Summary

Mathematical modelling is an important activity in environmental science. Models are used for understanding, prediction, design and optimization. A mathematical model is always a simplified representation of the natural system it attempts to describe. It represents the conceptual thinking about the system processes in a mathematical formulation and translates this into programming code. Once a suitable model has been identified, it becomes a powerful tool for both scientists and engineers.

There is no such thing as the *super-model*, applicable to all situations. Nature is a highly heterogeneous system, which requires a tailor-made description to be effective. The appropriateness of a model structure needs to be sufficiently evaluated taking into account the modelling purpose and the available observational data.

Determining a priori which model structure is most appropriate for a given model application, is a challenging problem. This makes the identification of a suitable model structure an iterative process. Each model structure represents a hypothesis which can be confirmed or rejected by the available observations.

In contrast to this need for adaptation and flexibility, a culture of monolithic model software applications with limited flexibility, arose. The same legacy models are used over and over again, ignoring the appropriateness of the model structure as correct system representation. It resulted in a practice of model parameters fitting instead of model structure identification.

The aim of this dissertation is to propose and apply a framework for improved model structure evaluation and identification. The proposed diagnostic approach combines the flexibility to continuously adapt model structures with the means to properly evaluate these alternative representations.

Flexibility in model development is provided by a wide range of existing software environments and frameworks, that however these do not always support a rejection framework. A minimal set of requirements that needs to be fulfilled is extracted: (1) the support to alternative representations of the considered processes, (2) the ability to construct alternative configurations, (3) a clear separation between the mathematical and computational model and (4) accessible and modular code implementations.

The model evaluation generalizes the idea of model calibration towards a combined and iterative process of parameter and process (model structural) adaptation. Practical identifiability, both in terms of parameters and model components, is the guiding principle during the evaluation. This means that model structures should contain sensitive parameters that are not cancelling each other out. In other words, process descriptions should have a clear function that can be consistently identified by the available observations.

The identification of parameters in complex models is supported by sensitivity analysis. Different methods for sensitivity analysis are audited and implemented as a modular and reusable set of functionalities to support the model evaluation process. To accommodate the variety of modelling purposes, the design is targeted to enable fast and easy construction of a wide range of aggregated performance metrics. Together, this provides a range of tools available to future modellers and initiates a library that can be further developed by and for the environmental modelling community.

In a first application, the identifiability and model calibration of a respirometric model with an additional time-lag component is analysed by the available tools. The analysis reveals that experimental data for which the ratio between the added substrate and the biomass is high enough need to be available to properly identify the time-lag component. The appropriateness of the model structure is confirmed and is in line with earlier studies, however subject to the assumptions taken.

For the remainder of the dissertation, lumped hydrological models are studied, describing the relationship between rainfall and runoff.

A first hydrological application studies an ensemble of hydrological model structure alternatives, representing different configurations of the already existing Veralgemeend Hydrologisch Model (VHM). Based on the observed runoff time series, the differentiation of the model structures is not feasible using the chosen set of performance metrics. A lack of parameter identifiability of the individual structures hampers the attribution of model performance to individual model decisions. Hence, there is no added value of creating an ensemble of highly alike structures when the identifiability of the model structures is not guaranteed. The identifiability of the individual model structures is a necessary condition to compare model structural alternatives in terms of performance.

To enable the interpretation of the appropriateness of model structural decisions when facing unidentifiability, a qualitative method for model component sensitivity analysis is introduced. The method enables to make qualitative statements about the relative influence of model structure components towards a chosen performance metric. The application on the ensemble of model alternatives results in actual suggestions for model structure adaptation.

The last application seeks to diagnose structural errors in two existing lumped hydrological models that are currently applied in operational water management (PDM and NAM). To comply to the requirements of the diagnostic approach, a conversion of both model structures is executed towards a system dynamics representation. It enables the decoupling of the mathematical and computational model and converts both models into a flexible entity supporting alternative model structure configurations.

Besides the implementation in a flexible modelling environment, a standardised matrix representation of lumped hydrological model structures is proposed. The latter provides a common format to communicate about the applied model structure, supporting a reproducible scientific application of lumped hydrological models.

To identify the model deficiencies, the DYNamic Identifiability Approach (DYNIA) is applied, a time-variant based method that screens the parameter identifiability as a function of time. In general, similar model performances are observed. However, the model structures tends to behave differently in the course of time. Based on the analyses performed, the probability based soil storage representation of the PDM model outperformed the NAM structure.

In a concluding perspective, a visionary roadmap towards an improved scientific practice in environmental modelling is given, relying on the capability of open science as the engine for collaborative development.