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-definedness 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 will be presented. Due to the complexity of ill-defined systems, it is not only necessary to describe the nature of models, but also to describe some procedures according to which the modelling will proceed. This will enable 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 serve as illustrations of the definitions given.

Introduction

In recent years, mathematical models have 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 modelling and simulation enterprise are given. Thereafter, a modelling procedure which may guide the modeller to find the "right" model, is presented. This modelling procedure consists of interactions between information sources and activities. These information sources and activities will be discussed. Models, the subset of the modelling enterprise, may be described in different formalisms. A common formalism classification will be presented.

Modelling and Simulation Concepts

One of the most important definitions in modelling and simulation is the definition of a *system*. A system is defined as a potential source of behaviour. It is *observable* when its behaviour can be transformed into data (information). Knowledge about given systems can be acquired through experiments. An *experiment* is defined as the process of causing (by known stimuli) and observing the behaviour of a system. In other words, given the inputs, the system outputs will be observed. In order to perform experiments on a system, its *experimental frame* has to be defined. 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.

A way to organise collected knowledge about a system, *given its experimental frame*, is by means of *modelling* and *models*. In a very broad sense, a model is anything which is capable of generating behaviour resembling the behaviour of a system (given its experimental frame). In this paper only parametric models will be discussed. A parametric model, is a model consisting of *parameters*, where parameters are defined as constants or an experiment.

All systems may roughly be divided into two subclasses: *well-defined* systems and *ill-defined* systems. However, there is a fundamental problem in classifying systems. All information of a system can only be given by means of a model. Therefore, in order to classify, one has to define the properties of a model describing the system. Klir [1] solves this problem by defining epistemological levels at which the system may be observed and Zeigler [5] postulates a Base Model, a hypothetical model capable of describing

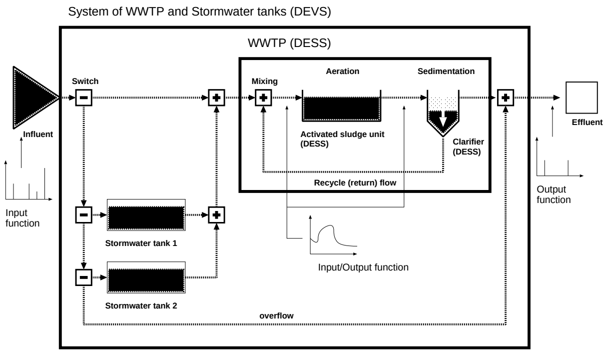

Figure 1: model formalisms in WWTP's

all possible behaviours of the system. Here, a well-defined system is 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, within a certain *accuracy*, *valid* model[1]. An ill-defined system can be defined as every system which is not a well-defined system.

The advantage of using a model to describe a system together with its experimental frame is that models are easier to experiment with. Experiments performed upon models are called *simulations*. Using simulations on a model instead of experiments on the system (and the experimental frame) it describes, has the advantage of *all* inputs and outputs being accessible. Hence, inputs or outputs can be applied to the model which lie outside the experimental frame of the system.

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 exist 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.

Model Formalisms

Before describing the process of model building first model formalisms [4] will be discussed. During the whole process of model building model formalisms play an important role. In order to get an overview of the existing model formalisms, they are often being classified. However, the defined classes will never contain all formalisms. A well known classification is a classification given by [5]:

- *Differential Equation System Specification (DESS)*: Assumes continuous independent variables. The models are specified in differential equations which express the rate of change in the state variables.

- *Discrete Time System Specification (DTSS)*: Assumes discrete independent variables. The models are specified in difference equations which express the state transition from one time (and space) instant to the next.

- *Discrete Event System Specification (DEVS)*: Assumes a constant time base (the only independent variable) but the trajectories are piecewise constant, *i.e.*, the dependent variables remain constant for a variable period of time.

An example of the use of these three model formalisms in wastewater treatment is given in Figure 1. At the highest 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. It may be modelled using the DESS formalism (PDE's or ODE's), or the DTSS formalism. Thus, within one system different formalisms may be used to describe its components and interactions.

[1]The concepts, formalisms and valid, will be explained in a later stage.

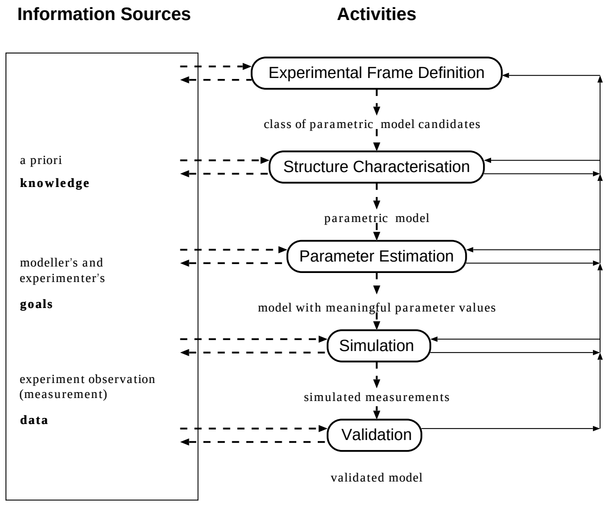

Figure 2: the process of model building

Another classification exists of (i) *deterministic*, (ii) *stochastic* and (iii) *probabilistic* classes. Whereas deterministic models originate from deductive modelling, probabilistic models originate from inductive modelling. Stochastic models can be seen as a combination of both. They assume one or more deterministic model attributes to have a statistical distribution.

The Process of Model Building

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 2.

From Figure 2 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 2 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.

The next sections describe the informations sources and activities.

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.

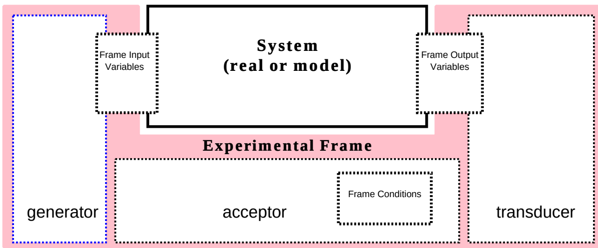

Figure 3: System versus Experimental Frame

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. Inductive modelling assumes the observed behaviour to be the most important information source. 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 acceptable results in modelling ill-defined systems. This implies that a good mix between the two approaches is needed.

A good mix may only be obtained by (i) letting both the a priori knowledge and the experimental data influence the whole process of model building, and (ii) define a model formalism which can be used during both modelling approaches. A step towards a more general formalism is the concept of *uncertainty* [2]. Experience with the use of deductive modelling methodologies to model ill-defined systems has led to the conclusion that the systems behaviour (experimental data) could never be duplicated by the model output. Uncertainty was introduced as a measure for modelling errors such as errors in the model structure or in the parameter values. This implies that uncertainty can also be seen as a measure of the probability that a model output is a plausible system output. This probability is completely defined by the *probability density function (pdf)* of the model output. In order to obtain the model output pdf one must assume that the modelling errors in the model obtained by deductive modelling have an a priori statistical distribution. This distribution may be obtained using inductive techniques.

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.

Referring to a limited set of circumstances under which a system is to be observed or subjected to experimentation, the experimental frame reflects the goals of the experimenter [5] (see Figure 3).

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 the system's output "fits" the conditions given.

For WWTP's inputs and outputs may, for example, respectively be defined as the incoming and outgoing wastewater flow, their substrate concentration and their dissolved oxygen concentration. However, the biomass within the aeration basin or the reaeration constant of the basin (in current models defined as a state variable and a parameter, respectively) may also be outputs. The conditions, which will be checked by the acceptor, may for example be defined as aerobic conditions. For example, consider the conditions being defined as aerobic and, during experimentation, it is measured that the oxygen concentration is zero. The acceptor will now conclude that the conditions do not hold at that particular time instant and the outputs measured in that time instant must not be taken into account during further analysis. In the observation of the behaviour of WWTP's often no generators are used; the inputs are not generated with known stimuli. An example in which transducers can be used is *risk analysis*. Here, the observer is, for example, only interested in all dissolved oxygen concentration below a certain threshold.

Structure Characterisation

Structure characterisation addresses the question of finding an adequate model structure.

Its aim is to reduce the class of models which are able to model the given system and experimental frame. The output class of structure characterisation may consist of more than one model structures, in which case each modelling activities (after structure characterisation) will be performed simultaneously for all model structures. In [3] 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.

Functions exist which, in order to reduce the class of models, will balance all or some of these principles. Such functions may, for example, be information criteria such as the AIC and BIC criteria. These criteria balance the fit and parsimony principles.

Furthermore, it has to be mentioned that structure characterisation issues cannot strictly be separated from other modelling activities, such as parameter estimation and validation.

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 some criterion defining the goodness-of-fit such as Least Squares, Maximum Likelihood, *etc.*. Estimating parameters of ill-defined systems often results in a set of parameter values which have an (almost) equal goodness-of-fit criterion. A measure for the quantity of the set is parameter uncertainty. If the obtained set is very large one speaks of the parameters being *unidentifiable*. The identifiability may be *theoretical* or *practical*. Theoretical identifiability gives an answer whether, given the model structure, the parameters are identifiable, whereas practical identifiability gives an answer whether, given the available experimental data, the parameters are identifiable. Practical identifiability can be increased by increasing the information contained in experimental data using *optimal experimental design*.

Simulation

As defined earlier, simulation is an experiment performed on a model. In most sciences simulation consist of, given the inputs, determining the output trajectory of a model. However, it may also consist of obtaining information about the model. For example, the number of state variables. 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 model, *i.e.*, generates data. Both the internal representation and solver depend on the model formalism [4]. Although these terms originate from computer science, they are generally applicable. For example, if one is able to solve a model analytically, the internal representation will be the model itself and the solver will be the person who solves the model.

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.

Validation

Validation refers to the capability of the model to, up to a certain level and within a certain accuracy, replicate the system. Three different levels of model validity may be identified [3]

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

With each ascending level, the validity of the model becomes stronger causing a growth in the need for information and justification. This implies that, with each ascending level validation becomes harder.

As defined previously a model describing an ill-defined system will never be valid. One may only falsify the model. Therefore, from a practical point of view one should better use the term *falsification* when referring to the "validation" of ill-defined systems. A common error among scientists it that, when they could not falsify the model at the replicative level, resulting in a high confidence level, start to use it at the predictive level. However, at predictive level the confidence level may well be very low.

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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