# The Process of Model Building and Simulation of Ill-defined Systems: Application to Wastewater Treatment

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ABSTRACT

In recent years, there has been a growing awareness of the ill-defined nature of environmental processes. To provide a frame of reference for discussions regarding ill-defined systems, a taxonomy and terminology of the modelling and simulation of systems is presented. Due to the complexity of ill-defined systems, it is not only necessary to describe the nature of models, but also to describe modelling procedures. This enables the modeller to obtain the model which best fits his goals (optimal model). For meaningful description of models, different model formalisms will be presented. Furthermore, modelling procedures will be described at a generic level and different model formalisms will be presented. Throughout this presentation, Waste-Water Treatment Plants and processes occurring within these plants will illustrate the definitions given.

**Key words**: mathematical modeling, simulation, ill-defined systems, wastewater treatment.

## 1 INTRODUCTION

In recent years, the use of mathematical models has gained importance in environmental studies. Environmental processes, such as those occurring in Waste-Water Treatment Plants (WWTP's), are often referred to as examples of ill-defined systems. Compared to the modelling of well-defined (*e.g.*, electrical, mechanical) systems, ill-defined systems modelling is more complex. In particular, the difficulty in choosing the "right" model is very apparent.

In the sequel a rigorous approach to modelling of ill-defined systems is presented. Illustrations are given for the case of WWTP's.

In order to develop a framework for the modelling of ill-defined systems, some definitions concerning the modelling and simulation enterprise are given. Thereafter, a procedure to guide the modeller in finding the "right" model is

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presented. This modelling procedure consists of interactions between information sources and activities. Models, the focal point of the modelling enterprise, may be described in different formalisms. A common formalism classification will be presented.

## 2 MODELLING AND SIMULATION CONCEPTS

In most sciences studying ill-defined systems, researchers have very different scientific backgrounds. In particular in the field of environmental sciences this is very apparent. Biologists and ecologists, need to collaborate with for example, mathematicians, statisticians or computer scientists. This diversity may result in very interesting approaches but also in communication difficulties [6]. The main goal of this section is to provide an unambiguous terminology. The understanding of the modelling and simulation definitions will also help scientists to better carry out their task. For an in depth presentation of modelling and simulation concepts the reader is referred to Klir [15] and Zeigler [34].

### 2.1 Basic Entities and Processes

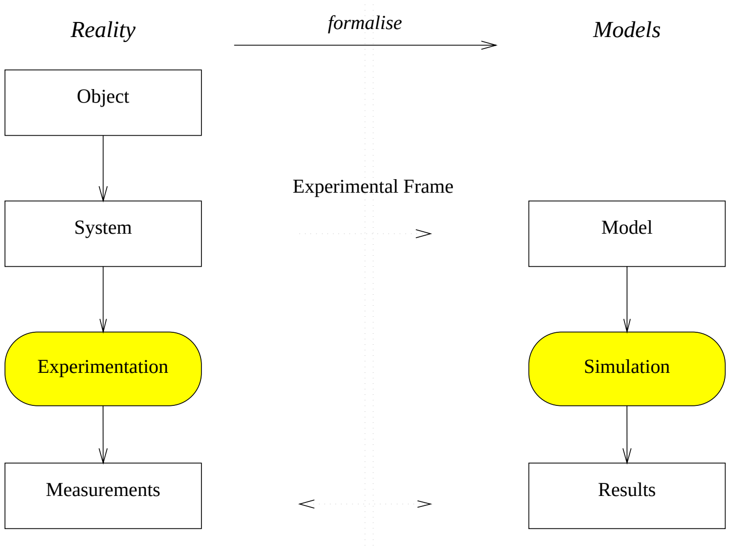


Fig. 1. The real world and its abstraction

In modelling and simulation three basic entities, *i.e.*, a *system*, an *experimental frame* and a *model*, as well as two main processes, *i.e.*, modelling and observation of behaviour, can be defined. A system, is defined as a potential source of behaviour. A system is an object in the "Real World" (figure 1), observed within a certain experimental context. An object is really a purely hypothetical concept because a perception of reality is determined by our own capacity for observation [25]. As such, we must always define the experimental frame within which reality is observed and modelled.

The concept of experimental frame refers to a limited set of circumstances under which a system is to be observed or subjected to experimentation. As such, the experimental frame reflects the objectives of the experimenter who performs experiments on a system [34] (see Figure 2).

In its most basic form, an experimental frame consists of two sets of variables, the *frame input variables* and the *frame output variables*, matching the systems inputs and outputs, and a set of *frame conditions*, matching the conditions under which the systems' behaviour is to be observed. On the input variable side, a *generator* describes the inputs or stimuli applied to the system or model during an experiment. On the output variable side, a *transducer* describes the transformations to be applied to the system outputs for meaningful interpretation. The *acceptor* will complete the experimental frame. It determines whether input/output pairs "fit" certain acceptance criteria (frame conditions) such as "goodness of fit".

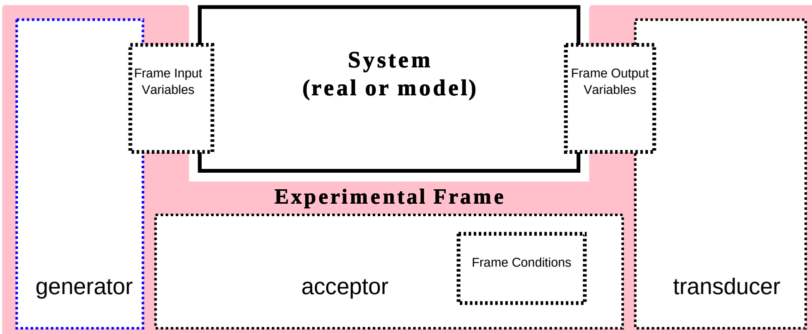


Fig. 2. System versus Experimental Frame

The third entity, a model, is an abstract representation of a system and its experimental frame. A model can be defined as anything which is capable of generating behaviour resembling the behaviour of a system within its experimental frame. The process of producing a model, for a given system and experimental frame is called modelling.

Systems as well as models are capable of generating behaviour. The processes of generating behaviour of systems and models are called experimentation and simulation, respectively. Simulation can be seen as experimentation on a model, *i.e., virtual experimentation*. Both experimentation and simulation result in (sets of) data.

The success of using models is mainly due to the relatively easy and cheap simulations. A model can be used to design a system, even before the system is built. A good example is the use of models to design the capacity of WWTP's. Moreover, models can be used to gain insight in a systems behaviour or to control it.

In the following two important model properties are defined. These properties lead to the definition of an ill-defined system.

### 2.2 Model Formalism and Validity

As a result of the various application areas, the different levels of a priori knowledge, the diverse goals, etc., a plethora of *model formalisms* were developed. Model formalisms play an important role in modelling and simulation of complex and ill-defined systems. In modelling, the most optimal model formalism must be chosen to describe the system. This choice has an impact on the simulation of the developed model. Currently, different formalisms require different simulation tools to simulate the model in an optimal way.

Some commonly used formalisms [27] are DAE (Differential Algebraic Equations), PDE (Partial Differential Equations), SDE (Stochastic Differential Equations), Bond Graphs[7], DEVS (Discrete Event System Specification) [34] and System Dynamics. Note that data can also be seen as a particular model formalism. In complex systems it is often necessary to combine different formalisms for different sub-systems. Figure 3 gives an example of such a system. At the top level, a system of WWTP's and storm-water tanks (buffer tanks) can be modelled using the DEVS formalism. Taking events (rain events, toxic discharges) into account, one must schedule the distribution of the wastewater loads between the WWTP and the tanks. In this case, a WWTP will be modeled as a "black box" with a given time delay and a given capacity. However, the WWTP can be seen as a system consisting of components such as aeration tanks and settling tanks. Those components can be modelled using the PDE or DAE formalism.

When a real world object is studied under particular experimental conditions, it is called a *system*. The experimental conditions are formalised in an *experimental frame*, and the system behaviour is formally represented as a *model*. different *model formalisms* may be used to represent a model. An *experiment* performed on a system can be reproduced in a *virtual experiment* or *simulation*. However, the question remains whether a specific model of a given system, under known experimental conditions is, through simulation, able to

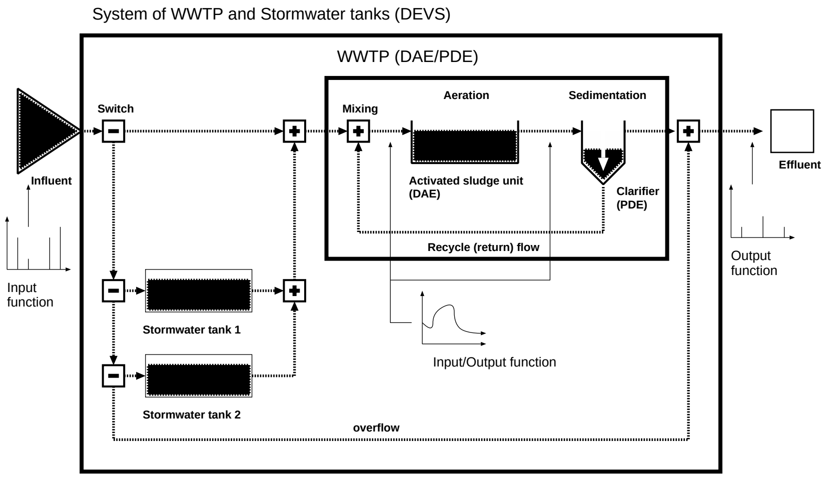


Fig. 3. model formalisms in WWTP's

*reproduce system behaviour* to a desired *level of uncertainty*. A model's ability to mimic system behaviour is referred to as "validity"[1]. Three different levels of model validity are defined [23]

- *replicative:* the model is able to reproduce the input/output behaviour of the system.
- *predictive:* the model is able to be synchronised with the system into a state, from which unique prediction of future behaviour is possible.
- *structural:* the model can be shown to uniquely represent the internal (structural) workings of the system.

With each ascending level, the validity of the model becomes stronger causing an increasing need for information and justification. Conversely, this implies that, for example, a replicatively valid model does not need to be valid at the predictive level.

### 2.3 Ill-defined or Well-defined

As mentioned before, "system" is a purely theoretical concept and will always be viewed through an experimental frame. Therefore, for classification purposes, one has to define the properties of a model describing the system. A well known and often used classification of systems is that between well-defined systems and ill-defined systems. General examples of well-defined and ill-defined systems are electrical or mechanical system and social or environmental systems, respectively. Both well-defined and ill-defined are often used terms but they also lead to confusion; an ill-defined system for one scientist may be well-defined for another. Hence, a definition of both well-defined and ill-defined must be given. Moreover, by understanding the definition of an ill-defined system one is aware of the pitfalls in using models for ill-defined systems.

A well-defined system can be defined as a system of which it is possible to build, within an experimental frame and given the current *formalisms* and techniques, a structurally and behaviourally completely specified and, up to a certain level of accuracy, *valid* model. An ill-defined system can be defined as every system which is not a well-defined system.

As an example, consider as a system and its experimental frame an aeration tank with a constant temperature and volume and as relevant variables the inflow ($Q_{in}$) and the outflow ($Q_{out}$). If one is only interested in the general flow this system is a well-defined system. Its internal workings can be described by the mass balance. The system will become ill-defined if the accuracy is refined, *e.g.*, one wants to describe the system on the level of internal flows (turbulence), or the output oxygen concentration is added as a relevant variable (change of experimental frame). Note that the well/ill-definedness of a system also depends on the current formalisms and techniques, *i.e.*, a currently ill-defined system may become well-defined in future by using a new formalism or technique.

Despite the ease of use and general applicability of models and simulation, one has to be cautious in using these to describe ill-defined systems. Being ill-defined implies that there will always be a chance that the behaviour (or structure) of the model describing the system will be different from the system itself, *i.e.*, that the model will not be valid.

## 3 THE PROCESS OF MODEL BUILDING

The process of model building is, in many ways, not unlike the process of software development. In both cases, very specific detailed knowledge must be acquired and represented. After development both the model and the software programme must meet strict requirements. Unlike the process of model building, the software development process has often been a topic for research. This resulted in software development models such as the "spiral model" [4] or the "entity process model" [13]. In [10] the spiral model is used as a methodology for the development of computer-based models of complex systems. The model building process given in this paper is more similar to an entity process.

Roughly defined, the process of model building consists of constant interactions between *information sources* and *modelling activities*. A schematic representation of the process of model building is given in Figure 4.

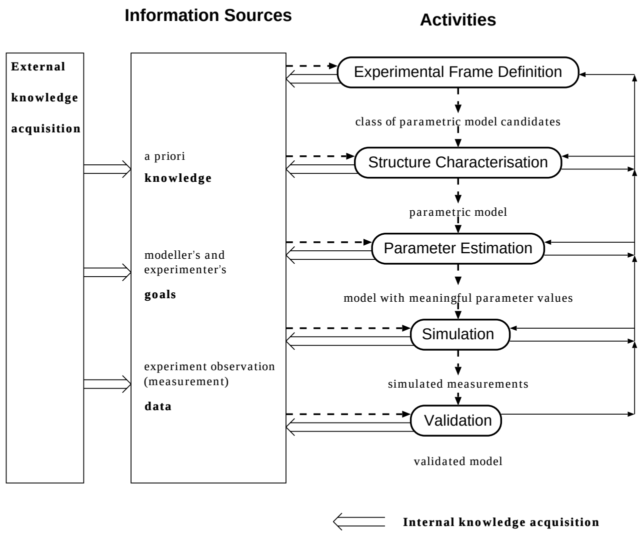


Fig. 4. the process of model building

From Figure 4 may be concluded that all activities have to be performed top down. However, a previously performed activity can be repeated depending on the outcome of the current activity. During the whole process of model building there exist constant interactions between activities and information sources. To ensure an equal importance of each information source, the modeller must justify each activity by using all information sources.

It has to be mentioned that since Figure 4 is a schematic representation (model) of a very complex and sometimes intuitive process (ill-defined system), it must not be taken for granted. Its only use lies in the rough guidelines it gives.

In the following the information sources and activities will be described.

### 3.1 Information Sources

Three major information sources can be identified:

- *Goals and purposes*
- *A priori knowledge*

- *Experimental data*

The *goals and purposes* of the model user will orient the modelling process. The goals will, for example, determine the complexity of the model. The *a priori knowledge* available reflects the knowledge already gathered. This a priori knowledge often consists of (physical) "laws", such as the mass conservation law. A priori knowledge not always has to be developed within the (scientific) field in which the system to be described lies. Especially in environmental sciences, which is a rather new science, some of the "laws" used have been developed in other sciences and subsequently been adopted to model environmental systems. The *experimental data* are the observations of the systems behaviour. Experimental data may be collected to guide the modelling process or to validate the developed model.

Depending on the importance given to a priori knowledge and experimental data, two different modelling methodologies have been developed: *deductive* modelling and *inductive* modelling. Deductive modelling assumes a priori knowledge as the most important information source. Starting from the a priori knowledge, a deductive modeller will develop a model by using mathematical and logical deductions. Experimental data is only used to accept or reject the model or the hypotheses made during the modelling process. The observed behaviour (data) is assumed to be the most important information source in inductive modelling. Whereas deductive modelling has its roots in physics, inductive modelling is based on statistics. Using the available data of a system, an inductive modeller will try to find a model describing the data. Often a part of the available data will be used to accept or reject the model or the hypotheses made during the modelling process.

Both deductive modelling and inductive modelling have a fundamental problem with the lack of a priori knowledge and data, respectively. Therefore, pure forms of both modelling approaches will seldom yield optimal results in modelling ill-defined systems. This implies that a good mix between the two approaches is needed.

During the last decades both deductive and inductive modellers are approaching this mix more and more closely. Deductive modellers have become aware that, for ill-defined systems, the measured data can never be duplicated by the simulated data. This led to an increase of statistical techniques and the concept of *uncertainty* [3]. Uncertainty is a measure of the probability that the simulated data match reality. Uncertainty and the analysis of uncertainty (uncertainty analysis) will play an important role during the modelling activities. As opposed to using more statistical techniques, inductive modellers' more and more use the a priori knowledge to compare their results with [31].

Before starting the modelling process one must acquire and structure the information sources (*external information acquisition*). The information sources can also be updated during the modelling process (*internal information acqui-*

*sition*). While modelling it is the modellers task to find a balance between the use of the a priori knowledge and the experimental data. This balance will, during each modelling activity, depend on the current availability of both information sources.

### 3.2 Modelling Activities

As mentioned before, five main modelling activities exist. All these activities will shortly be discussed below.

*Experimental Frame Definition*
As a model describes a system *together with its experimental frame*, the experimental frame definition must be the first modelling activity.

By defining an experimental frame, the modeller must define the systems inputs, outputs, and frame conditions. These can be accompanied by generators (inputs), transducers (output) and acceptors (conditions).

Actually, if the main focus is to model a system, the first experimental frame definition is not oriented towards defining the exact properties of the experimental frame. The exact properties only need to be specified before doing an experiment on the system or model. From a computer scientists' point of view one might say that the first experimental frame definition is the definition of the *experimental frame class* whereas experiments are done using *objects* of this class[1].

In activated sludge systems [12], the inputs and outputs may, for example, be defined as the flow rate and the concentrations of dissolved substances (such as dissolved oxygen), particulate substances and inert substances. Conditions are defined as, for instance, constant temperature and/or constant and neutral pH. The main inputs and outputs in water quality systems [26] are dissolved oxygen and biochemical oxygen demand. In order to couple (connect) models (such as WWTP's with receiving waters) the experimental frame classes of both models must be the same. Moreover, the units of all inputs and outputs must be the same. Conversion of units can be performed by transducers. Since the experimental frame classes of activated sludge systems and water quality systems are not the same, coupling of the models of these two systems has appeared to be rather difficult. Currently, research is being done to unify the experimental frame classes of WWTP's and, respectively, sewers [11] and receiving waters [18, 20, 22].

*Structure Characterisation*
Structure characterisation (or structure identification) addresses the question

[1] Viewing the experimental frame as a model the first definition is to define the structure of the frame. An experiment is done using this model with known parameter values.

of finding an adequate model structure. Its aim is to reduce the class of models which are able to mimic the given system and experimental frame, its internal structure and behaviour. In [23] some guiding principles for structure characterisation are given:

- *physicality*: A model must bare close resemblance to reality.
- *fit*: The experimental data available should be explained by the model as well as possible.
- *identifiability*: After structure characterisation, it must be possible to estimate the parameters.
- *parsimony*: The most simple explanation for phenomena must be found.
- *balanced accuracy*: The most useful model is often a balanced compromise of the previous principles.

The principles of physicality and fit are closely related to two information sources, a priori knowledge and the data, respectively. As a proper mix of the available information sources is needed to derive an optimal model, a proper mix of the above principles is needed to arrive at an optimal model structure.

The principles of identifiability and parsimony are closely related together. A structure containing an unidentifiable parameter is often assumed to be superfluous. However, if unidentifiability occurs not only the model structure, but also the information source used for identifying the parameters, need to be questioned.

In practice, structure characterisation techniques can be classified into two main classes; *a priori* techniques and *a posteriori* techniques. A priori techniques are capable of selecting models without the need of fitting the model(s) to the available data. These techniques include techniques which select models based upon the available a priori knowledge and the given experimental frame [8], techniques based on neural nets [30] and techniques using observers or filters [2, 24, 32].

In contrast with a priori techniques, a posteriori techniques do need the parameters to be estimated before selecting a model. These techniques are most widely used and include criteria such as the well known AIC, FPE [16] or BIC [19]. Other techniques included are, for example, statistical hypothesis tests (F-test) or analysis of residuals [21]. Using a biological process, a comparison of techniques, including both a priori and a posteriori ones, is given in [29].

As may be concluded from the above, structure characterisation issues cannot strictly be separated from parameter estimation. Another modelling activity closely related to structure characterisation is model validation. Both activities may, approximately, use the same techniques. However, while structure characterisation is focused on the selection of a model structure among other structures, model validation is focused on finding flaws in the developed model.

*Parameter Estimation*
Parameter estimation will provide parameter values (and values for initial conditions) for a chosen model structure. Parameter estimation aims to reduce the class of parameters, using the fit principle defined previously. It is based on the optimisation of a criterion defining the goodness-of-fit. Well known criteria are maximum likelihood and minimum variance[2].

Estimation of parameters can either be done recursively (on-line) or not recursively (off-line). Recursive estimation updates the estimation of the parameters every time a new observation is available. One of the best known recursive estimation algorithms is the extended Kalman filter [14]. Non-recursive estimation will use a batch of data to estimate the parameters. The criterion is minimised using optimisation algorithms such as simplex [17] or direction set methods [5].

An important concept in parameter estimation is that of identifiability (see the above on structure characterisation). By identifiability is meant the ability to estimate (identify) an (almost) unique value for the parameter, using the given model and observations. A parameter is said to be unidentifiable if only a large set of parameter values can be identified. Identifiability of parameters may be *theoretical* or *practical*. If a parameter is theoretical unidentifiable, *i.e.*, it can not be identified given only the model structure, one needs to return to the structure characterisation. Practical unidentifiability occurs if the parameters are unidentifiable given the model structure *and* the available data. In this case, one may be able to increase the information contained in the available data using *optimal experimental design* [28].

*Simulation*
An experiment performed on a model, a virtual experiment, is called simulation. It consists on generating and observing the behaviour of a model together with its *completely specified* experimental frame. Simulation is used to gain information about the model and, if the model is validated, to gain information about the system described by the model. After validation, simulation results can be used to design, analyse or control a system.

Simulation is performed by a *simulator*. A simulator consists of an *internal representation* and a *solver*. The internal representation is a representation of the model which can be understood by the solver. The solver "solves" the

[2]If the model is deterministic the criterion reduces to the least squares criterion.

model, *i.e.,* generates behaviour. Both the internal representation and solver depend on the model formalism [27].

Simulation is often said to be optimal if it can be done within a certain *accuracy* and *time instant*. Thus, within a given time instant, the simulator must provide output which resembles the "real" model output within a given accuracy. Both the accuracy and time instant depend on the goals and purposes of the modeller and user, the formalism and the current techniques.

Due to the ability of duplicating the complex system's behaviour and activities at a high speed and accuracy, computer software are mostly used as simulators. Earlier, simulators were rather isolated, *i.e.,* only capable of simulation. However, nowadays simulators often are embedded in a software tool for both modelling and simulation [9].

*Validation*

As validity is the model's ability to mimic system behaviour, validation is the process in which the validity of a model is determined. Some principles for model validation are given in [1]. Three levels of validity can be identified namely the replicative (reproduce data), the predictive (predict behaviour) and the structural (describe internal structure) level.

According to the definition of ill-defined systems, a model describing such a system can not be validated *i.e.,* it will never be valid. Therefore, in modelling ill-defined systems, the term "falsification" is preferred over "validation". With falsification is meant the process of trying to falsify (to find errors in) the model. If it appears to be very hard to falsify the model, the confidence in the model might increase (decrease of uncertainty) but validity will never be proven.

The most common falsification (validation) of models describing ill-defined systems is that on the replicative level. A model is tested using the same batch of data used for structure characterisation and parameter estimation. Falsification on a predictive level is often done using two data sets. The model is developed using one data set and validated using the other (*cross validation*). Concerning the level of validity, one must be aware that a high confidence level on the replicative level does not imply a high confidence level on a higher level (predictive or structural).

Methods used in validation often are the same as those used in structure characterisation. These include statistical hypothesis tests (F-test), residuals tests [21] and tests using different observers or filters [33].

After having tested the model's ability to mimic the system's behaviour it can be tested (validated) whether the model fits the goals of the user. These tests include tests for technical applicability, universality and uncertainty.

## 4 CONCLUSIONS

In recent years more and more different scientific fields have been involved in the modelling and simulation of systems. Moreover, the complexity of ill-defined systems has made it necessary to describe a procedure according to which the modelling will proceed.

By presenting both a taxonomy of modelling and simulation of systems and a modelling procedure, the above has provided a frame of reference for further discussions and research.

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