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Good modeling practice of water treatment processes

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Abstract. Models for water treatment processes include simulation, i.e., modelling of water quality, flow hydraulics, process controls and design. Water treatment processes are inherently dynamic because of the large variations in the influent water flow rate, concentration and composition. Moreover, these variations are to a large extent not possible to control. Mathematical models and computer simulations are essential to describe, predict and control the complicated interactions of the water treatment processes. An accurate description of such systems can therefore result in highly complex models, which may not be very useful from a practical, operational point of view. The main objective is to combine knowledge of the process dynamics with mathematical methods for processes estimation and identification. Good modelling practice is way to obtain this objective and to improve water treatment processes (its understanding, design, control and performance- efficiency). By synthesize of existing knowledge and experience on good modelling practices and principles the aim is to help address the critical strategic gaps and weaknesses in water treatment models application.

Keywords: good modeling practice; integrated modeling; model application; process control; process dynamics; water treatment process

1. Introduction

Every system can be accurately described by a model. A numerical model is model within a mathematical framework where equations of various types are defined to relate inputs, outputs and characteristics of a system (Jeppsson 2017). The act of simulation describes the use of a numerical model within a software package (called a “simulator”) (Rieger *et al*. 2013). A model is a “simplified representation of a system (or process) intended to enhance our ability to understand, predict, and possibly control the behavior of the system”, In the real world it must be realized that a model is always a simplification of reality. Model is actually a reflection of the modeler’s understanding of reality, its components and their interrelations, described in a relatively simple, yet accurate enough to serve his purpose (Ani 2016). Model results are only useful in practice if the model predictions are reliable (Issa 2009).

Models for water treatment processes can be used for different purposes like understanding of water treatment processes; optimization of water treatment plant design; optimization of process

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control (active control); predictions of the treatment plant performance under changing conditions (scenario studies) (Rietveld 2005, Rietveld *et al*. 2010). With drinking water standards becoming more rigorous, models will become an important tool to assess water treatment plant performance. Simulations using verified and accurate models can be used to obtained valuable information about a process far quicker than experiments and with minimal cost, and will lead to better water quality, reduction in capital expenditure, and more stable performance of a plant due to the increased understanding of the phenomena occurring. However, the future of models and their value to the water field are a function of their proper application and knowledge of their limits.

The behavior of real water treatment processes occurring in a water treatment reactor is complex and difficult to describe mathematically (Akinmolayan 2017, Ani 2016). In many cases, the modeler has to balance complexity with computational efficiency (Wicklein *et al*. 2016). Some of the major problems when trying to model water treatment processes are (Jakeman *et al*. 2018):

- lacking process knowledge (e.g., coagulation, flocculation, settling and filtration mechanism characteristics);
- several different unit processes interconnected by various internal feedbacks;
- highly non-linear processes;
- non-stationary processes;
- time varying process parameters;
- practically non-controllable and highly variable process inputs;
- lack of adequate measuring techniques.

As a general tool which can be of assistance in improving water treatment, the modelling of water processes has confronted many challenges (Serdarevic and Dzubur 2016). Unfortunately, there has been little application of water treatment modeling yet, especially in comparison with wastewater programs. Since the treatment processes involved are physically and chemically heterogeneous, the water and process parameters are generally complex and their mutual interactions nonlinear. Also, despite the long history of water treatment processes, their mathematical analysis is not a mature scientific discipline as possibly expected (Jusic *et al*. 2019).

The existing modeling environment was found to have varying availability and documentation. Processes modelled were also skewed towards those prevalent in the country where each program was produced (Juntunen *et al*. 2012). Good modeling practice (GMP) is a possible way for improvement of modelling development and application in water treatment sector. In this paper the principal features, trends and research needs, of GMP (generally and for water treatment processes) are outline briefly.

2. Water treatment processes modelling

2.1 Processes and mechanizms of water tretament plant

The main task of water treatment plant (WTP) is to produce drinking water quality according to water quality standards which continue to become more stringent. The quality of drinking water is an important matter, because water of low quality may cause health-related and economic problems which have a considerable impact on people’s daily lives (Jakeman *et al*. 2018).

A typical water treatment plant has the combination of processes needed to treat the contaminants in the source water treated by the facility. Water treatment is based on a wide range of unit processes, each contributing to some degree of removal or inactivation of contaminants from the raw water. As a "treatment train", conventional drinking water treatment plant compounds of many unit processes (Fig. 1). Within a perspective of sustainable development, treatment plants must be designed on the basis of technical, economic and environmental criteria (Yoann 2013, Jakeman *et al*. 2018).

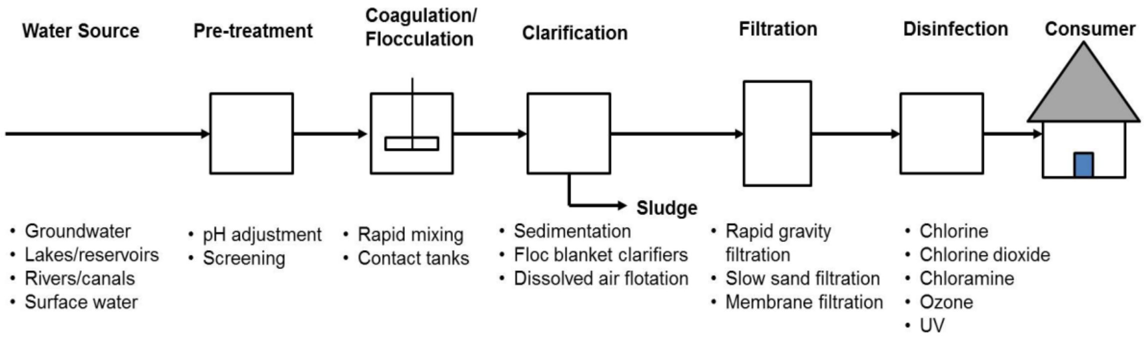

Fig. 1 Typical unit process diagram for clean water treatment plant (with examples of variations) (Akinmolayan 2017)

A water treatment unit process consists of the following mechanisms:

- Flow of water containing (pollution) compounds through the reactor,
- Equilibrium between water and gas or solid phase,
- Transfer of compounds to gas or solid phase,
- Decay in the water and/or solid phase,
- Mass balance between water and gas and solid phase (continuity law).

The number of reactions and different mechanisms that are involved in the water treatment processes are very large. Water treatment unit processes involve a complex interaction of fluid of fluid, mechanical, biological, and chemical processes. Water quality models attempt to simulate mechanisms and changes in the concentration of pollutants as they move through the environment or a reactor (Rietveld, 2005). Most reactions of importance in water treatment occur in more than a single phase, i.e., multiphase reactions.

To achieve an accurate and adequate design of efficient WTPs operating at optimum conditions, commercial simulation software has been developed (Dudley and Dillon 2014). Different models are developed to maximize treatment objective and minimize risk as the basic principle of optimization. Each of these units, its design and operation, could be optimized by modeling. The modeling itself resulted in new knowledge about the treatment processes and proposals for improved operation and design.

2.2 Water treatment model selection

Information Technology (IT) tools for water treatment modeling has formed the link between data, model, active control, research, education/training and design (Fig. 2). People involved in a modelling project - the stakeholders - can be split into modelers and non-modelers. Modelers are defined as a group that have a thorough understanding of the models and their use, whereas non-modelers might not know about the details of the models and how to simulate. Important

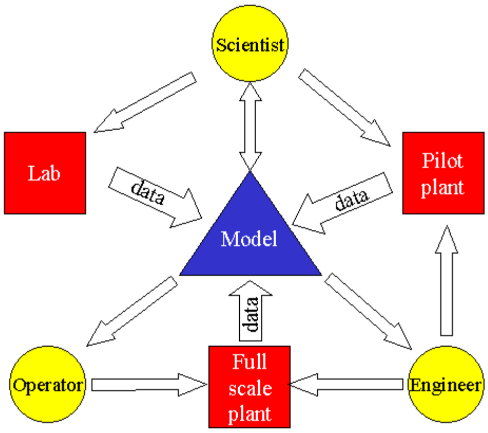

Fig. 2 Linking research to design and training (Rietveld 2004)

considerations for modelers are to set realistic expectations for the modelling and to ensure that model outputs are communicated clearly, and in such a manner that non-modelers are properly engaged and informed in the modelling project objectives and scope.

The knowledge of operators, designers and researchers (non-modelers stakeholders) is based on different information. Where operators get information from the full-scale plant, designers obtain their data from pilot plants and researchers experiment on lab scale (Rietveld *et al*. 2004). Web based, predictive and integrated computer models enabling control and optimization of existing water supply systems with respect to water quality, reliability, customer service level, environmental impact and costs.

Models can be categorized in a number of different ways (Jakeman *et al*. 2018), including by:

• type (e.g., empirical, conceptual, physical, numerical, analytical);
• treatment of space (e.g., non-spatial models, lumped spatial models, grid spatial models);
• treatment of time (e.g., non-temporal, steady state, lumped discrete, dynamic);
• composition (e.g., coupled, integrated); and
• execution (e.g., distributed, web-based).

Various considerations influence the modeler's choice of the most appropriate model. First of all, the model needs to have the ability to estimate the parameters/variables of interest for the study at an appropriate scale and resolution (i.e., temporal, spatial, and thematic) which matches the rate of change in the system of interest (Jakeman *et al*. 2018). Finally, there are contextual factors (e.g., past experience of the modelling team, previous investments in modelling platforms) and constraints (e.g., the requirement to use the same model across the region for consistency) that can be influential in model selection. Some of these models commonly used for water treatment processes are briefly presented below.

Empirical models (EM) are sometimes called "best fit" modeling and is contrasted with mechanistic process-based modeling (Voinov 2008). In best-fit or empirical models, mathematical relationships are derived from data; they may or may not represent actual physical relationships between those factors. They are often used early in modeling projects to explore, interpret and understand available quantitative data. These models are sometimes referred to as black-box models, because they operate as closed devices that process information with no explanation of processes or parameters involved. The empirical nature of the coagulation and flocculation models

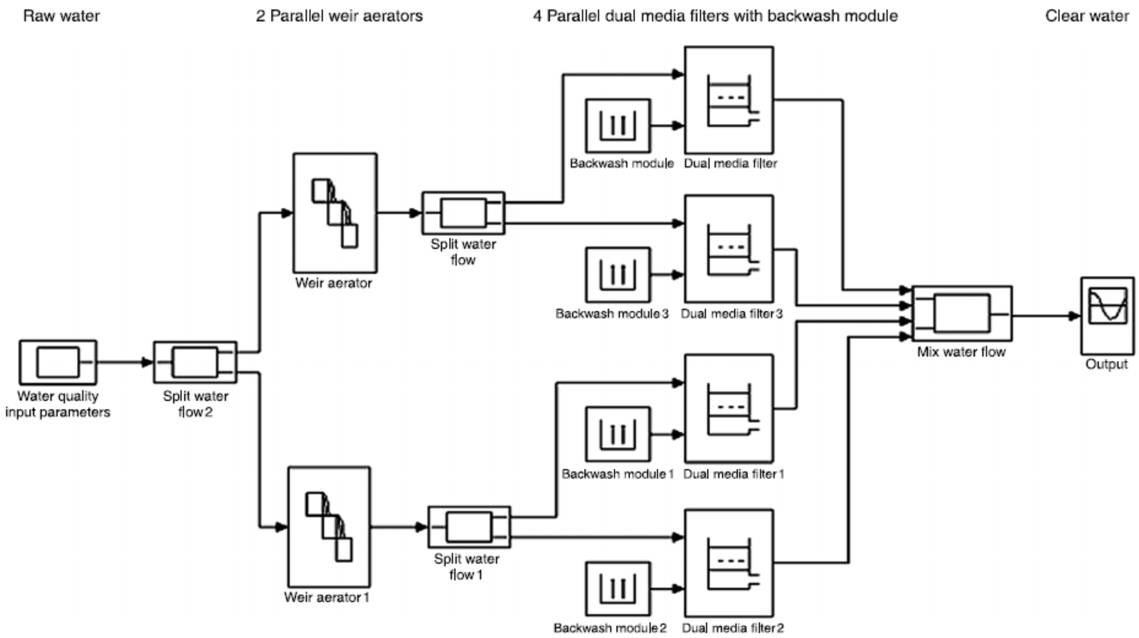

Fig. 3 Example of conection of unit model into integrated model - Stimela environment (Dudley *et al*. 2008)

has meant that the calibrated models could not be applied much outside the calibration region, restricting the degree of optimisation that could be studied. Also, models for Desinfection By-Products (DBP) formation contain empirical equations requiring extensive data for calibration. In the water treatment simulation, the balance between empirical approach and formal mathematical (dynamic and integrated) modelling must be reconsidered (Voinov *et al*. 2018).

System dynamics (SD) is a simulation-based method used to articulate and understand the causal interactions that explain how the system behavior changes over time. Key to the SD method is the representation of a system in terms of stocks (where material, energy, or items are stored and accumulated) and flows (which are rates of exchange between stocks). An SD model provides useful insights into the feedbacks, delays, and nonlinear interactions helping decision makers to see the long-term, system-wide, and sometimes counterintuitive, outcomes of their decisions. Computational fluid dynamics (CFD) modelling in the water treatment field is continuing to grow and be used to solve increasingly complex problems (Wicklein *et al*. 2016).

Also, one of the main problems with the existing work on dynamic modelling water treatment processes individually is a lack of understanding as to how these models fit together to develop a complete water treatment plant. An optimal operation of a water treatment plant requires, as first step, the understanding of the flow behavior along the treatment facility. Water treatment plants are strongly known with the complexity of the model structures and the large number of states and parameters (Ani 2016).

Modelling of the individual steps in clean water treatment has received some attention in terms of design and operation; however, very little has been considered in terms of the integration of the individual steps to create a representation of the overall plant performance which can be used for operational management. The knowledge and understanding of the individual unit gained can direct the efforts in the production of complete water treatment plant models (Fig. 3).

Integrated modeling (IM) is a way of building models by combining or coupling existing models used as components to represent complex systems (Voinov *et al*. 2018). Output from one model becomes input for another model (Fig. 3). Since component models can come from different disciplines, IM is often seen as transdisciplinary exercise. Complex and powerful simulation models can be created by finding existing well-tested modules and plugging them together to represent the systems of interest. With properly documented models and with appropriate user-friendly interfaces, this could potentially be done on the fly, with stakeholder participation. It was expected that an integrated model of the entire water treatment plant could be used as an instrument for operational support and process control to further improve the operation of a drinking water treatment plant, making maximal use of the installed infrastructure and postponing new investments.

Traditionally, the water industry has been sitting within the civil engineering domain rather than the chemical engineering domain, the search for efficient methodologies for operational management and mitigation of risk has led some to consider the use of *Process Systems Engineering (PSE) methods*, in particular, detailed modelling from first principles, which have been highly successful within the chemical industries. The use of PSE methods for design and control within water treatment has been shown to lead to better water quality, cost reduction and to a greater stability performance of the plant as well as to an increased understanding of the individual (unit) treatment processing steps (Akinmolayan 2018, Rietveld *et al*. 2010).

2.3 Processes modeling - trends and research needs

There are a large number of methods and tools that have been used for water treatment processes modeling (Voinov *et al*. 2018). Combining several methods is quite common but replacing one method for another is not. In operational research of water treatment processes, the mixing of integrated and dynamic methods has been viewed as a positive trend. Also, several important trends have been observed in the use of process modelling in recent years. Some of the most important amongst these include (Riegeretal *et al*. 2013):

- The increased use of whole plant models that enable process engineers to investigate interactions between unit processes;
- There is a need for more dynamic and integrated (mechanistic) models for water treatment (Ulinici *et al.* 2014). Increasingly dynamic simulations are being used for optimization and control design. The use of improved online instruments provides the data necessary for dynamic simulations and this trend will continue.

The potential of integrated and dynamic models in water treatment applications is great. However, to date this potential has not been fully exploited. One of the reasons for this, next to lack of training for practitioners, is lack of guidance of good modeling practice with respect to computational fluid dynamics (CFD) for water applications (Wicklein *et al.* 2016).

3. Good modeling practice

3.1 Purpose, objectives and protocol of good modelling practice

According to Black *et al*. (2011), "best practice modelling can be defined as quality assured model implementation to deliver a credible, robust model that is fit for purpose, and its application

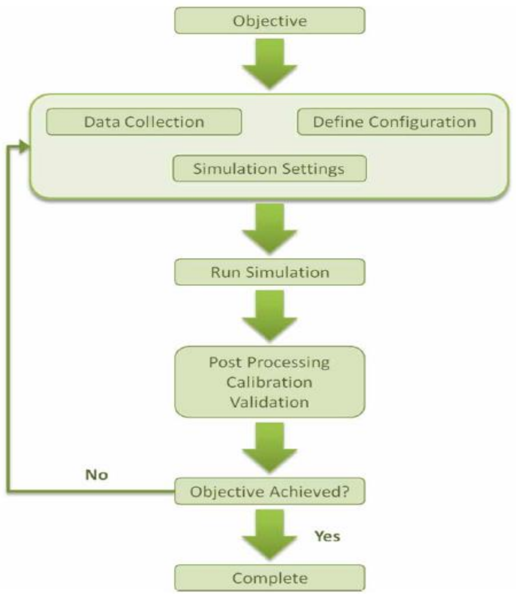

Fig. 4 Overview of the different components of a general modelling process (Wicklein *et al.* 2016)

to deliver results, using methodology that is transparent, defensible and repeatable" (Alwazae *et al*. 2015). Best practice means the best achievable procedures and outcomes taking into account intended modelling purpose, and trade-offs in knowledge, data, resource and time constraints.

Yet it is difficult to identify the best strategy or good modeling practice (GMP) for deciding on what methods and tools and/or combinations are most appropriate. Unfortunately, promoting the correct use of models and assuring quality and modelling efficiency were identified as problematic issues (Riegert *et al*. 2013). It was identified that model quality needed to be improved, reproducibility was lacking and standardized procedures were not available. Generally, development of good modelling practice means a review of existing water treatment simulators, to identify what would be needed for a new system. Good modelling practice should include learning from previous work.

GMP comprises a 'proven-to-work' routine that improves a model's quality and results. The aim is to develop purposeful, credible models from data and prior knowledge, in consort with end-users, with every stage open to critical review and revision. Best practices should be proven-to-work practices for managing common problems encountered throughout the modelling process (Swan 2015).

General components of GMP for any modelling exercise are illustrated in Fig. 4 (Wicklein *et al*. 2016). This modeling process consist of five steps, including the interaction between stakeholders (modelers and non-modelers):

- Project Definition (clearly defining the objective of the modeling task with all stakeholders);
- Data Collection and Reconciliation: defining the model configuration (e.g., level of detail of the model, spatial discretization or mesh generation);
- Plant Model Set-up: running the simulations (steady state, dynamic);
- Calibration and Validation;
- Simulation and Result Interpretation.

GMP should cover the complete process from objective definition to problem solution and visualization of results. GMP can be employed at every phase and step in the modelling process. The purpose and objectives of water treatment modeling should include a clearly articulated set of user data requirements, processes to be represented, questions, functionalities, system boundaries and predictive quantities of interest (Rietveld 2005, Yoann 2013). Typically, numerical models have to be calibrated to one or more data sets before they can be applied. Ideally, this is then followed by a validation step which ensures that the model can be used to predict the behavior of the system under different conditions. The quality and outcomes of a modelling process largely depend on the modelling practices that are undertaken at every step.

Fig. 5 presents proposed GMP unified protocol, defined by Refsgaard *et al*. (2005). Each step includes several tasks. Each task has an internal structure i.e., name, definition, explanation, interrelations with other tasks, activities, activity related methods, references, sensitivity/pitfalls, task inputs and outputs. Each step has to be reviewed and agreed upon with the stakeholders before the next step is carried out (decision boxes in black). This review is based on reports and other documents that are generated during the last task of a step. The protocol calls for a final report that encapsulates the outputs from all modelling steps, usually in summary form with the detailed reports from each step-in appendix.

3.2 Good modeling practice development

The goal of continued "good modeling practice" development is to improve modeling methodology an application of models through enhanced evaluation and interpretation of model performance as well enhanced communication of the performance to decision-makers and other modeling stakeholders (Harmel *et al*. 2014). The search for ways to improve the way modelling is conducted is not new (Jakeman *et al*. 2018). Several attempts have been made to investigate and identify 'best', 'good' and 'core' practices. Identifying best practices helps to provide guidelines for improved modelling practice. Such improvements will ultimately lead to more accurate, credible and useful models, more insightful model-based recommendations, better-informed model adoption, and more importantly improved decision-making.

For example, a study group of experts in water management in The Netherlands addressed these concerns by producing a Good Modelling Practice Handbook (Van Waveren *et al.* 2000). The GMP handbook consists of a clear demarcation of the types and domains of models for which it is intended, a glossary of all concepts, a structured ontology of the modelling and simulation process, a checklist and summary, a tool to document and archive the many steps and tests in the modelling and simulation process, the collective experience of large group of modelers on pitfalls and sensitivities in general and for specific modelling domains and finally references to specific literature and addenda on specific problems.

Enhancing model credibility was also one of the objectives of the European Union funded Project HarmoniQuA (http://harmoniqua.wau.nl/), which led to the development of quality assurance guidelines and a modelling support tool to provide guidance and a quality assurance framework in water management.

According to Black guidance on quality assured model application for water resources management planning (Black *et al.* 2014) is principally intended for practicing modelers, and also for peer reviewers and stakeholders such as managers, decision makers, and community-based groups. This guidance is based on the concept of achieving best practice. Adoption strategies and recommendations for future directions are also discussed. The emphasis is on scenario modelling

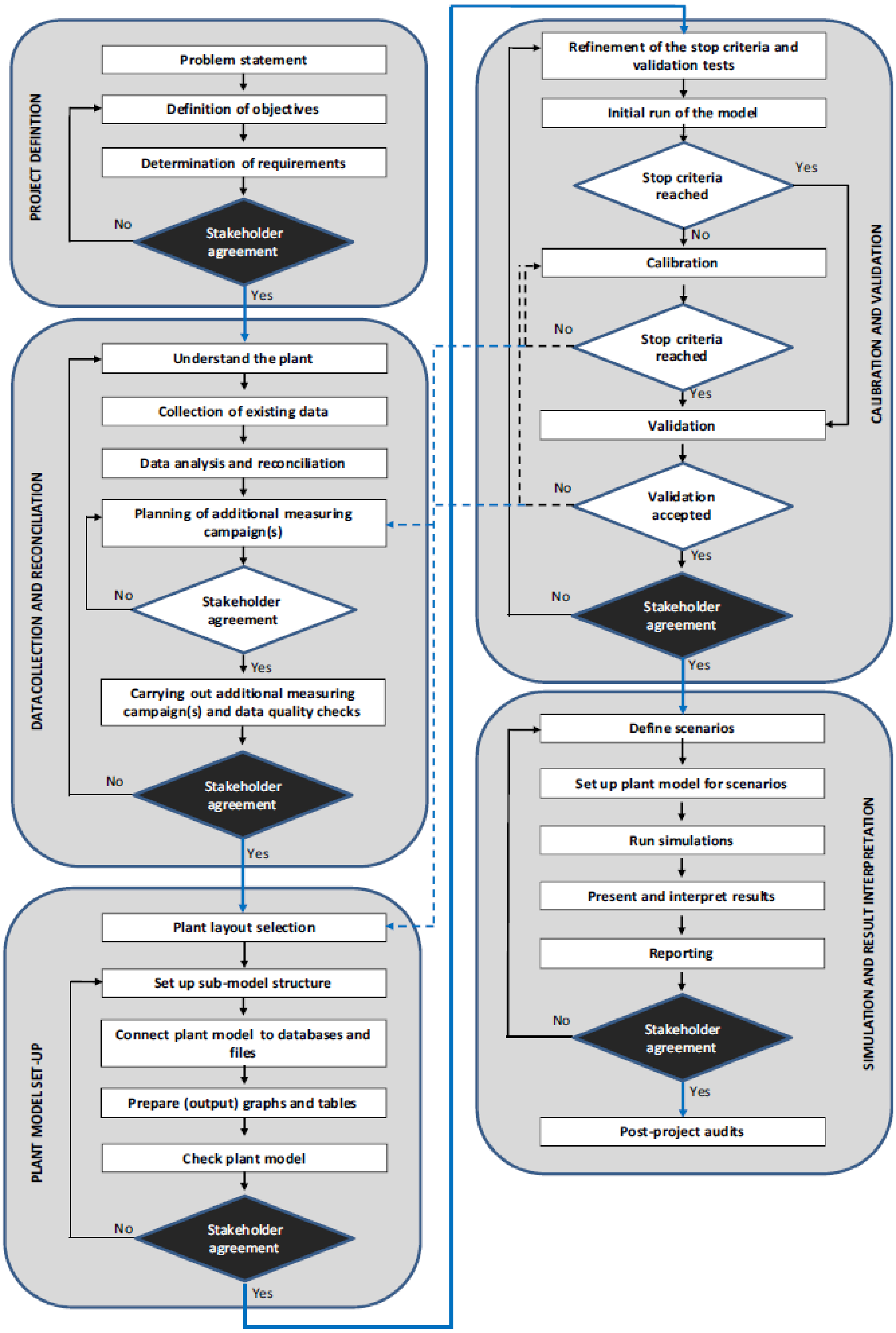

Fig. 5 The proposed GMP Unified Protocol (Rieger *et al.* 2013)

and evaluation of modelling results. An essential step in conceptual modelling consists of the definition of the boundaries: what has to be included and what not, which peripheral processes are relevant and what kind of interactions have to be modelled. It is important to find a balance between the degrees of detailing of the various elements of the model. Essential elements of a conceptual model are both the structure (which (state) variables, which input) and the relations between these.

Another corroborating viewpoint of good model development and evaluation practice is in Jakeman *et al.* (2018) who outline ten basic steps of good, disciplined model practice towards building credible models. The authors state that good practice modelling must:

- clearly identify the clients and objectives of the modelling exercise;
- document the nature (quantity, quality, limitations) of the data used to construct and test the model;
- provide a strong rationale for the choice of model family and features (encompassing review of alternative approaches);
- justify the techniques used to calibrate the model and conduct detailed analysis, testing and discussion of model performance; and
- make a resultant statement of model assumptions, utility, accuracy, limitations, and scope for improvement.

It is crucial to document the practices employed throughout the modelling process in a systematic and transparent way that helps decision-makers form their own judgment about the model's results and improves their confidence in using the model as a decision-aid. A checklist of modelling practices can be an effective means to document and report the modelling efforts and help distinguish between good and poor modelling practices. Such a checklist is a minimum requirement for evaluating the modelling process and informs sources of model uncertainties.

A 'practices description template' (Alwazae *et al*. 2015) is another useful tool for describing the detail of the practices implemented, including items, including the rationale for practice use, the steps carried out in the implementation of the practice, and references to data sources used to carry out the practice.

A new modelling support tool (MoST) aimed at facilitating better quality assurance of the modelling process (Scholten *et al.* 2007). MoST comprises a Knowledge Base with guidelines on good modelling practise for seven scientific domains. It supports multi-domain modelling and working in teams of different user types (water managers, modellers, auditors/reviewers, stakeholders and members of the public). The key functionality of MoST is to: (a) Guide to ensure that a model has been properly applied; (b) Monitor to record decisions, methods and data used in the modelling work and in this way enable transparency and reproducibility of the modelling process; (c) Report to provide suitable reports on what has been done by the various actors.

Various considerations influence the modeler's choice of the good modeling practice. The use of practice documentation tools such as checklists and templates are suggested to document the modelling efforts and help distinguish between good and poor modelling practices (Jakeman *et al*. 2018).

3.3 General benefits of using modelling guidelines of GMP

The use of a structured simulation protocol has great potential to improve the quality of modelling results and to reduce the required effort due to rework (Riegert *et al*. 2014). The GMP Unified Protocol structures the interaction between modeler, client, and other stakeholders and helps to define responsibilities and set clear objectives. Some of the main benefits are:

• a protocol leads to results that are typically more comparable, reproducible and transferable.

• a protocol can provide guidance that clearly defines requirements, limitations and expectations.

• standardised procedures should lead to improved quality assurance/quality control.

• standardised steps will aid inexperienced modelers, clients and other involved stakeholders through the project.

• standardised reporting will speed up documentation and communication with the client,which will aid knowledge transfer.

• the standardisation of a modelling protocol will benefit all the stakeholders involved in any modelling project be they practitioners, operators or regulators because the procedures undertaken to arrive at a conclusion will be understood.

• a simulation protocol should lead to improvements in simulation project quality and efficiency.

• newly developed technologies might require new models and a state-of the-art simulation protocol should develop with time and include new, improved models.

A standardized procedure is not without risk however. One of the disadvantages of using a standardized protocol is that it may block innovative and more cost-effective solutions. A structure common for all modelling projects is suggested, but the modeler should feel free to decide on the best methods and models available for the project's specific objectives. Furthermore, the modeler should not follow a protocol blindly.

Because modelling is as much an art as a science, and involves many choices at every step, progress in achieving best practice is best facilitated by undertaking case studies and sharing the lessons. An even more desirable outcome would be to achieve best practice across an issue that encompasses all the major domains that would lead to cultural change in modelling practice and its associated multiple benefits.

4. Conclusions

Models for water treatment processes are a reflection of the knowledge of the water treatment system. The more widespread modelling becomes, the more it highlights gaps in current knowledge and areas where models could be enhanced or improved. Even the potential role of modelling, itself, has been questioned, with decision makers often viewing models as "black boxes" which cannot be fully understood and trusted.

Although continuous progress has been made in recent years in improving the accuracy of mathematical models to predict water treatment processes, much research work still needs to be carried out. The most notable observation about this paper is that, although some attention has been given to defining good modelling practices in water treatment, there is still little progress across the globe in putting these into actual and routine practice-despite the critical need for such practices in coupling and integrating models.

Much of the discourse around adopting good modelling practices is still conducted at a high level, such as general advice around comprehensive testing, without much drilling down into the details of implementing these recommendations.

It is a big challenge to define, identify, and document GMP for different purposes of water treatment processes modeling application. This will increase trust in these models and allow the exploitation of their full potential in the future. To ensure the successful implementations of mathematical models in the water industry, regulators, water companies and modelling experts need to come together to develop formal guidance on good modelling practices which describe how models must be used in water companies. The recommendation is to focus on the transparent description of modelling practices at an appropriate level of detail to allow knowledge sharing and effective communication between all stakeholders (not only among the modelling community, but also among modelers, end users and decision makers).

This will lead to cost effective, high performance, stable and reliable treatments.

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