' \equiv \left.\frac{dC}{dx}\right|_{x=x_L} \tag{8.34}$$

Finally, we can take any combination of value and derivative. If the system is unbounded ($x_L \to \infty$), the coefficient A_i in Eq. (8.30) which is associated with an eigenvalue λ_i with a positive real part must be zero. Otherwise, the solution $C(x)$ becomes infinite for $x \to \infty$. Explicit expressions for A_i for all these possibilities are compiled in Table 8.3.

Table 8.3: *Coefficients A_i of the solution of the steady-state linear transport/transformation equation (Eqs. 8.29 and 8.30) for different boundary conditions at $x=0$ and $x=x_L$.*

Boundary conditions[a]	A_1	A_2
(1) C_0, C_L	$\frac{\left(C_L-\frac{J}{k_r}\right)-\left(C_0-\frac{J}{k_r}\right)e^{\lambda_2 x_L}}{e^{\lambda_1 x_L}-e^{\lambda_2 x_L}}$	$\frac{-\left(C_L-\frac{J}{k_r}\right)+\left(C_0-\frac{J}{k_r}\right)e^{\lambda_1 x_L}}{e^{\lambda_1 x_L}-e^{\lambda_2 x_L}}$
(2) C_0', C_L'	$\frac{C_L'-C_0' e^{\lambda_2 x_L}}{\lambda_1 (e^{\lambda_1 x_L}-e^{\lambda_2 x_L})}$	$\frac{-C_L'+C_0' e^{\lambda_1 x_L}}{\lambda_2 (e^{\lambda_1 x_L}-e^{\lambda_2 x_L})}$
(3) C_0, C_0'	$\frac{C_0'-\lambda_2\left(C_0-\frac{J}{k_r}\right)}{\lambda_1-\lambda_2}$	$\frac{-C_0'+\lambda_1\left(C_0-\frac{J}{k_r}\right)}{\lambda_1-\lambda_2}$
(4) C_0, C_L'	$\frac{C_L'-\left(C_0-\frac{J}{k_r}\right)\lambda_2 e^{\lambda_2 x_L}}{\lambda_1 e^{\lambda_1 x_L}-\lambda_2 e^{\lambda_2 x_L}}$	$\frac{-C_L'+\left(C_0-\frac{J}{k_r}\right)\lambda_1 e^{\lambda_1 x_L}}{\lambda_1 e^{\lambda_1 x_L}-\lambda_2 e^{\lambda_2 x_L}}$
If the system is unbounded on one side (e.g. $x_L \to \infty$), the solution is determined by a single boundary condition, either C_0 or C_0':		
(5) C_0	0	$C_0 - J/k_r$
(6) C_0'	0	C_0'/λ_2

[a] See definitions in Eqs. (8.33) and (8.34). Note that the two missing combinations (C_L, C_L' and C_0', C_L) follow from the other four simply by exchanging the boundaries ($x=0$ becomes $x=L$ and vice versa)

Example 8.3: Radon-222 in the ocean

The decay of radium-226 (^{226}Ra) in deep sea sediments produces the radioactive noble gas radon-222 (^{222}Rn, half-life $\tau_{1/2} = 3.8$ d). Radon diffuses from the sediment surface into the water with a flux F (constant per time and area). Once in the water, it is distributed by turbulent diffusion. We are interested in the steady-state radon profile as a function of the vertical distance h from the sediment $C(h)$. J_{Ra} is the production of ^{222}Rn in the water column per volume and time from the decay of dissolved ^{226}Ra. Because as a first approximation we can describe the sediment surface as an infinitely large horizontal plain, the horizontal concentration gradients and therefore the horizontal diffusive fluxes are zero. The average vertical advective flow v_z is also zero, since the sediment is neither a source nor a sink of water.

With $v_z = 0$, and according to Eq. (8.29), the steady-state vertical transport/transformation equation for the concentration C of ^{222}Rn is:

$$\frac{\partial C}{\partial t} = K_z \frac{\partial^2 C}{\partial h^2} - \lambda_{Rn} C + J_{Ra} = 0 \tag{8.35}$$

h(m):	Height above sediment
K_z(m^{2}d^{-1}):	Vertical turbulent diffusion coefficient (instead of D_z)
k_{Rn}(d^{-1}):	Decay constant of ^{222}Rn (see Eq. 4.45) $k_{Rn} = \ln 2/\tau_{1/2} = 0.693/3.8 \text{ d} = 0.18 \text{ d}^{-1}$
C(Bq m^{-3}):	Activity of ^{222}Rn in the water (1 Bq = 1 Becquerel = 1 decay per second)
J_{Ra}(Bq m^{-3}s^{-1}):	In-situ production of ^{222}Rn through decay of ^{226}Ra

The eigenvalues of Eq. (8.35) follow from Eq. (8.32):

$$\lambda_i = \pm (k_{Rn}/K_z)^{1/2}$$

Since ^{222}Rn decays rather rapidly compared to the vertical mixing time in the deep ocean, the water column can be seen as infinitely deep. Thus A_1 (corresponding to the positive eigenvalue λ_1) in Eq. (8.30) must be zero. To determine the remaining coefficient A_2, we express the vertical ^{222}Rn flux at the sediment surface (h=0), F_{Rn}, in terms of Fick's first law (Eq. 8.5):

$$\left.\frac{\partial C}{\partial h}\right|_{h=0} = -\frac{F_{Rn}}{K_z} \tag{8.36}$$

According to Table 8.3 (case 6) and Eq. (8.30), the solution is[11]:

$$\begin{aligned} C(h) &= \frac{J_{Ra}}{k_{Rn}} - \frac{F_{Rn}}{K_z \lambda_2}\ \mathrm{e}^{-(k_{Rn}/K_z)^{1/2} h} \\ &= \frac{J_{Ra}}{k_{Rn}} - \frac{F_{Rn}}{(K_z k_{Rn})^{1/2}}\ \mathrm{e}^{-(k_{Rn}/K_z)^{1/2} h} \end{aligned} \tag{8.37}$$

---

[11] Note that $\lambda_2 = -(\lambda_{Rn}/K_z)^{1/2}$.

The ^{222}Rn activity above the sediment falls exponentially towards the constant value $C_\infty = J_{Ra}/k_{Rn}$. In Problem 8.4 we will look into how ^{222}Rn measurements can be used to determine the vertical turbulent diffusion coefficient in the ocean.

8.3.3 Spatial Structures: Péclet und Damköhler Numbers

We want to bring out the influence of the eigenvalues λ_i on the spatial structure of the solution of Eq. (8.29) more clearly. To do so, we introduce the non-dimensional spatial coordinate $\xi = x/x_L$ which normalizes the distance between the two boundaries $x = \{0, x_L\}$ onto the interval $\xi = \{0, 1\}$.[12] To write the solution (8.30) in terms of the new spatial coordinate, we only have to multiply the eigenvalues with x_L, since $\lambda_i x = \lambda_i^\star \xi$:

$$\lambda_i^\star = \lambda_i x_L = \frac{x_L v_x}{2D_x}\left[1 \pm \left(1 + \frac{4D_x k_r}{v_x^2}\right)^{1/2}\right] \qquad [\text{-}] \tag{8.38}$$

The $\lambda_i^\star$ are the non-dimensional eigenvalues. The solution of Eq. (8.30) is now:

$$C(\xi = x/x_L) = A_1\,\mathrm{e}^{\lambda_1^\star \xi} + A_2\,\mathrm{e}^{\lambda_2^\star \xi} + \frac{J}{k_r} \tag{8.39}$$

Since ξ only varies between 0 and 1, the size of $\lambda_i^\star$ determines the influence of the spatial functions $\exp(\lambda_i^\star \xi)$ on the shape of $C(\xi)$. For instance, if $|\lambda_i^\star| \ll 1$, then $\exp(\lambda_i^\star \xi)$ barely varies with ξ and is about 1 everywhere. If, on the other hand, $(-\lambda_i^\star) \gg 1$, then $\exp(\lambda_i^\star \xi)$ drops off from 1 (at $\xi = 0$) to 0 over a very short distance. In other words, the spatial variation of this term is limited to a small zone close to the boundary while over the rest of the interval the term is zero.

To systematically discuss the different patterns of spatial behavior of Eqs. (8.30) and (8.39), we rewrite the non-dimensional eigenvalues in terms of two non-dimensional numbers, `Pe` and `Da`:

$$\lambda_i^\star = \frac{\mathtt{Pe}}{2}\,[\mathrm{sgn}(v_x) \pm (1 + 4\,\mathtt{Da})^{1/2}], \quad i = 1, 2 \tag{8.40}$$

Here, $\mathrm{sgn}(v_x) =$ is the sign of v_x. `Pe` and `Da` are defined as follows:

$$\mathtt{Pe} \equiv \frac{|v_x| x_L}{D_x} \geq 0 \quad \text{Péclet number} \tag{8.41}$$

---

[12] Note that the following considerations are only valid if the extent of the system is finite, i.e. if it is enclosed by finite boundaries.

$$\mathtt{Da} \equiv \frac{D_x k_r}{v_x^2} \geq 0 \quad \text{Damköhler number}^{13} \tag{8.42}$$

In Problem 8.5 we will show that the Péclet number `Pe` can be seen as a measure for the relative velocity of advection versus diffusion in the interval x_L (for $\mathtt{Pe} \gg 1$, advection is faster than diffusion and vice versa). The Damköhler number `Da` measures the ratio between diffusive and advective transport during the average life span of the reactive substance, k_r^{-1}.

The Péclet and Damköhler numbers measure the relative influence of directed transport, diffusive transport, and transformation.

Figure 8.8 gives an overview of the influence of `Pe` and `Da` on $\lambda_i^\star$ and schematically shows the shape of the steady-state concentration profile $C(x)$ between $x = 0$ and $x = x_L$. We can divide the extreme cases into four groups (explained in more detail on the next page, following Fig. 8.8).

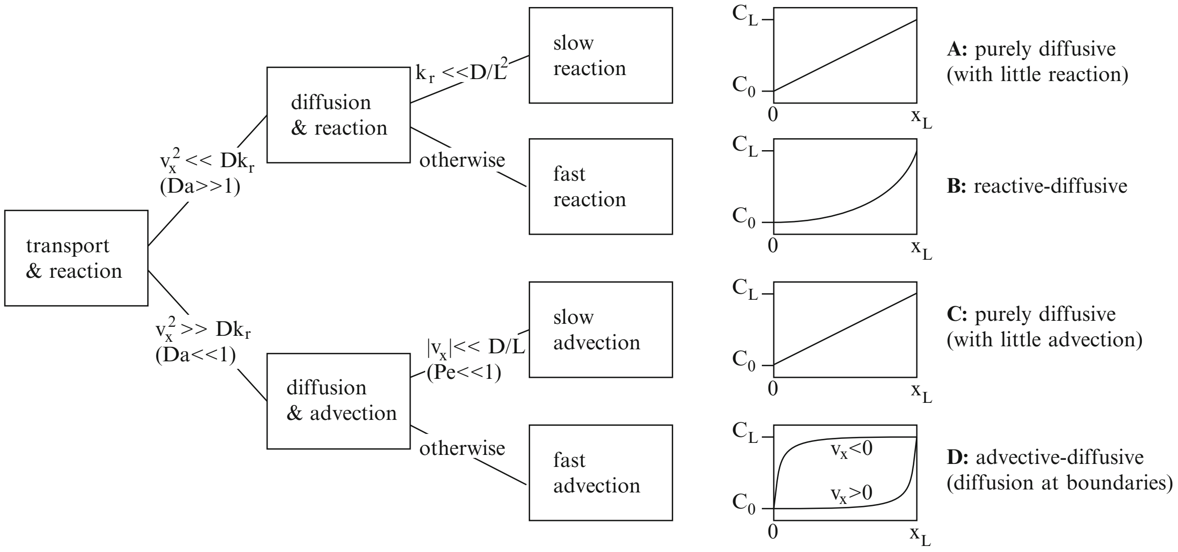

Fig. 8.8: *One-dimensional diffusion/advection/transformation profiles at steady-state: the non-dimensional Péclet and Damköhler numbers determine both the form of the profile and the influence of diffusion (coefficient D_x), advection (velocity v_x) and the specific reaction (rate k_r). See text for further explanations*

If $\mathtt{Da} \gg 1$ (i.e. $v_x^2 \ll D_x k_r$), according to Eq. (8.40) the non-dimensional eigenvalues are virtually independent of v_x: $\lambda_i^\star \sim \mathtt{Pe}(\mathtt{Da})^{1/2} = (k_r/D_x)^{1/2} x_L$. Therefore we call this the *diffusion and reaction regime.* It can be further subdivided:

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[13] In the literature, we find different types of Damköhler numbers, see e.g. Domenico and Schwartz (1998). For our purposes, the definition in Eq. (8.42) is the adequate form.

Case A: Purely Diffusive Regime: $\mathtt{Da} \gg 1$ and $k_r \ll D_x/x_L^2$

The reactivity is too slow to significantly alter the linear diffusion profile (which therefore looks similar to e.g. Fig. 8.5).

Case B: Reactive-Diffusive Regime: $\mathtt{Da} \gg 1,\ k_r$ is not $\ll D_x/x_L^2$

The time needed for diffusion over the distance x_L is large enough to allow for a significant reaction during diffusive transfer (Example 8.3 belongs to this category).

If $\mathtt{Da} \ll 1$ (i.e. $v_x^2 \gg D_x k_r$), the substance behaves approximately conservative ($k_r \sim 0$). In this case, which we call the *diffusion and advection regime*, the size of the Péclet number decides whether diffusion or advection is the dominant transport process.

Case C: Purely Diffusive Regime: $\mathtt{Da} \ll 1,\ \mathtt{Pe} \ll 1$

The substance is quasi-conservative throughout its transport ($\mathtt{Da} \ll 1$); the transport process is determined by diffusion ($\mathtt{Pe} \ll 1$).

Case D: Advective-Diffusive Regime: $\mathtt{Da} \ll 1,\ \mathtt{Pe}$ not $\ll 1$

As in case C, but advection dominates except near the boundaries.

To summarize, we can say that the structure of a concentration profile is determined by the eigenvalues of the linear second-order differential equation (8.29). The eigenvalues themselves are determined by Eq. (8.32), which depends on the three coefficients D_x, v_x und k_r. k_r is a substance-dependent property, v_x a property of the system, and D_x generally a property of both. This means that in a given system with its distinct transport regime, different substances experience different transport/transformation ratios. In a system with (substance-independent) turbulent diffusion, the Péclet number is only a property of the system. The following example illustrates this.

Example 8.4: Vertical transport in the ocean

In the Atlantic and Pacific oceans, there is a depth zone (typically between 1 and 5 km depth, see Fig. 8.9), in which water flows upward extremely slowly (called *upwelling*). This happens as a compensation for deep water formation in the North Atlantic and in the Antarctic Circumpolar Current. This depth zone is also affected by vertical turbulent diffusion, compared to which molecular diffusion can be neglected.

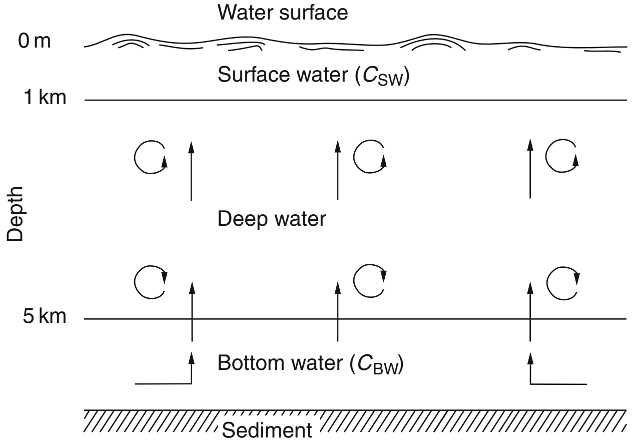

Fig. 8.9: *A simple model of the vertical water column in the Atlantic and Pacific Oceans. The deep water is bounded by the bottom water and the surface water. Water slowly moves upwards through the deep water layer (upwelling), while turbulent mixing takes place simultaneously*

We consider the steady-state vertical profiles of two dissolved radioactive isotopes, radium-226 (^{226}Ra, $\tau_{1/2}$ =1,600 year) and the heavy hydrogen isotope tritium (^{3}H, $\tau_{1/2} = 12$ year). We assume that the concentrations at the lower deep water boundary are controlled by the bottom water, and at the upper deep water boundary by the surface water. These concentrations are constant. Radium diffuses out of the sediment, its concentration in the surface water is zero ($C_{SW} = 0$). Tritium enters the surface water via the atmosphere and then diffuses downwards. In the bottom water there is no tritium ($C_{BW} = 0$).[a]

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[a] Of course, these assumptions strongly simplify the real picture. In particular, atmospheric tritium concentration, primarily determined by human activities, has changed significantly over the recent past. Furthermore, we don't take into account the production of radium from the decay of uranium in the water column (i.e. $J = 0$).

Numerical values used:

$K_z = 1\ \text{cm}^2\text{s}^{-1} = 3.2 \times 10^3 \text{m}^2\text{year}^{-1}$	Vertical turbulent diffusivity
$v_z = 2\ \text{m year}^{-1}$	Speed of upwelling
$k_{Ra} = 0.693/1,600\,\text{year} = 4.3 \times 10^{-4}\text{year}^{-1}$	Decay constant of ^{226}Ra
$k_T = 0.693/12\,\text{year} = 0.058\,\text{year}^{-1}$	Decay constant of tritium

Coordinate system: positive upwards, $\xi = 0$ at the lower boundary, $\xi = 1$ at the upper boundary, $x_L = 4\,\text{km} = 4 \times 10^3\,\text{m}$.

Radium-226
We normalize the concentrations with the lower boundary concentration C_{BW}. In other words, we set $C_0 = C(\xi = 0) = 1,\ C_L = 0$. We then

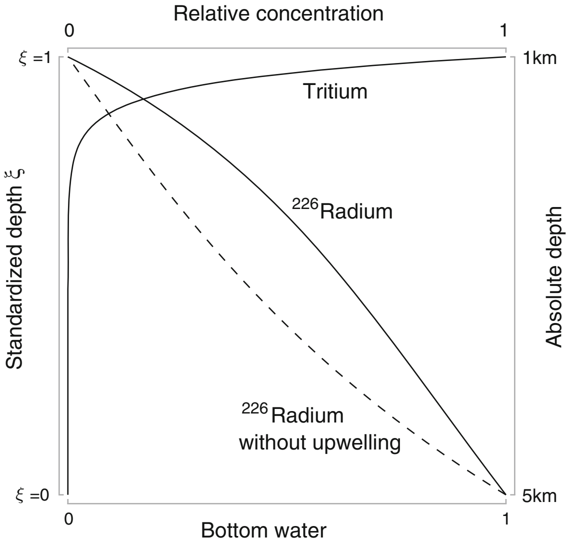


Fig. 8.10: *Relative vertical concentration profile of two radionuclides in the deep water of the Pacific Ocean (see Fig. 8.9). The short-lived tritium ($\tau_{1/2}$ =12 year) is barely influenced by the upwelling. For the long-lived radium-226 ($\tau_{1/2}$ =1,600 year) however, there is a clear difference between the profiles with and without upwelling*

calculate the non-dimensional parameters:

$$\mathtt{Pe} = \frac{v_x x_L}{K_z} = \frac{2\ \text{m year}^{-1} \times 4 \times 10^3\text{m}}{3.2 \times 10^3\text{m}^2\text{year}^{-1}} = 2.5$$

$$\mathtt{Da} = \frac{K_z k_{Ra}}{v_z^2} = \frac{3.2 \times 10^3\text{m}^2\ \text{year}^{-1} \times 4.3 \times 10^{-4}\ \text{year}^{-1}}{(2\ \text{m year}^{-1})^2} = 0.344$$

$$\text{Eigenvalues}: \quad \lambda_1^\star = 3.18, \quad \lambda_2^\star = -0.68$$

From Table 8.3, case (1) with $C_0 = 1,\ C_L = 0,\ J = 0$:

$$A_1 = -0.0217, \quad A_2 = 1.0217$$

The normalized radium profile thus has the form:

$$C_{Ra}(\xi) = -0.0217\text{e}^{3.18\xi} + 1.0217\text{e}^{-0.68\xi} \tag{8.43}$$

The profile is shown in Fig. 8.10. To illustrate the effect of upwelling, the corresponding profile without upwelling ($v_z = 0$) is included in the figure. It becomes clear that, due to upwelling, at a given depth the concentration is shifted to higher values.

Tritium (^{3}H)
Boundary conditions: $C_0 = 0, \quad C_L = 1$

$$\mathtt{Pe} = 2.5 \quad (\text{as for } ^{226}\text{Ra})$$

$$\mathtt{Da} = \frac{3.2 \times 10^3\text{m}^2\text{year}^{-1} \times 0.058\ \text{year}^{-1}}{(2\ \text{m year}^{-1})^2} = 46.4$$

Eigenvalues[14]: $\lambda_1^\star = 18.3, \quad \lambda_2^\star = -15.8$

$$A_1 = \frac{1}{e^{\lambda_1^\star} - e^{\lambda_2^\star}} \sim e^{-\lambda_1^\star} \qquad (\text{note: } e^{\lambda_1^\star} \gg e^{\lambda_2^\star})$$
$$A_2 = -A_1 \sim -e^{-\lambda_1^\star}$$

The standardized profile therefore has the form:

$$\begin{aligned} C_T(\xi) &= e^{-\lambda_1^\star} e^{\lambda_1^\star \xi} - e^{-\lambda_1^\star} e^{\lambda_2^\star \xi} \sim e^{-\lambda_1^\star} e^{\lambda_1^\star \xi} = e^{-\lambda_1^\star (1-\xi)} \\ &= e^{-18.3(1-\xi)} \end{aligned} \tag{8.44}$$

The profile corresponds to an exponential curve that rapidly declines in negative ξ direction, with the boundary value $C_T(\xi = 1) = 1$. The influence of upwelling on the tritium profile is weak.

Sustaining the radium and tritium profiles at a steady state implies that there is a continuous flux of isotopes from and to the deep water across its upper and lower boundaries. In Problem 8.8 we will discuss the relative size of these boundary fluxes and compare them to the loss of isotopes due to radioactive decay.

8.4 Time-Dependent Solutions of the Transport/Transformation Equation

As we already noted at the outset of Chap. 8, spatially continuous models lead to partial differential equations. These equations can only be solved algebraically in special cases. The dynamic equations for fluids,[15] the so-called Navier-Stokes equations, which are particularly important for natural systems, unfortunately *don't* belong to the category of generally solvable partial differential equations. In fact, the numerical analysis of the coupled ocean-atmosphere system is one of the major challenges for computational science and supercomputing. Thus, neither the weather nor the climate are easily predictable.

Dealing with such models lies beyond the scope of this book. However, we don't want to conclude this chapter without at least throwing a glance at some specific time-dependent solutions of the transport equation. We will begin with the one-dimensional case.

8.4.1 The One-Dimensional Diffusion Equation

We consider the one-dimensional diffusion equation with constant diffusion coefficient D_x. This equation results from Eq. (8.26) by dropping the derivatives with respect to y and z (Fick's second law):

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} \tag{8.45}$$

---

[14] Since the Damköhler number `Da` $\gg 1$, the eigenvalues would approximately be $\lambda_i^\star = \pm x_L (k_r/K_z)^{1/2} = \pm 17$.

[15] "Fluid" is used here as a general expression for liquid and gaseous systems. The most important fluid systems on Earth are the ocean and the atmosphere.

The solutions of Eq. (8.45) depend on the initial and boundary conditions. We assume that the system is infinite in both directions along the x-axis, i.e. the substance described by the concentration C can spread along the x-axis from $-\infty$ to $+\infty$. We'll now look at two different initial conditions.

(1) The Delta Function

At time $t = 0$, the substance mass m is concentrated entirely at point $x = 0$.[16] To concentrate a finite mass onto a point with (by definition) no spatial extent, mathematicians created the delta function δ. It is defined as follows:

$$\delta(x) = \begin{cases} 0 & \text{for} \quad x \neq 0 \\ \infty & \text{for} \quad x = 0 \end{cases} \quad \text{where} \quad \int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x = 1 \tag{8.46}$$

The initial condition of Eq. (8.45) is thus:

$$C(x, t = 0) = m\,\delta(x) \tag{8.47}$$

We now claim that the solution of Eq. (8.45) with the initial condition Eq. (8.47) has the following form:

$$C(x, t) = \frac{m}{2(\pi D_x t)^{1/2}} \exp\left(-\frac{x^2}{4 D_x t}\right) \tag{8.48}$$

You can verify that this is indeed a solution of Fick's second law by inserting Eq. (8.48) into Eq. (8.45) (see Problem 8.9). $C(x, t)$ is a normal distribution with the variance:

$$\sigma_x = (2 D_x t)^{1/2} \tag{8.49}$$

The normal distribution (also called Gaussian distribution), a probability distribution often used in statistics for random variables distributed around an average value, is defined in Appendix E.1. The total substance mass (calculated from the integral of $C(x, t)$ between $x = -\infty$ and $+\infty$) is m, i.e. constant with respect to time. This result is not entirely surprising; we already saw in Example 2.7 (the bed of nails) that random processes lead to a normal distribution whose standard deviation increases with time.

For $t = 0$, σ_x and the denominator of Eq. (8.48) become zero, i.e. $C(x, t = 0)$ describes a normal distribution with variance $\sigma_x = 0$. The delta function introduced in Eq. (8.46) can be defined as the limit of a normal distribution with $\sigma_x \to 0$, thus, Eq. (8.48) does indeed fulfill the initial condition of Eq. (8.46).

---

[16] Note that for the one-dimensional case, m has the dimension $[ML^{-2}]$ (mass per area perpendicular to the x-axis).

Example 8.5: Substance spreading in a canal

Due to an accident, a certain mass M of the herbicide atrazine enters an abandoned canal with stagnant water. It rapidly expands across the canal's cross section (width w, average depth h). Mixing along the canal axis takes place by turbulent diffusion (turbulent diffusion coefficient K_x). How long will it take for the atrazine concentration $C(x,t)$ to drop below the tolerance value for drinking water C_{tol} along the entire length of the canal?

Numerical values: $M = 1\,\mathrm{kg},\ C_{tol} = 0.1\,\mu\mathrm{g/L} = 10^{-4}\,\mathrm{g\,m^{-3}}$

$$w = 50\,\mathrm{m},\ h = 8\,\mathrm{m},\ K_x = 0.1\,\mathrm{m^2\,s^{-1}}$$

We assume that the atrazine enters the canal at $x = 0$ and neglect the time needed to distribute it homogeneously across the canal's cross-section. Its further spread can be described by Eq. (8.45) and the initial condition Eq. (8.47), where the initial mass per cross-sectional area is:

$$m = \frac{M}{w\ h} = \frac{10^3\mathrm{g}}{50\mathrm{m} \times 8\mathrm{m}} = 2.5\,\mathrm{g\,m^{-2}}$$

Note that the concentration maximum remains at the location of inflow $x = 0$, where its time-dependent value is:

$$C(x=0,t) = \frac{m}{2(\pi K_x t)^{1/2}}$$

We are looking for the time t_0 at which $C(x = 0, t_0) = C_{tol}$:

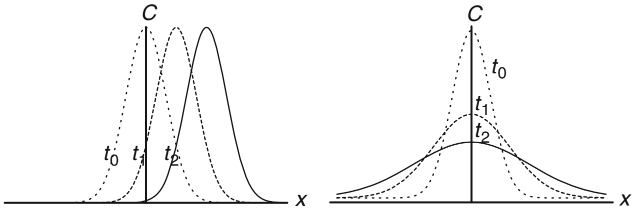
$$C_{tol} = \frac{m}{2(\pi K_x t_0)^{1/2}}$$

Solving for t_0 yields:

$$t_0 = \frac{m^2}{4\pi K_x C_{tol}^2} = \frac{(2.5\,\mathrm{g\,m^{-2}})^2}{4\pi \times 0.1\,\mathrm{m^2 s^{-1}}(10^{-4}\,\mathrm{g\,m^{-3}})^2}$$
$$= 5.0 \times 10^8\,\mathrm{s} \sim 16\mathrm{year}\ (!)$$

This unrealistically long time indicates that the herbicide's disappearance is probably not determined by diffusion but rather by other processes (chemical conversion, sorption on suspended particles and the sediment surface). In Example 8.7 we will show that diffusive dispersion in two and three dimensions radically reduces the diffusion time t_0.

We can easily generalize the solution of this problem to the case where in addition to horizontal diffusion, a longitudinal flow with velocity v_x exists. The maximum of the concentration distribution shifts according to



Advection: directed transport (in one direction)

Diffusion: "undirected" transport (against the gradient)

Flow	$F = vC$	$F = -D\frac{\partial C}{\partial x}$
Concentration	$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x}$	$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$
Mixing time	$\tau_{mix} = L/V$	$\tau_{mix} = L^2/D$

Fig. 8.11: *Effects of advection and diffusion on concentration: advection moves the center of the curve without changing its form (left), while diffusion broadens the distribution without moving its center. Because the underlying equations are linear, the two processes can be superimposed*

the equation $x_m = v_x t$, while the distribution relative to x_m keeps the form of Eq. (8.48). Written out, the solution is (see Problem 8.9):

$$C(x,t) = \frac{m}{2(\pi D_x t)^{1/2}} \exp\left(-\frac{(x - v_x t)^2}{4D_x t}\right) \tag{8.50}$$

Note that the flow has no influence on the time calculated in Example 8.5, but only moves the location of the concentration maximum along the x-axis. The effects of advection and diffusion are compared in Fig. 8.11.

(2) Diffusion with Constant Boundary Concentration

A second type of solution for Eq. (8.45) results if the initial concentration is a step function (see Fig. 8.12):

$$C(x, t = 0) = \begin{cases} C_0 & \text{for} \quad x \le 0 \\ 0 & \text{for} \quad x > 0 \end{cases} \tag{8.51}$$

It describes an initial situation with two regions separated by a boundary: a region with constant concentration C_0 on the left-hand side and a region with zero concentration on the right-hand side. At time $t = 0$, transport across the boundary at $x = 0$ begins. The substance can now diffuse from the left ($x < 0$) to the right ($x > 0$). It is further assumed that the stock of substance on the left side of the boundary is large and transport towards the boundary fast enough so that the boundary concentration at $x = 0$ remains constant at C_0: $C(x < 0, t) = C_0$.
The problem can be solved by way of the superposition principle, which we know to be valid for linear equations (see Appendix E.3). The result is:

$$\begin{aligned} C(x,t) &= \frac{C_0}{(\pi D_x t)^{1/2}} \int_x^\infty \exp\left(-\frac{\xi^2}{4D_x t}\right) \mathrm{d}\xi \\ &= C_0 \ \mathrm{erfc}\left(\frac{x}{(2D_x t)^{1/2}}\right) \ ; \ x \ge 0 \end{aligned} \tag{8.52}$$

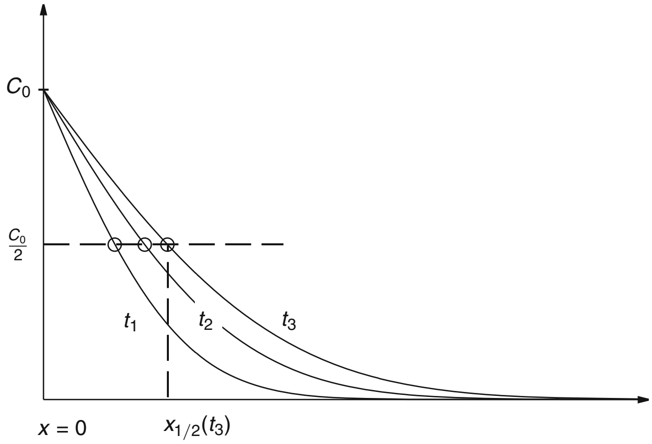


Fig. 8.12: *Diffusion from a boundary with constant concentration: the concentration profile constantly advances into the (initially empty) right section (Eq. 8.52). The point $x_{1/2}$ where the concentration reaches half of the boundary value moves to the right with a velocity proportional to $t^{1/2}$ (Eq. 8.54)*

erfc is the *complementary error function* (see Appendix E.2), which has the value 1 for $x = 0$ and 0 for $x \to \infty$.[17] As shown in Fig. 8.12, the solution (Eq. 8.52) consists of concentration profiles which—starting from the boundary value C_0 at $x = 0$—intrude further and further into the positive section. One way to quantify the speed of this process is by following the migration of the distance $x_{1/2}(t)$ at which the concentration is half the value at the edge, i.e., $C_0/2$. We can calculate $x_{1/2}(t)$ from the following equation:

$$\operatorname{erfc}\left(\frac{x_{1/2}(t)}{2(D_x t)^{1/2}}\right) = 0.5 \tag{8.53}$$

The erf and erfc functions are given in tables in most mathematical handbooks. In such a table we can find that erfc(y) has the value 0.5 if $y = 0.48$. Thus:

$$0.48 = \frac{x_{1/2}(t)}{2(D_x t)^{1/2}}$$

Solving for $x_{1/2}(t)$, we get:

$$x_{1/2}(t) = 2 \times 0.48(D_x t)^{1/2} \sim (D_x t)^{1/2} \tag{8.54}$$

Except for a numerical factor, the movement of the "half-concentration front" with time thus follows the Einstein-Smoluchowski relation (Eq. 8.9).

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[17] Note that in the definition of erfc the spatial variable x appears as the lower boundary of the integral while ξ is just an auxiliary integration variable.

Example 8.6: Oxygen diffusion in a pipe

An abandoned, water-filled vertical groundwater pipe (length: 8 m) is opened at time $t = 0$ and brought into contact with the atmosphere. Molecular oxygen (O_2) diffuses into the initially completely oxygen-free water inside the pipe (molecular diffusivity of O_2 at T=10 °C: $D = 1.5 \times 10^{-5}\,\text{cm}^2\,\text{s}^{-1}$, O_2 equilibrium concentration in water in contact with the atmosphere at T=10 °C: $C_w^{eq} = 11.3\,\text{mg/L}$).

We want to answer two questions:

(a) How long will it take for the O_2 concentration 1 m below the water surface to reach the value $0.1\,C_x^{eq}$?

(b) How long does it take to reach $0.5\,C_x^{eq}$?

Since the atmospheric O_2 concentration and thus the O_2 concentration in the water at the upper end of the pipe ($x = 0$) stays constant, the oxygen begins to propagate as per Eq. (8.52) as soon as the pipe is opened to air. For the moment, let us assume that the pipe is infinitely deep. We will later check whether the finite pipe length (8 m) substantially changes the result.

(a) $0.1C_w^{eq}$ is reached when erfc is $\left(\frac{x}{2(D_x t)^{1/2}}\right) = 0.1$. According to an erfc table, this is equivalent to $\frac{x}{2(D_x t)^{1/2}} = 1.15$. Solving for $t = t_{0.1}$ with $x = 1\,\text{m}$, $D_x = 1.5 \times 10^{-5}\,\text{cm}^2\,\text{s}^{-1} = 1.5 \times 10^{-9}\,\text{m}^2\,\text{s}^{-1}$ results in:

$$t_{0.1} = \frac{x^2}{(2 \times 1.15)^2 D_x} = \frac{1\,\text{m}^2}{(2.3)^2\, 1.5 \times 10^{-9}\,\text{m}^2\,\text{s}^{-1}} = 1.3 \times 10^8\,\text{s} \sim 4\,\text{a}\,(!)$$

(b) The answer of the second question follows directly from Eq. (8.54):

$$t_{0.5} = \frac{x^2}{D_x} = \frac{1\,\text{m}^2}{1.5 \times 10^{-9}\,\text{m}^2\,\text{s}^{-1}} = 6.7 \times 10^8\,\text{s} \sim 21\,\text{a}\,(!)$$

Note that at that time (after 21 years) the O_2 concentration at $x = 8\,\text{m}$ would be (Eq. 8.54):

$$\begin{aligned}\frac{C(x = 8\,\text{m}, t_{0.5})}{C_0} &= \text{erfc}\left(\frac{8\,\text{m}}{2(1.5 \times 10^{-9}\,\text{m}^2\,\text{s}^{-1} \times 6.7 \times 10^8\,\text{s})^{1/2}}\right) \\ &= \text{erfc}(4) < 10^{-5}\end{aligned}$$

In other words, after 21 years the concentration at the lower end of the pipe would still be so small that the diffusion process doesn't really "feel" the finite length of the pipe yet. Therefore, it is justified to assume an infinite pipe length and to use Eq. (8.52).

Note that the calculated times ($t_{0.1}, t_{0.5}$) are so large that we should really question the validity of our assumptions. Any kind of tiny convective movement (caused e.g. due to small temperature and thus density gradients along the pipe) would reduce the calculated times by several orders of magnitude.

8.4.2 Multi-dimensional Diffusion

To conclude, we will briefly touch on multi-dimensional diffusion. For a constant diffusion coefficient $D_x = D_y = D_z = D$ (isotropic diffusion), we have already derived the three-dimensional version of Fick's second law (Eq. 8.26). By dropping one of the three terms, we also get a two-dimensional variant.

For the case of a (two- or three-dimensional) point-shaped initial condition[18] the solutions are (not surprisingly) two- or three-dimensional normal distributions of the following form:

2-dimensional:

$$C(x,y,t) = \frac{m^{(2)}}{4(\pi Dt)} \exp\left(-\frac{x^2+y^2}{4Dt}\right) \tag{8.55}$$

3-dimensional:

$$C(x,y,z,t) = \frac{m^{(3)}}{8(\pi Dt)^{3/2}} \exp\left(-\frac{x^2+y^2+z^2}{4Dt}\right) \tag{8.56}$$

Note that $\mathrm{m}^{(2)}$ has dimension $[\,\mathrm{ML}^{-1}\,]$, while $\mathrm{m}^{(3)}$ has dimension $[\,\mathrm{M}\,]$. The concentration distributions are circularly or spherically symmetric.

In Example 8.5 we've seen that in the one-dimensional case the maximum concentration of a point source drops with $t^{-1/2}$, i.e. rather slowly. As we can see from Eqs. (8.55) and (8.56), the coefficient declines with t^{-1} in the two-dimensional case and with $t^{-3/2}$ in the three-dimensional case. Let's therefore have a last look at the behavior of a pollutant, but this time for the case of two-dimensional diffusion.

Example 8.7: Pollutant dispersal in a lake

We want to examine how quickly diffusive horizontal isotropic mixing lets the concentration of a pollutant fall below a critical value. To do so, we will modify Example 8.5 (atrazine in a canal) as follows: At time t_0, the amount M of the herbicide atrazine enters the surface layer of a lake, is rapidly distributed vertically within the epilimnion (height h) and then further spreads through isotropic horizontal diffusion ($K_x = K_y = K$). How long will it take for the atrazine concentration to fall below the tolerance value for drinking water C_{tol} throughout the lake?

Numbers: $M = 1\text{kg},\ C_{tol} = 0.1\,\mu\text{g/L} = 10^{-4}\,\text{g}\,\text{m}^{-3}$
$h = 10\text{m},\ K_x = 0.1\ \text{m}^2\text{s}^{-1}$

---

[18] We get a three-dimensional point from the product of three delta functions: $C(x,y,z,t=0) = \mathrm{m}^{(3)}\delta(x)\delta(y)\delta(z)$, whereby $\mathrm{m}^{(3)}$ has the dimension of a mass.

We assume that the horizontal concentration distribution initially corresponds to a two-dimensional delta function with the total mass per depth $m^{(2)} = M/h = 10^3\,\mathrm{g}/10\,\mathrm{m} = 100\,\mathrm{g\,m^{-3}}$. The horizontal concentration distribution is then described by Eq. (8.55). The maximum concentration at $x = y = 0$ as a function of time is:

$$C_{max}(t) = \frac{m^{(2)}}{4\pi K t} = C_{tol}$$

Solving for $t \equiv t_0$:

$$\begin{aligned} t_0 &= \frac{m^{(2)}}{4\pi K C_{tol}} = \frac{100\,\mathrm{g\,m^{-1}}}{4\pi \times 0.1\,\mathrm{m^2\,s^{-1}} \times 10^{-4}\,\mathrm{g\,m^{-3}}} \\ &= 8.0 \times 10^5\,\mathrm{s} = 9\,\mathrm{d} \end{aligned} \tag{8.57}$$

Compared to one-dimensional mixing, this time is much smaller. Of course, the atrazine could be moved by advection in addition to diffusion. As we showed in Eq. (8.50) for the one-dimensional case, this does not change the value of C_{max}, but only the location where it occurs.

8.5 Questions and Problems

Question 8.1: Why do models that are continuous in time and space lead to partial differential equations?

Question 8.2: What is the difference between diffusive and advective transport?

Question 8.3: Define typical times for diffusion, advection and transformation.

Question 8.4: The ratio between mixing time τ_{mix} and transformation time τ_r determines whether spatial differentiation is appropriate when modeling a system. What is the decision criteria?

Question 8.5: Give examples for processes that can be described by an exchange model.

Question 8.6: What are some of the commonalities and differences between molecular and turbulent diffusion?

Question 8.7: Explain the meaning of the divergence theorem.

Question 8.8: Explain the meaning of the Péclet and Damköhler numbers.

Question 8.9: What is the difference between the diffusive-advective and the diffusive-reactive regime of a space/time model?

Question 8.10: The Einstein-Smoluchowski relation states that diffusion in one dimension spatially advances at the speed of $t^{1/2}$. What does this mean for the maximum concentration of a substance which is initially concentrated in one point? In two and three dimensions, this effect is in play across multiple dimensions simultaneously. What then is the corresponding rule for the maximum concentration in two- or three-dimensional diffusion?

Question 8.11: How must we modify Eqs. (8.55) and (8.56) in order to also include the influence of advection?

Problem 8.1: Tetrachloroethene in a pond

We consider a pond with little through-flow (volume $V = 2 \times 10^4 \mathrm{m}^3$, surface $A = 5 \times 10^3\,\mathrm{m}^2$). Due to an accident, a small amount $M = 2\,\mathrm{kg}$ of tetrachloroethene (a substance used to clean electronic components) is introduced. Tetrachloroethene is a volatile substance; its atmospheric concentration is small and can be neglected in the calculation of gas exchange.

(a) How long will it take until the average concentration in the pond falls below the value $C_{\mathrm{crit}} = 0.1\,\mu\mathrm{g/L}$, if the average gas exchange velocity of tetrachloroethene at the pond's surface is $v_{\mathrm{W/L}} = 0.4\,\mathrm{m\,d^{-1}}$? No other elimination processes of tetrachloroethene play a role in the pond. Furthermore, you can assume that tetrachloroethene rapidly becomes completely mixed in the water body.

(b) By how much is this time shortened if we also take a through-flow of Q =2,000 m^3 per day into account?

Problem 8.2: Dissolved oxygen in a lake
In Example 8.2 we assumed that the O_2 concentration in the well-mixed surface layer of the lake remains roughly constant ($C_A = 12\,\mathrm{mg/L}$), while the deep water remained anoxic (oxygen-free), i.e. ($C_B \to 0$). Assess whether this assumption makes sense, using the following information:

$3.0\,\mathrm{g\,m^{-2}\,d^{-1}}$: O_2 production via photosynthesis in the surface layer

$9\,\mathrm{mg/L}$: O_2 equilibrium concentration with the atmosphere (at 20 °C)

$v_{\mathrm{W/L}} = 0.6\,\mathrm{m\,d^{-1}}$: Water-air exchange velocity at the lake surface

As a reminder: The O_2 flux through the thermocline into the deep water is initially $0.72\,\mathrm{g\,m^{-2}d^{-1}}$ and then rises up to about $1.4\,\mathrm{g\,m^{-2}d^{-1}}$ when C_B drops to zero.

Problem 8.3: Geothermal heat flux at the bottom of a lake
To determine the geothermal heat flux through a lake's sediments, a measuring rod with attached thermistors is pushed into the sediment. After waiting long enough, a steady-state temperature profile will be reached along the rod (that is, along the vertical axis). From this temperature profile we can calculate the geothermal heat flux F_{th} (unit: Wm^{-2}), if we assume that the sediment predominantly consists of water. This is an acceptable assumption, since fresh sediment consists of 85–95 % water. The heat transfer can be described by Fourier's law, which has the same form as Fick's first law:

$F_{\mathrm{th}} = -\gamma_{\mathrm{th}} \frac{\mathrm{d}T}{\mathrm{d}x}$, γ_{th}: Thermal conductivity $[\mathrm{Wm^{-2}\,K^{-1}}]$

$\gamma_{\mathrm{th}}(\text{Water, } 4\,°\text{C}) = 0.58\,\mathrm{W}m^{-1}\,\mathrm{K}^{-1}$

(a) Determine the heat flux F_{th}.

(b) Calculate the vertical temperature gradient in the water column above the sediment which is in equilibrium with F_{th}. Assume that we are dealing with a hypothetical lake with vertical walls. The vertical turbulent diffusion coefficient in the water column is $K_z = 0.05\,\mathrm{cm^2\,s^{-1}} = 5\times10^{-6}\,\mathrm{m^2\,s^{-1}}$.

Temperature data from the sediment

Depth in the sediment [cm]	T [°C]
0	4.250
10	4.269
20	4.285
30	4.304
50	4.342
100	4.425

Problem 8.4: Vertical turbulent diffusivity

In a 50 m deep lake with a flat bottom, the following profile of the radioactive noble gas radon-222 is measured at the deepest spot:

Height above ground [m]	^{222}Rn activity [Bq/Liter]
0.5	53
1.0	47
2.0	37
3.0	30
4.0	25

The in-situ production of ^{222}Rn from ^{226}Ra decay is $J_{Ra} = 1.8\,\mathrm{BqL^{-1}d^{-1}}$.

(a) Calculate the vertical turbulent diffusion coefficient K_z above the lake floor by using a one-dimensional diffusion/reaction model.

(b) How large is the flux F_{Rn} of ^{222}Rn from the sediment (expressed in $\mathrm{Bq\,m^{-2}\,d^{-1}}$)? The decay constant of radon-222 is $0.181\,\mathrm{d^{-1}}$.

Note: As per Eq. (8.37), the "excess activity" of radon, $C_{\mathrm{exc}} \equiv C - J_{Ra}/\lambda_{Rn}$, is an exponential function. Therefore $\ln(C_{\mathrm{exc}})$ should be a linear function of height h with slope $-(\lambda_{Rn}/K_z)^{\frac{1}{2}}$. With λ_{Rn} known we can therefore determine K_z. The flux follows from Eq. (8.36).

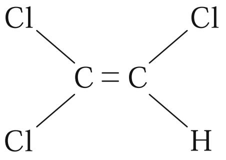
Problem 8.5: Péclet and Damköhler numbers

Use the concepts we developed in Sects. 8.2.1 and 8.2.2 for mixing times and transport distances to show that

(a) The Péclet number (Eq. 8.41) is the ratio of diffusive to advective mixing time over the distance x_L;

(b) The Damköhler number (Eq. 8.42) is the square of the quotient of diffusive and advective transport distance in time $\tau = k_r^{-1}$.

Problem 8.6: Volatile substance in the groundwater



Trichloroethene

A leaking tank at an electronics plant causes the volatile organic solvent trichloroethene (TCE) to enter the groundwater beneath the plant, where a concentration of $25\,\mathrm{mg\ m^{-3}}$ is measured. The water table is at 4 m below the surface.

Via gas exchange, TCE enters the air-filled pore space of the so-called vadose zone (also called unsaturated zone), and from there, diffuses into the free atmosphere. The atmospheric TCE concentration is very small and can be neglected. The non-dimensional Henry coefficient between air and water (see Eq. 3.2) for TCE at a water temperature of 10 °C is $K_{a/w} = 0.22$. The effective diffusion coefficient of TCE through the air filled pores of the vadose zone is $D_{ground} \sim 7 \times 10^{-3}\ \mathrm{m^2d^{-1}}$. Note that for the diffusion through the gas phase only 15 % of the total cross section is available.

(a) Calculate and draw the steady-state TCE profile from the groundwater up to the surface assuming that TCE is not degraded in the soil.

(b) Sketch the steady-state concentration profile of TCE, assuming that it degraded while migrating upwards through the soil. Compare the two profiles (a) and (b).

(c) Calculate the steady-state flux of TCE from the groundwater into the atmosphere per surface area (m^2) and day for case (a) (no decomposition). Remember that only 15 % of the cross section is available for the diffusion of TCE through air.

(d) Using Eq. (8.10), estimate the time τ_{stat} needed for a steady-state TCE profile to develop.

(e) The answer to question (d) will show that the time to reach a diffusive steady state is several years. We should therefore additionally consider the influence from vertical air flow, as can result from air pressure differences. This might significantly alter the flux calculated in (c) and the time calculated in (d). Investigate this question for the case of a small air current of $0.1\,\mathrm{m\,d^{-1}}$. Calculate the modified values for F und τ_{stat}. Calculating the Péclet number may be helpful for this.

Note: This problem is explored in more detail in Schwarzenbach et al. (2003, Illustrative Example 19.2).

Problem 8.7: Transport and reaction in a lake's water column
The measurement of four different volatile chemicals in a lake results in distinct vertical steady-state concentration profiles (see Fig. 8.13). Note that in order to interpret and understand these profiles, the scale and units of the coordinates are not relevant and thus omitted. The following simplified assumptions can be made:

1. Vertical transport of the chemicals is by turbulent diffusion only, with a diffusion coefficient which is constant across the whole water column (it simplifies the mathematics, although physically it's not very realistic!).

2. The lake consists of an oxic upper and an anoxic lower layer. Anoxic means that the concentration of dissolved molecular oxygen (O_2) is zero.

3. All substances enter the lake by air-water exchange at the water surface. The exchange rate is assumed to be fast, so that the surface concentration in the water is in equilibrium with the atmosphere and constant with time. (Note that in Fig. 8.13 the surface concentrations of all chemicals are drawn at the same value for convenience, although in reality they may be different. We can do that because the concentration axis has no absolute scale.)

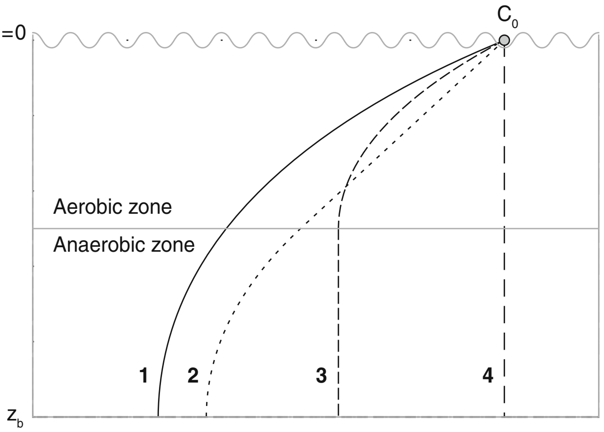


Fig. 8.13: *Concentration profiles of four different volatile chemicals in a lake*

4. The lake bottom acts like an impermeable boundary. The chemicals can neither enter the sediments nor is there a flux out of the sediments.
5. The four chemicals A, B, C, D have the following specific properties: A is inert (no reaction in the water). B is degraded in the anoxic part by a first-order reaction, but it is inert in the oxic layer. C is degraded by a first-order reaction in the *oxic* layer, but inert in the *anoxic* layer. D is degraded in both layers; the first-order reaction rate is independent of the O_2 concentration, i.e. it is equal in the whole water column.

Answer the following questions:

(a) Identify the profiles shown in Fig. 8.13 by the four chemicals A, B, C, and D.

(b) Derive the analytical solutions for the curves of chemicals A and D. Use K_z and k_r as vertical diffusivity and first-order reaction rate constant.

(c) How do the profiles for chemicals B, C, and D qualitatively change if k_r is increased? Go to the limits of an extremely fast reaction.

Problem 8.8: Radium and tritium in the ocean deep water
In Example 8.4 we discussed the steady-state concentration profiles of ^{226}Ra and tritium in the deep water of the ocean. The calculated profiles (Eq. 8.43 for ^{226}Ra, Eq. 8.44 for tritium) correspond to an equilibrium between mass flows at the upper and lower boundaries of the deep water and the radioactive decay within the deep water. Establish a mass balance of the deep water column consisting of the following components for each of the two radioactive isotopes:

1. Flux between surface and deep water, divided into the contribution of diffusion and advection;
2. The same, but for the flux between bottom and deep water;
3. Radioactive decay.

Note: To calculate the flux per surface, use the standardized concentration profiles. Choose the sign so that all fluxes into the deep water are counted positively in the balance while all fluxes out of the deep water appear as negative numbers. The radioactive decay is also a negative contribution to the balance.

Problem 8.9: Time-dependent diffusion/advection equation

(a) By forming the corresponding spatial and temporal derivatives, show that Eq. (8.48) is indeed a solution of Fick's second law in the one-dimensional case (Eq. 8.45).

(b) Show that the pure advection equation $\partial C/\partial t = -v_x \frac{\partial C}{\partial x}$ has solutions of the form $C(x - v_x t)$, whereby $C(x)$ is the initial concentration.

(c) Confirm that the combination of (a) and (b) equates to Eq. (8.50).

Problem 8.10: Symmetrical diffusion at a boundary surface

Look for solutions of the differential equation (8.48) for the initial condition Eq. (8.51), which represents a concentration jump from C_0 to 0 at $x = 0$. Unlike in the solution Eq. (8.52), the concentration in the left section does not stay constant.

Note: Use the method from Appendix E.3. The diffusion of the mass element $C_0\,\mathrm{d}\xi$ now proceeds in both directions. Using qualitative considerations, first make a sketch of the distribution of $C(x)$ through the boundary surface at $x = 0$.

Appendix A

List of Symbols

Only symbols that appear more than once are listed here.

A, A_i	Area $[\,\mathrm{L}^2\,]$
$\mathbf{B}(\boldsymbol{\mathcal{V}}^{\mathbf{k}})$	Jacobian matrix, calculated at the fixed point $\boldsymbol{\mathcal{V}}^{\mathbf{k}}$
C	Concentration $[\,\mathrm{ML}^{-3}\,]$
C^0	Initial concentration
C^∞	Steady state concentration
C_X	Concentration of substance X $[\,\mathrm{M}_X\mathrm{L}^{-3}\,]$
C_{aq}	Concentration in water $[\,\mathrm{ML}^{-3}\,]$
C_{in}	Concentration in the inflow $[\,\mathrm{ML}^{-3}\,]$
C_{air}	Concentration in air $[\,\mathrm{ML}^{-3}\,]$
C_{sed}	Concentration in sediment $[\,\mathrm{MM}_{sed}^{-3}\,]$
D	Diffusion coefficient
$\mathtt{Da}$	Damköhler number (Eq. 8.42)
F_i, F	Flux
F_{ad}	Advective flux
F_{diff}	Diffusive flux
$F_{i,j}$	Mass flux from box j to box i in a multi-dimensional model $[\,\mathrm{MT}^{-1}\,]$
I	Inhomogeneous term in discrete models
J_p	Zero-order production process
J_l	Zero-order loss process
$J^\star$	Zero-order net process
J_{in}	Substance input $[\,\mathrm{MT}^{-1}\,]$
J_{out}	Substance output $[\,\mathrm{MT}^{-1}\,]$
$K_{A/B}$	Chemical distribution (or partition) coefficient between A and B
K_d	Distribution coefficient between particles and water $[\,\mathrm{L}^3\mathrm{M}_{sed}^{-1}\,]$
$K_{a/w}$	Non-dimensional air/water distribution coefficient (or non-dimensional Henry coefficient)
K_x	Turbulent diffusion coefficient in direction x
L_{diff}	Characteristic diffusion distance

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M	Mass $[\,\mathrm{M}\,]$
N	Quantity, e.g. of individuals or atoms
$\mathbf{P}$	Coefficient matrix, $\mathbf{P} = (p_{i,j})$
$\mathtt{Pe}$	Péclet number (Eq. 8.41)
Q	Flow rate $[\,\mathrm{L}^3\mathrm{T}^{-1}\,]$
Q_{ex}	Exchange rate $[\,\mathrm{L}^3\mathrm{T}^{-1}\,]$
$\mathcal{R}, \mathcal{R}_i$	External relation
T	Period of a periodically fluctuating input $[\,\mathrm{T}\,]$
V	Volume $[\,\mathrm{L}^3\,]$
V_E	Volume of the epilimnion $[\,\mathrm{L}^3\,]$
V_H	Volume of the hypolimnion $[\,\mathrm{L}^3\,]$
$\mathcal{V}$	Generic system variable
$\boldsymbol{\mathcal{V}}$	Vector of the system variable $\boldsymbol{\mathcal{V}} = (\mathcal{V}_i)$
$\mathcal{V}_i$	i-th system variable in a multi-dimensional model
$\mathcal{V}^0$	Initial value of the system variable $\mathcal{V}$ at time $t = 0$
$\mathcal{V}^\infty$	Steady state value of the system variable $\mathcal{V}$

a_i	Coefficient in discrete models
$a_{i,j}$	Coefficients of the solutions of linear differential equations
$f(\mathcal{V})$	Change function for an autonomous system
$g(\mathcal{V}, t)$	Change function for a nonlinear differential equation
j_{in}	Substance input set in relation to the system's volume $[\,\mathrm{MT}^{-1}\mathrm{L}^{-3}\,]$
j_0	Mean value of a periodically fluctuating input $[\,\mathrm{MT}^{-1}\mathrm{L}^{-3}\,]$
j_1	Amplitude of a periodically fluctuating input $[\,\mathrm{MT}^{-1}\mathrm{L}^{-3}\,]$
k	$k = -k^\star$ $[\,\mathrm{T}^{-1}\,]$
$k^\star$	Net first-order coefficient describing substance conversion $[\,\mathrm{T}^{-1}\,]$
$k_{ex,E}$	Exchange rate from epilimnion into hypolimnion $[\,\mathrm{T}^{-1}\,]$
$k_{ex,H}$	Exchange rate from hypolimnion into epilimnion $[\,\mathrm{T}^{-1}\,]$
$k_{i,j}$	Specific exchange rate from box j into box i
k_p	First-order production or growth rate $[\,\mathrm{T}^{-1}\,]$
k_r	Linear reaction rate $[\,\mathrm{T}^{-1}\,]$
k_s	Sedimentation rate $[\,\mathrm{T}^{-1}\,]$
k_{tot}	Specific total rate $[\,\mathrm{T}^{-1}\,]$
k_l	First-order coefficient describing a loss process $[\,\mathrm{T}^{-1}\,]$
k_w	Specific flow rate $k_w = \frac{Q}{V}$ $[\,\mathrm{T}^{-1}\,]$
m	Mass per area
k_λ	Radioactive decay rate $[\,\mathrm{T}^{-1}\,]$
p	Model parameter
$p_{i,j}$	General model parameter in a multi-dimensional model
t	Time $[\,\mathrm{T}\,]$
t_n	Time steps in discrete models
t_0	Starting time from which the system is modeled
$v_{A/B}$	Exchange velocity between A and B
$v_{w/a}$	Water/air exchange velocity $[\,\mathrm{L}^{-1}\,]$

v_x	Advective velocity in direction x
x	Spatial coordinate (usually horizontal)
$x_{1/2}$	Distance at which concentration has half of the boundary value
y	Spatial coordinate (usually vertical)
y_i	Generic variable in a differential equation
z	Vertical spatial coordinate, e.g. depth in a lake $[\,\mathrm{L}\,]$

β	Growth rate of an exponentially growing input $[\,\mathrm{T}^{-1}\,]$
$\beta' = -\beta$	Reduction rate of an exponentially falling input $[\,\mathrm{T}^{-1}\,]$
γ	Stratification parameter
ε	Positive parameter (usually small)
κ	Relative convergence towards an equilibrium concentration
λ_i	Eigenvalues of the coefficient matrix
ω	Angular frequency of a periodically fluctuating input $(\omega = \frac{2\pi}{T})$ $[\,\mathrm{T}^{-1}\,]$
τ_κ, $\tau_{5\,\%}$	Adjustment time to κ or to $5\,\%$ $[\,\mathrm{T}\,]$
$\tau_{1/2}$	Half-life of a radioactive isotope $[\,\mathrm{T}\,]$

det(..)	Determinant of a matrix
tr(..)	Trace of a matrix
Δ(..)	Discriminant of a matrix

Indices

$i, j, \ldots$	Subscript: variable or box number
$(n), (k), \ldots$	Superscript: iteration step of a discrete variable
$\circ, \infty$	Superscript: initial value or steady-state/fixed-point value

Appendix B

Dimensions and Units

B.1 Dimensions

Mathematical models tie together various measured quantities. These quantities usually have a dimension. The basic dimensions in physics are (indicated with capital letters):

$[\mathrm{L}]$	Length	$[\mathrm{M}]$	Mass
$[\mathrm{T}]$	Time	$[\mathrm{Q}]$	Electric charge

Other common dimensions include:

$[\mathrm{K}]$	Temperature
$[\mathrm{N}]$	Number (of individuals, atoms, etc.)

All further dimensions can be composed from these basic dimensions, as the following examples demonstrate:

$[\mathrm{LT}^{-1}]$	for velocity
$[\mathrm{MLT}^{-2}]$	for force
$[\mathrm{ML}^{2}\mathrm{T}^{-2}]$	for energy or work
$[\mathrm{ML}^{-1}\mathrm{T}^{-2}]$	for pressure

Occasionally it can make sense to add an index to the dimensions, such as:

$[\mathrm{M}_A\mathrm{L}^{-3}]$	concentration of substance A
$[\mathrm{L}_r^3]$	volume of the reactor
$[\mathrm{L}_w^3\mathrm{L}_{tot}^{-3}]$	porosity, i.e. water volume per total volume

If dealing with indexed dimensions, only quantities with the same index can be reduced.

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B.2 Units

From the dimensions we arrive at units by choosing a specific system of measurement, for instance the metric system. The metric system leads us to the SI units, which are the international standard and commonly used in most scientific fields:

m	Meter for length [L]
kg	Kilogram for mass [M]
s	Second for time [T]
C	Coulomb for electric charge [Q]

The units derived from the basic dimensions usually have their own names:

Newton N	for $\mathrm{kg\,m\,s^{-2}}$	(force)
Joule J	for $\mathrm{N\,m}$ or $\mathrm{kg\,m^2\,s^{-2}}$	(energy, work)
Watt W	for $\mathrm{J\,s^{-1}}$ or $\mathrm{kg\,m^2\,s^{-3}}$	(power)
Pascal Pa	for $\mathrm{N\,m^{-2}}$ or $\mathrm{kg\,m^{-1}\,s^{-2}}$	(pressure)
Liter L	for $\mathrm{dm^3}$	(volume)
Becquerel Bq	for $\mathrm{s^{-1}}$	(radioactive activity)
Curie Cu	$1\ \mathrm{Cu} = 3.7 \times 10^{10}\mathrm{Bq}$	(radioactive activity)

Temperature (in degrees Celsius °C or Kelvin K) is a bit of a special case. It is an intensive quantity, that is, energy per volume. In practice, K is often treated as another basic dimension (and basic unit).

Appendix C

Formulary

C.1 Linear Inhomogeneous First-Order Differential Equation

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}t} = J(t) - k(t) \cdot \mathcal{V} \tag{C.1}$$

In the most general case, the coefficients J and k can be time-dependent. J is the inhomogeneous term. The solution is

$$\mathcal{V}(t) = \mathcal{V}^0 \mathrm{e}^{-\varphi(t)} + \mathrm{e}^{-\varphi(t)} \int\limits_0^t \mathrm{e}^{\varphi(t')} J(t') \mathrm{d}t' \tag{C.2}$$

with the exponent $\varphi(t)$ defined as

$$\varphi(t) = \int\limits_0^t k(t') \mathrm{d}t' \tag{C.3}$$

and the initial condition

$$\mathcal{V}^0 = \mathcal{V}(t = 0) \tag{C.4}$$

C.1.1 Special Cases

Homogeneous Equation: $J = 0$

The solution for a constant k is

$$\mathcal{V}(t) = \mathcal{V}^0 \mathrm{e}^{-k \cdot t} \tag{C.5}$$

For a time-dependent k, it is

$$\mathcal{V}(t) = \mathcal{V}^0 \mathrm{e}^{-\varphi(t)} \tag{C.6}$$

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Inhomogeneous Equation with Constant Coefficients J and k

$$\mathcal{V}(t) = \mathcal{V}^{\infty} + \left(\mathcal{V}^{0} - \mathcal{V}^{\infty}\right) \mathrm{e}^{-k\cdot t}, \quad \text{with steady state} \quad \mathcal{V}^{\infty} = \frac{J}{k} \tag{C.7}$$

Inhomogeneous Equation with Constant k but Time-Dependent External Parameter $J(t)$

The general solution is

$$\mathcal{V}(t) = \mathcal{V}^{0}\mathrm{e}^{-k\cdot t} + \int_{0}^{t} \mathrm{e}^{-k\cdot(t-t')} J(t')\mathrm{d}t' \tag{C.8}$$

With expontentially growing input $J(t) = J(0)\mathrm{e}^{\beta t}$ it is

$$\mathcal{V}(t) = \mathcal{V}^{0}\mathrm{e}^{-kt} - \frac{J(0)}{k+\beta}\mathrm{e}^{-kt} + \frac{J(0)}{k+\beta}\mathrm{e}^{\beta t} \tag{C.9}$$

And finally, with periodically fluctuating input $J(t) = J_0 + J_1 \sin \omega t$ we get

$$\begin{aligned}\mathcal{V}(t) = {} & \frac{J_0}{k} + (\mathcal{V}^{0} - \frac{J_0}{k})\mathrm{e}^{-kt} + \\ & + \frac{J_1}{\sqrt{\omega^2 + k^2}} \sin(\omega t - \arctan \frac{\omega}{k}) + \frac{J_1 \omega}{k^2 + \omega^2}\mathrm{e}^{-kt}\end{aligned} \tag{C.10}$$

C.2 System of Two Linear First-Order Differential Equations

By writing

$$\dot{\mathcal{V}}_i = \frac{\mathrm{d}\mathcal{V}_i}{\mathrm{d}t} \tag{C.11}$$

the following system of equations results:

$$\begin{aligned}\dot{\mathcal{V}}_1 &= J_1 + p_{1,1}\mathcal{V}_1 + p_{1,2}\mathcal{V}_2 \\ \dot{\mathcal{V}}_2 &= J_2 + p_{2,1}\mathcal{V}_1 + p_{2,2}\mathcal{V}_2\end{aligned} \tag{C.12}$$

The solution for constant coefficients J_i and p_{ij}, if $\det(\mathbf{P}) \neq 0$ is

$$\begin{aligned}\mathcal{V}_1(t) &= a_{1,0} + a_{1,1}\mathrm{e}^{\lambda_1 t} + a_{1,2}\mathrm{e}^{\lambda_2 t} \\ \mathcal{V}_2(t) &= a_{2,0} + a_{2,1}\mathrm{e}^{\lambda_1 t} + a_{2,2}\mathrm{e}^{\lambda_2 t}\end{aligned} \tag{C.13}$$

The eigenvalues λ (characteristic rates) are thereby

$$\lambda_{1,2} = \frac{1}{2}\left[(p_{1,1} + p_{2,2}) \pm \sqrt{(p_{1,1} - p_{2,2})^2 + 4p_{1,2}p_{2,1}}\right] \tag{C.14}$$

If both eigenvalues are real and negative, the model has the following steady state:

$$
\begin{aligned}
a_{1,0} = \mathcal{V}_1^{\infty} &= \frac{p_{1,2}J_2 - p_{2,2}J_1}{p_{1,1}p_{2,2} - p_{1,2}p_{2,1}} \\
a_{2,0} = \mathcal{V}_2^{\infty} &= \frac{p_{2,1}J_1 - p_{1,1}J_2}{p_{1,1}p_{2,2} - p_{1,2}p_{2,1}}
\end{aligned}
\tag{C.15}
$$

The elements of the matrix $A_{i,j}$ are calculated as follows:

$$
\begin{aligned}
a_{1,1} &= q \cdot \left[(p_{1,1} - \lambda_2)(\mathcal{V}_1^0 - a_{1,0}) + p_{1,2}(\mathcal{V}_2^0 - a_{2,0})\right] \\
a_{1,2} &= -q \cdot \left[(p_{1,1} - \lambda_1)(\mathcal{V}_1^0 - a_{1,0}) + p_{1,2}(\mathcal{V}_2^0 - a_{2,0})\right] \\
a_{2,1} &= q \cdot \left[p_{2,1}(\mathcal{V}_1^0 - a_{1,0}) + (p_{2,2} - \lambda_2)(\mathcal{V}_2^0 - a_{2,0})\right] \\
a_{2,2} &= -q \cdot \left[p_{2,1}(\mathcal{V}_1^0 - a_{1,0}) + (p_{2,2} - \lambda_1)(\mathcal{V}_2^0 - a_{2,0})\right]
\end{aligned}
\tag{C.16}
$$

with

$$
q = \frac{1}{\lambda_1 - \lambda_2} = \frac{1}{\sqrt{(p_{1,1} - p_{2,2})^2 + 4p_{1,2}p_{2,1}}} = \frac{1}{\sqrt{\Delta}}
\tag{C.17}
$$

C.3 General Solution of the Linear Second-Order Differential Equation with Constant Coefficients

The inhomogeneous differential equation of the function $f(x)$

$$
a\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + b\frac{\mathrm{d}f}{\mathrm{d}x} + cf + d = 0, \quad a, c \neq 0
\tag{C.18}
$$

can be transformed by using $g = f + \frac{d}{c}$ into the homogeneous equation

$$
a\frac{\mathrm{d}^2 g}{\mathrm{d}x^2} + b\frac{\mathrm{d}g}{\mathrm{d}x} + cg = 0
\tag{C.19}
$$

It has the solution

$$
g(x) = A_1\mathrm{e}^{\lambda_1 x} + A_2\mathrm{e}^{\lambda_2 x}
\tag{C.20}
$$

where λ_1 and λ_2 are

$$
\lambda_1 = \frac{1}{2a}\sqrt{-b + (b^2 - 4ac)} \quad \text{and} \quad \lambda_2 = \frac{1}{2a}(-b - \sqrt{b^2 - 4ac})
$$

The solution for $f(x)$ is therefore

$$
f(x) = A_1\mathrm{e}^{\lambda_1 x} + A_2\mathrm{e}^{\lambda_2 x} - \frac{d}{c}
\tag{C.21}
$$

The parameters A_1 and A_2 are determined by the boundary conditions, such as

$$f(0) = f_0, \quad \text{thus} \quad g(0) = f_0 + \frac{d}{c}$$

$$f(x_L) = f_L, \quad \text{thus} \quad g(x_L) = f_L + \frac{d}{c}$$

With these boundary conditions, the following results for the parameters A_1 and A_2:

$$\begin{aligned} A_1 &= \frac{(f_L + \frac{d}{c}) - (f_0 + \frac{d}{c})\mathrm{e}^{\lambda_2 x_L}}{\mathrm{e}^{\lambda_1 x_L} - \mathrm{e}^{\lambda_2 x_L}} \\ A_2 &= \frac{(f_0 + \frac{d}{c}\mathrm{e}^{\lambda_2 x_L}) - (f_L + \frac{d}{c})}{\mathrm{e}^{\lambda_1 x_L} - \mathrm{e}^{\lambda_2 x_L}} \end{aligned} \tag{C.22}$$

C.3.1 Special Case: $b = 0$

The differential equation (C.18) then has the form

$$a\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + cf + d = 0 \tag{C.23}$$

The approach to the solution is the same, except that λ_1 and λ_2 are calculated as follows:

$$\lambda_1 = \sqrt{-\frac{c}{a}} \quad \text{and} \quad \lambda_2 = -\sqrt{-\frac{c}{a}} \tag{C.24}$$

C.3.2 Non-dimensional Description of the Solution

With the following definitions we can describe the solution of Eq. (C.18) within the interval $[0, x_L]$ in a non-dimensional form:

$$\xi = \frac{x}{x_L}, \quad \mathtt{Pe} = -\frac{x_L b}{a}, \quad \mathtt{Da} = -\frac{ac}{b^2} \tag{C.25}$$

The new non-dimensional quantities Pe and Da are the Péclet and Damköhler numbers, respectively. The non-dimensional spatial coordinate ξ varies between 0 and 1 if x remains limited to the interval $[0, x_L]$. The following now holds:

$$\begin{aligned} \frac{\mathrm{d}g}{\mathrm{d}x} &= \frac{\mathrm{d}g}{\mathrm{d}\xi} \cdot \frac{\mathrm{d}\xi}{\mathrm{d}x} = \frac{1}{x_L}\frac{\mathrm{d}g}{\mathrm{d}\xi} \\ \frac{\mathrm{d}^2 g}{\mathrm{d}x^2} &= \frac{1}{x_L^2} \cdot \frac{\mathrm{d}^2 g}{\mathrm{d}\xi^2} \end{aligned} \tag{C.26}$$

With this, we can rewrite Eq. (C.19) with ξ as

$$\frac{\mathrm{d}^2 g}{\mathrm{d}\xi^2} - \mathtt{Pe}\frac{\mathrm{d}g}{\mathrm{d}\xi} - \mathtt{Pe}^2\mathtt{Da}g = 0 \tag{C.27}$$

The solution then becomes

$$g(\xi) = A_1 \mathrm{e}^{\lambda_1^* \xi} + A_2 \mathrm{e}^{\lambda_2^* \xi} \\ \text{with} \quad \lambda_i^* = \frac{\mathtt{Pe}}{2}(1 \pm \sqrt{1 + 4\mathtt{Da}}) \tag{C.28}$$

For the Damköhler number `Da` we can now distinguish between the following two extreme situations:

- $|\mathtt{Da}| \ll 1: \quad \begin{array}{l} \lambda_1^* \approx \mathtt{Pe} \\ \lambda_2^* \approx -\mathtt{DaPe}, \quad |\lambda_2^*| \ll |\lambda_1^*| \quad (\text{use: } \sqrt{1+\varepsilon} \approx 1 + \frac{\varepsilon}{2}) \end{array}$

  If simultaneously, $|\mathtt{Pe}| \ll 1$, then the exponential functions $\mathrm{e}^{\lambda_i^* \xi}$ barely vary in the interval $\xi \in [0, 1]$, i.e. the function $g(\xi)$ is practically constant.

- $|\mathtt{Da}| \gg 1: \quad \lambda_i^* = \pm \mathtt{Pe}\sqrt{\mathtt{Da}}$

  If simultaneously, $|\mathtt{Pe}| \approx 1$ or larger, then the large sizes of the eigenvalues λ_i^* entail strong variations in the solution function $g(\xi)$ in the interval $\xi \in [0, 1]$.

C.4 Solution of Linear Differential Equations with Imaginary Eigenvalues

The solution of a two-dimensional system of linear differential equations with the imaginary eigenvalues $\lambda = \pm \mathrm{i}\omega$ has the form (see Eq. 5.55)

$$y_j(t) = a_{j1}\, \mathrm{e}^{\mathrm{i}\omega t} + a_{j2}\, \mathrm{e}^{-\mathrm{i}\omega t}, \qquad j = 1, 2 \tag{C.29}$$

With Euler's formula

$$\mathrm{e}^{\mathrm{i}\omega t} = \cos \omega t + \mathrm{i} \sin \omega t \tag{C.30}$$

we can bring Eq. (C.29) into the form

$$y_j(t) = b_{j1}\, \cos \omega t + b_{j2}\, \sin \omega t, \qquad j = 1, 2 \tag{C.31}$$

The $b_{i,j}$ are defined as

$$\begin{array}{ll} b_{11} = (a_{11} + a_{12}), & b_{12} = \mathrm{i}(a_{11} - a_{12}) \\ b_{21} = (a_{21} + a_{22}), & b_{22} = \mathrm{i}(a_{21} - a_{22}) \end{array} \tag{C.32}$$

Finally, we can also write Eq. (C.31) as a single trigonometric function with phase shift φ_j, e.g. as

$$y_j(t) = c_j\, \sin(\omega t + \varphi_j), \qquad j = 1, 2 \tag{C.33}$$

where c_j and φ_j are

$$c_j = (b_{j1}^2 + b_{j2}^2)^{1/2}) \quad ; \quad \varphi_j = \mathrm{arctg}\left(\frac{b_{j1}}{b_{j2}}\right), \qquad j = 1, 2 \tag{C.34}$$

Usually, the system variables $y_j(t)$ are real functions, which means that the coefficients b_{j1}, b_{j2} and c_j are real and the pairs $(a_{j1},\ a_{j2})$ are conjugate-complex. All these coefficients are calculated from the initial conditions y_1° and y_2°.

Let's consider an example. We will use the equations of the harmonic oscillator (Example 5.11, Eqs. 5.73 and 5.77):

$$\frac{\mathrm{d}y_1}{\mathrm{d}t} = y_2 \quad ; \quad \frac{\mathrm{d}y_2}{\mathrm{d}t} = -\omega^2\, y_1 \tag{C.35}$$

The initial values are $y_1^\circ = A$, $y_2^\circ = B$. The eigenvalues are $\lambda = \pm\,\mathrm{i}\omega$. If we insert the general solution (Eq. C.31) into the differential equations (Eq. C.35) and compare the coefficients of $\cos\omega t$ and $\sin\omega t$ on both sides of the equals sign, we get

$$\begin{array}{lcl} b_{11} = A & ; & b_{12} = \frac{B}{\omega} \\ b_{21} = B & ; & b_{22} = -\omega\, A \end{array} \tag{C.36}$$

This means that $y_1(t)$ and $y_2(t)$ are

$$\begin{array}{lcl} y_1(t) & = & A\,\cos\omega t + \frac{B}{\omega}\,\sin\omega t \\ y_2(t) & = & B\,\cos\omega t - \omega\, A\,\sin\omega t \end{array} \tag{C.37}$$

The solutions, as per Eq. (C.33), are then

$$\begin{array}{ll} y_1(t) = (A^2 + \frac{B^2}{\omega^2})^{1/2}\,\sin(\omega t + \varphi_1), & \varphi_1 = \mathrm{arctg}\left(\frac{A\omega}{B}\right) \\ y_2(t) = (\omega^2\,A^2 + B^2)^{1/2}\,\sin(\omega t + \varphi_2), & \varphi_2 = -\mathrm{arctg}\left(\frac{B}{A\omega}\right) \end{array} \tag{C.38}$$

Finally, we can also write the solutions in the form of Eq. (C.29) as

$$\begin{array}{l} y_1(t) = 1/2\,(A - \mathrm{i}\frac{B}{\omega})\mathrm{e}^{\mathrm{i}\omega t} + 1/2\,\left(A + \mathrm{i}\frac{B}{\omega}\right)\,\mathrm{e}^{-\mathrm{i}\omega t} \\ y_2(t) = 1/2\,(B + \mathrm{i}\omega A)\mathrm{e}^{\mathrm{i}\omega t} + 1/2(B - \mathrm{i}\omega t)\mathrm{e}^{-\mathrm{i}\omega t} \end{array} \tag{C.39}$$

The coefficients are, as mentioned, complex numbers.

Appendix D

Eigenvalues

D.1 The n-Dimensional System

The system consists of the n differential equations

$$\frac{\mathrm{d}\mathcal{V}_i}{\mathrm{d}t} = \mathcal{R}_i + \sum_{j=1}^{n} p_{ij}\mathcal{V}_j, \quad i = 1, \cdots, n \tag{D.1}$$

In vector and matrix form, and with $\dot{\mathcal{V}}_i = \frac{\mathrm{d}\mathcal{V}_i}{\mathrm{d}t}$, we can write it as

$$\dot{\mathcal{V}} = \mathbf{R} + \mathbf{P}\mathcal{V}$$

$$\mathbf{R} = \begin{pmatrix} \mathcal{R}_1 \\ \vdots \\ \mathcal{R}_n \end{pmatrix} \quad \mathcal{V} = \begin{pmatrix} \mathcal{V}_1 \\ \vdots \\ \mathcal{V}_n \end{pmatrix} \quad \mathbf{P} = \begin{pmatrix} p_{11} & \ldots & p_{1n} \\ \vdots & & \\ p_{n1} & \ldots & p_{nn} \end{pmatrix} \tag{D.2}$$

With the matrix $\mathbf{U}$ we introduce n new variables Z_i:

$$\mathbf{Z} = \mathbf{U}^{-1}\mathcal{V}, \quad \text{or} \quad Z_i = \sum_{j=1}^{n} (U^{-1})_{ij}\mathcal{V}_j \tag{D.3}$$

If we multiply Eq. (D.2) on both sides from the left with $\mathbf{U}^{-1}$ and add the identity matrix $\mathbf{E} = \mathbf{U}\mathbf{U}^{-1}$ in between $\mathbf{P}$ and $\boldsymbol{\mathcal{V}}$ on the right-hand side, then it follows that

$$\mathbf{U}^{-1}\dot{\mathcal{V}} = \mathbf{U}^{-1}\mathbf{R} + \mathbf{U}^{-1}\mathbf{P}(\mathbf{U}\mathbf{U}^{-1})\mathcal{V} \tag{D.4}$$

or, in terms of $\mathbf{Z}$,

$$\dot{\mathbf{Z}} = \mathbf{U}^{-1}\mathbf{R} + \boldsymbol{\Lambda}\mathbf{Z} \quad \text{with} \quad \boldsymbol{\Lambda} = \mathbf{U}^{-1}\mathbf{P}\mathbf{U} \tag{D.5}$$

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With a well-chosen transformation matrix $\mathbf{U}$, the new system matrix $\mathbf{\Lambda}$ becomes diagonal[1]:

$$\mathbf{\Lambda} = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix} \tag{D.6}$$

The λ_i are the eigenvalues of the matrix $\mathbf{P}$. The corresponding eigenfunctions are the column vectors of the matrix $\mathbf{U}$.

As per Appendix C.1, the diagonalized system (Eq. D.5) can now be solved row-wise. For instance, for

$$\dot{Z}_k = T_k + \lambda_k Z_k, \quad T_k = k\text{-th component of the vector } \mathbf{U}^{-1}\mathcal{R} \tag{D.7}$$

we get the solution

$$Z_k(t) = Z_k^\infty + (Z_k^0 - Z_k^\infty)\mathrm{e}^{\lambda_k t}, \quad Z_k^\infty = -\frac{T_k}{\lambda_k} \tag{D.8}$$

Through the inverse transformation $\mathbf{V} = \mathbf{UZ}$ we can calculate the time-dependent solutions $\mathcal{V}_i(t)$ from the solutions in Eq. (D.8).

D.2 Explicit Solution for the Two-Dimensional System

D.2.1 The Eigenvalues

The eigenvalues λ_i are calculated with the so-called characteristic equation of $\mathbf{P}$,

$$\det(\mathbf{E}\lambda - \mathbf{P}) = 0 \tag{D.9}$$

In the above equation, det(..) is the determinant and $\mathbf{E}$ the two-dimensional identity matrix, which is

$$\mathbf{E} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{D.10}$$

Written out, Eq. (D.9) thus has the following form:

$$\det \begin{pmatrix} \lambda - p_{1,1} & -p_{1,2} \\ -p_{2,1} & \lambda - p_{2,2} \end{pmatrix} = 0 \tag{D.11}$$

To determine the two eigenvalues λ_1 und λ_2, Eq. (D.11) leads to the quadratic equation

$$\lambda^2 - \lambda(p_{1,1} + p_{2,2}) + p_{1,1}p_{2,2} - p_{1,2}p_{2,1} = 0 \tag{D.12}$$

---

[1] If one or more of the eigenvalues λ_i are identical, the diagonalization no longer succeeds completely, but only up to the diagonally arranged sub-matrices. This case is not discussed here.

The solution of the quadratic equation can be written as

$$\lambda_i = \frac{1}{2}\left[\mathrm{tr}(\mathbf{P}) \pm \sqrt{\Delta(\mathbf{P})}\right], \qquad i = 1, 2 \tag{D.13}$$

Here $\mathrm{tr}(\mathbf{P})$ is the so-called trace of the quadratic matrix, i.e. the sum of its diagonal elements:

$$\mathrm{tr}(\mathbf{P}) = p_{1,1} + p_{2,2} \tag{D.14}$$

$\Delta(\mathbf{P})$ is the discriminant of the quadratic equation:

$$\begin{aligned}\Delta(\mathbf{P}) &= (p_{1,1} + p_{2,2})^2 - 4p_{1,1}p_{2,2} + 4p_{1,2}p_{2,1} \\ &= (p_{1,1} - p_{2,2})^2 + 4p_{1,2}p_{2,1} \\ &= \mathrm{tr}(\mathbf{P})^2 - 4\det(\mathbf{P})\end{aligned} \tag{D.15}$$

D.2.2 Properties of the Eigenvalues λ_i

Mass balance models lead to distinct systems of differential equations, i.e. to certain properties of the matrix **P** and its eigenvalues λ_i.

Conservative Equations (Homogeneous)

The system of equations is homogeneous if $\mathbf{R} = 0$. The matrix **P** then has the following properties:

- The diagonal elements p_{ii} are negative. All elements outside of the diagonal, p_{ij} with $i \neq j$, are positive or zero.
- The sum of all elements in one column of **P** is zero (as should be expected for a conservative mass balance). From this it follows that the matrix is singular, i.e. its determinant is zero.

These properties are responsible for the fact that **P** has one eigenvalue $\lambda = 0$. The corresponding transformed variable $\mathbf{U}^{-1}\mathbf{y}$ is the sum of all y_i, that is, the total mass in the system (which is constant). All other eigenvalues λ_i are negative, i.e. there is a steady state.

Non-conservative Equations (Inhomogeneous)

Not all $x_i = 0$. In addition, at least one sum of column elements is negative. Then, the matrix **P** is not singular, i.e. the inverse matrix $\mathbf{P}^{-1}$ exists. It can be used to calculate the steady state with the relation

$$\mathbf{y} = -\mathbf{P}^{-1}\mathbf{x} \tag{D.16}$$

Because the p_{ij} are still constrained,

$$p_{ij}\begin{cases} < 0 & \text{for } i = j \\ > 0 & \text{for } i \neq j\end{cases}$$

Therefore all eigenvalues λ_i are negative, so that a steady state exists in this case, too.

D.2.3 Eigenfunctions

The eigenfunctions of the matrix $\mathbf{P}$ are only determined up to a constant (positive or negative) factor. For instance, they can be written as

$$\begin{aligned} z_1 &= p_{2,1}\mathcal{V}_1 + (\lambda_1 - p_{1,1})\mathcal{V}_2 \\ z_2 &= (\lambda_2 - p_{2,2})\mathcal{V}_1 + p_{1,2}\mathcal{V}_2 \end{aligned} \tag{D.17}$$

Written in the new variables z_i, the system of homogeneous differential equations becomes

$$\begin{aligned} \frac{\mathrm{d}z_1}{\mathrm{d}t} &= \lambda_1 z_1 \\ \frac{\mathrm{d}z_2}{\mathrm{d}t} &= \lambda_2 z_2 \end{aligned} \tag{D.18}$$

with the solutions

$$z_1(t) = z_1^o e^{\lambda_1,t} \qquad z_2(t) = z_2^o e^{\lambda_2,t} \tag{D.19}$$

The initial values z_i^o can be calculated from the transformation equations (D.17) by inserting $\mathcal{V}_1^o$ and $\mathcal{V}_2^o$ into them. The inverse transformation to Eq. (D.17) is

$$\begin{aligned} \mathcal{V}_1 &= \frac{1}{D}[p_{1,2}z_1 - (\lambda_1 - p_{1,1})z_2] \\ \mathcal{V}_2 &= \frac{1}{D}[-(\lambda_2 - p_{2,2})z_1 + p_{2,1}z_2] \end{aligned} \tag{D.20}$$

with

$$\begin{aligned} D &= p_{1,2}p_{2,1} - (\lambda_1 - p_{1,1})(\lambda_2 - p_{2,2}) \\ &= -2\det(\mathbf{P}) + \lambda_1 p_{2,2} + \lambda_2 p_{1,1} \end{aligned} \tag{D.21}$$

Note that we used the following relation: $\lambda_1\lambda_2 = \det(\mathbf{P})$.

Appendix E

Time-Dependent Diffusion Equation

We will look at some mathematical functions that are useful for the explicit time-dependent solution of the diffusion equation. More can be found in Crank (1975) and in Schwarzenbach et al. (2003, Chaps. 18 and 22).

E.1 The Normal or Gaussian Distribution

Figure E.1 shows the Gaussian distribution $G(x)$ (often also called the normal distribution).

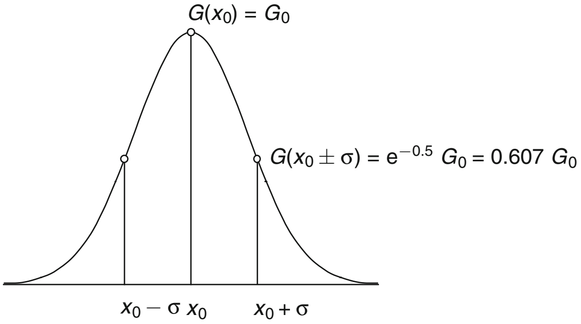

Fig. E.1: *Gauss or normal distribution around the mean value x_0 with variance σ*

The mathematical formulation is

$$G(x) = \frac{1}{\sqrt{2\pi}\ \sigma} \exp\left(-\frac{(x - x_0)^2}{2\sigma^2}\right) \tag{E.1}$$

where x_0 is the mean value of the distribution and σ is the variance. The Gaussian distribution $G(x)$ is standardized, so

$$\int_{-\infty}^{\infty} G(x)\mathrm{d}x = 1 \tag{E.2}$$

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The values the distribution takes on for $x_0 \pm 2\sigma$ and $x_0 \pm 3\sigma$ are

$$G(x_0 \pm 2\sigma) = \mathrm{e}^{-2}\ G_0 = 0.135\ G_0$$
$$G(x_0 \pm 3\sigma) = \mathrm{e}^{-9/2}\ G_0 = 0.011\ G_0$$

The area between the edges $x = x_0 - \sigma$ and $x = x_0 + \sigma$ is 68.3 % of the total integral of $G(x)$ standardized to 1. The area between $x = x_0 \pm 2\sigma$ encompasses 95.4 %. The special solution of the diffusion equation is thus a Gaussian distribution with the time-dependent variance

$$\sigma(t) = \sqrt{2Dt} \tag{E.3}$$

From it, we can determine the diffusion coefficient D as

$$D = \frac{1}{2}\frac{\mathrm{d}\sigma^2}{\mathrm{d}t} \tag{E.4}$$

E.2 The Error Function

The error function $\mathrm{erf}(x)$ is defined as

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp\,(-\xi^2)\mathrm{d}\xi \tag{E.5}$$

The complement of the error function is

$$\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty \exp\,(-\xi^2)\mathrm{d}\xi \tag{E.6}$$

The error function has the following properties:

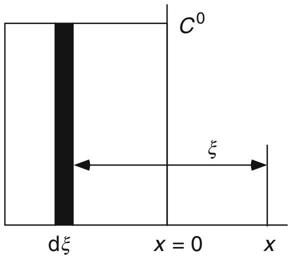
$$\begin{aligned} &\mathrm{erf}(x=1) = 1, \quad \mathrm{erfc}(x=1) = 0\\ &\mathrm{erf}(x=0) = 0, \quad \mathrm{erfc}(x=0) = 1 \end{aligned}$$

Its values can be looked up in tables in the literature, for instance in Abramowitz and Stegun (1972).

E.3 The Principle of Linear Superposition

The influence of the layer $\mathrm{d}\xi$ on the concentration at point x is calculated from Eq. (8.48) with $m = C_0 d\xi$. Because the concentration only moves in positive x direction (for $x < 0$, $C = C_0$ =constant), the factor 2 disappears in the denominator of Eq. (8.48). Thus the influence of the layer $\mathrm{d}\xi$ can be described by

$$\frac{C^0\mathrm{d}\xi}{\sqrt{D\pi t}}\exp\,(-\frac{\xi^2}{4Dt})$$



The superposition of all dξ sections results in

$$C(x,t) = \frac{C^0}{\sqrt{D\pi t}} \int\limits_x^\infty \exp{(-\frac{\xi^2}{4Dt})} \mathrm{d}\xi \tag{E.7}$$

Note: the integration boundaries in (E.7) result because the smallest distance of an element dξ to the point x is given by x, the largest distance by ∞.

Equation (E.7) can be transformed by the substitution of the variable ξ with $\eta = \frac{\xi}{2\sqrt{Dt}}$ and thus $\mathrm{d}\xi = 2\sqrt{Dt}\ \mathrm{d}\eta$:

$$C(x,t) = \frac{2C^0}{\sqrt{\pi}} \int\limits_{\frac{x}{2\sqrt{Dt}}}^{\infty} \exp{(-\eta^2)} \mathrm{d}\eta = C^0\ \ \mathrm{erfc}(\frac{x}{2\sqrt{Dt}}) \tag{E.8}$$

The function erfc is the complement of the error function (see Sect. E.2):

$$\mathrm{erfc}(\frac{x}{2\sqrt{Dt}}) = 1 - \mathrm{erf}(\frac{x}{2\sqrt{Dt}}) \tag{E.9}$$

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