Good Modelling Practice Handbook

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Good Modelling Practice Handbook

GMP is an AQUEST project

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Good Modelling Practice Handbook

This Handbook comprises the following sections:

- Foreword
- Introduction
- Scope
- Glossary and Conceptual framework
- Part I: Modelling step-by-step, with separate:
    - Checklist and Flow chart
    - Templates
- Part 2: Pitfalls and sensitivities
- Bibliography
- Appendices
    - Scales
    - Data assimilation
- Templates stored on disk

The authors would like to keep the Handbook dynamic, making it not only a Handbook for modellers but also one by modellers. All users are therefore requested to send their experiences, proposals for improvement and any other notes to the address mentioned below so that these may be processed in the next version.

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This Handbook can also be downloaded from the internet: http://waterland.net/riza/aquest/

Good Modelling Practice Handbook

Foreword

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Foreword

On 4th February 1997, a meeting was held within the Aquest framework, discussing the topic of a Standard Framework for models in Dutch water management. The idea behind this is that major efficiencies can be attained by coordinating or even integrating the numerous separate developments in this domain. Important players in Dutch water management attended the meeting (Dutch Department of Public Works, Provinces, Water Boards, STOWA, RIVM, Staring Centrum, NITG-TNO and various consultants involved in one of the LWI programmes at that time (WL | DELFT HYDRAULICS, DHV, EDS and Aquasense/ECOSYS).

At this meeting, all parties involved expressed the intention to achieve closer co-operation regarding a Standard Framework for models and it was agreed that the consultations would be continued. This has resulted in the establishment of three study groups: ‘Generic Tools’, ‘Good Modelling Practice (GMP)’ and ‘IT Model Coupling’. The Generic Tools study group has made an inventory of the tools available in the Netherlands (and in other countries), which may serve as building blocks for a Standard Framework for models. Meanwhile, this stock-taking has been completed and the study group recently started the exploration of the technical feasibility of the construction of a Standard Framework, which was in fact recently renamed Standard Water Framework (SWF). For this purpose, an IT architecture is being designed, including a technical description of the interfaces.

The IT Model Coupling study group is not an official study group under the Standard Water Framework, but rather an existing group which was involved in the LWI project called ‘Architectural design of complex model systems’. This project concentrates on the link between the complex SIMONA 2D/3D hydrodynamic models by the Dept. of Public Works and Delft 2D/3D by WL|DELFT HYDRAULICS. The LWI project has been completed by now and the co-operating parties have initiated a follow-up project.

At this moment a fourth group is actively involved in the Standard Water Framework. Their field of study is the problems regarding the copyrights of software and databases.

The Good Modelling Practice (GMP) study group has started a project for the development of a GMP Handbook. The objective of this project was to stimulate the proper manner of dealing with models. The project set out in August 1998, was financed by the Dutch Department of Public Works, STOWA and DLO Staring Centrum. The project was executed by Wageningen Agricultural University, NITG-TNO and DLO Staring Centrum under the management of WL | DELFT HYDRAULICS and was supervised by a broad group of representatives from water managers, universities, scientific institutes and engineering offices.

The project started with an inventory, in which relevant literature was consulted and the experiences from the organisations involved were charted. This formed the basis for the first draft of the ‘Good Modelling Practice’ Handbook. Next, the usability of the draft Handbook was verified by both inexperienced and experienced modellers at various water management institutions. The test period was concluded with a workshop at which the testers’ experiences were discussed. The final version of the Handbook now presented to you is based on the findings during the test period.

The Handbook is primarily intended to support the modeller. It deals with all major steps in the modelling process and is therefore very suitable for use as a checklist. Recording the procedures of the checklist (for instance in the forms appended) will create a model journal which renders this model study reproducible and transferable, allowing other parties involved to get an idea of the model study executed more easily. In this sense, the Handbook is explicitly not intended as a compulsory straitjacket to the modeller, but rather as a technical tool.

The members of the project team, whose names are given on the first page of this Handbook, were supported and advised by a supervisory committee consisting of the following persons:

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It would not have been possible to develop the first GMP Handbook without the commitment of the testers who were the pilot users of the Handbook and provided valuable feedback on its usability.

Finally, we would like to thank the numerous experts of WL | DELFT HYDRAULICS, NITG-TNO, Alterra (former DLO Staring Centrum), STOWA, LUW, RIKZ and RIZA for their contributions to the pitfalls and sensitivities contained in Part 2 of the Handbook and all other persons for their support in whatever form towards the realisation of the Good Modelling Practice Handbook.

GMP Handbook

Introduction

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Introduction

Background to the Handbook

Models have become an essential tool in the modern world of water management. They are used extensively and play an important auxiliary role in fulfilling the core tasks of water management, in policy preparation, operational water management and research, and in the collection of basic data (monitoring), among other things.

Besides the fact that the use of models is becoming increasingly common in water management, a development can also be discerned in terms of increasing co-operation in the modelling field. Gone are the days when every manager or institute developed its own models. This is reflected, for example, in the willingness to develop the Standard Water Framework by a large number of parties involved in Dutch water management. The Standard Water Framework (for models, databases and IT tools such as presentation programs in water management) is intended to provide water managers with an integrated system in which models and other information systems can easily be 'coupled' or 'decoupled', depending on the type of problem requiring attention. This allows for efficient use of the know-how developed elsewhere and of the available financial means.

However, when models can be deployed in such a flexible manner, this also increases the risk of inexpert use. This may be the result of errors in the software or incomplete manuals, though the cause may equally lie with the modeller himself. Careless treatment of input data, insufficient calibration and validation, working outside the scope of the model, inaccurate model hypotheses, these are all errors which can lead to the results of model calculations being unreliable. This can have far-reaching consequences, certainly when considering the important role played by models in modern-day water management.

Objective

In order to stimulate the correct use of models, the initiative has been taken to develop a 'Good Modelling Practice' Handbook, a list of guidelines for the use of models. GMP can also improve the reproducibility and transferability of model studies. There were previously no guidelines for GMP supported by all the parties involved in water management, though some institutes did have their own guidelines. To summarise, the objective of the GMP Handbook is to:

- take the initiative on guidelines with regard to model use, which are supported by all parties in water management;
- stimulate more careful use of models in water management;
- to improve the reproducibility and transferability of model studies.

The Handbook is intended in particular to support the modeller. It deals with all major steps in the modelling process and is therefore very suitable for use as a checklist. Recording the procedures of the checklist (for instance in the forms appended) will create a model journal which renders this model study reproducible and transferable, allowing other parties involved to get an idea of the model study executed more easily. In this sense, the Handbook is explicitly not intended as a compulsory straitjacket to the modeller, but rather as a technical tool.

Target groups and use of the Handbook

The Handbook is intended for all water management parties involved in modelling. There is a number of specific target groups, each of whom will probably use the Handbook in its own manner. That is the reason for the choice of a loose-leaf system, so that each user of the Handbook can organise it to suit his or her purposes.

The main target group for the Handbook is the (non-programming) *modeller* who carries out modelling projects. The various components of the Handbook provide an *inexperienced modeller* with a clear and step-by-step plan in order to carry out a modelling project in a careful, reproducible and transferable manner. More *experienced modellers* will probably mainly use the checklist to check whether all steps in the modelling process have been or will be paid sufficient attention.

Upon contracting out a modelling project, a *client* will benefit particularly from the checklist and the concepts and backgrounds described in parts 1 and 2. In assessing the completed modelling projects, the client can make good use of the forms (possibly) filled in, which describe the backgrounds to the results achieved and therefore improve the transferability and reproducibility of the model study.

The Handbook may well become part of the quality system in *institutes and companies* in the future, regardless of whether they are acting as a client or an executive party. Finally, the Handbook can be used as a study and reference book in the training of modellers.

However the Handbook or parts of it are used, it is essential that each of the individual steps is followed. The client and modeller can confer on which steps will have priority and/or extra attention in any particular modelling project. There may well be good reason to agree to pay certain steps little or no attention. The speed with which the various steps are followed will generally depend on the complexity of the modelling project

All users are advised to at least read the glossary of terms and the scope of the Handbook, as this can avoid unnecessary misunderstandings.

On the whole, the Handbook is expected to be a useful tool in decreasing the gap and confusion which often occurs between client, executing party and modeller. More efforts will be required in order to remove barriers completely, particularly in the personal communication between client and modeller.

Layout of the Handbook

The core of the Handbook comprises two sections:

Part I: a step-by-step plan of all activities involved in working with models in water management (from 'problem' to 'interpretation' and 'documentation');

Part II: a summary of the pitfalls and sensitivities for models, for a total of 13 different domains of application, varying from groundwater quality models to surface water quantity models, and from ecological models to models for water related economic sectors.

Both Part I and Part II include literature references for supplementary information. A series of forms has been included with the Handbook, both on paper and diskette, for the recording of modelling projects. There is a form for each step in the first Part. A glossary of terms has also been included. This has been compiled on the basis of all existing lists (recorded, for instance, within the framework of the National Study Programme on Dehydration and the inventory of Generic Tools under the scope of the LWI) and the (international) literature in this field, whereby concepts are described 'over the full width of water management'.

Dynamic character

The Handbook in front of you is not a static item. Although it is based on an extensive testing period, broader and more intensive use of the Handbook will inevitably lead to supplements and improvements. Hence the loose leaf layout of the Handbook. The idea is to keep the Handbook dynamic and to regularly distribute extensions or adaptations based on experience gained in practice. Of course, the feasibility of this plan depends greatly on the response by the users. The authors therefore invite all users to pass on any experiences, suggestions for improvements and any other general comments, to the address given in the front of this Handbook.

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Good Modelling Practice Handbook

Scope

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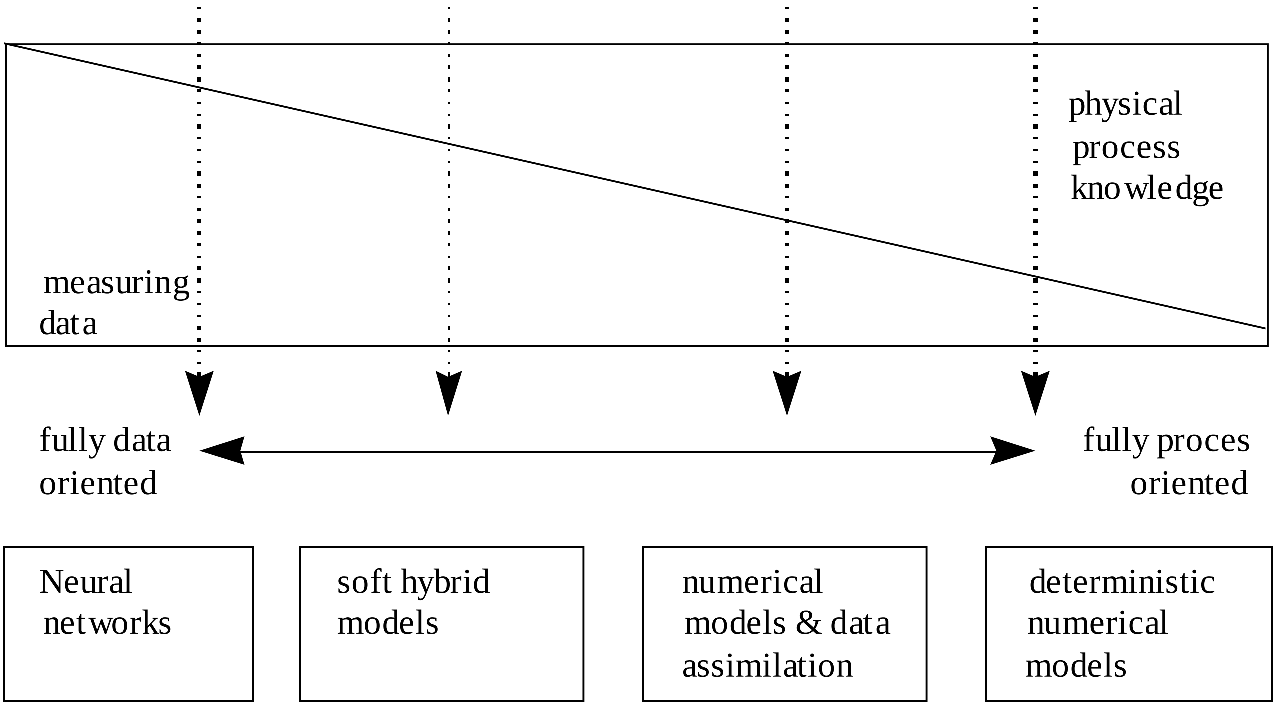
Scope

To what types of models does this Handbook apply?

The concept of a 'model' is a very broad one. This paragraph indicates which types of models are covered by this Handbook and which are not. On the one hand, this means defining the scope of this Handbook, on the other hand a detailing of the concept of a 'model'. More general information on the terms used in the Handbook can be found in the glossary and the related conceptual framework.

Scope

The questions from policy and management practice often concern the behaviour of a water system, the system parameters or influencing factors of certain system parameters. The key question is generally: *Given the need for information and required accuracy contained in the question, what is the most suitable source of information to answer a question.* There are, in principle, two possible approaches, which can be seen as the extremes of a spectrum. Firstly: fully data oriented (field measurements) and, secondly, fully process oriented (use of a deterministic model based on physical process knowledge). This has been visualised in the figure below.



As usual, all kinds of combinations are possible, between these extremes. In many cases, the use of a model alone or measuring data alone will not result in the answer required. In making a rough subdivision, the range of opportunities lie in the following classes:

Neural networks, whereby a relationship is derived between cause and effect, based on purely statistical grounds. The correlation between the input and the output variables is derived via calibration on the basis of data sets comprising a representative set of input – output relationships. The calibrated neural network can then predict the output for new values of input variables.

Soft Hybrid models, whereby physical concepts are processed in a neural network, for example by not only limiting the calibration to the input-output combinations but rather also including physical concepts such as the conservation of equations as a precondition. The physical concepts used thereby supplement the knowledge contained in the measuring data.

Numerical models with data assimilation, whereby the basis is formed by the physical process knowledge stored in the numerical models, supplemented with field measurements which are added to the model via data assimilation (see the glossary and appendix 2).

Deterministic numerical models, whereby all knowledge of the system is stored in the model in the form of equations and the accessory parameters and knowledge of the system environment is supplied in the form of time series. In these types of models, the physical process knowledge is assumed to be fully known.

Water management mainly makes use of the latter category: deterministic numerical models. Numerical models with data assimilation are also applied, but only by a select group of specialist users. The GMP Handbook mainly discusses the deterministic numerical models (the right hand side of the figure). The limit has been set at the numerical models with data assimilation. Consequently, Soft Hybrid models and neural networks, which are regularly used in ecology for example, are not discussed.

Detailing of the concept of ‘model’

Besides the above classification of models, determined by the degree to which physical process knowledge is the basis for the model, many other classifications are possible. A number of these classifications will be dealt with in this paragraph, without any claim of being exhaustive. The Handbook can be used for all these models, as long as they comply with the scope described in the previous paragraph.

In Part 2 of this Handbook, ‘Pitfalls and sensitivities’, a classification of models was chosen on the basis of domains of application. Based on this classification, attention is paid to specific pitfalls and sensitivities of models used in water management. The following domains of application can be distinguished:

- groundwater models for the saturated zone (quantity and quality);
- groundwater models for the unsaturated zone (quantity and quality);
- precipitation runoff models;
- water distribution models;
- hydrodynamic models;
- high water forecasting models and operational models;
- calamity models;
- morphological models;
- surface water quality models;
- waste water purification models;
- ecological models;
- models for water related economical sectors;
- emission models.

Models can also be classified on a more general basis, such as the spatial dimension to which they apply.

- 0D (point models);
- 1D;
- 2D;
- 3D;

We sometimes also refer to quasi 2D or quasi 3D models. These are not separate dimensions but rather refer to a manner of schematization, by modelling a 2D system as a series of coupled line elements, for example.

Carrying on from the spatial dimensions, a distinction can also be made in models for the local, regional, national and international scale.

The resolution in time is comparable to the spatial resolution. The main distinction made here is whether a model is stationary or dynamic. The mathematical solution mechanism also often plays a role here. In turn, this leads to another sub-division, which varies from purely analytical to fully numerical, and everything in-between of course.

Finally, models can also be distinguished on the basis of the reason for their application, varying from policy analytical (rough and broad) to scientific research models (detailed and narrow). In-between, we find the operational models (for real-time control of structures, for example) and the calamity models. In fact, it is not always possible to clearly distinguish between these fields. In past years, it has become increasingly apparent how the models for the various domains begin to overlap.

The five classifications given above (domain of application, space, time, mathematical solution mechanism and reason for application) are partly separate but also partly linked to one another.

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Good Modelling Practice Handbook

Handbook Glossary

Conceptual framework

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1 Glossary

concept		meaning
algorithm		sequence of steps for solving a problem in a computer program
analytic element method		calculation method for groundwater flows based on the superimposition of analytical solutions of the Poisson’s equation (for spatially variable vertical flow and for the storage term for non-stationarity) which apply to infinite or finite areas in several linked or non-linked layers
auxiliary variable		variable whose value is not dependent on its value at a previous value of the independent variable (e.g. not dependent on its value at an earlier point in time)
calibration		activities to obtain a previously determined degree of similarity between model and measurements in the field by the (systematic) change of uncertain factors (often parameters), followed by analysis of the residual errors
conceptual model		description of a system structure with qualitative dependencies
constant		a quantity whose value is accurately known
data		items of information
data assimilation		approach which integrates data in a physical/chemical process description to allow for the information contents of both data and process description being made explicit and weighted
dependent variable		variable which changes versus one or more independent variables
deterministic		without randomness (the opposite of stochastic)
dimension		1. length, width, height 2. (dimension analysis) unit in which a quantity is expressed
dimension analysis		test to verify the correctness of all dimensions in the model equations
discretisation		the conversion of a continuous model (in time and space) into a model which describes the system in discrete (not infinitely small) steps in time and space
domain		science domain, in this Handbook sub-domains of water management
dynamic model		model in which time is an independent variable
energy budget		balance of energy flows
entity		independent quantity with its own meaning
finite difference method		transformation of (partial) differential equations which are continuous in time and/or space into discrete difference equations to solve these numerically with the aid of a discrete grid
finite element method		transformation of (partial) differential equations which are continuous in space into discrete equations to solve these numerically with the aid of discrete elements, viz. spatial compartments

concept		meaning
fuzzy logic model		model with descriptions on the basis of fuzzy logics, e.g. with intermediate values between yes and no (maybe)
global behaviour test		test to verify whether the rough operation of the model meets with expectations
heuristic method		non-formal method to reach an objective which is not precisely known in an explorative and continuously evaluating manner in accordance with a specific criterion
identification		calibration in order to determine unambiguous values of all parameters and other calibration factors
independent variable		variable versus which changes in a dynamic system are described; e.g. time, three spatial dimensions
integrate		solving differential equations
integration algorithm		algorithm to (numerically) solve differential equations
interpretation		interpretive explanation
Jacobian matrix		matrix of partial derivatives from individual residues to the (model) parameters
mass balance		balance of material flows
mathematical model		the mathematical translation of the conceptual model
meta information		data on data (location of data, measured how and by whom, what accuracy, etc.)
model		collective term for representations of essential system aspects, with knowledge being presented in a useful form. Note: In this Handbook, ‘model’ is often referred to as a computer program (a model program) with corresponding input. However, the word ‘model’ may also refer to some notes on paper, a mathematical model, a diagram or a figure
model program		mathematical representation in the form of a computer program, intended to build models through the input of data
model project form		GMP Handbook form to describe the modelling project as completely as possible
modeller		1. the developer of a model 2. someone working with a model
modelling		1. making a model 2. working with a model
modelling process		all steps which have to be or can be taken when making and working with models
modelling project		project in which working with a model is an important feature
neural network model		model which describes the relations between input and output by means of a network of nodes with their own weight, to allow the neural network to produce known output data on entering known input data
non-stationary model		model in which time is an independent variable (see dynamic model)
objective function		quantification of the model error with the aid of field measurements

concept		meaning
observation		field measurement, hence observation at the system which is represented by the model
optimisation		determination of those parameter values which minimise the predefined objective function
parameter		quantity which is supposed to be a constant, but which is not exactly known
partial differential equation		differential equation with more than one independent variable
problem definition		a clear, precise (not necessarily quantitative) specification of the known problem details and the calculations to be made
programmer		someone who writes or adjusts computer programs. Note: some (programming) modellers write their own programs, but this is not very common
residual		residual error
residual analysis		(statistical) analysis of residuals
residual error		difference between the model results and field measurements
robustness test		test to verify whether the model is resistant to extreme input data
schematisation		simplified representation of the spatial and temporal distribution of variables and parameters
scope		the set of conditions under which a model may be applied
sensitivity analysis		research into the relation between changing factors (often parameters) and model output
simulate		imitation of a part of reality or a system (conceptual model, physical model, computer model)
soft-hybrid model		data oriented model (e.g. a neural network) in which physical concepts are included (e.g. through calibration)
stability		quality of differential equation and/or integration method reducing the error in each integration step
standard input		the input data of a standard test (e.g. from the Handbook of the model program or a simple case) of which the corresponding output is known
state		a set of variables in the system at a specific point in time which contains all information of the past which is relevant for the future of the system. The state is not always a unique set of variables: several sets may satisfy the definition
state variable		a variable which is part of the state of the system
stationary (static) model		model which is not dynamic; changes in time are not examined
statistical distribution		probability distribution of a random sample
stochastic		randomly
system		a whole (often a part of reality) consisting of interrelated entities
system definition		a textual description of a system

concept		meaning
uncertainty analysis		activities to estimate the reliability of a model following calibration (and/or validation)
unit		predefined unit to express or measure a quantity
validation		comparison of model output with an independent (i.e. not yet used in calibration) set of measuring data in order to determine whether the model is 'good' (or whether the concept is good, whether the model is able to reproduce the past with the required accuracy and whether the model is suitable to answer all the questions)
variable		quantity whose value may change
verification		check of the correct implementation of the mathematical model into a computer program and the computer program into a computer

2 Conceptual framework

2.1 Introduction

In practice, the language used by modellers in water management is not always univocal and often gives rise to confusion. To prevent such confusion, this Handbook contains a glossary with unequivocal definitions. In addition, an attempt is made to present these concepts a more contextual manner in the following paragraphs, in order to give the individual concepts more coherence.

2.2 The concept scope of modelling and simulation

This Handbook uses the word ***model*** as a collective term for 'representations of essential system aspects, with knowledge being presented in a workable form'. This frequently refers to a computer program (a ***model program***) with corresponding input. However, the word 'model' may also refer to some notes on paper, a mathematical model, a diagram or a figure, representing the system. In this context, a ***system*** is a part of reality (isolated from the rest) consisting of ***entities*** with their mutual relations (processes) and a limited number of relations with the reality outside the system. A ***model*** is a representation of a system if it describes the structure of the system (entities and relations). A system is referred to as an object system when it is converted into a model. In this context, ***modelling*** means the construction of a model, but this concept is also used for working with a model. ***Simulation*** is a similar term and is generally used for 'doing something with the model on a computer'. However, the concept is also used in a wider sense, meaning 'to imitate the system on a computer' (i.e. the whole system). This practically always implies making a number of assumptions which render the model more simple, but also less realistic. This simplification makes the model more workable, though.

Models can be depicted in all kinds of presentations: ordinary language, figures, mathematics, etc. ***A mathematical model*** is the mathematical translation of the conceptual model. Examples of ***mathematical models*** are: algebraic equations, differential equations, ordinary differential equations, partial differential equations, ***neural networks***, statistical models and combinations of these.

A model is ***dynamic*** if it describes changes over time; it is ***stationary*** or ***static*** if it does not. A mathematical model has one or more ***independent variables*** and one or more ***dependent variables***. In a dynamic model, time is the minimum independent variable present. In a spatial model, at least one spatial dimension is another independent variable. A dynamic 3D model has four independent variables: time and three spatial dimensions

Dynamic models on the basis of a 'hard' non-stochastic representation are referred to as ***deterministic models***: the knowledge of the modelled system is fully determined in the model and repetitive use of the model produces the same results. Just like the system of which is it a representation, a model has a model structure (state variables and relations which are defined by auxiliary variables) and a model behaviour (how does the model behave along the axis or axes of the independent variables: what are the changes in the result of a model over time and/or along the spatial axis (axes)).

This Handbook only discusses mathematical models, consisting of (partial or ordinary) differential equations and/or algebraic equations. The term mathematical model then refers to a set of one or more mathematical equations. The logics used in this model are usually crisp (yes-no; do-don't; black-white), sometimes they are ***fuzzy logics*** (yes-maybe-no; newborn-young-middle aged-old-ancient).

Non-mathematical representations of a model are often called ***conceptual models***: the structure has been defined but the elements of the model and the relations have not (all) been quantified. The mathematical equations in a model may be solved in an analytical manner (allowing for the exact value to be derived for each point in the domain) or a numerical manner (allowing for a numerical approach of the exact value for each point in the domain).

The entities in a mathematical model are represented by means of one or more ***state variables*** and the relations between the entities by means of ***auxiliary variables***. The state variables determine the state of the model. Changes in state variables are defined by means of (partial) differential equations. Auxiliary variables are defined by means of algebraic equations or are directly allocated a value (input). Equations may make use of state variables, auxiliary variables, ***parameters*** (constant over time), or other ***model components***.

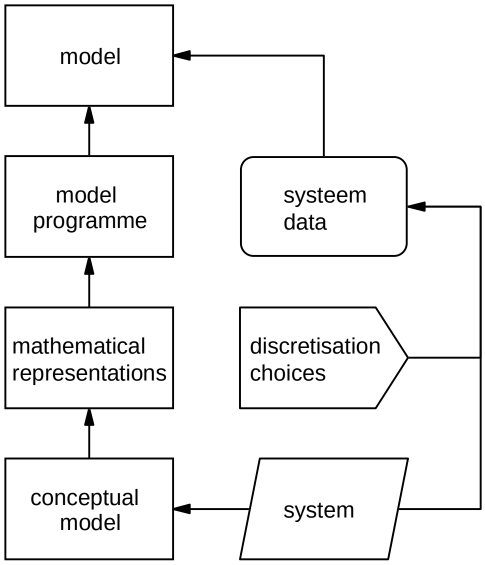
The conceptual model is converted into a computer model by entering data in a ***model program*** (a mathematical model in the form of a computer program, intended to build models through the input of data). For this purpose, choices have to be made, including those required for spatial ***schematization***. Apart from the choices made concerning ***discretization***, system data must be supplied to or included in the model program with which the model is to be built. The procedure of checking the proper implementation of the model on the computer is called ***verification***.

Following the input of a model in the computer, the resemblance between model and system has to be aligned, in other words, the similarity of model behaviour and system behaviour must be improved. This process is called ***calibration***; it is performed by changing the parameter values and subsequently comparing the model results with the field measurements. The process often uses ***optimisation*** techniques. Using the same techniques as those used in calibration, sometimes allows for ***identification*** of the model (if the model is not too complex and the system is known by measurements), meaning that univocal values of all parameters and other calibration factors are found. ***Sensitivity analysis*** may serve to identify the uncertain factors, which have to be adjusted during calibration to obtain greater similarity. Following calibration, the remaining differences may be investigated and the remaining uncertainties in the model predictions may be quantified in an ***uncertainty analysis***. In addition to being calibrated, the model may also be validated. In the ***validation*** process the model results (the results of the uncertainty analysis) are compared with an independent set of observations (i.e. not used in calibration) of the real system to verify whether the model describes the system (behaviour) correctly.

The whole set of procedures and actions involved in modelling and simulation in order to solve a specific problem is called the ***modelling project***.

2.3 Coherence on the basis of the 'model' concept

The figure below shows the relationship between the various representations of a model.



The conceptual model is developed on the basis of knowledge of the system and serves as the basis for a mathematical model. This model may be solved either analytically or numerically. In the latter option a number of choices are made, based on the system, to numerically imitate the mathematical model (discretization), and numerical algorithms are coupled to enable discretization over time. The model thus created is further refined into a model program and finally into a computer model by entering the proper input data.

Literature

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Good Modelling Practice Handbook

Part I: Modelling

Step-by-step

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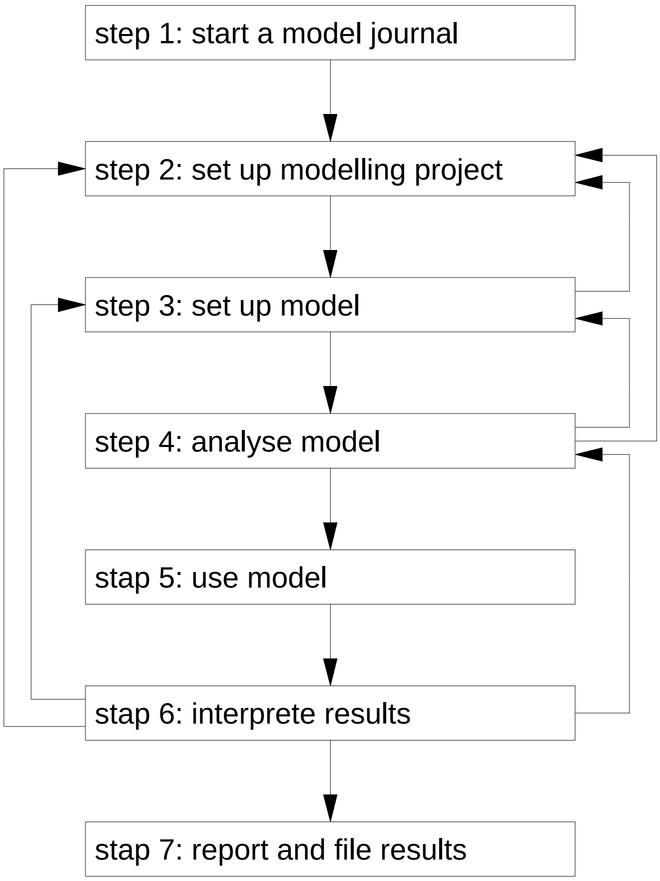
Contents:

Step 0 The modelling process

Making, studying and working with models can be seen as a network of activities and products. This section of the Handbook presents a method for supervision of the modelling process. The process has been divided into seven steps for that purpose, namely:

1. Start a model journal;
2. Set up the modelling project;
3. Set up the model;
4. Analyse the model;
5. Use the model;
6. Interpret the results;
7. Report and file the results.



The modelling process has many feedbacks to moments at which a step in the process indicates deficiencies in previous steps. These feedbacks make the modelling process an iterative procedure.

Part I of the Handbook deals with each step in a separate chapter. Per step or activity, the following matters are generally dealt with:

- what is it?
- who does it?
- why is it done (objective)?
- what are the products?
- who uses the products?
- what methods are used (standard/different)?
- where is it all described?

The steps given in the Handbook are not all relevant at all times. Some parts of the process can simply be skipped for certain applications. Even if one and the same method is always used (according to a protocol), this can be referred to, so that the recording of activities need not give too much work in practice. The result is a description of all which has been done in the modelling project and the results thus achieved.

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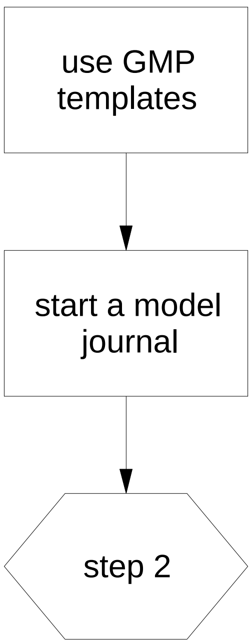
Step 1 Start a model journal

One of the main problems of model studies is that it is often difficult to determine whether the quality of the study is adequate to solve the problem for which the study was intended. It is also often impossible for third parties to continue from the point at which the study left off. Both problems are caused by a lack of information on how the study has been carried out. In other words, the study is not (fully) reproducible. What was the pattern of thought followed? Which concrete activities were carried out? Who carried out which work? Which choices were made? How reliable are the end results? These are all questions which can be answered if a daily model journal is kept. This is often neglected under the pressure of time, also because it is not rewarding work. In order to make life somewhat easier, a number of templates have been designed and included in this Handbook. These templates can be used to enter information in the model journal. They proceed through the complete model study step by step, thus giving a description as they go along. We shall come back to the question of reporting in the final step of this GMP Handbook.

step 1



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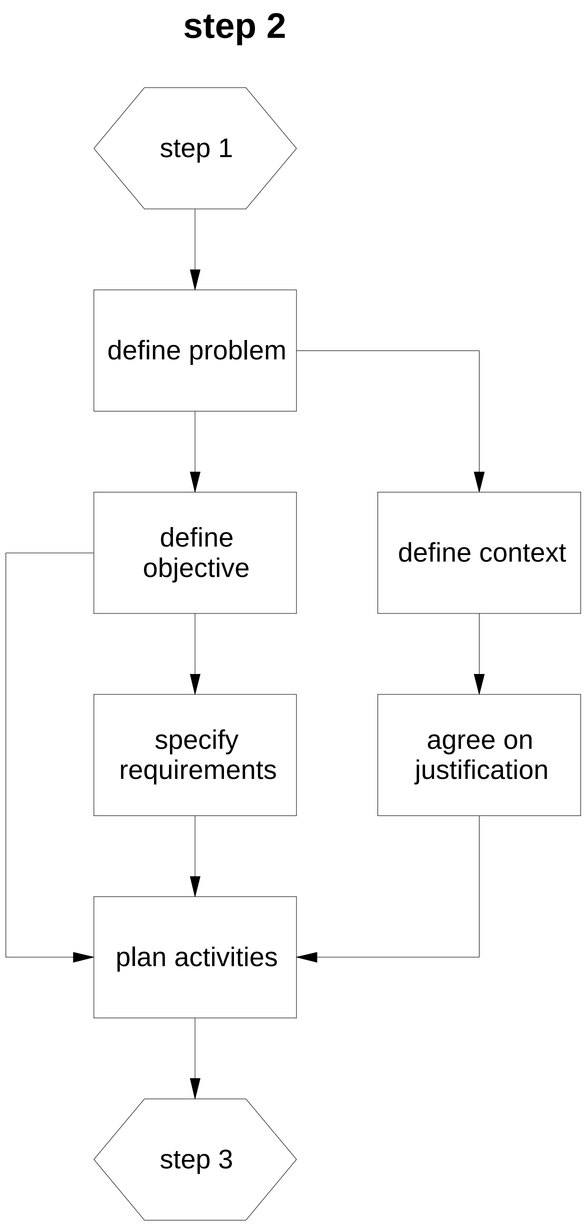
Step 2 Set up the modelling project

2.1 Describe the problem



Someone somewhere has detected a problem for which a model would seem to provide a useful contribution to solving the problem. One of the first steps to be undertaken is analysis of the problem. This analysis of the problem generally needs to take place at two levels: at the client level and at the level of the modeller. Of course, the two levels are inter-related but there are also often major differences between the perception of a policymaker and that of a technician. They must consult to arrive at an effective problem description for the modeller, eventually establishing a working plan which is acceptable for both parties. The problem area must first be defined. To which domain does the problem belong? In which characteristic time scale and spatial scale does the problem occur? And also: which physical processes play a role, and must therefore eventually be described along with the model? A brief description of the problem in text will also be required. The question of the various time and spatial scales is described in great detail in appendix 1.

Details do not belong here, neither do detailing and interpretation of the model. However, serious attention must be paid to the fact of whether a model is the right medium for solution of the problem. What are the alternatives?

2.2 Define the objective

If a model seems to be the right tool to solve the problem, the objective of this project must be defined. The objective must be described in terms of:

- the domain and the problem area;
- the reason for solution of the problem by means of a model;
- the questions to be answered by the model;
- the scenarios to be calculated.

The latter is a profession in itself and is potentially a great source of misunderstanding between the client and modeller. This will therefore be dealt with in great detail in step 5. At various moments during the project, it must be checked whether the objective is being met.

2.3 Analyse the context and reach agreements on the justification

2.3.1 Context

The use of a model nearly always takes place within a broader context: a project, a study, routine activities, etc. The model itself will sometimes also be part of a larger whole, such as a network of models which use each others' results.

2.3.2 Justification

In many cases, an internal or external client will put a problem to a person who must solve the problem. This means that the activities required to solve the problem (within the modelling project) must be justified towards this client. Agreement must also be reached on how this justification must take place. Are intermediate reports required, is there an official completion of the modelling project, is verification by third parties required, etc.? It is particularly important to record beforehand at which moments the client must approve the results. It must also be recorded during the process that this approval has indeed been gained. Finally, it is also sensible to reach agreement with the client on the template, scope and contents of the report (also what type of 'pictures'). This cannot yet be agreed in detail of course, it will therefore be a point of recurrence throughout the project.

2.4 Specify the requirements

2.4.1 Quality requirements

This may well be the most difficult step of the entire modelling process. When is something adequate or inadequate? This may be clear right from the start, but usually the quality requirements can only be determined following lengthy consultation between the client and modeller. And even then, it often becomes apparent during or after the modelling process, that the quality requirements demand slight adjustment or are simply unattainable, so that the entire process must begin again. It is therefore sensible not only to work through this step right at the beginning of the modelling process but also to continue to maintain close contact with the client throughout.

What quality requirements should be concerned? There are a number, which are actually all inter-related.

- requirements with regard to the quality of the answer to the question posed;
- requirements with regard to the quality of the analyses to be carried out using the model;
- requirements with regard to the quality of the model;
- requirements for the calibration, particularly with regard to when calibration can be ceased.

2.4.2 Expertise requirements

In order to solve a certain problem with a model, those involved must have expertise in the study discipline. The form of expertise required must have been determined beforehand, as well as whether this can indeed be provided by the project participants. If that is not the case, there must be an indication of how the expertise can be acquired after all.

2.4.3 Estimated capacity/manpower requirement

Just like any other project, an estimate must be made beforehand of how much capacity is required to complete the project. Sometimes there may be external forces or other reasons which restrict the amount of time/manpower available. This must be taken into account when planning the project. There must be a clear relationship between the size of the project (in manpower) and the level of ambition of the modelling project. An indication (and no more than that) of the global time required could then be as follows:

·	start a model journal	0 %
·	define the modelling project	10 %
·	make the model	25 %
·	analyse the model	30 %
·	use the model	10 %
·	interpret the results	5 %
·	report	20 %

Due to feedback links, some ‘steps’ (or ‘sub-steps’) are performed more than once (see the figure for step 0: The modelling process). The time expenditure given here refers to the total time to be spent. Occasionally, there may be a ready-made model which can be directly deployed. Steps 3 and 4 will take much less time then, of course

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2.4.4 Communication and reporting

A note must be made of how and with whom there will be communication regarding the project (meetings, workshops, study days, etc.) The requirements set for reporting of the project are as follows:

· what needs to be reported?

· to whom?

· when?

It must be established beforehand how these requirements will be met in this project, so that this cannot become a subsequent bone of contention. In small, routine projects, a simple report and possible production of the results may be sufficient, whereby the recording of the project through the Handbook guidelines (the templates) is generally adequate.

It is often useful to appoint a supervisory committee in order to monitor the quality of the process. Some clients demand this in fact.

2.4.5 Other requirements

Supplementary requirements may be formulated in some projects. One could think in terms of:

- use of the results from other models and the requirements which must be set for that purpose;
- supply of the results of this modelling project for use by other models;
- scientific reporting;
- the hypotheses on which the model is based;
- the quality of the field data;
- formulation of responsibilities for the purpose of final completion;
- evaluation of two or more different approaches (with various models and/or model programmes);
- completion of an implemented model for the client;
- processing of the model results into a policy advice;
- provision of digital files of (part of) the results.

2.5 Draw up a working plan and a budget

Depending on what is common practice, the activities must be carried out in the form of a project (plan, project management, administration, etc.). In the approach taken towards a project, there will in any case be a working plan established according to normal methods (common practice in the organisation), which includes:

· problem definition (step 2.1);

· objective of the project (step 2.2);

· agreements on the justification (step 2.3);

· what quality requirements must be made of the end results (step 2.4.1);

- what requirements must be made of the people carrying out the project (step 2.4.2);
- required capacity of people and other resources (step 2.4.3);
- requirements made of communication and reporting (step 2.4.4);
- other requirements made of the project (step 2.4.5);
- how the project will be carried out.

Furthermore, the working plan must contain the following components:

- possible sub-division of the modelling project in sub-projects;
- time scheduling;
- allocation of the tasks to project team members.

At the end of this step, the project must have been recorded as clearly as possible. There must always be the opportunity to react to unforeseen circumstances and insights, of course. The idea is not to have the project fully airtight at this stage.

Use of ISO 9001 is certainly advisable. These standards of the International Organisation for Standardisation concern the requirements made of organisations involved in matters varying from design and development to production, installation and service.

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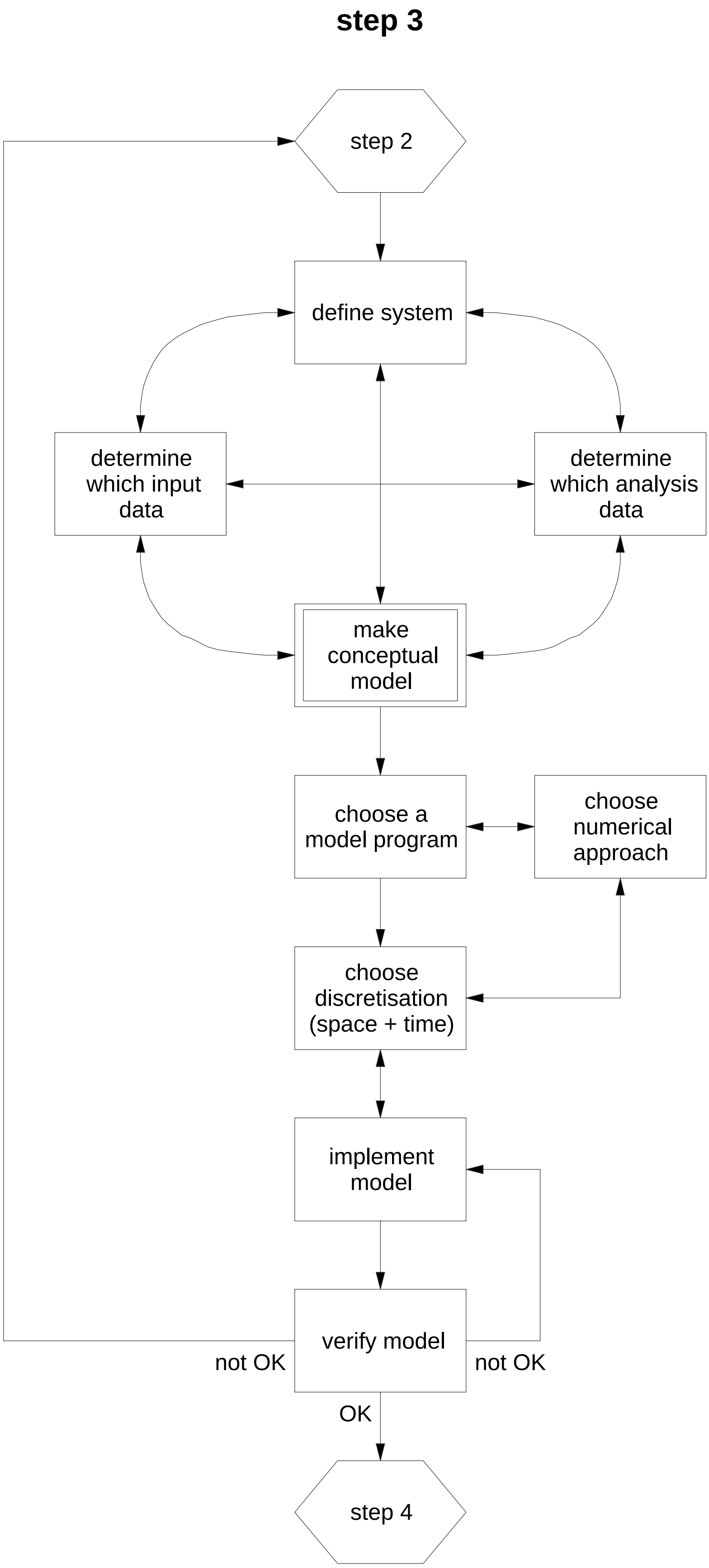
Step 3 Set up the model



3.1 Choose the beginning: data analysis, system definition or conceptual model

The design of a model begins with analysis of the available and necessary data, description of the system and the design of a conceptual model. The sequence taken for these 4 steps can vary depending on the case and the modeller, and is not really of any importance. It is often an iterative process. In this Handbook, analysis of the data is the first step taken but the choice could equally have fallen upon a system definition or establishment of the conceptual model to start off this step.

3.2 Analyse the data

3.2.1 Determine which data is needed to make and use the model

Lots of data is needed in order to make and use a model. It may concern:

· schematization data (physical area data, peripheral data);

· input data (initial values and input time series);

· (process) parameters;

· data for scenarios and decision support (combinations of the above).

At this stage, we need to know the exact nature of the data required in order to solve the problem. Of course, this step cannot always been seen separately from the (conceptual) model and the model program with which you want to work in the end, but in this stage it is important to think in terms of the physical processes such as those defined in the problem definition (step 2.1). They eventually form the basis for the choice of a model program. In an iterative process, you can come back to this step later, once the final choice has been made for a certain program.

3.2.2 Determine which data is needed to analyse the model

For analysis of a model (sensitivity analysis and calibration, for example), more data must be collected along with the input data. It concerns three aspects:

- measurements (system observations) for comparison of the model results (not necessary for sensitivity analysis);
- knowledge on the parameters: which are known and which are not precisely known;
- statistical distributions (often only a range) of all parameters which are not accurately known.

Not only must an inventory be made of this data (what is available and where is it) but it must also actually be collected (for later).

3.2.3 The availability of data and meta-information

At this stage of the project, it is actually enough to know the following about the data required:

- the data is available;
- where the data can be found;
- whether the data is available in digital form;
- what are the approximate values;
- how to deal with serious outliers;
- how to deal with missing values;
- the quality of the data;
- who is responsible for supply of the data.

This knowledge is therefore global knowledge and meta-knowledge (where is the data, measured how and by whom, which level of accuracy, etc.). In fact, it is often useful to actually start collecting the data at this stage of the project.

Finally, we recommend paying attention to the copyrights of the data and the legal aspects.

3.3 Make a system definition

If there is reasonable perception of the problem, the objective of the project and what data is available, a definition can be made between which matters can be modelled and which cannot. This is generally a physical part of reality.

The system definition can be made as follows:

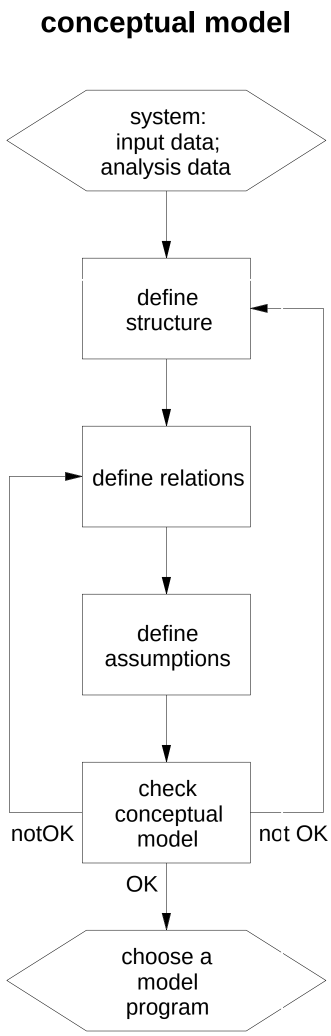
- sum up all relevant parts (components) of the system;
- describe the mutual relationships between the components (the processes);
- describe the relationships between the system components and the environment (= everything which is not part of the system).

The system boundary is the dividing line between the system and the environment. It may often suffice to clearly define the system boundary, preferably in such a manner that the dividing line between the system and the environment is characterised by a clear transition from processes inherent to the system to processes not inherent to the system.

3.4 Make a conceptual model

3.4.1 Working towards a conceptual model

The first real modelling step is the construction of a conceptual model (or model concept). This conceptual model describes the functional relationships between components with which the system (reality) will be simplified to a model, in text or in mathematical equations. This may possibly be supported by means of drawings, graphs and diagrams. The result is a model without everything being explicitly described in mathematical terms.



The importance of a conceptual model is particularly that the idea on which the model is based is described and can be provided as information to other people.

Definition of the boundaries of the model is an essential step in formation of the conceptual model: what is to be included and what not, how far beyond the target area (in space and time) is to be included, which processes occur at the periphery and how is the interaction with the environment translated (per section of the limit).

It is important to make a choice here in terms of the degree of detailing, particularly with regard to the question of which processes are to be included in the model. An initial choice must also be made with regard to time and space. This will be dealt with in more detail in step 3.6 and in appendix 1. The detailing in components and processes (aggregation level of the model) needs to be chosen at the time of construction of the conceptual model.

This first modelling step and the other steps within this chapter are also paid plenty of attention in Part II of this Handbook (Pitfalls and sensitivities) for all types of models. This includes an indication of the basis on which the choices described in this chapter can be made, in which situations certain choices are out of the question or actually preferable, and what consequences are attached to the choices made.

3.4.2 Describe the structure

The structure of the model must, in any case, be recorded in the conceptual model. In other words, the network of components from which the model is built must be described here, as well as the relationships between the components (usually ‘processes’). This concerns the following components:

- input variables (= interpolated input data);
- state variables;
- other variables.

3.4.3 Choose the type of model

In this step, the independent variables must first be chosen. In a dynamic model for example, these would be time and 1 or more spatial dimensions. After determining the independent variables, the type of model must be chosen. That is particularly dependent on the domain of application (chemical, physical, ecological, etc.) but also on time and space, among other things. If time is the only factor which plays a role, it is a dynamic model for a point in space (0D). If space and time are the independent variables, the model can be 1D, 2D or 3D.

In this step, we advise you to consult the manual of a specific model program in support of your choice.

3.4.4 Define the relationships between variables

The relationships show which variable affects one or more other variables. These may be state variables, input variables or other variables. Insofar as this has not taken place elsewhere or by others, a record must be made here of how the relationship is defined mathematically (or textually).

3.4.5 Establish the assumptions

Each model concept implicitly contains a (large) number of assumptions. Evaluation of the success or failure of a modelling project will not work without the opportunity to use the suppositions and hypotheses in the concept in order to interpret the results. A list of all assumptions must therefore be made, with a note of why this assumption was made or why it is justified. Do not forget to explicitly state how definition of the model came about. Reference to another model study (with the same assumptions) is sometimes also justifiable.

3.4.6 Verify the conceptual model

If there is a conceptual model, we now need to consider whether this concept is the best one, given the problem, the objective of the model and the available data and techniques. This can be determined in a variety of manners, none of which are particularly formal. The best method is to compare a number of concepts with one another in an experimental manner (i.e. make and analyse the model in accordance with the various concepts and then compare the results). A less time consuming method is to submit the conceptual model to experts (meeting, workshop, client, supervisory committee or such).

If inconsistencies (matters which are in conflict) are found in the conceptual model, or if there are other reasons to find the conceptual model unacceptable, you need to move back to earlier steps.

3.5 Choose from existing model programs

In the previous steps the criteria to be met by a model are defined as clearly as possible. These criteria can now be used to look for suitable model programs (i.e.: a mathematical model in the form of a computer program, intended for the construction of models by means of data input). Alternatively, new software could be developed, though this is generally not advisable, unless you have sufficient know-how and experience or there really is no other option.

The choices to be made here are partly determined by the choice of the type of model, depending on the dimensions in space and time. The series of available model programs from which to choose will differ for a 0D model or a 3D model, for example.

The choice may be further determined by project based matters and the computer. Examples include:

- the available hardware platform;
- the available operating system;
- the available expertise;
- the available time;
- the modeller's personal preferences with regard to interfaces;
- the client's wishes or requirements;
- what is available in the organisation.

Finally, an important practical criterion is whether there is an accessible manual for the model program and a help desk for any future problems. In the future, such matters will probably be arranged via the STOWA hallmark for model programs. By then, a simple recommendation to choose programs with a STOWA hallmark will suffice.

3.6 Choose a discretization for the model in space and time

A 0D, a 1D, a 2D or a 3D approach has been chosen, depending on the objective of the model and the available data. This leaves the actual schematization (the spatial structure of the model) to be selected. The rest of the discretization (choices of spatial and temporal resolution) must now also be chosen.

Of course, the objective and the available data are once again of importance, but attention also needs to be paid to the available time and manpower (= money). Very often, the actual discretization is also related to the choice of the model program.

The final choices with regard to the discretization are made after selecting the numerical approach (step 3.7).

3.7 Choose a numerical approach

In certain model programmes, a choice can be made between various methods of solving the (differential) equations numerically (or analytically). Analytical methods are generally much quicker but by no means always available. Numerical methods are therefore often applied.

The various methods can be distinguished in terms of discretization (finite differential method, finite elements method or analytical elements method). A choice can sometimes also be made from a variety of numerical integration algorithms in order to solve the differential equations over time.

Both choices are closely related to the stability of the solution, the discontinuities (possible rigidity of the system), the desired accuracy and efficiency. These are matters covered by numerical mathematics which fall largely outside of the scope of this Handbook. Part of this problem is also related to the final discretization (step 3.6) and to the opportunities offered by the software.

3.8 Implement the model

In this step, the model is 'put into' the computer by means of the chosen model program. This is actually a straightforward step but it may entail a great deal of work (depending on the model program). This step must certainly take place with great care, as errors made here can be difficult to trace.

It is important to read the manual of the model program carefully before beginning, in order to be aware of the areas requiring attention during implementation. Only those people with great expertise in the use of the model program in question will manage to arrive at a good product (= model) without needing to use such a working aid.

3.9 Verify the model

3.9.1 Verification versus validation

Verification is the step in which you check whether the mathematical model (and therefore also the conceptual model) has been effectively converted into a computer program. An interpretation check as it were. ***Validation***, on the other hand, is used to check the suitability of the model to simulate an independent data set (i.e. not yet used in calibration). See step 4.5. This also determines the suitability of the model in relation to the objective (can it answer the questions which may be put to the model; step 2.2).

A simple ***verification*** process may comprise the following components:

- a check of the prescriptions of the model program used (step 3.9.2);
- dimension/unit analysis (only for programming modellers; step 3.9.3);
- run a sample model (with schematization/discretization) which is supplied along with the model program (step 3.9.4);
- check the spatial schematization (step 3.9.5).

Verification will never give certainty with regard to correct implementation. It can, at most, increase confidence in the implementation process.

3.9.2 Check the implementation instructions of the model program used

Once the model has been implemented, it is sensible to check that no errors have occurred during that implementation process. Any problems can generally be solved with assistance from the producer of the model program or a more experienced user.

3.9.3 Dimension analysis (only for programming modellers)

A second step in the verification of a model can be a dimension analysis. It is not only the dimensions which are verified, but also whether the correct units have been applied. This step will therefore not only detect incorrect dimensions/units (W versus J, for example) but also errors in units and conversion factors (kg m^2 s^{-1} en kg m^2 h^{-1}).

3.9.4 Run a simple, familiar sample

Some model programs include a simple model for testing purposes, i.e. a simple schematization, input, etc. of which the output is already known. If the program does not include such a sample model, the modeller can define his own simple case, of course, the required results of which are already known to him or her. In the run with standard input, the idea is that the model should not crash, that the results are comprehensible and also that they are in keeping with expectations.

3.9.5 Check the spatial schematization

The spatial schematization must always be checked. Some model programs can make their own summaries of the schematization, such as total values of the surfaces and the volumes. Making a picture is often also very useful for purposes of insight.

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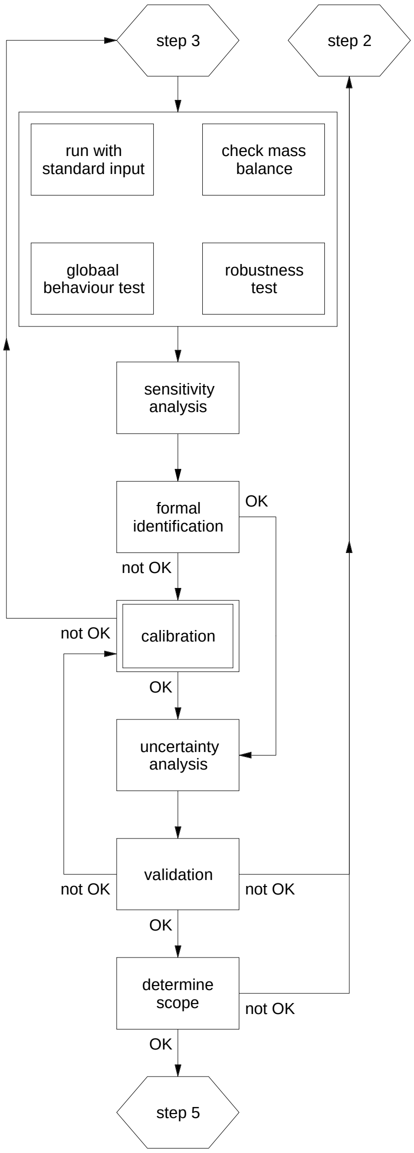
Step 4 Analyse the model

4.1 Make a planned approach for the analysis activities

step 4



Once a model has been developed (step 3) in which there is reasonable confidence, it can then be studied in more detail. The first step is to set up a plan in which a summary is given of the analyses to which the model is to be subjected. There must also be a note of the qualitative requirements to be checked in each analysis.

Analysis of the model can vary in nature, from very simple to very comprehensive and complex. Depending on the options and requirements, the following tests can/must be carried out:

- global analyses (step 4.2);
- run with standard input (step 4.2.1);
- global behaviour test (step 4.2.2);
- verification of mass balances (step 4.2.3);
- robustness test (4.2.4);
- sensitivity analysis (step 4.3);
- (formal) identification (scarcely applicable to most models, step 4.4);
- calibration (step 4.5);
- uncertainty analysis (step 4.6);
- validation (step 4.7).

Once the above activities have been completed, the scope of the model can be determined (step 4.8) followed by a final check whether the objective has actually been achieved.

This plan must not only determine which analysis techniques are to be used but also how much time is to be spent on the analysis and the quality of the results. It is important to keep a record, per step, of what has exactly taken place, by whom, when, using what input data, etc.

4.2 Make a general analysis of the model

As described in the previous paragraph, there are four, mainly simple tests used to gain a general impression of whether the model works correctly. These tests are:

- a run with standard input (step 4.2.1);
- global behaviour test (step 4.2.2);
- verification of mass balances (step 4.2.3);
- robustness test (step 4.2.4).

The various tests will be described below.

4.2.1 Carry out a run with standard input

The most common test is to carry out a single run using so-called ‘standard input’ material. This is generally a simple case of which the modeller knows the exact results in advance. Obviously, this need not be done if it has already taken place in step 3.9. A standard run must be well documented: what model version was used (program with supplementary data as input in the previous step), what is the input for the test calculation and what are the results?

4.2.2 Carry out the global behaviour test

The global operation of each model needs to be checked. This means that the model must translate any changes in the input or in the operating variables into an altered output, which describes the behaviour of the system in an expected manner.

4.2.3 Check the mass balances

Most model programs have provisions to reach and maintain the mass balance (or energy balance). However, this must be checked in order to be certain. If there are no such provisions, the modeller must carry out the test himself.

4.2.4 Carry out a robustness test

In a robustness test, the model is fed with extreme values in order to find out which conditions cause it to crash (or show other undesirable behaviour). Most of the work involves the choice of a limited number of interesting input sets. This exercise is not really necessary in commonly used models, because the scope of the model is then known precisely, i.e. there is knowledge of the conditions under which the model may be used (step 4.8). The model program manual can also (partially) provide directional instructions for this process.

4.3 Carry out a sensitivity analysis

The next step is the systematic testing of the model behaviour in reaction to changes in the input, the initial conditions and parameters. This can be done manually or using programs written specially for this purpose (see 4.5). The model behaviour must be studied on the basis of changes in the output variables. The results of this step give information with regard to the accuracy required for input, initial conditions and parameters. On the other hand, it indicates which parameters benefit from parameter estimation.

When changes in input, initial conditions and parameters lead to either no change or extreme changes in model behaviour, the model structure may require reconsideration. However, the results only apply to the range covered by the test.

The changes implemented in input, initial conditions and parameters must be realistic, of course. A fixed percentage of a nominal value is often used, or a percentage of the standard deviation. Testing of minimum and maximum deviations is sensible in non-linear models. Changes can be studied one by one or in combination with other changes. Finally, a choice needs to be made on the assessment of the model behaviour. Besides the choice of (the weights attached to various) variables, the choice of period is equally important; an average, a set moment or the largest deviation? Initial conditions, for example, will play a less important role as the period lengthens or the reference point lies further away.

Numerous studies have been carried out into the what, why and how of sensitivity analyses. Generally speaking, there are various options:

- ***an analytical sensitivity analysis***: if the model equations can be analytically solved, the effect of changing factors (parameters, for example) on the model results can be directly calculated and graphically represented;

- ***individual variation of a number of assumedly independent factors***: in this approach, the factors are changed one by one. The main disadvantage of this method is that no attention is paid to the effects of interactions between the factors;

- ***classic sensitivity analysis***: the model is linearised around the nominal values of the factors, so that the derivative to a factor can be traced in one single run at any time and for any state variable, in order that the sensitivity of the model can be simply determined. This method is only applicable if the factors may only deviate very slightly from the nominal value and the result will depend strongly on the chosen nominal value. Another disadvantage is that interactions between factors are hardly taken into account;

- ***'Response Surface' Method***: a meta-model is made of the model, which is linear in the coefficients and often comprises a first or second order of Taylor series approach. Interactions between the factors are not accounted for in the former case, but are accounted for in the latter. However, the meta-model must still be validated, through cross validation, for example.

- ***'Monte Carlo' analysis***: all factors to be varied are varied simultaneously sampled from their statistical distribution), therefore not systematically. A relatively large number of runs are required and linear regression is subsequently applied to determine the relationship between the model results and the factors. Unlike the classic sensitivity analysis, no assumptions need be made beforehand with regard to linearity.

- 'Regionalized Sensitivity Analysis': by running the model a number of times (Monte Carlo) and segmenting the runs into acceptable and unacceptable, two empirical distributions are found, after which the distributions can be used further in order to estimate a value for the sensitivity.

All these options cannot be described in full here, but a number of references have been included in the literature list (Beck, 1987, Janssen, 1990a, 1990b, Kleijnen & Groenendaal, 1988).

An analytical approach is seldom possible, but is certainly very preferable to any other method when it is possible. Independent variation of factors is simple to carry out but ignores the interaction between factors (co-variance).

Whatever the method applied, the results of the sensitivity analysis must be translated into a sensitivity measure . The following are options (depending on the method): partial derivatives, regression coefficients and degree of discrepancy. Once again, a full description cannot be given of all these options, references have therefore been included in the literature list.

4.4 Carry out (formal) identification (if possible)

Ideally, a model should be 'constructed' on the basis of the knowledge available on the system (= the field situation). Slightly less extreme: the parameter values of a model must be able to be determined with great accuracy if sufficient measurements/observations have been made in the field. In practice, this is hardly possible. There are usually too few field observations, the time series are too short or the number of parameters to be identified too large. In that case, calibration offers a solution (step 4.5).

4.5 Calibrate the model

4.5.1 Introduction

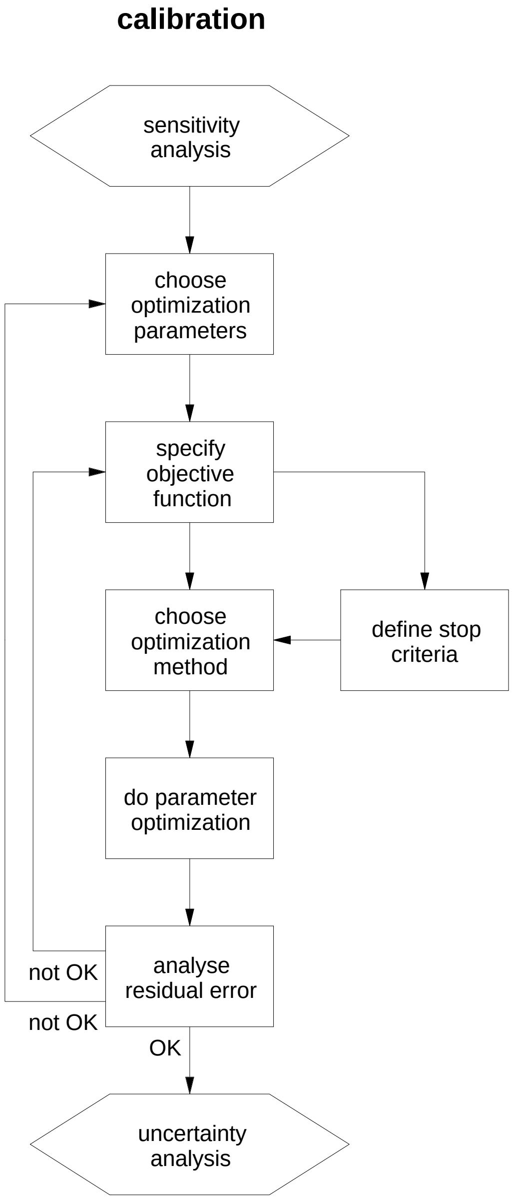
If a model cannot be fully identified (step 4.4), calibration becomes essential. There will then at least always be a certain degree of fit between model results and measurements in the field. Criteria must be defined beforehand (step 2.4.1) in order to be able to carry out an uncertainty analysis (step 4.6) to check whether the model offers sufficient certainty for the problem to be studied, following calibration. This paragraph gives a global description of the principle of calibration. However, good and efficient calibration is also a question of experience.

Section 2 of this Handbook (Pitfalls and sensitivities) includes an extensive summary of experiences of modellers with all types of models in water management.

There is extensive literature on the calibration of models, varying from very advanced mathematical processes to an application described for a specific discipline. Hemker provides a very readable introduction (1997).

Calibration focuses on the comparison between model results and field observations. An important principle is: the smaller the deviation between the calculated model results and the field observations, the better the model. This is indeed the case to a certain extent, as the deviations in a perfect model are only due to measurement errors. In practice, however, a good fit is by no means a guarantee of a good model.

The deviations between the model results and the field observations are determined by a large number of factors. These factors can be divided into groups (possible software errors are not taken into account here).



Conceptual errors. These are inaccuracies in the model definition, such as the (conscious) simplification of complex structures, neglecting of certain (sub-)processes, errors in the mathematical description or in the numerical method applied.

Parameter values. Many models entail a large number of parameters whose value is not exactly known.

Errors in the driving forces. This is expressed, for instance, in errors in the boundary conditions of the model.

Measuring errors in the field observations.

In modelling practice, the above sources of errors are by no means always explicitly quantified. Data Assimilation is an approach in which all sources of errors can be integrally included. A disadvantage of many Data Assimilation techniques, however, is that they are often complex and are not always described in literature which is easily accessible to modellers. In the text box in this paragraph and in appendix 2, the concept of Data Assimilation is explained in more detail. Te Stroet (1995) gives a good summary of Data Assimilation options in calibration. In general terms, the calibration process can be split into three parts, whereby the cycle is generally repeated a number of times, using different choices for the parameters to be optimised.

- choice of the parameters to be optimised;
- calculation of the optimal values;
- analysis of the results of the optimisation.

4.5.2 Choose the parameters to be optimised

Many models have large numbers of parameters which may or may not be spatially distributed and/or correlated. In virtually all cases, the amount of field data does not permit all parameter values to be optimised, however. Consequently, the number of parameters to be optimised must be reduced in one way or another, by choosing which parameters (or combination thereof) are to be optimised. This can be done in many ways, by including the ‘well known’ parameter values as known constants, by making groups of parameters values equal to one another (zoning) or by assuming a (geostatistic) relationship between parameters.

The choice of parameters to be optimised can be based on the results of the sensitivity analysis. The modeller also often has the expertise required to choose the right parameters for calibration purposes. On the one hand, they must have considerable influence on the final model results and, on the other hand, they must be visible throughout the measurements.

Data Assimilation

An important characteristic of Data Assimilation is that it tries to make optimum use of both the process definition and the measuring information. The quantification (in terms of probability distributions) of all sources of uncertainty is an essential precondition. Data Assimilation can be used both in the calibration and estimation of the model results in the use phase (state estimate). The advantages of Data Assimilation are that:

- process definition and measuring information (statistic) are optimally combined both for the calibration and the state estimate;
- the uncertainties in the calibration and state estimate are explicitly quantified.

The influence of field observations (both in time and space) on the calibration and the state estimate are explicitly included and quantified. This may be used for measuring network design and measuring network evaluation.

4.5.3 Calculate the optimal values

Establishing the objective function

During calibration, a description will be made, in some manner, of the differences between the field observations and the model results, in the form of an objective function (penalty function). The objective function can be mathematically formulated in many ways, depending on which factors are explicitly included. All deviations between the model and field observations will be processed, at all times and in all spatial positions (where applicable) for one or more (state) variables. Simple, commonly used forms for the objective function in the univariate case (one unknown variable/parameter with supplementary field data) are:

- the relative error;
- the average value of the residual error;
- the maximum residual error;
- the quadrates of the residual errors (sum of least squares).

Each of these has advantages and disadvantages, but these will not be discussed in this Handbook. In the multivariate version too (number of unknown parameters/variables with field data), the objective function can be expressed in a single figure (value). This can be done by taking the maximum or the average of all values determined per variable, for instance. If necessary, the objective functions can be expanded by weighting the various terms in order to emphasise certain aspects to a greater or lesser extent, and by adding additional conditions (constraints). In practice, the choice of the objective function is often determined by the model program used.

Choose a method for optimisation

The essence of the objective function is that its value decreases along with the decreasing deviations between the field observations and model results. Minimisation of the objective function is therefore the target during calibration. While this is reasonably simple in the univariate case, it soon becomes impossible to keep track of the situation when a number of parameters needs to be optimised.

Many methods have been developed to find the minimum of the objective function. A distinction can be made between ***manual optimisation*** and ***automatic optimisation.*** These two techniques can also be combined, of course.

Manual optimisation attempts to find the minimum through trial and error, hoping for the best. The results of earlier runs are used to gain insight into the influence of the various parameters on the value of the objective function. The parameter values are constantly adjusted until the objective function falls within acceptable limits. The advantage of manual optimisation is that the modeller gains great feeling with the characteristics of the model (see also the sensitivity analysis). However, although an experienced modeller can achieve good results for problems which are not too complex, this approach is not particularly reproducible. Moreover, it will seldom result in the true optimum of the objective function.

An alternative for manual optimisation is automatic optimisation, whereby the minimum of the objective function is sought systematically in an iterative process. The modeller therefore no longer needs to adjust the parameter values during the process.

This actually makes the optimisation process a parameter estimation process, a search in the parameter space (searching in an ***n*** dimensional space, whereby ***n*** is the number of parameters to be estimated). Working from a certain state of affairs (a certain fit between the model and field situation, or from a certain value of the objective function at that point in time), the modeller can determine whether the situation can be improved. Often a certain mathematical technique is applied to determine the direction in which the parameter values must be adjusted, and how great that adjustment must be. Calculation of the model continues using the new parameter values, the objective value is re-assessed. The modeller checks whether the value of the objective function meets the pre-set criteria (i.e. is it small enough). If this is indeed the case, the process can be halted, if not, then one or more new vectors will be chosen again. Etc.

A main advantage of automatic optimisation is that many methods also generate information on the reliability (uncertainty) of the model. This information can be used in the uncertainty analysis.

Although there are great variations in the methods nowadays, all derived from the world of '(global) optimisation', only a limited number of these are used in the world of water management. A full list cannot possibly be given here, and a limited number of possibilities will therefore be discussed.

The methods can be divided into two groups: ***stochastic*** and ***deterministic***. The stochastic ones are usually simple to implement, require no particular mathematical structure (no partial derivatives of the parameters in order to determine the direction of adjustment), but there is also no guarantee that the (best, global optimum) solution sought will be found in a finite period of time. Deterministic methods are much more difficult to implement. They are most simple when incorporated in the model program used, but there are also programs on the market (PEST, 1994 for example) which can be coupled to model programs.

A number of ***stochastic methods*** will be briefly described here. PRS (Pure Random Search) is a method whereby the parameter vectors are drawn randomly from the probability distributions of the individual parameters. The model is then run using a new parameter vector, and the fit is determined. This continues until optimisation is complete. This is also exactly what happens in a Monte Carlo approach. Variants are the CRS (Controlled Random Search) which differs from PRS in the way in which a new parameter vector is chosen. CRS therefore converges more quickly, though the properties of the posterior parameter vectors are somewhat less attractive. The Genetic Algorithms (GA) method resembles this; it has less useful methods for drawing new parameters, but more provisions for controlling the optimisation process. Unified Covering by Probabilistic Rejection (UCPR), a recently developed method, converges reasonably quickly and, in the end, has a set of parameter vectors with attractive properties (being uniformly distributed).

Deterministic methods use the mathematical structures in one way or another. Partial derivatives (to the parameters) can thus be determined and used. Relevant methods for the type of problems handled in this Handbook will be summed up below. Many of the methods make use of the Jacobian. These include the Gauss-Newton method and the related Levenberg-Marquardt method (which can also deal with singular matrices). These methods use the ‘sum of least squares’. More simple in use are the direct search methods, such as Nelder-Mead or Powell’s method, but these often result in local optima. There are also those methods which are in-between the direct search methods and those methods based on the Jacobian, such as the method referred to as DUD (Doesn’t Use Derivatives) which was developed by Ralston and Jenrich. They estimate the Jacobian instead of calculating it. Finally, there is the commonly used ‘adjoint method’ developed by Carrera-Neuman.

In practice, the modeller will often be limited to the built-in calibration options and will choose one of those. When more than one method has been included, it may be worth while to compare the methods.

Define criteria to stop optimisation

The best way of determining when optimisation can be stopped is to use a pre-determined criterion for the objective function. This is the case when a parameter vector is found with which the model deviates less from the field data than the criterion. Or (in another method), when all parameter vectors give results which meet the criterion. The process of automatic optimisation is often stopped once the successive iterations do not change any more than a pre-determined criterion. It is then assumed that the objective function is close enough to the minimum. However, don’t forget that the minimum found applies to the chosen set of parameters. It is quite possible that a different choice of parameters to be optimised will give a smaller value than the objective function. The results of the optimisation must therefore always be analysed.

Optimisation does not necessarily result in a satisfying set of parameters. In this sense, there is a differences between manual and automatic optimisation. An automatic procedure cannot converge to the correct minimum if, for instance, the objective function is relatively insensitive to the parameters to be optimised, or if the number of parameters to be optimised is too large. In manual optimisation, the modeller runs the risk that errors resulting from too many parameters to be optimised are not detected, so that the model appears to be effective but in fact is not.

In practice, there are various other criteria used for stopping. For example, a pre-set number of iterations or a pre-set number of man days to be spent on calibration. This can lead to very undesirable results and is therefore strongly advised against.

4.5.4 Analyse the results of the optimisation

Two requirements must have been met once optimisation has been completed:

- the stop criterion must have been met (see step 4.5.3);

- the residual errors must be small and may not be systematic (i.e. the residual errors must actually be 'random'; see Hemker, 1997).

For example: a hydrodynamic model may seem excellent because all the calculated model values are smaller than a certain criterion, for example deviating x centimetres from the measured values. If, however, all the calculated points are consistently x centimetres too high, then we refer to this as a systematic error.

If the model concept is good and the right choice has been made for the parameters to be optimised, the residual errors will be acceptable. If the residual errors are unacceptable, there are various options available to progress further. These are:

other calibration factors (parameters) without a new sensitivity analysis (return to step 4.5.2);

other calibration factors (parameters) based on a new sensitivity analysis (return to step 4.3);

- going back and changing 'the model', for example the:
- discretization (return to step 3.6);
- numerical approach (return to step 3.7);
- conceptual model (return to step 3.4.1);
- quality requirements (the criteria) (return to step 2.4.1);
- collection of more or other field data (return to step 3.2.2).

When a model cannot be calibrated acceptably, the imperfect or unsatisfactory calibration results may well still be used in certain cases. It is then ultimately important that the remaining uncertainty be estimated as realistically as possible, in order to avoid the model being afforded too much confidence.

4.6 Carry out an uncertainty analysis

In this step of the simulation and modelling process, the remaining uncertainties must be estimated. This step resembles the sensitivity analysis, except that the attention has now shifted to the total effect of uncertain factors on the model results, rather than the (relative) sensitivity of factors. In brief, this means that the uncertainty in the calibrated parameters (and other sources of uncertainty which have been explicitly included: the uncertainty in conceptual errors and errors in driving forces) are translated into the uncertainty in the model results. Some calibration methods support this step (Price's CRS, for instance). Results of a calibrated model may actually only be presented with inclusion of the reliability of the model results.

The method used for analysis depends strongly on the calibration method chosen or applied. In a straightforward approach to the uncertainty analysis, the uncertainty in the calibrated parameter vector (and other sources of uncertainty) can be characterised by a variance-covariance matrix. This can then be translated with the model to give an uncertainty interval (confidence interval) in the model results. This approach is often not too simple in practice, however. An alternative choice is the min-max approach (which closely resembles a sensitivity analysis) or an uncertainty interval constructed using a Monte Carlo Simulation.

Uncertainty intervals are actually not conclusive, however, as an interval is created following a number of choices. It will often only reflect the uncertainty as a result of parameter ranges, for example. These may become insignificant in relation to uncertainty in future input. The uncertainty interval also depends on a number of assumptions regarding the statistical distribution of the calibrated parameter. A common assumption is that the error in the parameter value has a (log) normal distribution.

4.7 Validate the model

In order to determine whether or not a manually calibrated model is ‘good’, it must be validated (see also 3.9.1). The calibrated model must be able to reproduce field observations from an independent data set (i.e. a data set not used in calibration) with a certain pre-set degree of fit (with or without uncertainty in the model and field observations). Validation can also be carried out for automatically calibrated models, as long as an independent data set has been kept aside for this purpose. However, all available data is often used in the automatic calibration process itself in order to arrive at the best possible results. The decision to leave out validation is then a conscious and justifiable one.

The ‘independent data set’ is often a measuring series from the same system as the series used for calibration, but then for a different year. It is even better if the model can simulate field observations of another highly similar system. Of course, the model may not be recalibrated.

An important note to be made here concerns the impossibility of proving that the model is ‘correct’in a philosohical sense. There is no means of proof. Confidence in the model can only be increased by experimenting with that model, i.e. by carrying out all kinds of validation tests. This is generally referred to as corroboration. After a sufficient number of successful tests, the model is not ‘valid’ or ‘good’ but rather ‘good enough’, whereby the ‘enough’ factor is determined by the requirements made beforehand (step 2.4.1). The model can then be regarded as having been validated (to a greater or lesser degree).

The impossibility of proving the correctness of a model must not be unattached from an important consequence: models (whether or not validated) may not actually be used to form extrapolations, neither in space, nor in time. This makes the use of models a tricky business (at least in theory). If validation has taken place, particularly for situations which closely resemble the situation on which the model is to make predictions, there may be some confidence that the prediction will be reasonably reliable, but this is by no means certain.

4.8 Determine the scope of the model

The final step in the analysis process is to determine under which circumstances the model may be used and particularly whether this can solve the problem for which the model was designed. This must also be clearly described. The scope is inextricably bound up with the model which has been developed and analysed.

A model may actually not be used for extrapolations as commonly applied in predictions and in scenario analyses, but that is often exactly the reason for development of the model. The model will be used after all in such cases, but a presentation of the results must pay extensive attention to the uncertainties attached to the use of the model for this application. Beck summarised the problem effectively in the following statement: ‘using scientifically based models, you will often predict an incorrect future with great accuracy, and when using complex, non-identifiable models, you may be capable of predicting the correct future with great uncertainty’.

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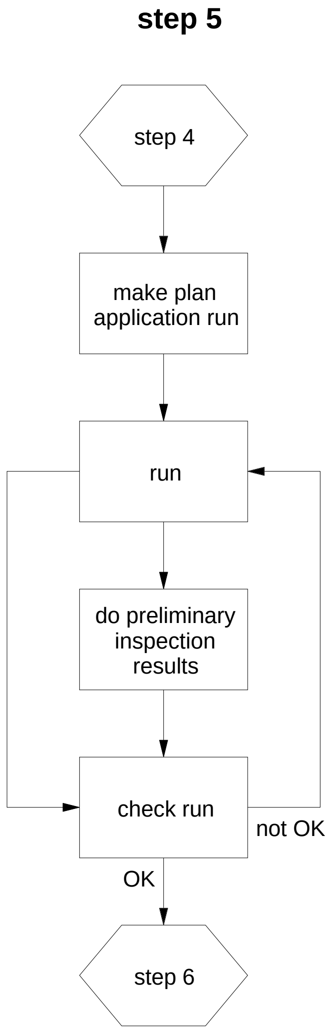
Step 5 Using the model



5.1 Make a planned approach for the simulation runs

Once the model has been thoroughly tested and the modeller is sufficiently confident of its operation, the model may be used for all kinds of applications. In this phase, it is sensible to design a planned approach, describing the exact implementation of the model. The plan defines:

- the input to be used;
- the (calibrated) version of the model to be used;
- the period to be simulated;
- the deviations to the reference run (the run with standard input);
- the quality of the results to be expected.

Designing the calculations to be made requires close co-operation with the client. The calculations to be made have been roughly described earlier, in step 2, but now that the model is ready to be applied, the arrangements must be reconsidered and further detailed. It is important that distinction be made between the questions posed by the client and their translation into questions for the modeller and the model. There sometimes is a major difference between the client's policy scenarios (which often only allow for a minor deviation from the present policy) and the modeller's analysis scenarios (which explore the band width of the wildest solutions), for example. Close co-operation in the 'same language' is essential to prevent confusion. Therefore, you should come to agreement with the client about an unambiguous conceptual framework. Before entering into consultation with the client, it may be useful to make a series of initial calculations in advance. This will give both parties an idea of what they are talking about.

5.2 Perform the eventual simulation runs

This important activity (this is what it is all about) is the next logical step in the procedure. Make sure that the output (the results) is suitably stored to allow for future reference for other purposes and for use with other tools, for instance further processing for a presentation and statistical analyses. Generally, model programs have various integrated storage options.

5.3 Verify the results

Immediately following the actual use of the model, the results must be verified to expose any extreme or impossible outcomes. Items to be paid attention include:

- any extremes and outliers;
- ranges of model output;
- unexpected results;
- indications of numerical errors.

5.4 Is this all?

In this phase of the modelling project, it must be determined whether all the planned activities have been performed and whether they have been performed in a sound way. Did the modeller use the correct version of the model, with the correct input, with all other correct settings, is the solution stable, are the mass balances correct, etc.

Use the modelling project templates to verify all the individual steps:

- does the model fulfil its purpose?
- are the quality requirements met?
- is all necessary data correct and was it properly used?
- is the system definition correct?
- is the conceptual model correct?
- were all hypotheses made correctly and justifiably?
- was the discretization in space and time chosen well?
- was the choice of the model restrictions correct?
- with retrospect, was the correct model and/or model program chosen?
- was the numerical approach chosen in a responsible manner?
- was the implementation performed correctly?
- what was verified regarding the implementation?
- was the manual of the model program adhered to?
- are the dimensions and units correct?
- which analyses were performed?
- are the mass balances correct?
- what are the sensitive parameters (and other factors)?

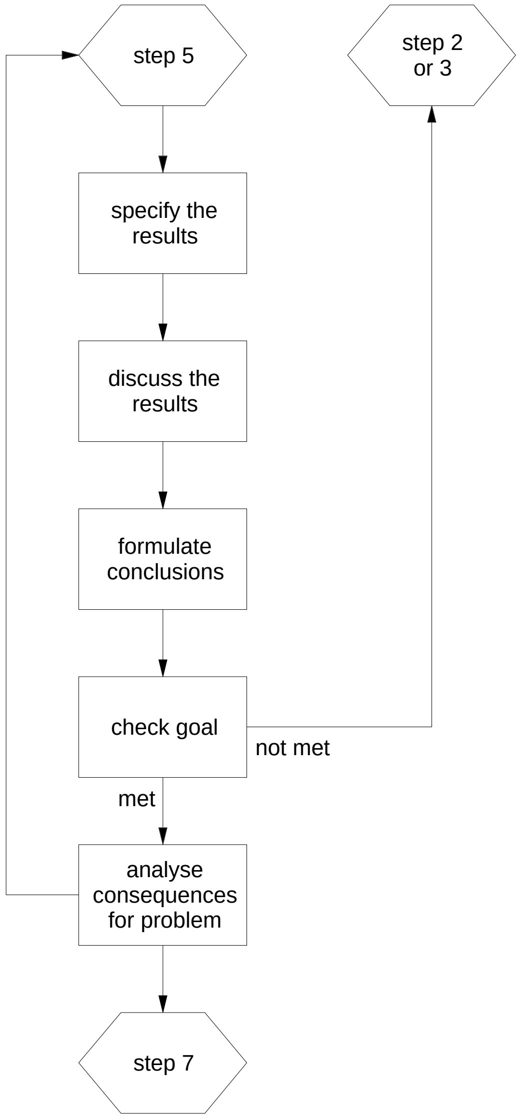
- how and with what result was the model calibrated?
- is this adequate given the pre-set (quality) requirements?
- was an uncertainty analysis performed?
- was the scope of the model defined accurately and in such a manner that the questions to be answered by the model may indeed be answered?
- did the execution of the runs, intended to find answers to the questions posed, take account of any uncertainties in the results?

Literature

none

Step 6 Interpret the results

step 6



6.1 Describe the results

Defining the exact interpretation of the results is crucial, in particular because some people will only (want to) look at the results, disregarding the way in which these were attained.

A prudent approach is to first describe the results without attaching any conclusions, consequences or statements to them. Use texts, figures and tables to give both a compact and a full description of the results (referring to appendices, annexes, other reports, databases, if possible). This description must be recorded in the modelling project templates, covering the entire modelling project. These template the basis for later reports and communications.

6.2 Discuss the results

In this step, the results are compared with those of other similar studies. Any unanticipated results must be discussed and supplemented with a (possible) explanation.

6.3 Describe the conclusions

The conclusions to be drawn from the results must be related to the objective of the model and the model calculations (step 2.2). In other words, there must be a direct link between the research question and the results.

6.4 Check whether the objective has been achieved

In this step (operational validation) the question must be answered, whether the procedure followed has resulted in a model with which it is possible to answer the questions posed in the objective. If this is not possible, then either the objective will have to be adjusted (no problem for the modeller, but often unacceptable to the client) or the model will have to be adjusted (which is likely to imply a load of work for the modeller and therefore extra costs for the client).

6.5 Summarise the results

People are often more willing to read information when it is presented in a concise form. Therefore, make a responsible (statistical) summary, explicitly indicating any restrictions of and uncertainties in the results. Compare the quality of the project results with common practices (of others) in the field of study.

6.6 Analyse the consequences for the research question

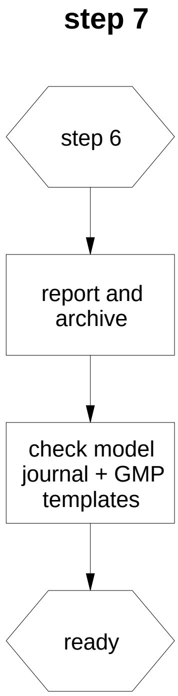
Unfortunately, the procedure followed will often produce an unsatisfactory solution, a compromise between feasibility and affordability. This may have various consequences:

- the response to the modelling project is negative (particularly if the modeller keeps too many options open);
- the modelling project exposes gaps in the domain knowledge, thus generating new research questions;
- the modelling project requires more field observations/measurements;
- a follow-up modelling project has to be initiated to thoroughly investigate all matters involved;
- the client is dissatisfied, or, quite the contrary, satisfied.

Literature

none

Step 7 Report and file



7.1 Report in the language of the target group

The road from science through the model to advice is veiled, and unambiguous road signs are lacking or illegible. To the client the origin, the status and the reliability of an advice are often absolutely inconceivable. Although the results of a model are very rarely used as the basis for policy, modellers have their own responsibility when it comes to translating the model results into policy supporting conclusions. Policymakers at management level, for instance, want clear answers to complex questions. Many of the scientifically justified marginal notes made when answering the question are not included in the executive summary which eventually forms the basis for decisions. Therefore, the translation of the model study conclusions must not only be scientifically justified, but also so crisply formulated (i.e. without jargon) that they are fully understood by the members of the target group (e.g. managers and policymakers), preventing them from having to convert the conclusions into a policy advice themselves.

Another aspect is the form in which the results are presented. If they are given as graphics, it is particularly important that the form be discussed in advance by modeller and client (step 2.3.2).

7.2 Make the model study reproducible

The report is based on the completed templates given elsewhere in this Handbook. They cover the entire modelling process, from problem definition to policy advice. Logically, a practical and preferably uniform structure and layout of the report will enhance the quality of the entire modelling project. All topics discussed in this general section of the Handbook must also be discussed in the report, even if - for good reasons - they were not executed.

The quality of this report should allow third parties to reproduce the model study (including its results) and/or proceed from the point where this study left off. The latter consideration therefore requires a clear indication of, for instance, the validity, usability and any restrictions of the model results.

The model study must not only be reported - as described above - but also be filed (on paper and electronically) in order that model studies from the past may be re-initiated or serve as a reference.

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Good Modelling Practice Handbook

Checklist

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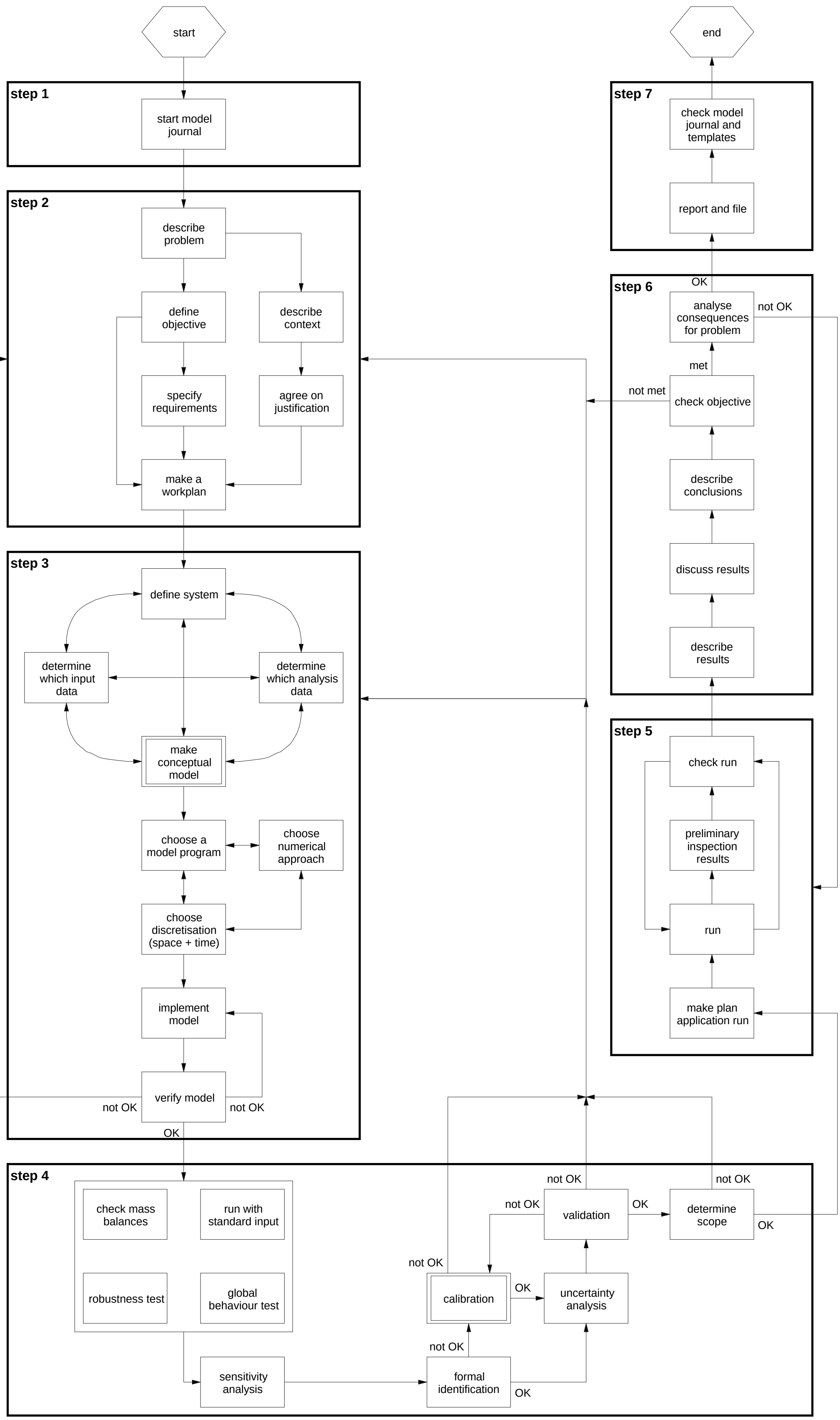
Good Modelling Practice - Checklist

Activity / Step	Performed?		
	Yes	No	n.a.
Step 1: Start a logbook (and continue using it)			
Step 2: Set up the modelling project:			
2.1 Describe the problem			
2.2 Define the objective			
2.3 Analyse the context and reach agreements on the justification:			
2.3.1 Context			
2.3.2 Justification / responsibilities			
2.4 Specify the requirements:			
2.4.1 Quality requirements			
2.4.2 Expertise requirements			
2.4.3 Estimated capacity/manpower requirement			
2.4.4 Communication and reporting			
2.4.5 Other requirements			
2.5 Draw up a working plan and a budget			
Step 3: Set up the model:			
3.1 Choose the beginning: data analysis, system definition or conceptual model			
3.2 Analyse the data			
3.2.1 Determine which data is needed to make and use the model			
3.2.2 Determine which data is needed to analyse the model			
3.2.3 The availability of data and meta-information			
3.3 Make a system definition			
3.4 Make a conceptual model (in words):			
3.4.1 Working towards a conceptual model			
3.4.2 Describe the structure			
3.4.3 Choose the type of model			
3.4.4 Define the relationships between variables			
3.4.5 Establish the assumptions			
3.4.6 Verify the conceptual model			
3.5 Choose from existing model programs			
3.6 Choose a discretization model in space and time			
3.7 Choose a numerical approach			
3.8 Implement the model			

3.9 Verify the model			
Step 4: Analyse the model:			
4.1 Make a planned approach for the analysis activities			
4.2 Make a general analysis of the model			
4.2.1 Carry out a run with standard input			
4.2.2 Carry out the global behaviour test			
4.2.3 Check the mass balances			
4.2.4 Carry out a robustness test			
4.3 Carry out a sensitivity analysis			
4.4 Carry out (formal) identification (if possible)			
4.5 Calibrate the model:			
4.5.1 Introduction			
4.5.2 Choose the parameters to be optimised			
4.5.3 Calculate the optimal values			
4.5.4 Analyse the results of the optimisation			
4.6 Carry out an uncertainty analysis			
4.7 Validate the model			
4.8 Determine the scope of the model			
Step 5: Use the model:			
5.1 Make a planned approach for the simulation runs			
5.2 Perform the eventual simulation runs			
5.3 Verify the results			
5.4 Is this all?			
Step 6: Interpret the results:			
6.1 Describe the results			
6.2 Discuss the results			
6.3 Describe the conclusions			
6.4 Check whether the objective has been achieved			
6.5 Summarise the results			
6.6 Analyse the consequences for the research question			
Step 7: Report and file:			
7.1 Report in the language of the target group			
7.2 Make the model study reproducible (file)			


start
end
step 1
start model journal
step 2
describe problem
define objective
describe context
specify requirements
agree on justification
make a workplan
step 3
define system
determine which input data
determine which analysis data
make conceptual model
choose a model program
choose numerical approach
choose discretisation (space + time)
implement model
verify model
not OK
not OK
OK
step 4
check mass balances
run with standard input
robustness test
global behaviour test
sensitivity analysis
formal identification
not OK
OK
calibration
OK
not OK
uncertainty analysis
validation
not OK
not OK
OK
determine scope
not OK
OK
step 5
check run
preliminary inspection results
run
make plan application run
step 6
describe results
discuss results
describe conclusions
check objective
not met
met
analyse consequences for problem
OK
not OK
step 7
report and file
check model journal and templates

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Good Modelling Practice Handbook

FORMS

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Step 1: Start a model journal

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- The following procedure(s) is (are) used in order to record all steps of the modelling project:

the templates of this Handbook	
your own model journal based on this Handbook	
your own model journal of your own design	
any other procedure (which one?)	
a quality system (which one?)	

Step 2: Set up the modelling project

This template has been filled in by	

2.1 Describe the problem

- Give a brief description, in words, of the problem (no details):

- Encircle the problem domain(s): (groundwater quantity models, groundwater quality models, precipitation runoff models, water distribution models, hydrodynamic models, high water forecasting models, morphological models, surface water quality models, emission models, ecological models, economic models, other models)?
- Fill in the following for the (physical) processes in this modelling project:

relevant processes?	characteristic time scale?	spatial scale?

- Is a model the only correct tool for solution of the problem?

- If not, what are the alternatives for a model based approach?

- What is the reason for application of the model (policy analytical, scientific, operational, calamities management)?

2.2 Define the objective

- What is the domain and the problem area?

- What is the objective of a model in this project?

- Which questions need to be answered using the model?

- Give an indication of the scenarios which need to be calculated using the model.

2.3 Analyse the context and reach agreements on the justification

2.3.1 Context

- The larger context (project, study, routine activities, research programmes, etc.) of the modelling project is:

- This modelling project must be carried out in combination with the following models (in a chain):

model	location

2.3.2 Justification

It has been agreed with the client to assess the following modelling project steps at the following decision moments:

decision moments	modelling project step

The following agreements have been made with the client on reporting and completion.

2.4 Specify the requirements

2.4.1 Quality requirements

- The analysed (calibrated) model must describe a specific data set with a specific accuracy: yes/no.
- If yes:

which data set: …….

with what accuracy: …….

2.4.2 Expertise requirements

- The following persons and their expertise will be deployed in the modelling project.

name of person	expertise

2.4.3 Estimated manpower capacity

- The following manpower is required for the modelling project:

discipline	time (days)	to be spent on step

2.4.4 Communication and reporting

- The following meetings, workshops etc. have been planned within the scope of the modelling project:

activity	when?	persons involved	subject

- Which reports must be made for the modelling project?

type of report (progress, interim report, final report)	when?	intended for whom?

2.4.5 Other requirements made of the modelling project

- From which other models does this modelling project use the results?

- What requirements are made of the results of other models (format, proper balance, calibration, discretization, meta-information, ...)?

- Who will supply the results of those other models, and when?

- Who will verify the results of those other models?

- Who will approve the results of those other models?

- How can the quality of the (field) data best be described?

  very incomplete/reasonably complete/complete

  poorly documented/reasonably well documented/well documented

- What else can be said about the quality of this data?

- Must alternative models or other methods (discretization, integration algorithms) be used in this modelling project in order to create a framework for comparison?

- If the results are to be processed in a policy advice, who is to do so?

2.5 Draw up a working plan and a budget

- Make a working plan of the modelling project on the basis of the above, and a planning schedule for the steps yet to be carried out. Add a budget.

Step 3: Set up the model

This template has been filled in by	

3.1 Choose the beginning

- The development of a model is an iterative process, whereby the following steps may be carried out one or more times.

3.2 Analyse the data

3.2.1 Basic data required for a run

spatial data	
time series	
begin values	
boundary conditions	
parameters	
scenario data	
other data	

3.2.2 Data required for analysis

observations of the system (field measurements)	
statistic distributions or ranges of non constant parameters	

3.2.3 Availability of data

is data available?	
where is the data?	
is the data available in a digital version?	
briefly describe the values of the data	
how to deal with outliers?	
how to deal with missing values?	
describe the quality of the data	
who is responsible for supply of the data?	

3.3 System definition

- The system is that part of reality simulated in the model (see Part I).

components of which the system is comprised	
the relations between the components	
the relations between the components and the environment (outside the system)	

3.4 Conceptual model

3.4.1 In words

- Describe the general conceptual model in words.

3.4.2 Structure

- If the structure of the model is not completely defined by the choice of model, describe this structure using words or diagrams.

3.4.3 Type of model

domain of application	
dynamic/stationary	
number of spatial dimensions	

Relationships3.4.4 entirely defined by the choice of model, describe them below.

3.4.5 Assumptions

- If implicit or explicit assumptions have been made (other than those in the model program in question and described in the Handbook), describe them below.

3.4.6 Verification of the conceptual model

- What action has been taken to determine that the conceptual model is consistent (no contrary issues) and in keeping with the solution to the problem?

3.5 Which existing model program or model?

which existing model program or model has been chosen?	
why was that model program or model chosen?	
is there any better option on the basis of content, and what would that option be?	
why has that better option not been chosen?	

3.6 Discretization in space and time

describe the spatial schematization	
where has this been recorded (in detail)?	
what choices have been made regarding the discretization in the time (related to numerical approach)	

3.7 Further numerical approach

which solution method (algorithm) has been chosen for the spatial integration step?	
is there any choice and is the choice made the best one in terms of content?	
if the choice is not the best one, why was it made?	
which solution method has been chosen for the integration in time?	
is there any choice and is the choice made the best one in terms of content?	

if the choice is not the best one, why was it made?	

3.8 Implementation of the model

how is the model implemented?	
on which points does it deviate from the manual of the chosen model program?	

3.9 Verification of the model

- Verification was carried out by:

internal check (included in the functionality of the model)	
manual check of I/O, other parts of the implementation	
manual or automatic check of dimension and units	
was a test run carried out using the sample supplied with the model program (or similar)?	
was the spatial schematization checked?	

Step 4: Analyse the model

This template has been filled in by	

4.1 Which analysis activities?

- Indicate which analysis activities were planned or why they were not carried out:

which	yes/no	comments
standard run		
global behaviour test		
mass balance check		
robustness test		
sensitivity analysis		
(formal) identification		
calibration		
uncertainty analysis		
validation		
determination of scope		

4.2 Make a general analysis of the model

4.2.1 Run with standard input

describe the input	
how did the run progress?	
are the results comprehensible?	
are the results in keeping with the expectations?	

4.2.2 Global behaviour test

- Which characteristic changes have been tested in order to check the model behaviour (effect of more load, more precipitation, more nutrients, no load, etc.):

- Carry out these runs and describe the result of these tests.

4.2.3 Mass balances

- How were the mass balances checked?

how?	yes/no	result
by the model		
manually		

4.2.4 Robustness test

was a robustness test carried out?	
which extreme values of parameters and other input were used?	
what were the results of this test?	

4.3 Sensitivity analysis

was a sensitivity analysis carried out, and if so, how?	
did this analysis pay attention to interactions between all uncertain factors or not?	
what measure was used for the sensitivity?	
sensitive factors (including parameters) are	
insensitive factors are	

4.4 Formal identification

is there enough data (observations and measurements) for identification?	
was the identification successful?	

4.5 Calibration

did calibration take place?	
how was the choice of factors to be calibrated made?	
which measure was used to determine the progress and the result of the calibration (objective function)?	
which method and/or package was used	

for calibration purposes?	
which criterion was used to stop calibration?	
describe the result of the calibration	
did it meet the criterion set beforehand?	
did residual error analysis take place?	
are the residual errors systematic?	
if calibration was not successful, to which previous step did the process return?	
how much time (in man days) was spent on calibration?	

4.6 Uncertainty analysis

was an estimate made of the uncertainty in the model results?	
the uncertainty analysis was carried out on the basis of a covariance analysis	
the uncertainty analysis was carried out differently, namely	

4.7 Validation of the model

are the results of the calibrated model compared with field measurementsother than the data used for calibration purposes?	
what were the results?	

4.8 Scope of the model

has the scope of the model been determined?	
how was the scope determined?	
what do you think to be the scope of the model?	

Step 5: Use the model

This template has been filled in by	

5.1 Describe the eventual simulation runs in terms of:

the input used	
the (calibrated) version of the model	
the simulation period	
the deviations from the standard run	
the expectations regarding the results	

5.2 Perform the eventual simulation runs

date	
person	
computer	
department	
institute	
where are the results stored?	

5.3 Verify the results

which extremes and outliers were found in the model output?	
did the model output ranges meet the expectations?	
which unexpected results were found in the results?	
are there indications of numerical errors (discretization in space and time) and if so, what are they?	

5.4 Is this all?

are there points on which the model does not meet the objective?	
what quality requirements are not met?	
which of the necessary data is incorrect and was used wrongly?	
in what sense is the system definition incorrect?	
in what sense is the conceptual model incorrect?	
which assumptions were made incorrectly or unjustly?	
was the discretization in space and time chosen well?	
with retrospect, was the correct model or model program chosen?	
is there a better model program or model?	
why was the better alternative not chosen?	
was the choice of numerical approach a sound one?	
can the implementation of the model be improved? if so, how?	
what was verified regarding the implementation?	
on which points does it deviate from the manual of the model program?	
was dimension and unit analysis carried out?	
which model analyses were performed?	
are the mass balances correct?	
what are the sensitive parameters (and other factors)?	
how and with what result was the model	

calibrated?	
is this adequate given the pre-set (quality) requirements?	
was an uncertainty analysis carried out and with what result?	
does the model cover the scope required by the problem?	
did the runs, intended to find answers to the questions posed, take account of any uncertainties in the results?	
what else can be noted about the modelling project?	

Step 6: Interpret the results

This template has been filled in by	

6.1 Describe the results

where can a description of the results be found?	
where are the simulation results stored and in what form?	

6.2 Discuss the results

in comparison with other studies	
unexpected results are	
can the unexpected results be explained?	
the model project is incomplete in the following points	
other points of criticism with regard to the modelling project	

6.3 Describe the conclusions

summarised, the conclusions are as follows	

6.4 Has the objective been met?

which points of the objective have been met?	
which points of the objective have not been met?	

6.5 Summarise the results

the *executive summary* of the modelling project is as follows	

6.6 Analyse the consequences for the research question

who has reacted to the modelling project and how (positive, cautious, negative)?	
what were the most important reactions?	
which gaps in the domain knowledge are detected by the modelling project and which new research questions are generated?	
was the number of observations and measurements sufficient for the modelling project?	
in a subsequent modelling project, the following issues would have to be paid further attention:	
what suggestions can you give for subsequent studies or other (similar) modelling projects?	
to what extent is the client satisfied?	

Step 7: Report and File the modelling project

This template has been filled in by	

7.1 Reporting

the report makes use of the templates of this Handbook	fully/partly/not at all
a report on the modelling project can be found	
will there be any further scientific reporting on the modelling project? if so, in which journal?	

7.2 Other documentation

a full description of the model used can be found	
which other internal memos (etc.) are there?	
where are the modelling project records stored?	

Good Modelling Practice Handbook

Part II

pitfalls and sensitivities

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Contents:

I Introduction

Part I of this Good Modelling Practice Handbook gives a step-by-step plan which a modeller can use in his work. This stepped plan mainly concerns the process to be applied in modelling work, more than the actual contents. This part, on the other hand, discusses the contents, by means of a description of pitfalls and sensitivities which the modeller may meet. This description of pitfalls and sensitivities does not in any way claim to be comprehensive. After all, pitfalls and sensitivities are often specific to a model. However, an attempt has been made to sum up frequently occurring problems.

Matters important to all models are discussed in chapter 2, with sub-division into the same steps defined in part I of this Handbook. Chapter 3 then describes the pitfalls and sensitivities for a total of thirteen different and specific domains of application, varying from groundwater models to ecological models and from water quality models to economic models.

Where possible, relevant literature references have been included for readers looking for specific details on a subject. This part can be regularly updated on the basis of experiences of modellers.

2 General pitfalls and sensitivities

This chapter gives a number of general pitfalls and sensitivities. It follows the steps of the modelling process as described in part 1.

Step 1: Start a model journal

The model journal has no direct influence on the modelling process. However, when passing on modelling tasks and when re-using the model and data files (after some time), the lack of full information can lead to incorrect interpretation. For example, because it is no longer simple to deduce which output is related to which input. The completion of a good model journal is a rarity. Two common pitfalls are:

- the model journal is incomplete,
- the model journal is incomprehensible, not only for third parties but often also for the author himself.

Both pitfalls have a lot to do with time and motivation. Little can be done about the latter, keeping a model journal is simply no fun. However, the time factor can be influenced, by planning sufficient time for this aspect beforehand, for example. It is also a question of investment. For the short term, keeping a model journal costs time, but this time will be earned back amply in the longer term, when looking to determine exactly what work has already been carried out.

Step 2: Set up the modelling project

The objective of the modelling process and the requirements which the modelling must meet cannot be recorded clearly enough. A pitfall when setting up the modelling project is that the method of recording the results is not determined until later on in the modelling project. When a model is part of a chain, it is particularly important that all relevant requirements are specified beforehand (including the resolution, boundary conditions, uncertainty and scale). The scope chosen must be large enough to allow the boundary conditions to be independent of what takes place in the field of study.

If the temporal and spatial scales of the problem have not be defined clearly enough, this will have consequences in the later phases of the modelling process. Consequently, the model scales may not be correspondent to the required answer. If the model scale chosen is too large, this will be translated in too general a schematization, so that relevant details can no longer be derived from the results. The problem could be schematized away, for example. If the chosen model scale is too small, irrelevant small-scale variations will be disproportionately weighted, which can lead to non-optimal calibration for the large-scale variations.

The user must be aware of the possibilities offered by the model. It occasionally occurs that a model is required to have more functionality than is possible (insufficient support in know-how, data, theory, etc.). In practice, the target of a modelling process is often also formulated at a ‘management’ level. This sometimes leads to communication problems in the translation to the ‘technical’ model level. Consequently, the modelling does not provide the answer required by the client in the end.

Step 3: Set up the model

A sensitive point in this step is the construction of a good model concept. A wrong choice of processes and the comparisons which describe the process, can lead to errors in the model which cannot be traced at a later date. This can occur, for example, if essential processes (chemical, for example) or driving forces (discharges, for example) are ignored. As the modelling progresses, there is a risk that wrong choices in the model concept may become ‘concealed’ by the method of calibration.

Another sensitive point is the construction of a very detailed model, while there is insufficient or no data available. In large , spatially organised models in particular, it is vital that the scale and the number of independent parameters (degrees of freedom) are chosen in accordance with the available data. If too many parameters are applied to a model, there is a risk of it appearing to work well (it follows the historical measurements) but that it is hardly or not at all suitable for interpolation or prediction. This can actually only be determined if adequate measuring data is available, i.e. with the right frequency in relation to the chosen time step. Measuring data is often interpolated in order to meet the temporal step of the model. The method of interpolation in particular can have major consequences. This must be taken into account upon construction of the model, as there is otherwise the risk that a model is constructed which cannot be calibrated. In a number of cases, incorrect estimation of a starting state (for example, the amount of pollution present), can lead to wrong conclusions.

Finally, knowledge of the various model programs available is also of great importance. Only too often however, the choice of model program is made because the modeller is familiar with that program. This does not necessarily mean that this is the most suitable program, of course.

Step 4: Analyse the model

The main pitfall in this step is that insufficient time is taken, despite the fact that virtually everyone agrees that this may well be the most important step in the modelling process. Practice wins over theory apparently, so that this step is pressurised by the fact that a final product must be delivered on time.

Assessment of whether a model is ‘good’ often does not take place objectively, on the basis of pre-set criteria. In many cases, this assessment depends on the expertise of the modeller. In complicated cases in particular, this expertise is therefore a sensitive factor.

In choosing the parameters to be calibrated (see the previous two steps), the number and the spatial distribution of the degrees of freedom (the model controls) must be geared to the amount of information available for calibration. Calibration of a model with too many degrees of freedom often results in a distorted picture of the truth. Errors in the model concept can be ‘calibrated away’ in this manner. In the previous point, there is the paradox that a model seems to fit better when there is less measuring data. In practice however, there is often a tendency to increase the number of parameters to be calibrated, in order to reduce the deviations between the measured and calculated values. There are theoretical concepts (‘observability’) to determine whether too many degrees of freedom have been defined, but these are not generally used in practice.

In a number of cases, estimates are calculated for the reliability of the calibrated parameter values. This is certainly recommendable. For that matter, unknown parameters can also be estimated by means of expert judgement. Default values are usually not adequate, because they apply to a (too) general or a single system.

Parameters may not be sensitive to the available observations (not at the locations or times at which there are observations). As a result, the sensitive parameters cannot be adequately calibrated.

Comparison of the model results and observations does not always take account of the differences in scale (see also appendix 1). A point observation is often directly compared with a model value which is representative of a certain volume or a certain time period. Calibration generally does not cover all the sources of uncertainty. Consequently, measuring errors may have a strong effect on a parameter value in small data sets.

Finally: a perfect ‘history match’ is, in itself, no guarantee of a good definition of the system.

Step 5: Use the model

Before starting the real calculations, there must first be certainty that the model is afforded sufficient run-in time. This may sometimes even be longer than the simulated period. We recommend that the run-in time be estimated on the based of residence time and processing speed, beforehand.

The main pitfall in modelling is that the model is used outside of the scope. This occurs, for example, when the model construction and analyses have taken place using data gained from another water management regime.

This usually occurs if the model is used for scenarios which represent the situation of measures yet to be carried out. This pitfall can be due to two things: either the model analysis (the previous step) was not carried out properly, or the results from the previous step have not bee applied effectively.

Step 6: Interpret the results

Take account of the uncertainty bandwidth when interpreting the results. Check, for example, whether a distinction can still be made between the results of various scenarios. When presentation packages are used, units or flow directions have been known to become switched. The absolute values may well be correct, but in the wrong direction.

Step 7: Report

Reporting must take place in the ‘language’ of the client. It is important that a correct balance is found between the (technical) details and the degree of usability for the client. In practice, reports are often incomplete, so that the modelling process is not reproducible on the basis of the report.

An essential pitfall often encountered by both the client and the modeller is that the transfer of knowledge often does not exceed beyond the completion of the report. Consequently, the information provided by the modeller may be incorrectly applied. While this, in theory, is prevented when a report is good, in practice it becomes apparent that a written report alone is hardly ever sufficient to provide a client with exactly the information required. Personal contact between the modeller and client is essential. It is the responsibility of the modeller to monitor whether the information provided by him has been used in the correct manner, insofar as he has any influence in this matter.

3 Pitfalls and sensitivities per domain

This chapter describes a number of common pitfalls and sensitivities per domain. One domain will be described per paragraph. The following domains will be covered:

- groundwater models for the saturated zone (quantity and quality);
- groundwater models for the unsaturated zone (quantity and quality);
- precipitation run-off models;
- water distribution models;
- hydrodynamic models;
- high water forecasting models and operational models;
- calamity models;
- morphological models;
- surface water quality models;
- waste water purification models;
- ecological models;
- economic models and use functions;
- emission models.

Each paragraph comprises two sections. The first section begins with a brief introduction to a number of relevant characteristics of the models. Examples are also given of model programs currently applied in the Netherlands. The second section gives the pitfalls and sensitivities per modelling step. This only concerns those modelling steps in which pitfalls and sensitivities actually occur.

3.1 Groundwater models for the saturated zone (quantity and quality)

3.1.1 General

There are many model programs available for a numerical approach to the *groundwater flow*. Without attempting to be comprehensive, the model programs used most frequently in the Netherlands are: MODFLOW, TRIWACO, MicroFEM, MLAEM and SIMGRO. Without exception, these programs are based on the elementary conservation of equations (Darcy's law and the continuity equation). The differences are mainly found in the method of discretization (finite differentiations, finite elements and analytical elements) and the way in which the user can define the boundary conditions.

Two classes of model programs can be distinguished in the *groundwater quality* models. The first class comprises the 'lumped' model programs in which chemical aspects are defined by strongly simplified parameters (dispersion, sorption, retardation). Well-known model programs in this class are: MT3D, HST3D, RT3D, MODWALK. Just like the groundwater flow models, the differences between the various programs lie mainly in the method of discretization and the way in which the user can define the boundary conditions. This mainly concerns the top system (the bed section with saturated groundwater flow above the first aquifer).

The second class of model programs explicitly describes the chemical reactions. Representatives of this class are FREEQM and CHARON. This type of model program cannot be used without considerable chemical expertise.

3.1.2 Pitfalls and sensitivities

Step 3: Set up the model

<u>Conceptual model</u>

A conceptual model is constructed prior to numerical modelling. This conceptual model defines, among other things, the global structures of the subsoil and the substances found in it.

The hydraulic properties play a particularly important role for the groundwater flow. The choices made in the conceptual model with regard to the limits of the model field, both horizontally and vertically, are generally not changed in the further course of the modelling process. The choice of the location and type of the boundary can greatly influence the model results and therefore requires effective underpinning.

The layers are often classified into aquifers and separating layers. The method of binding of these layers greatly influences the simulated flow field, and thereby the model results.

Another important aspect is the existence of hydraulic short circuits or blockages. These phenomena occur in separating layers, fracture systems (open or closed), sand and gravel banks and dams. Information on these phenomena is often not explicitly included or is insufficiently known. Non-recognition of these structures can lead to incorrect interpretation of the results during the further course of the modelling process. Moreover, the negligence of density variation can lead to completely incorrect flow directions and calibrated constants. In the coastal areas of the Netherlands in particular, the effects of density variation due to deviations in the salt content will have to be taken into account. This also applies at waste dump sites and other locations with strongly polluted groundwater.

For the total sediment discharge, it is particularly the estimation of local heterogeneity which is important. These help to determine the travelling times and breakthrough curves. Also vital is a good hypothesis of the geo-hydrochemical processes. Examples of important aspects are the sorption processes (balance or imbalance, linear or non-linear), the presence of decomposition, the geochemical conditions (for example rich or poor in oxygen), the presence of organic matter in the sediment, etc. The limited observation material is often not adequate to be able to distinguish between various processes in the calibration phase, so that the modelling is strongly dependent on the expertise in the conceptual phase.

Choice of the model program

The choice of model program is not particularly critical for the final results of a model for groundwater flow, at least not in the models generally used in the Netherlands. However, the modeller must be aware of the underlying assumptions and the usage limitations of the various model programs. The top system (small surface waters, drainage and unsaturated zone) may be defined in more detail in one model than in another, for example. The approach to modelling in MLAEM varies quite strongly from that in the other modelling programs (there are no element grids, for example, and a choice must be made from various types of analytical elements).

In the modelling of total sediment discharge, the differences between the various model programs may be very relevant, however. There is numerical dispersion in most of the model programs based on finite elements and finite differentials. The mass balance is often not guaranteed in model programs based on the finite elements approach. This may result in major errors, particularly when there are strong gradients in the concentration, due to the model incorrectly distributing the flux and the concentration over a large surface area.

Besides physical and chemical considerations, practical considerations also play a role in the choice of model program. The more organised the input of parameters and options, the less the chance of practical usage errors. Moreover, the calculating time and the memory required may also play a role in the more complex (unsteady) problems.

Step 4: Analyse the model

Sensitive parameters

In groundwater flow models, the sensitive factors often depend on the objective of the model. For many models, the degrees of resistance of separating layers are sensitive parameters as they are more difficult to estimate (variation of 10 or 100) than, for example, the permeability of aquifers (variation of 2). Local holes in separating layers have much larger regional effects than local areas with high permeability. Conversely, areas with a much higher local resistance in the separating layer, hardly have any influence at all, while local areas with high resistance in aquifers are generally relevant.

The lack of flow over a separating layer means that the value of the resistance is not important, but does make it almost impossible to determine the resistance. Once flow has been applied over this layer in a scenario (through extraction, for example), the resistance may well be a dominating factor (if it is relatively great, for instance).

The most sensitive parameters for total sediment discharge models depends on the type of substance being described and on the local situation. For those substances which adsorb to organic matter, the retardation factor and the organic matter content can often be noted as being sensitive parameters (NOBIS, 1995).

Discretization

The spatial and temporal discretization must be small enough to minimise numerical errors. Generally speaking, this means that smaller steps must be taken when the gradients become steeper. The steepness of the gradients is partly determined by the hydraulic properties of the system and can often be characterised by the composite leakage factor (see Maass, 1996). Elements must generally be smaller than this leakage factor. This therefore also applies to surface waters where there are hardly any resistance layers at all. The errors made in such cases can lead to both incorrect flows in the model and to incorrect hydraulic parameters in the calibration.

Many total sediment transport models are very sensitive to the grid size in terms of the numerical dispersion. The discretization suitable for a flow model is not automatically also suitable for a total sediment discharge model based on the speed field of the flow model in question. The time step and grid distances can be chosen independently of one another. Some model programs automatically determine the (maximum) time step. If this is not the case, major numerical errors may occur.

Reduction of the grid distances and the time steps will not automatically produce better model results. A very fine grid may give the impression of a very detailed and therefore accurate model. Unless information is added on the right scale however, the only added value of a finer grid is its ability to prevent numerical errors. In combination with overly detailed parameterisation, a finer grid may even provide less information. Conversely, too coarse an elements network can lead to ‘stable’ calibration results, which are incorrect due to insufficient possibilities for simulation of variations in hydraulic head and flux.

One of the main pitfalls in the modelling of boundaries is the definition of a closed boundary or fixed hydraulic head at the location of a catchment boundary under an infiltration area. That boundary and therefore the flow and the hydraulic head change as the circumstances change. The same applies in modelling a freshwater-salt water boundary area, this cannot be seen as a closed boundary either if the circumstances in its vicinity change.

Special attention is required for the discretization in the vertical. A quasi 3D approach is an effective one for modelling for regional flow. Quasi 3D means that the vertical differences in the hydraulic head within an aquifer are neglected in the calculations. This does not mean that there can be no vertical flow component within the aquifer. In such cases, great care must be exercised with the schematization in aquifers and separating layers, as incorrect connections can lead to major errors in the model. Moreover, in local problems and in flows in heterogenic packages, this approach may lead to relevant errors, particularly in the calculated flow distribution and the total sediment discharge.

Parameterization

A numerical groundwater flow model or a groundwater transport model comprises many spatially distinguishable units (blocks, elements). In principle, each unit is attributed a value for the parameters (permeability, storage co-efficient, dispersion co-efficient, sorption, etc.) This results in many (often tens of thousands of) degrees of freedom. Given the limited availability of information, both in terms of the geological definition as the observations of the dynamics (hydraulic head and concentration measurements), it is essential that the number of degrees of freedom be reduced. This takes place through a certain form of processing of the parameter values. Common methods include zoning, whereby a certain zone is attributed the same value and a geostatistic interpolation.

A pitfall of parametrization is that the structures which are modelled are too detailed and cannot be adjusted in the course of the modelling, due to a lack of field observations (see also calibration), so that they in fact begin to lead a life of their own. Another important point is that the scale on which information on the parameter values is available is not always in keeping with the model discretization. This applies to geological information from drilling, for example, and to geohydrological information from pumping tests (see also appendix 1). The parameters in the grid blocks must become ‘block effective’ values. The point observations therefore need to be scaled up. The method of scaling may be very sensitive, particularly when there is great heterogeneity. If a ‘simple’ mathematical average or a linear interpolation of the point values is used in such cases, major errors may be the result, particularly with regard to the breakthrough curves and residence times. It is difficult to determine beforehand which method should be used, but there must in any case be careful verification in relation to observations from the field.

Boundary conditions

An important component of the modelling process is formulation of the boundary conditions. These are not only the conditions concerning the physical external boundaries of the model but also the conditions concerning the so-called interior boundaries (extraction points, drains, etc.). It is essential to include as many observations of fluxes (discharges) alongside the potentials (measured or estimated hydraulic heads and groundwater levels). Hydraulic parameters in a model without given fluxes cannot, in principle, be defined, as they may otherwise be attributed any possible value (and therefore also useless ones) in a calibration procedure.

Calibration & Scaling up

Measurements with which a model is calibrated (hydraulic head, fluxes and concentrations) are often point observations in relation to the ‘block effective’ values which the model calculates. When there is great small-scale variability in particular, it is very questionable to what extent a calculated head or concentration in a grid block or element must meet the measured point value. The trend must generally be in keeping, though even this need not always be the case. Prior effective (geostatistic) analysis of the representativeness of the measuring points is therefore always recommendable.

Calibration & Minimization criteria

Calibration (both manually and using calibration programs) is carried out by changing parameter values in order to gear the model results to observations. A squares sum or a variance is often used as a measure for calibration. A large number of calibration procedures is based on unweighted criteria. In other words, all measurements are attributed equal importance. This can lead to imbalanced calibration, for example in areas where there are clusters of observations with a great deal of superfluous information. The cluster then weighs disproportionately heavy in relation to a single measuring point at a different location. If the scope of the variables’ values is very diverse (in concentration measurements, for example), there is a risk that a peak in the observations will be disproportionately weighted.

Calibration of steady models

Steady models are commonly used in the geohydrological practice. These models neglect the effect of storage and can only describe an ‘average’ flow, and are therefore usually only applied for modelling of the quantity. The principle behind steady models is that a balanced situation is described, i.e. a situation in which the effects of changes in time can be neglected with regard to the effects to be calculated. There are a number of pitfalls here, particularly for the description of the groundwater flow (flow direction and residence times). There is often less sensitivity for the effects in terms of groundwater levels or hydraulic head.

The observations used in the calibration come from a dynamic system. Observations from a so-called ‘average hydrological year’ are often applied, and this can lead to serious errors (also in terms of hydraulic head) in systems with a long-term ‘memory’ (great inertia). For calibration of the hydraulic parameters of the quantity, it is often more advisable to look for an almost steady state (i.e. a state in which the storage variation is negligible) such as that found at the end of the rainy season, and to take the average of this over a number of years.

In order to calibrate a steady model effectively (i.e. usable for calculation of an average flow situation), the steady values must be calculated for the observations from the dynamic system (hydraulic head, concentrations, precipitation, surface water levels, etc.). A rule of thumb in this is to take the average over approx. 4 times the correlation length (the period within which the variables to be modelled still show cohesion). Consequently in many situations in the low Netherlands, a 5 to 10 year period with representative head observations may well suffice. In the higher Netherlands, the period required is much longer (often > 40 years).

Calibration of unsteady models

If there is little dynamics in the calibration phase, it is difficult to determine the parameters which influence time-dependent behaviour (storage). If possible (in groundwater decontamination for example), great dynamic variation should be applied to the starting state, for the benefit of calibration of the model.

Step 5: Use the model

In the user phase (forecasting), the model results are often sensitive to different parameters when compared with the calibration phase (present state). A well-known example is that a model calibrated for an average state cannot effectively be applied to a dry or wet state. Another example is that the groundwater flow is often strongly dependent on the feed from the top system. Due to the complexity of the top system, many model studies invest a great deal of energy in its calibration. However, if the model is intended for analysis of the effects of a change in deep groundwater reclamation, the separating layers between the aquifers may be equally important.

One of the best-known pitfalls in separating layers is that the calibration phase is generally dominated by a small hydraulic gradient, to the extent that its resistance cannot be calibrated, while that resistance may be a deciding factor when reclamation is increased in the new situation. Measures in the top system often lead to a change in the representative resistance of that top system. It also occurs that a change in the flow (direction and volume) alters the hydraulic properties of layers. Examples include:

- a change in the entrance resistance under surface waters due to the turning of seepage into infiltration or to dredging work.
- strong increase in the resistance of a separating layer through an increased flow due to extraction.

The spread length changes in such cases, requiring verification that the element sizes are even smaller than this leakage factor.

For total sediment discharge models too, the conditions (in terms of flow and discharge) may be quite different in the user phase than in the calibration phase. Diffusion and decomposition may have an important effect on the total sediment discharge in the calibration phase for example, while convective transport is much more important in the user phase. What is needed in that case is modelling outside of the scope of the calibration.

Generally speaking, the dynamic variation is different and more limited in the starting state than in the user phase. A change in the direction of flow (horizontal and/or vertical) can have major consequences for the parameter values determined by the calibration (for example those for retardation and sorption).

3.1.3 References

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3.2 Groundwater models for the unsaturated zone (quantity and quality)

3.2.1 General

LEACHM, MUST, DEMGEN, MOZART, SWIF, WATBAL, SWACROP, SWAP, ANIMO and STONE are commonly used model programs for the calculation of water transport and sometimes also the total sediment discharge in the unsaturated zone of the bed. The model programs vary in the way in which the flow equations (Darcy equation combined with the continuity equation to the Richards equation) are solved. Generally speaking, this can be done via the following methods:

- Balance approach (tipping bucket) of which WATBAL is an example. This is in fact the most simple version. Often, only 1 or 2 soil compartments are used (above and underground). The result is that there is a relatively limited need for data, but also that the results gained have relatively little detail. This type of model program is often used on larger scales in order to gain a general impression of water transport. Sediment transport is not included.

- Pseudo steady approach, combination of balance and dynamic model program. MUST is an example of this type. A distinction can be made in terms of various soil compartments. This type of model program is somewhere between the balance approach and the dynamic model programs. Sediment transport is not generally included.

- Dynamic model programs in which the Richards equation is solved. SWAP is an example of this type. The programs use soil compartments of variable thickness, 1 cm close to ground level, and 25 cm deeper in the profile for example. The result is that there is a relatively large need for data, and that the results gained have relatively great detail. This type of model program is often used on smaller scales (field scale) in order to gain a detailed impression of water transport. Sediment transport is included in a general manner.

3.2.2 Pitfalls and sensitivities

Step 3: Set up the model

Virtually all of these types of models are sensitive to schematization and boundary conditions. Splitting of the vertical soil compartment generally takes place in 1 cm layers over the first 15 cm below ground level, via 5 cm layers to 25 cm layers on the lower side of the unsaturated system. In the horizontal sense, the combination of soil maps and files on measured physical characteristics of the soil tend to be the practical begin of schematization of physical soil properties in the unsaturated zone, and consequently form the input for calculations. The models are nearly all based on the assumption that the unsaturated zone is a homogenous, anisotropic medium. In practice however, matters such as hysterisis in the water retentivity curve, preferred flow and swelling and shrinkage phenomena are the rule rather than the exception.

In the detailed dynamic models, these processes are often included as separate modules in the model, but this then leads to the problem of how to generate input data for these modules. One could say that the 'model crisis' is sometimes replaced by the 'data crisis' and that the problem is therefore not really solved.

Blooper: "We've introduced the ditch factor in the calibration".

"In calibration of our nutrients drainage and leaching model, the prediction was not at all in keeping with the measurements. There was a factor 2 difference each time. Upon further analysis, it became apparent that processes take place at the transition from unsaturated groundwater to surface water in particular, i.e. in the ditches and canals, which result in enormous retention. Those processes were not included in our model. We were in a hurry and therefore could not adapt the model. We introduced a 'ditch factor' of 0.5. The model then made perfect sense!"

Step 4: Analyse the model

Physical soil properties (water retention and saturated and unsaturated permeability) are always sensitive parameters.

This type of model almost always defines water and/or mass balances. These balances must be correct. Any balancing errors caused by computer inaccuracies should preferably be found in the results.

Just like in the saturated zone, total sediment discharge models for the unsaturated zone are sensitive to the initial values, to sorption processes (balance or imbalance, linear or not linear), the presence of decomposition, aeration state and the presence of organic matter. Independent measuring values are often indispensable. However, the measurements are often not representative. Spatial and temporal scales play a particularly important role here, because the top system is often quick to react (the top system is that part of the soil with saturated groundwater flow above the first aquifer). If the initial values are not known or poorly known, an adjustment calculation time of a number of weeks is recommendable.

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3.3 Precipitation/run-off models

3.3.1 General

Common model programs in the Netherlands are SOBEK-RR, RAM, AQUARIUS, SIMGRO, MIKE-SHE, MODFLOW, J-model. Precipitation run-off models simulate regional groundwater flow and water levels in the surface water. They often take account of aspects such as water retention in the unsaturated zone, sprinkling irrigation, underground irrigation and condensation reduction.

The models distinguish between hardened and non-hardened sites. They also account for the type and capacity of drains and the processing capacity of water purification plants. In greenhouse horticultural areas, they must take account of basin management.

The flow in the surface water can be calculated in a number of different manners. The most common are: steady, pseudo steady, unsteady or by means of catchment characteristics. The models are often part of a larger model train, centred around a theme such as dehydration.

3.3.2 Pitfalls and sensitivities

Step 3: Set up the model

The main pitfalls and sensitivities are described in the sections on surface water models and models for the unsaturated zone. However, a number of additional points can be mentioned. There must be certainty beforehand that this type of model is suitable, for example. This is not the case in areas where there is significant surface run-off. The slope and micro-relief are important influencing factors.

The effect of the fluctuation of the lower boundary condition (regional influence) for the modelling of the unsaturated zone is often also underestimated. The regional groundwater system must be included in some cases, both saturated and unsaturated. This type of model is often applied for extreme conditions. However, estimation of the initial conditions of the unsaturated zone in particular is as difficult as it is important. In that case, the water content measured or knowledge of the progress of pressure heads in relation to depth are very valuable indeed. Also important is good estimation of drainage resistance as a function of the groundwater level.

Blooper: “A ‘safe’ design, but unnecessarily expensive”.

“After construction of a large retention basin, it proved to never fill more than halfway, even following extremely heavy rainfall. Upon checking the design calculations, it became apparent that the assumption was made that all precipitation would run off quickly. Precipitation losses were not taken into account and neither was a tardy run-off component via the groundwater. The result was a somewhat oversized basin. “They developed a ‘safe’ design, but it was unnecessarily expensive!”

Step 4: Analyse the model

Specific calibration parameters

(See also surface water models and models for the unsaturated zone). The most important calibration parameter is the percentage of open water. The size and the moment of run-off peaks are often used for calibration purposes. The storage co-efficient in the unsaturated zone is usually poorly known and is therefore often calibrated. The drainage resistance is also often hard to measure autonomously and is therefore often obtained via calibration of groundwater levels. A common pitfall for this type of model is that modellers often attempt to compensate errors in the modelling of the unsaturated zone by altering other parameters (such as the drainage resistance). Finally, the last pitfall is that the models require a sufficiently long adjustment period (a number of weeks) in order to arrive at reliable calculation results if the initial conditions are uncertain.

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3.4 Water distribution models

3.4.1 General

Commonly used models are DM, DIWA, HYDRA, TAUWSIM, RIBASIM, AAD (ARIADNE), CONVER. Water distribution models are often used for planning in the field of water demand situations, while hydrodynamic models are mainly used for water surplus (flood) situations. Water distribution models mainly use steady calculations, while dynamic calculations are preferably carried out using a hydrodynamic model.

3.4.2 Pitfalls and sensitivities

Step 3: Set up the model

The interpretation of input data requires expertise from the model user. The ‘bookkeeping’ approach in this type of models often deviates somewhat from the practical situation and requires careful reshaping of practical data into input quantities for the model (from infrastructure to model schematization, from management measure to model calculation, etc.). Coupling with districts (district models) is often essential.

Water distribution models make calculations using steady situations. The time steps chosen must therefore not be too short. In a water distribution model without volumes (some water distribution models have volumes in reservoirs), the water has no ‘run time’, the water comes directly from its source at the mouth of the river. This implies that water distribution models can/may only be applied for planning projects, and therefore not for ‘real-time’ studies. Inaccuracies in water distribution models are often linked to exceeding of the maximum applicable time step.

Blooper: “The error in the measurement was sevenfold”.

“We were assigned to analyse a water movement model in which Chloride was also modelled, to determine how a certain salt discharge could be compensated. The salt discharge gave around 1% increased concentration, which needed to be cancelled out using water management measures. However, the measuring error for the salt concentration was 7% in itself, while the model also had an uncertainty margin of more than 10%. Our model was therefore totally unsuitable for such issues. Our client was adamant, however. He wanted the calculations and that was that. We did it in the end, but can it have helped him much?”

Step 4: Analyse the model

Input errors are simple to find by defining balances (great advantage of water distribution models versus hydrodynamic models).

Calibration parameters

The main calibration parameters in this type of model are:

- measured discharges (and/or water levels) in rivers and channels;
- long-term balances, check these against characteristic parameters such as the annual average discharge and such;
- water level management and management rules for water distribution;
- unknown balance items can often be adequately estimated using the model;
- take account that the practical situation is often dynamic however, due to cessation of pumping, for instance.

Blooper: "The water was sucked out of the sea and disappeared in the extraction".

"We had carried out calibration using a calibration tool. What we hadn't realised however, was that the tool only presented the absolute value of the discharge. The discharge presented therefore said nothing about the DIRECTION of the flow. Due to considerable extraction somewhere in the middle of the project area, the situation could arise whereby, after calibration, the water was 'sucked' out of the sea, flowed up the mountain and disappeared into the 'extraction point'. The absolute value of the calibrated discharges was pretty much in keeping with the measured values, however! Warning: this error/pitfall could even occur when using a 'normal' presentation tool, because the user can input the positive flow direction per branch/segment of a schematization."

Step 5: Use the model

Initial conditions often play a limited role in a model, though the starting volumes in any reservoir may be of importance.

3.4.3 References

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3.5 Hydrodynamic models

3.5.1 General

Hydrodynamic models are often deployed at the beginning of a chain of simulations, such as water movement => water quality or water movement => morphology. This often takes place on the basis of sequential coupling, whereby simulation of a module is not started before the previous is fully completed. In certain cases however, coupling is implicitly or explicitly required at the time step level, such as water movement <=> salt | temperature. Similarly, calculations using a hydrodynamic model are sometimes coupled to a precipitation run-off model. Once again, sequential simulation is the rule of thumb, but in flat areas a direct coupling between groundwater and surface water is desirable.

Hydrodynamic models are based on schematizations of one or more dimensions. The choice of the amount of detail with which the calculations are carried out is mainly based on the calculation times produced from the schematization. At present, 1D models are often deployed for analysis of the behaviour of a system over a number of years. The following step is normally to determine the statistic parameters of the behaviour of the system. For instance: sewer systems are currently designed on the basis of simulations of the overflow behaviour for a 10 year precipitation series. The statistical parameters are then the overflow frequency per location and the distribution of overflow volumes. 1D models are often used for design, forecasting, operational management, optimisation of systems and policy studies. Model programs currently used include: SOBEK (with the River / Low Land / Urban lines), DUFLOW, ISIS, MIKE11, MOUSE and HYDROWORKS.

2D schematizations are applied where detailed insight is required into the speed field and/or the water levels in the horizontal axis and where the variation of variables over the vertical axis has no significant influence on the result of the calculations. 2D models are generally deployed for the supervision of design and execution and for detailed morphological studies and water quality studies. Simulations are generally defined for a selected set of events. Current model programs in this field are packages such as MIKE21, Delft3D, WAQUA and DUCHESS.

3D simulations are carried out in similar projects to the 2D simulations, namely in situations where the distribution of the important variable values along the vertical axis makes discretization along this axis essential. Generally speaking, this is the simulation of distributions of temperature, salt and other water quality parameters. Current model programs are Delft3D, MIKE3 and TRIWAQ. The less common 2DV schematizations are also simulated using these packages.

3.5.2 Pitfalls and sensitivities

Step 3: Set up the model application

System behaviour

The model schematization should not be set up without having good insight into the behaviour of the system to be modelled. It may be useful to first set up a pilot model, whereby a number of calculations can be made on the basis of a rough estimate of model data. Sensitivities can be studied, such as the degree of influence of boundary conditions, sensitivity of certain physical model parameters such as friction or storage, damping of the dynamic phenomena in the system, etc. Always check which terms are important in the equations used.

Modelling scale

The choice of scale is particularly important in 2D and 3D modelling. Are important physical processes described on the chosen grid? Is the required dynamics passed on in successive calculations, such as morphology, water quality? Which time scale is chosen, via filtering of tides, for instance?

As far as the latter is concerned, there was once a case when, during adjustment of a tidal model, water levels apparently did not vary. Due to the low frequency of sampling, a calculating time step of 12 hours had been chosen, which is exactly one tidal movement. A calculating time step of an hour gave much better results.

Blooper: "The first ship to come along very nearly rammed the bridge".

We used our new 1D hydrodynamic model to design a channel which was to be used mainly for shipping. The flow rates had to be limited therefore. The design indeed made to restrict the flow rate to 1 m/s maximum. After the channel had been opened with great pomp and circumstance, the first ship to pass very nearly rammed the bridge. It had become almost uncontrollable due to the high flow rate. What was the problem? The bridge caused a narrowing of the channel, which also happened to be located in the bend in the channel. While the average flow rate was indeed still 1 m/s, it was 5 m/s locally under the bridge. We should have used a 2D model in this case."

Boundary conditions

Are the boundaries of the model far enough apart? The principle is that, when studying changes in the physical system, the results remain as independent as possible of those defined at the boundaries. In a river, for instance, this means that the lower boundary must be so far downstream from the study area that the back water curve caused by an error in this boundary condition is not passed on in the model results of the area where the measures were taken. The pilot model can be useful in checking the chosen location of the boundaries.

Salt and temperature differences

These have great effects in the hydrodynamic detailed calculations (2D and 3D). Their influence on the results is often limited in 1D models. However, do not forget the effect on dispersion co-efficients.

Storage and discharge capacity

This is particularly important in 1D calculations. 1D systems can generally be seen as a combination of storage and discharge capacity. How sensitive is our system to these two parameters? How does this sensitivity vary throughout the model area? Concentrate on this when carrying out sensitivity analyses with the pilot model. Do not forget to correct errors caused in the storage and discharge capacity by slimming down a network (sewer pipes, polder ditches).

Mass or volume balance

Not all available models guarantee a correctly calculated mass balance. However, this may well be vital when applying the model results. This is the case when the storage parameter is strongly non-linear in nature, such as in sewer systems. If comparative calculations are made to simulate the effect of retention basins, a balancing error in the mass balance will have great effect on the design and therefore the costs of the project to be implemented. Another good reason for correct mass balance (or volume balance) occurs where the hydrodynamic calculation is used as part of water quality simulations. The importance of a correct volume balance must also be set off against the accuracy with which certain data is known. Uncertainties in lateral discharges and the topography of the high water bed in high water predictions are notorious. In such a model, a volume error of a few percent caused by the calculation method is therefore not really a problem.

Garbage in - garbage out

Do not be put off by this well-known slogan in choosing the model. What costs are involved in gaining better data? How is the quality of the data passed on in the model results? What are the options for improvement of wrongly measured model parameters or boundary conditions on the basis of interpretation of calibration results? For instance: application of neural networks in precipitation run-off calculations leads to recognition of extrapolation errors in the stage-discharge curve which is used in the transition of water levels in discharges. Surely our own neural network (common sense) enables us to detect such an error and consequently to make assumptions which lead to improved extrapolation?

Numerical parameters

Care must be taken in choosing the numerical parameters. An important factor is the number of calculation points on the wave length to be simulated, both in terms of space and time. Make sure there are sufficient calculation points per wave length, whose effects must be included in the calculation. The model will otherwise often filter out these wave components. Equal density in the spatial and temporal definition is optimal. This often means that a Courant figure (relationship between the numerical time step and the travelling rate of a wave through a distance step) greater than one. Also check the chosen spatial discretization on the basis of a sufficiently accurate definition of the topography and special local phenomena, such as back water curves. A model is often used in order to compare situations. Make sure the Courant figure always remains the same. 2D and 3D models often use hidden interim steps in time. Check whether the numerical processing cannot lead to strongly deviating values of the model variables. This is particularly the case in the larger Courant figures. It is always sensible to check the model for sensitivity in the choice of the numerical parameters.

Step 4: Analyse the application

Initial values

Check the length of calculation required in order to be rid of the influence of incorrect or inconsistent initial values. Generally speaking, the following applies for tidal areas: water levels approx. 2 tides, speeds and discharges approx. 4 tides and residual flows approx. 12 tides. In rivers, the adjustment time needed to let errors work themselves out of the model depends on the travel time of the wave through the model. Remember that this is governed by the storage factor. Always start a high water calculation with water only in the summer bed, therefore. Also remember that in systems with little friction, the assumed initial values work through in the simulation for a long time (in sluice chambers for instance).

Calibration

Resistance co-efficients are essential. They cannot be measured and must therefore be derived. Verification takes place on the basis of water levels (discharges are less accurately measured than water levels). Take account of the wind effects on the water level. Translation of water levels into discharges can lead to incorrect discharges.

In tidal areas, the uncertainties mainly lie in defining the effective depth. Resistance co-efficients then become less important. When the choice of grid size does not allow for the realistic inclusion of sandbanks in the model, a useful and effective depth needs to be chosen in order to be able to take account of the effects as a result of the location of the bank. In storm surge models, the greatest uncertainty lies in the wind forcing. Kalman filtering may play a role here.

In river models based on quasi steady states, always begin with the lowest discharge. The calibrations for the higher water levels are carried out in the sequence of increasing discharges.

Make sure you limit the spatial variation in the parameter values. This can be achieved by dividing up the area into larger sub-areas with the same parameter values. This area classification can be made either on the basis of direct spatial distribution or on the basis of area characteristics (ecotopes). Too much variation in parameter values leads to excessive parametrization.

Check whether steering of the engineering works has no disturbing effect on the consistency of calibration data.

Detailed calibration is thought less important for certain calculations. In the sewers world, for instance, a reference calculation is generally made on the basis of the data file of the sewers system and standard friction values. The only important thing is how the new situation deviates from the existing one. In high water calculations for our rivers, compensation calculations are made on the basis of a comparison of a reference calculation and the new situation. Once again, the calibrated model is not constantly adjusted to the changes.

Validation

Do not underestimate the importance of model validation. First and foremost, validation serves to provide insight into the process of excessive parametrization. Extrapolations soon become unreliable. A good principle would therefore be to use an extreme situation in a set of field observations initially to validate the calibration on the basis of the other data sets.

Step 5: Use the model

Take care in choosing the boundary conditions for which a model is implemented. Pay attention to the choice of combinations and take note of the dependent factors (precipitation and wind direction, for instance) in particular. Also check whether simulation is required with boundary conditions being defined on the basis of statistical pre-processing or whether actual time series are given at the boundaries and the statistical processing takes place on the basis of model results. The latter is becoming increasingly common in the application of 1D models, due to the increasing speed with which computers can calculate.

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3.6 High water prediction models and operational models

3.6.1 General

As it is not always simple to distinguish between high water prediction models and operational models, a joint inventory has been made of the pitfalls and sensitivities with regard to these models. Steering on the basis of water quality through the use of operational models is not really applicable in the Dutch situation. Steering often takes place on the basis of measurements rather than on the basis of model calculations (see: calamity models). High water prediction and operational models mainly comprise a combination of a precipitation run-off model and a water movement model. At present, there are mainly one dimensional model programs in use for the water movement, such as DUFLOW and SOBEK.

3.6.2 Pitfalls and sensitivities

Step 3: Set up the model

In setting up and choosing the model, it is very important to know the characteristics of the system. These determine the required data density and frequency. Sewer systems have a very short response time for instance, so that the effect of brief but heavy rain showers is important. This requires great detail in terms of space and time. In polders, it is the amount of precipitation which is important, while the distribution of the precipitation in time (and space) plays a less important role. In river basins, the distribution of the precipitation in terms of space and time is important, as well as the direction of the shower, for example. Sloping areas and flat areas require their own specific approaches.

Avoid setting up models which are ‘hungry for data’. This includes systems which expect supply of current data in a period of time or at a detailed level which is not realizable in practice. Take account of the types of emergency situations for which models may be deployed. What data is required? When and how is it supplied (telephone lines may not be operational, for instance)? Keep the schematization as simple as possible. You will often only be interested in specific locations in the system. You are not interested in changes as the result of measures taken, such as in planning studies or environmental effect studies, but rather in the effects of a discharge wave on the existing system. When rules of thumb are apparent, they must be applied. The speed of calculation is also important! Of course, the model results for the selected locations must be in keeping with the actual situation.

Blooper: “The model was too good”.

“For years, we had worked with a certain high water model, which we knew to generally predict slightly higher water levels than actually occurred in practice. In time, we produced a new model which predicted the water levels almost exactly. The consequences: a year later there was a flood, with relatively great damage. What had happened? The local councils always assumed that our old model’s prediction would be a standard half metre too high. For the sake of convenience, they had also deducted a half a metre from our new prediction. Now that the prediction was accurate, nobody was prepared for the resultant flood.”

The acceptable prediction period of models depends primarily on the response time of the system. The response time determines whether you can or indeed must base the model prediction on ‘historical’ sets of measurements, current precipitation figures or weather forecasts. The shorter the response time, the shorter the prediction period and/or the greater the inaccuracy of the prediction. Of course, this is also related to the area for which the predictions are to be made. In the upstream area of a river basin, there is usually little 'historical' data available and the response time is short, for areas further downstream, the upstream data can always be used.

The model results can be strongly influenced by errors or inaccuracies in the schematization of the infrastructure. Failing to notice a bridge or incorrect input of dike heights can lead to completely different flow or even flood patterns! When a dike is breached, the model results will also no longer be usable, of course.

The initial water level in reservoirs and storage basins can have a great effect if the retention volume is significant in relation to the volume of the discharge peak.

Water movement models are dynamic models and therefore generally not very sensitive to the initial conditions, though this depends on the response time of the system.

Step 4: Analyse the model

Calibration in sloping areas takes place mainly on the basis of discharges and in flat areas on the basis of water levels. There is often not much measuring data pertaining to extreme discharge situations. This makes it difficult to calibrate models effectively.

As far as input data is concerned, the model is generally most sensitive to the precipitation data. It is also very important to know whether the precipitation falls in the form of rain or snow. The defined soil conditions determine how quickly the water will run off. The precipitation/run-off part is often the most sensitive part of high water prediction models and operational models. These are mainly event models which depend greatly on the initial conditions.

3.6.3 References

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3.7 Calamity models

3.7.1 General

Calamity models currently used are: Version 3 of the Rhine alarm model (DBAM shell based on Delft Tools (analytical solution 1.5D)); MARS and RAMFOS (particle models for the North Sea based on the DELPAR model program); TRANSPILL (2D analytical model for suspended solids on the North Sea without tide); Meuse alarm model (1D analytical mode).

Calamity models are often specific **operational** models which are quickly ready for use and require little (additional) information. Most of the work is involved in setting up such a model. In emergency situations, it must be possible to simulate using a limited amount of data material. The estimation of the travel time (in river modelling or 1D modelling) is generally thought much more important than the maximum contents of discharged substances which will occur: what is important is the time the manager needs to protect and/or close potable water intake points. In 2D calculations, there is also uncertainty as to **where** the discharge will pass by and end up: the tide, wind force and wind direction are all important factors here. Inclusion of the dispersion in the modelling is very important in order to gain insight into the concentrations which will occur in the surface water.

In calamities, there is always a need for detailed information on the nature and the type of substances discharged (toxicity). Information on volatility and/or speed of decomposition are usually slightly less urgent because a **worst case** analysis is generally carried out (no decomposition, sedimentation or evaporation). Detailed information on substances is stored in a number of databases, including one managed and kept up to date by the Dutch organisation for applied scientific research.

Detailed sampling of discharge/calamities is very important for the calibration of this type of models under various hydrological and meteorological circumstances.

3.7.2 Pitfalls and sensitivities

Step 3: Set up the model

Handling of the dispersion term can have a major influence on the final result. Processes and phenomena which are strongly related to silt and adsorbed substances can often be less accurately reproduced using a model.

Step 4: Analyse the model

The calculated results are always strongly dependent on the uncertainty of the input data: emissions and water quantity (travel time) are particularly crucial. If there is measuring data available pertaining to earlier calamities, that will help to considerably improve the certainty/accuracy of the calculated result.

Step 5: Use the model

When using a calamity model, take account of the fact that a model is usually subjected to a reasonably specific time scale. That time scale lies between a few days and a few weeks for the Rhine alarm model, for example.

3.7.3 References

Spreafico, M. and A. van Mazijk, 1993.

3.8 Morphological models

3.8.1 General

Unlike hydrodynamics for instance, morphology entails much more uncertainty with regard to the processes which occur and the way in which the system reacts to them. Just like ecology, morphology is at the end of a chain:

water levels => transport => flow rates => morphology

The complexity and inaccuracy increase greatly the further down the chain we move. A clear distinction can be made between river systems on the one hand and tidal systems on the other. In river systems, the morphological end situation is much more clear than in tidal systems and the time scales studied are often longer. This requires a different approach to morphological modelling. Model programs currently used include: SOBEK (1D), DELFT 3D, MIKE 21, UNIBEST, ESTMORE, EMPREL.

3.8.2 Pitfalls and sensitivities

Step 3: Set up the model

Dominant discharge

Calculations with a variable discharge are preferable because it is theoretically impossible to choose such a constant discharge (‘dominant discharge’) that this results in the same soil situation as a series of varying discharges. A varying discharge is nowadays generally used in one dimensional calculations, though a constant discharge is still usually applied in two and three dimensional models, for the sake of practicality. A discharge is therefore chosen which gives the same annual sediment transport as the hydrograph of varying discharges. In tidal models, a representative ‘morphological tide’ is defined, analogous to the ‘dominant discharge’. The inaccuracy thus introduced is then taken into account in the interpretation.

Quasi steadiness

A common assumption in morphological calculations of lowland rivers is that the water movement is quasi steady. When compared with the morphological changes in the river, the water movement adapts so quickly to the new boundary conditions that the hydrodynamic unsteadiness of this adaptation is negligible. This means that the flow can be calculated using a steady water movement model. Varying discharges can therefore be calculated using a series of steady discharge levels. In tidal areas, the concept of *quasi periodicity* is applied, based on the fact that morphological time scales are much larger than the time scales which apply to the water movement.

Feedback in estuaries

An extra complication in the hydrodynamic boundary conditions for models with tidal flow is that the volumes of water flowing through an estuary during a tidal cycle are not an independent parameter but rather are influenced by the morphological development in the estuary. Moreover, in tidal models, the morphological changes are linked to the residual transports during a tidal cycle. These residual discharges are the net effect of inward transports during flood and outward transports during ebb. The definition of sediment transport therefore requires much greater accuracy for estuaries than for rivers.

Step 4: Analyse the model

In morphological models, the water movement must always be calibrated first. In one-dimensional models, the water levels can be adjusted using the bed roughness co-efficients. In two-dimensional models, flows can also be adjusted using bed roughness co-efficients and turbulent diffusion co-efficients.

Morphological calibration can then initially take place for the bed situation: the *bed length profile* in one-dimensional models, the *bed topography* in two- and three-dimensional models. In the case of graded sediment, there must also be calibration of the *composition* (characteristic sediment grain size) of the top bed layer. Calibration based on sediment transport is not a suitable method.

Measured and calculated bed length profiles can be compared on the basis of average positions. Filtration therefore takes place, of:

- dunes and sand waves from the measurements;
- bed waves caused by one-dimensional schematization from the calculation results.

Quantitative criteria for calibration of bed topographies can be related to cross bed drops in bends and locations of bend transitions (which are more or less linked to the length of the sand banks in the inside bends).

One-dimensional morphological models of branching rivers are extremely sensitive to the empirical junction relations to be defined, which indicate how, on arrival at a junction, the sediment splits and is divided among the river branches (see PAO syllabus ‘River morphological boundary conditions – continued’, pages 6 and 8 and the literature references given therein).

Very important parameters in two- and three-dimensional morphological models are the co-efficients for the effect of bed slopes on the sediment transport. Also important is that the parameter for numerical stability in fact entails modification of the co-efficient for the effect of longitudinal bed slopes on the sediment transport. Spatial variations in sediment grain size and bed roughness also have a great influence on two- and three-dimensional morphological calculations. As yet, there are no effective techniques for measurement of these spatial variations in the field, to allow for good calibration. Modules to calculate these spatial variations are currently under development.

Step 5: Use the model

Subsequent expansion of a calibrated flow model with a morphological module does not generally result in a good morphological model. Such cases require full re-calibration and possibly even definition of a new schematization.

Step 6: Interpret the results

Calculated initial erosion and sedimentation which do not obey a general trend have no physical significance. They are the result of an adaptation of the bed situation to the schematization.

3.8.3 References

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3.9 Water quality models

3.9.1 General

Water quality models are models which are able to simulate the (generally chemical) quality of water systems. This is usually done on the basis of water and silt movements, emissions and (chemical) processes. Water quality models are roughly divided into two categories:

- ‘Near field’ models, for determination of local effects (mixed zone approach). These are practically always steady models, due to their small temporal and spatial scale, which are mainly used for licencing purposes.
- ‘Far field’ models, for calculation of an entire water system. These are often dynamic models, as processes and transport through flow play an important role here. They are also used for policy analyses, comparing the effectiveness of measures/scenarios.

Common water quality model programs are: DELWAQ (including SOBEK, DBS and Delft3D), DUFLOW, Mike*, Nuswa, PcDitch, PcLake, SOM3 and IMPACT. These programs can also be used for pesticides. SLOOT.BOX and TOXSWA (plot ditch, for admission) are additional specific model programs for pesticides.

A special category of models which is strongly related to water quality models, are the sediment models. Sometimes they are separate model programs (such as Horizon), sometimes they are integrated modules, e.g. the Switch module in DBS.

There are model programs which do not calculate water and/or silt movements themselves, but rather receive this data from other models. However, programs are increasingly showing a trend towards integration of hydrodynamics, morphology and water quality. DUFLOW, SOBEK and Mike are examples of such integration. Programs such as Nuswa, PcDitch and PcLake apply a simplified water movement.

The various water quality model programs vary strongly in terms of (the number of) substance groups included. Some model programs only focus on pesticides, for instance, while other programs theoretically aim at all substance groups (nutrients, metals, organic micro-contiminants, pesticides,etc.) and the attendant process models (e.g. re-aeration from the atmosphere, net sedimentation of algae and detritus, mineralization, nitrification and denitrification, sedimentation, resuspension, chemical and biological decomposition, adsorption and desorption and volatilization). Regarding eutrophication, biological processes (algae) are included in addition to chemical processes. Certain model programs allow for the input of new processes by the user.

Blooper: “Negative concentrations”.

“Upon completion of a water quality model, the nitrogen concentrations (nitrate and ammonium) in the boundary layer between water and bed showed severe oscillations. Further investigation proved that this happened around the value 0, and that the model in fact calculated negative nitrogen concentrations. This was due to the integration algorithm chosen on the one hand, and the absence of a mechanism to prevent this, on the other. When this situation was remedied, the performance of the model became much better.”

3.9.2 Pitfalls and sensitivities

Step 3: Set up the model

Just like in any other type of model, it is necessary to analyse whether sufficient data is available before starting the actual water quality modelling. In this case the most relevant data includes:

- water movement (see 3.4 and 3.5 of Part II);
- emissions (see 3.13 of Part II);
- silt transport (for silt-bound substances);
- processes (including parameter values);
- measuring data.

Quite frequently, a splendidly detailed model is constructed, while there is little or no measuring data available to calibrate the model.

Emissions data is faced with a similar problem. Diffuse sources, in particular, are difficult to quantify, and even if they are quantifiable, the figures are not very reliable. In these situations, constructing a extremely detailed water quality model is a waste of time. If discharges are easily mixed over the entire width of the flow, an 1D model will suffice. In stagnant situations and in local-scale models, a 2D model is preferable.

When constructing the model, the modeller should take account of the fact that the time scales of some processes vary largely. An example is the sedimentation process under the influence of the tide, where the difference in time scales entails a number of time steps. The numerical approach may then prove extremely difficult, unless the model program includes the option to calculate various processes with different (numerical) time steps.

Finally, the treatment of the dispersion term may greatly affect the end result.

Step 4: Analyse the model

When analysing the model, it is sensible to verify the correctness of the model by means of a number of test calculations. In this case, relevant data includes the mass balances and the displacement characteristics, in particular. Even a simple sum with a conservative substance may provide much insight. Great prudence is required if the results fail to meet (part of) the expectations. In that case the cause must be investigated in detail.

To verify the stability and accuracy of a model application, the time step/place step ratio should be varied in order to check whether a critical boundary is exceeded or approached. This should be taken into account in the case of some rapid processes (re-aeration, bacterial decomposition), in particular. Some solution models are hardly or not affected at all by this, but others may show large oscillations (see the Blooper on the previous page).

Blooper: "A continuously failing nitrogen balance".

"We repeatedly failed to reach a nitrogen balance. Whatever we tried, there would always be a nitrogen surplus or deficit, while carbon and all the other nutrients worked out perfectly. It took a balance analysis of many days for the truth to come out. The nitrogen equations included the option of the adsorption of ammonium and nitrate by algae. The choice had been defined with an 'if then' statement with a threshold value for the concentration of ammonium. There was not a single common numerical system which was able to handle such a typical definition of the ecological modelling of this substance flow. By replacing this definition by a continuous equation, the problem was soon solved. Two years later, another workshop, another institute, it happened again. Being forewarned, we quickly solved the problem.'

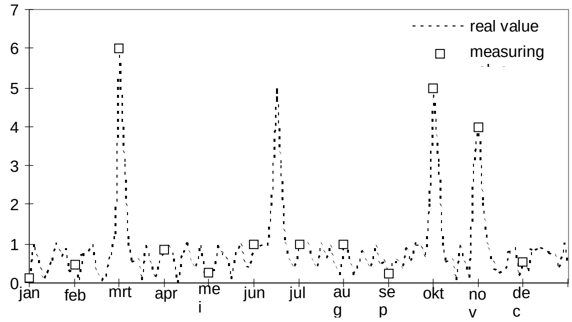
When analysing the model, the influence of the initial situation on the end result must also be investigated. The required run-in time may sometimes even be longer than the simulated period. In addition, the effect of the boundaries on the end result must be established. is the distance between the boundaries and the model area to be studied sufficiently great?

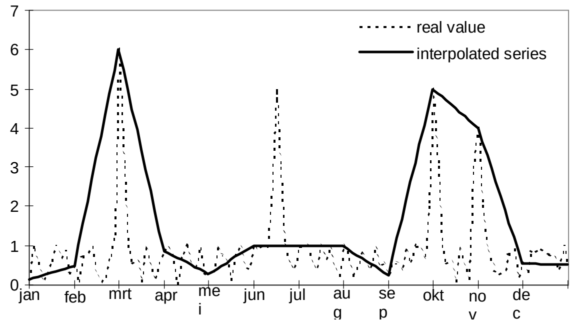
Following global analysis of the model, calibration can take place. Calibration of a model is preferably started with a sensitivity analysis and adjustment of the model using the major parameters.

The calibration variables include:

- process co-efficiënts;
- transport variables (water, silt/suspended solids);
- emissions.

Of the above variables, the transport variables and emissions are often (though not always!) very sensitive (see 3.4/3.5 and 3.13). However, in practice most energy is devoted to the proper setting of the process co-efficients. This is only useful, though, if the other variables are properly taken into account as well. Unknown parameters can be estimated by means of expert judgement. Default values are usually not adequate, because they apply to a general/single system. Literature values may be misleading for the same reason, for that matter. Poorly understood/poorly defined processes (BOD) or processes with a 'dustbin' character always require more calibration (extinction, mineralization, sedimentation).





A notorious pitfall concerns the interpolation of the measuring data used for calibration. Linear interpolation is the most simple way to deduce a measuring series from measuring values. However, one should be aware of the existence of peaks in the parameter chosen and whether these peaks are actually present in the measuring values. An incorrect interpolation method may result in a severe overestimation or underestimation of the transport load, as illustrated by the diagrams on this page.

The last potential pitfall which must be eliminated when analysing the model, concerns the phenomenon of 'shooting water'. In a water quality model with a simple container set-up, the water volume input and output is calculated for each time step, including the relevant concentration of substances. This is the basis for the calculation of the new concentration in the container. This method works fine, as long as the flow rate is not too high. At times of high discharges, however, the water volume flowing through the container per time step may be greater than its contents. This is called 'shooting water' and it yields very strange calculated concentrations. It is always sensible to check whether the discharge per time step is smaller than the capacity of the containers.

Step 5: Use the model

Prior to the actual use of the calibrated model, the run-in time must be checked once again. The residence time and processing speed usually give an indication of the length of this period. As said before, the run-in time may be longer than the simulated period and therefore cause major errors.

When constructing a water quality model, the modeller should take account of the fact that a model is usually designed for a relatively specific time scale. This holds good for processes as well as for the period within a year. To start with the former: sediment models are sometimes designed for time scales varying from tens to hundreds of years. Obviously, this type of models should not be deployed for on-line predictions. Regarding the period within the year: chemical processes may depend strongly on meteorological circumstances (temperature, precipitation/flow rate). Consequently, measuring data describing the situation in de project area over a period of at least 12 months will enhance the reliability/accuracy of the calculated result considerably.

Step 6: Interpret the results

Take account of the uncertainty bandwidth when interpreting the results. Check, for example, whether a distinction can still be made between the results of various scenarios and whether the measuring error in the field observations does not exceed the uncertainty margin of the model.

3.9.3 References

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3.10 Waste water purification models

3.10.1 General

The available model programs for waste water purification must clearly be distinguished into static and dynamic models. The static models are used for designing purposes only. The dynamic models are used for optimisation of existing waste water purification plants, development of regulating strategies, optimisation of sub-aspects in design studies and training. Dynamic modelling is frequently used for scenario studies.

Static modelling

The most commonly used model program in the Netherlands is DenNi, which is based on the HSA method (HochSchulAnsatz). Another program, also based on the HSA method, is ARA-BER which is used by a number of engineering offices in the Netherlands. With the effluent quality as a starting point, a static model may calculate the required volume, the required oxygen capacity and the silt production. This Handbook does not expand on static modelling, also because apparently there are hardly any bottlenecks.

Dynamic modelling

In 1995, it was decided, within the STOWA framework, to switch to the standardised use of a single model for the active silt system and a single simulation program, instead of using dynamic modelling for the active silt system. The choice fell upon the SIMBA (SIMulation von BelebungsAnlagen) simulation program, in which the IAWQ model[1] serves as an active silt model. The IAWQ model is an internationally accepted model program and is widely applied. The SIMBA program operates under the simulation environment of MATLAB and SIMULINK. As early as in 1996, by far the greater part of all water quality managers, engineering offices and research institutes had bought SIMBA and had gained vast experience with its use.

Comments

In 1999, a SIMBA protocol will be drafted for users within a STOWA project. It will describe all pitfalls, bottlenecks, sensitivities and inaccuracies concerning the modelling of active silt systems. STOWA already issued a manual for the determination of the influent characteristic in 1996. Within the scope of the modelling of waste water purification systems, all this results in a more responsible use of models.

3.10.2 Pitfalls and sensitivities

Step 2: Set up the modelling project

Interpreting the model results into a practical application involves taking decisions which may have major financial consequences or may put the guarantee of a certain effluent quality at stake. Accepting a specific measuring effort is therefore a precondition for the realization of effective usage. For waste water purification, this means that particular attention must be paid to thorough influent characterization and the determination of the hydraulic pattern. If this effort is not made, the model results will be unreliable and the model will theoretically only be suitable for training purposes.

[1] *Within the context of the terminology of this Handbook, the IAWQ model is actually a model program; however, since 'IAWQ model' is a generally accepted concept, this term is also used in the continuation of this paragraph.*

Step 3: Set up the model

When setting up the model, check to some degree whether the purification is fully mixed or whether it has a clogged flow character, as this determines the number of compartments chosen for the model and may have great influence on the model results. There also has to be some knowledge of the possible presence of an oxygen profile over the length and/or the depth of the reactor, in order to establish the totally aerated and non-aerated area of the reactor.

When setting up the model, various resedimentation tank models may be selected, one having a more dynamic pattern than the other. The reliability of resedimentation tank models still leaves much to be desired. Therefore, careful consideration must be given to the intended purpose when selecting such a model.

The IAWQ model has been developed for the purification of waste water from households, because this waste water served as a model substrate in the determination of the default parameters. Most domestic waste water compositions are covered by the IAWQ model range. If a large part (>70%, arbitrarily chosen) of the waste water consists of industrial waste water, this may lead to inaccuracies. This also implies that the IAWQ model is not directly suited for industrial waste water (usually higher pollution load, presence of toxic components and absence of certain nutrients). Following specific research, the IAWQ model may be adapted to become suitable for a specific type of industrial waste water, but it will in fact only be suitable for this type of industrial waste water.

The IAWQ model is a biological model, meaning that physical and chemical processes such as adsorption, coagulation, flocculation and stripping are not defined. A number of chemical reactions have been included though, for the purpose of chemical phosphate removal (restricted to Fe^{3+}). Once more, this indicates that the IAWQ model is not directly suited for model studies with industrial waste water. Apart from the biological aspect in the active silt system, purification also comprises a number of mechanical process components and silt processing. The latter two cannot be modelled with the IAWQ model, but this is not absolutely necessary anyway. Characterization of the originating water flows is usually enough to assess their influence on biological purification.

The IAWQ model has been set up for a temperature range of 10 to 20 ^{o}C and a neutral pH. Simulations beyond these ranges may lead to a certain degree of inaccuracy. The temperature has a constant value per simulation, so that a sudden drop in temperature in the reactor, caused by rain water, cannot be processed.

As mentioned before, the SIMBA resedimentation tank models are not so very advanced as yet. This means that expectations of predictions regarding the suspended solid content in the effluent must not be set overly high. For the time being, this can better be determined by empirical relations from practice between the influent discharge and the suspended solid content in the effluent. Since SIMBA runs on a MATLAB/-SIMULINK platform, this can be relatively easily implemented in the design of the model. For the dissolved substances, the choice of a resedimentation tank model is less sensitive.

Blooper: “Practice is unmanageable”.

“When setting up the model, the purification must be divided into compartments. For a waste water purification plant with nitrification and denitrification, this means that the model must be divided in a number of aerated and non-aerated compartments. The model fully mixes the compartments and does not take account of oxygen profiles over the depth. In practice, oxygen profiles over the depth may certainly occur, however, and if they are not defined in practice, this will result in an incorrect model construction and inadequate calibration.

If, in practice, the upper half of an aerated nitrification area has an oxygen content of >0.5 mg O_2/l, the lower half will be non-aerated, resulting in denitrification. During calibration, practice will show higher denitrification levels when compared to the model, because the compartments are fully aerated in the model. When compared with the practical situation, the model thus contains too little denitrification area and the parameters of the denitrification process must now be disproportionately adjusted in order to make the model correspond with practice.”

Step 4: Analyse the model

Important calibration variables are:

- hydraulic pattern of the entire purification;
- influent characteristic;
- mixing character (fully mixed or clogged flow);
- silt production measured;
- organic dry matter content versus total dry matter content;
- temperature.

The calibration of an active silt model for nitrogen removal is based on NH_4 and NO_3 content in the effluent, and on silt production and possibly oxygen consumption. In the case of an active silt model with phosphate removal, calibration must also be based on the PO_4 content in the discharge of the anaerobic reactor and in the effluent.

Static calibration assumes a constant influent flow rate and a constant waste water composition. Taking daily samples is sufficient for this purpose. Dynamic calibration assumes a variation in influent flow rate and waste water composition. This requires a higher sampling frequency (for the hyfraulic influent pattern, in any case).

Since the various processes in the active silt process encroach upon one another, the sequence of the calibration steps is essential. In order to prevent errors and inaccuracies in the simulation, the silt production must first be calibrated, next the nitrification and finally denitrification. By following that sequence, a ‘trial and error’ calibration procedure is avoided. During calibration, the user’s technological background must constantly be addressed in order to keep the parameters within a rational bandwidth. Therefore, automatic calibration programs are highly unadvisable as a user with inadequate technological knowledge would be provided with an instrument which makes him lose track of reality completely. Still, as in most calibration procedures, the majority of calibration errors are cumulated in processes of which the least knowledge is available. In active silt systems, this involves the hydrolysis process which is an important factor in the availability of CZV for micro-organisms.

3.10.3 References

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3.11 Ecological models

3.11.1 General

Describing general pitfalls and sensitivities for ecological models is difficult because:

- 'ecological models' is a collective name for a highly diversified group of models;
- the ecological processes to be modelled are generally very complex and the uncertainties great;
- ecological models are often deployed at the end of a 'model chain' and are therefore highly dependent on the assumptions made in other models, along with the accompanying inaccuracies.

The following types of ecologocal models can be distinguished:

- ***Ecological substance flow models*** which focus on modelling of the food flow to the 'primary consumers'. Examples of model programs are ERSEM, PCLAKE, GEM and DBS;
- ***Cycle or food web models*** for the modelling of complete food chains. These models are considered to include ecotoxicological models. Examples of programs are CHEOPS, CATS and MC^2;
- ***Energy models*** which focus on energy flows instead of substance flows. These models are hardly applied in the Netherlands as yet;
- ***'Probabilistic models'*** is a collective name for highly diverging expert and empirical models which are hard to be grouped together. Examples of such programs are: DEMNAT, NTM, NICHE, MOVE, LEDESS, ICHORS, ITORS, LARCH, METAPHOR and MORRES.

3.11.2 Pitfalls and sensitivities

Step 2: Set up the modelling project

The use of ecological models requires a multi-disciplinarian approach. Therefore, ecological models need to be used by well-versed experts or model users who are supported by a multi-disciplinarian team. If this is not the case, there is the risk of solution directions being exclusively sought in the field of knowledge of the model user.

When ecological models are deployed as part of a model chain, it must be thoroughly investigated whether the space and time scales used in the other models are applicable to the ecological models. The user must also be able to judge the quality of the results of the other models which serve as input for the ecological model.

Blooper: "The algae refused to grow".

"We had made a model in order to observe algae into more detail. However, the algae refused to grow. Upon closer consideration, it appeared that the residence time of the lake (?) was less than one day. Consequently, the algae did not have the chance to grow in the model. In a similar model, the algae would not grow because.... the initial algae concentration was set to zero. You don't have to be a biologist to see that algae will not grow/multiply when there are no algae in the first place!"

Before making a start in the first place, think carefully whether the deployment of a model is useful and, in particular, whether the modeller has sufficient knowledge to handle the model responsibly. In fact, only a very limited percentage of the natural processes is known for practically all ecological models. Consequently, the modeller will soon want to modify the processes. This type of work and correct interpretation of the results requires much expertise.

The more complex, the better, is not generally applicable in the case of ecological models. Often even the converse is true. Since only a limited number of processes is known, it is better to opt for a simple approach allowing insight, than for a complex system with a jumble of known processes, unless the modeller has vast experience with the model.

Step 3: Set up the model

With the exception of bacteria and algae models, spatial and temporal scales are particularly essential. The response time of various vegetation types and organisms generally varies greatly. Therefore, it is vital that a suitable time scale be used when setting up and applying ecological models.

Step 4: Analyse the model

Given the great uncertainties soon encountered when using ecological models, verification with the personal (domain) knowledge is an absolute prerequisite. Prior to making calculations, one should contemplate the results you expect.

Numerous abiotic factors usually serve as boundary conditions. They must be correct, because otherwise the starting points for the ecological calculations will be incorrect.

In systems with long-term time scales, the initial state is generally decisive for the results. They must therefore be accurately defined in ecological models. When they are not known, a sensitivity analysis is necessary.

The calibration of ecological models is generally not isolated from the calibration of the other models in the chain.

Blooper: "The model ecosystem operated excellently, but the mussels did not have enough to eat".

"In ecological substance flow models, it may be justifiable to use forcing functions for biological variables. These forcing functions influence the model system, but the biological variables themselves are not influenced by the model system. A model to which the filtration of phytoplankton by mussels has been applied as a forcing function, was calibrated automatically. Excellent results were produced for the calibrated variables of the model ecosystem. During the workshop in which the results were demonstrated, an experienced modeller noted that the results looked excellent, but that in the real ecosystem the mussels would die. It turned out that the model system was not able to produce sufficient algae as food for the mussels, while the filtration pressure remained too high due to the forcing function. This was caused by the absence of feedback information on the growth of the mussel biomass. Six weeks of re-calibration, including another workshop, followed. Afterwards the model was also adjusted for the mussel food supply."

There are no additional remarks about the calibration variables in a general sense. They are highly dependent on the ecosystem or the types/variables to be modelled.

Substance flow models

The water and substance balances must be correct. Users generally tend to pay (too) much attention to concentrations and too little to process speeds, as these are difficult to verify.

Expert and empirical models

Ecological expert models often contain many assumptions which are not always fully documented. When using these models, knowledge about the assumptions on which the model is based, is a prerequisite. Calibration is only possible on the basis of the 'real vegetation', for example from FLORBASE for terrestrial nature. However, much information is not available on a national scale.

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3.12 Economic models and use function models

3.12.1 General

Although economic aspects are extremely important in water management, there are few widely supported models and model programs. There are, however, very many, often tiny models and spreadsheets for sub-domains, often per use function. In addition, there are macroeconomic models such as 'Athena', used by the economic planning office of the Dutch government. They often include input/output analyses in the form of cross reference tables. In a cross reference table, the production of a specific branch of industry is related to the production of the supplying companies. In addition, there is the environmental cost model (MKM spreadsheet) which considers the aggregated environmental costs on a national scale without passing them on to other sectors.

As far as the function models are concerned, these include model programs for recreation (e.g. for the WGI, TOUR and SEO model), inland navigation (PAWN-Scheepvaart), potable water (Atlantis and DRISIM) and agriculture (Agricom, DEMGEN).

A final important instrument is the so-called MIOW analysis which is primarily intended to determine the (changing) competitive position of companies or sectors under the influence of, for instance, environmental measures. They may put a heavy financial burden on companies, and this instrument can determine whether the costs exceed the financial resources of a company or sector.

3.12.2 Pitfalls and sensitivities

Step 3: Set up the model

Particularly the interest and inflation aspects must be properly defined, though temporal and spatial scales are also very important. An example is the comparison of unlike variances such as dredging (discontinuous in time) and purification by industry (continuous process with permanent effects). Extensive attention is also often paid to the scope of analysis: the scale is important. For instance, VAT is not important on a national scale (input equals output), but it may be important for a specific branch of industry. An exhaustive survey of the costs involved in the analysis (both direct and indirect costs) is essential to be able to assess the significance of the results. In the macroeconomic sphere, 'substitution effects' are important: locally, the construction of a shopping centre will often have great economic significance, but it will only have a draining effect on the region.

The collection of data suitable for this type of model is a serious problem. It must often be obtained from the corporate sector. Therefore, it is crucial that (representatives of) use functions participate in the development of the model. There must be agreement on this before the modelling is started; otherwise the modelling is of no use at all. It stands to reason that the objectivity of the study must still be guaranteed.

Finally, the scenarios of the government economic planning office, which are published every five years on average, are also an important source of input for economic models. However, these scenarios are often so general that conversion into water and water-relevant use functions is necessary. This is a step which is generally performed by specialised offices or institutes and which is quite costly.

Step 4: Analyse the model

A major problem in the use of economic models is that there are few of no calibration variables available. A good sensitivity analysis is of utmost importance. Of course, it is possible to verify on the basis of historic data (trends), but the sensitivity for the (uncertain) economic scenarios in particular, is so great that it is often only possible to give a development bandwidth. Entering into too many details must therefore be prevented, as the uncertainties are too great for that.

As to the function models, they allow for reasonable verification of the characteristic aspects for the various use functions. For inland navigation, for instance, this is the number of navigating movements per ship category, for potable water the cubic metres of potable water, for agriculture the crop yield and for recreation the number of recreation days per type of recreation. For that matter, one must be aware of an overly rough approach of this last category of models. The various types of recreation are so diverse, that a distinction must be made between, for instance, recreational shipping, sunbathing and swimming, and angling.

Calibration and validation on the basis of expert judgement is often the best method to arrive at a good model result. Once again, it is highly recommended that co-operation be sought with specialised agencies and the corpoarate sector (the branches in question).

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3.13 Emission models

3.13.1 General

Emission models are models with which emissions to the surface water can be calculated. They are often used for quantification of diffuse sources, which are usually not measurable. Emission models are also used for analysis of the effect of emission reducing measures, for instance the effect of an extra purification phase. Attempts are made to determine the sources and the various emission routes for each substance, and therefore the starting points for measures.

Most emission models have two main variables: the emission explicative variables and the emission factors. By multiplying these two, an emission figure is reached. An emission explicative variable is the phenomenon which causes the emission (the source), for instance, a cow in the case of nutrients emissions or a ship if it concerns the extraction of PAC from ships' coatings. An emission explicative variable produces a certain amount of (waste) material. However, that need not be entirely emitted into the surface water. Thanks to all kinds of chemical, physical and biological processes, only a very limited part of the manure produced by a cow actually ends up in the surface water. Only a limited percentage of the PAC smeared on a ship's hull will be leached each year. The percentage which eventually ends up in the water is referred to as the emission factor.

Both the emission descriptive variables and the emission factors form starting points for measures to limit emissions. Total emission can be limited by reducing the number of cows or navigational movements, but attempts can also be made to reduce the emission factor. If the cow manure is used on land for sweet corn, for example, a trapping crop could be set out between the sweet corn in order to increase the biological absorption of nutrients, therefore reducing the percentage which leaches to the surface water. In ships' coatings, a coating can be chosen whose component parts are less quickly leached, or which contains less PAC.

Although emissions have been a priority agenda point in water management for decades now, there is a limited number of emission models. Commonly used model programs are Promise and the WLM (Waste Load Model). Pesticides are covered by the PESCO model, which is based on a spreadsheet. There has also been regular emission modelling carried out within the framework of Emission Registration, a co-operative project of the Ministry of Housing, Regional Development and the Environment and the Ministry of Transport and Public Works in the Netherlands. The results are used for annual filling of the ER-C (Emission-Registration Collective) database which, in principle, contains all emissions of all sources for all Dutch surface waters, also the diffuse sources, though the data is sometimes very aggregated.

A very special group of emission models is that of the groundwater quality models, particularly those for the unsaturated groundwater. They define the emission routes via the groundwater, along which substances finally end up in the surface water. These are important emission routes for nutrients and some pesticides in particular. Commonly used nutrients models and model programs are ANIMO/STONE, FUSSIM-2, FLUSIM, NITSOL-PHOSOL, NITRIK-C, NPK and WAVE. A model program commonly used for the flushing and leaching of pesticides is PESTLA.

As far as the nutrients models in particular are concerned, various research and advisory groups use a reasonably large diversity of simulation models. The models vary greatly in terms of the degree to which they describe leaching to the groundwater and surface water. Reasons for this are:

- the model targets with regard to the type of answers required;
- the resolution of the expected answers and the comprehensiveness of the issue (e.g. only the nitrate content due to manure, or all the nutrient emission routes due to soil, crops and water management);

- experimental and literature information available;
- ambitions and personal preferences of the researchers.

The choice ranges from simple calculation rules or regression relationships to detailed deterministic models. A description of the scope of the range has been given below, in order to illustrate the great degree of variation, in model programs for nutrients in particular.

- *In flat surface area:* from a few m² to the whole of the Netherlands;
- *In the depth:* from the root zone and approximately the phreatic surface to around 50 metres under ground level (in deep groundwater systems);
- *In the time:* from one growth season (for calculation of the nutrient absorption of a crop or leaching in a validation study) to approximately 100 years (for prediction of the subsequent effects of manure reduction in relation to phosphate leaching and organic matter development);
- *In embedding:* from scant studies which only monitor the effect of a change in the amount of manure on a plot of land, to integral studies in which nutrients emission is calculated as a link in a long model chain (EU politics => change in farm structure => change in nutrients flows at a farm => fertilisation on a field => nutrient leaching to field and plot ditches => water quality on a regional scale => water quality at the national scale => loads to the North Sea);
- *Complexity:* from a limited model output (of nitrate concentration in groundwater, for instance) to a full list of all the nutrients flows in various environmental compartments, including the relationship between the balance items.

3.13.2 Pitfalls and sensitivities

Step 2: Set up the modelling project

With a view to the complexity of emission models, model studies require a clear picture to be formed with regard to the research issue. In practice, the original research issue has been known to develop into a much more comprehensive matter (spatial resolution, temporal resolution, integral character, emission routes, processes).

Before starting modelling, four aspects must be paid careful attention:

- what are the sources;
- what are the emission routes;
- what are the emission explicative variables;
- what are the emission factors (an emission factor usually comprises a number of sub-factors in an emission route).

Knowledge developed elsewhere can be applied here, though it often proves very difficult to gain a complete picture of the above aspects, more so when diffuse sources are involved. And that is in fact the first pitfall: pay careful thought to whether modelling has any use if there is doubt as to the comprehensiveness of the above data.

Step 3: Set up the model

Once the decision has been taken to start modelling, the necessary data must be collected. Many emission models require enormous amounts of input data before a simulation can be carried out at the field scale or regional scale. Models can also often be used to derive such data, in the form of simulation models (hydrology as pre-processing) or in the form of regression relationships (pedo-transfer functions). Much of this information therefore relies on estimates and processing of other sources of information. These methods can actually also be included under the models, seeing as the models make use of these estimates and processing. A model therefore not only comprises a description of a concept in the form of mathematical equations but also those methods upon which the input data is based.

Blooper: "Phosphate and phosphor are two totally different things".

"NO END of errors are made with units in the emission issue. In (artificial) fertiliser, a common mistake is to forget to convert P_2O5 to P, the same applying to NO_3 to N. This can lead to gross underestimation or overestimation of the results."

Once again, it is the diffuse sources which are particularly problematic, both in terms of recognition of the source, of gaining insight into the correct emission routes and also the determination of the emission factors. The latter is generally the most troublesome.

It is important to make a good estimate of the contributions to be made from the various sources, beforehand. There is no point in investing lots of time in collecting data for a source with a relatively small emission if data on large sources is lacking. And even if that data is available, it is not always necessary to spend lots of time on collection of data for sources which make little contribution to the total emission.

A final pitfall in setting up a model is the negligence to examine whether there is sufficient material available for verification of the quality of the model to be constructed. Very often, there is little or no data available, necessitating deviation to other methods, such as expert judgement, for instance.

Step 4: Analyse the model

The main problem in analysis of an emission model is often the shortage or total lack of measuring data. While point sources can be measured, diffuse source generally cannot. They can only be indirectly measured through, for example, measuring the water quality and relating it back to the emissions. However, that determines the composite sum of all sources, while you are often interested in the individual sources. If there is no awareness of this beforehand, the entire model project may prove to be very disappointing. The central question of which sources require action then cannot be answered.

Defining emission factors is a point which requires great scientific research. It is relatively simple to take measurements before and after purification, in order to determine the emission factor. However, factors such as flushing or leaching are much more complex and often also determined locally. A number of model outputs can be validated for specific field studies. However, the individual process descriptions in deterministic/dynamic models are almost impossible to validate. In regional studies, a statistical validation will sometimes be possible, whereby the distribution of measured values is compared with a distribution of calculated values.

Due to the wide diversity of substances, emission routes, emission factors and emission explicative variables, we cannot possibly sum up all the important calibration factors. We shall therefore limit ourselves to the nutrient models below. Specific calibration parameters are then:

- The nitrate concentrate in the groundwater;
- The phosphate state of the soil;
- The nutrients drainage in the field;
- The nutrients discharge of farms (agricultural statistics);
- To a lesser degree: the nitrogen and phosphate concentration in the surface water.

In order to calculate good results for nutrients models, reliable data must be available on the following critical factors:

- All factors which lead to a certain manure surplus at the field level (fertilisation minus crop absorption);
- Biological/chemical factors in the soil (mineralization, denitrification, binding and fixing of phosphate);
- Hydrological factors (groundwater level variation, distribution of water discharge among various means of drainage, depth of the system under consideration);
- Initial conditions. Estimation of the initial conditions is often part of the model itself in regional model studies. A strategy must be developed for this purpose which depends on the model and the basic data available.

Step 6: Interpret the results

Due to emission models being generally difficult to calibrate, interpretation must be carried out with the utmost care. The main error which can be made is to miss out this step. In practice however, it is regularly skipped due to a lack of time, as in the other models.

Step 7: Report

Just like the previous step, very careful reporting is necessary, due to the often great uncertainties. They must also be clearly communicated to the client.

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Good Modelling Practice Handbook

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