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Wastewater Treatment Process Modeling

SECOND EDITION

Water Environment Federation® (WEF®)

WEF MANUAL OF PRACTICE No. 31

Chapter 6

Overview of Available Modeling and Simulation Protocols

1.0 INTRODUCTION

The quality of simulation studies can vary depending on project objectives, resources spent, and available expertise. Consideration should be given to model accuracy and the amount of time required to carry out a simulation project, with the goal of producing the accuracy required. A variety of approaches and insufficient documentation make quality assessment and comparability of simulation results difficult or almost impossible. A general framework for the application of activated sludge models is needed to overcome these obstacles.

During the last few years, several guidelines have been developed around the world focusing on different aspects of simulation projects. To synthesize the available experience into an internationally recognized industry standard, the International Water Association (IWA) formed a task group on good modeling practice (GMP), known as the GMP Task Group. The objective of the GMP Task Group was to prepare a scientific and technical report that describes GMP with activated sludge systems (http://iwa-gmp-tg.irstea.fr/). The report was published in 2012 (Rieger et al., 2012).

2.0 AVAILABLE PROTOCOLS

2.1 Protocols Dedicated to Wastewater Treatment Modeling

Several groups working on wastewater treatment have proposed activated sludge modeling and simulation protocols. The following four protocols have reached a level of application such that they are now considered standards in the field:

- STOWA (Hulsbeek et al., 2002; Roeleveld and van Loosdrecht, 2002)
- Water Environment Research Foundation (WERF) (Melcer et al., 2003)
- BIOMATH (Vanrolleghem et al., 2003) and extensions (e.g., Corominas et al. [2011])
- HSG (Langergraber et al., 2004)

A comparison of these four protocols can be found in works by Sin et al. (2005) and Corominas (2006). Protocols with less international scope or coverage have been proposed by Frank (2006), Japan Sewage Works Agency (2006), and Itokawa et al. (2008). Guidance for water resource recovery facility modeling can also be found in many publications presenting case studies (e.g., Meijer et al. [2002]), different books (e.g., Henze et al. [2008] and Makinia [2010]), simulator manuals, or proprietary company guidelines.

2.2 Protocols from Related Fields

In fields other than wastewater treatment, promoting the correct use of models and ensuring quality and modeling efficiency have also been studied (e.g., Scholten et al. [2000], Refsgaard et al. [2005], and U.S. EPA, 2009). A working group in The Netherlands published *Good Modeling Practice Handbook* (Van Waveren et al., 2000) for the water management field. Enhancing model credibility was also one of the objectives of the European project, HarmoniQuA (http://harmoniqua.wau.nl/), and led to the development of quality assurance guidelines and a modeling support tool, MoST (Version 3.1.5; http://harmoniqua.wau.nl/public/Products/most.htm).

2.3 Comparison of Existing Protocols

This section highlights the main features of the different protocols to identify specific items that should be included in a unified protocol.

The HarmoniQuA project suggested the following classification scheme for modeling quality assurance guidelines (Refsgaard et al., 2005):

- Type 1—internal technical guidelines developed and used internally
- Type 2—public technical guidelines
- Type 3—public interactive guidelines

The last two types are developed in a public consensus-building process. Type 3 guidelines also include organization of the interaction between the modeler and the client. Moreover, the HarmoniQuA project also discussed establishment of performance criteria and reviews of the different phases of the modeling project.

The four main activated sludge modeling guidelines (STOWA, WERF, BIOMATH, and HSG) are Type 2 and the other protocols are Type 1. All protocols have been developed in a mature scientific discipline and a mature market, as can be seen in the now widespread use of activated sludge models in engineering practice.

The main emphasis of STOWA is to help end users model their nitrogen removal facilities using Activated Sludge Model No. 1 in a systematic and standardized way. An essential part of this protocol was the development of an easy-to-use wastewater characterization procedure. As part of the development, user groups were set up and the outcome was the result of an extensive consensus-building process. The STOWA guideline is regarded as an international standard because of its ease of use and widespread application. Unfortunately, only a summary is available in English in the form of two journal publications (i.e., Hulsbeek et al. [2002] and Roeleveld and van Loosdrecht [2002]).

The WERF guidelines (Melcer et al., 2003) are based on experiences from a large market (mainly North America), with authors from consulting companies, software developers, and universities. Targeted users are municipalities and consulting engineering companies, including junior and intermediate modelers. The development consisted of research on wastewater characterization methods and a consensus-building process involving a large international reviewer group. The 575-page final report includes an extensive overview of knowledge, experience, and data and became a standard reference for wastewater characterization and simulation procedures.

BIOMATH at Ghent University (Ghent, Belgium) proposed a generic calibration procedure (Vanrolleghem et al., 2003) using state-of-the-art parameter estimation methods for step-wise calibration/validation of models, with a focus on the biokinetic model and sections on settling, hydraulics, and aeration. The protocol requires a high level of experimental results and takes advantage of systems analysis tools (see Chapter 5). The protocol summarizes the work of the BIOMATH research group and is mainly dedicated to experienced modelers. It has been applied in academic research projects to increase process understanding or during development of new models.

The HSG protocol (Langergraber et al., 2004) is a generic procedure to guide modelers through all steps of a modeling project. The HSG protocol gathers the experience of specialized researchers from German-speaking countries. The focus is on a standardized structure for modeling projects. An objective-oriented approach is encouraged, but deviations from the full procedures need to be explained and documented. The importance of data quality is highlighted. The HSG protocol targets modelers from consulting firms, water boards, and municipalities. An eight-page journal publication is publicly available.

Regional protocols (e.g., the Japan Sewage Works Agency [2006] protocol; http://www.sbmc.or.jp/) often focus on specific issues and constraints and may not allow for generalization. Company protocols (e.g., Frank [2006]) are often proprietary and not easily accessible. The focus of both types of protocols is typically on practical use. Software manuals are focused on explaining the use of respective software, but often provide a relevant source of information on how to apply models. Some software companies provide additional support to clients in their modeling work. Published case studies (e.g., Meijer et al. [2002] and Third et al. [2007]) can be used as another source of guidance, but are often too specific to be used as general guidance on activated sludge modeling.

2.4 Toward a Unified Protocol

The GMP Task Group analyzed existing protocols looking for agreements and differences to identify the strengths of each protocol, with the goal of combining them in one unified protocol. When comparing protocols, agreements outnumbered differences and, where differences were evident, they were mostly in the level of detail and foci. This can be related to the background of the authors (e.g., researchers, consulting engineers, and roundtables and the field of their expertise, e.g., process engineering or water management) and the targeted users. Differences may also be linked to the fact that the objectives of model use are different (i.e., mainly for design/redesign purposes in North America and for optimization or controller studies that require more dynamic simulations in Europe) (Hauduc et al., 2009).

All discussed protocols show some similarities in the following tasks that should be considered for inclusion in a unified protocol:

- Objectives definition
- Data collection and reconciliation strategies
- Model selection and setup
- Plant model calibration/validation, including parameter selection
- Documentation
- Interaction between modelers and end users (establishment of performance criteria and reviews of the main steps of the protocol)

The main differences of the discussed protocols are the design of measuring campaigns; experimental methods used to characterize influent, hydraulics, settling, and aeration and to estimate stoichiometric/kinetic parameters; and the procedure to calibrate and validate the plant model.

3.0 GOOD MODELING PRACTICE UNIFIED PROTOCOL

The GMP Task Group proposed the GMP Unified Protocol (Rieger et al., 2012), which combines the key aspects of the protocols discussed in the preceding sections. The GMP Unified Protocol includes interactions of stakeholders and identifies substeps in which the client should be involved in the decision-making process.

An important aspect of the GMP Unified Protocol is that every step is linked to an application matrix to assist modelers in considering the level of effort required to carry out a simulation project depending on the particular objective. The GMP application matrix provides 12 typical modeling objectives for domestic water resource recovery facilities (WRRFs) and two additional ones for industrial facilities.

3.1 Outline of the GMP Unified Protocol

The goal for the GMP Task Group was to develop a Type 3 protocol according to Refsgaard et al. (2005), that is, a protocol based on a broad international consensus and including the interaction between modelers and clients. The proposed protocol is illustrated in Figure 6.1. It comprises the following main steps, which have to be reviewed and agreed on with stakeholders before the next step is carried out (decision boxes are in black):

- Step 1—project definition
- Step 2—data collection and reconciliation
- Step 3—plant model setup
- Step 4—calibration and validation
- Step 5—simulation and result interpretation

3.2 Protocol Steps

3.2.1 *Step 1—Project Definition*

On the basis of requirements (why use modeling, to answer which questions, what model quality required) and of available data, the objectives of the project are defined in close cooperation with stakeholders. Boundaries and layout of the system to be modeled have to be agreed on. Performance criteria (e.g., data quality requirements or "stop criteria" for calibration) should be set at this stage, responsibilities should be defined, and required data should be identified to decide on the budget and schedule.

3.2.2 *Step 2—Data Collection and Reconciliation*

Data collection refers to existing (process-related and historical) and missing (measuring campaign setup) data. Because data collection and reconciliation represent the most time-consuming step (30 to 60% of the total effort) (Hauduc et al., 2009),

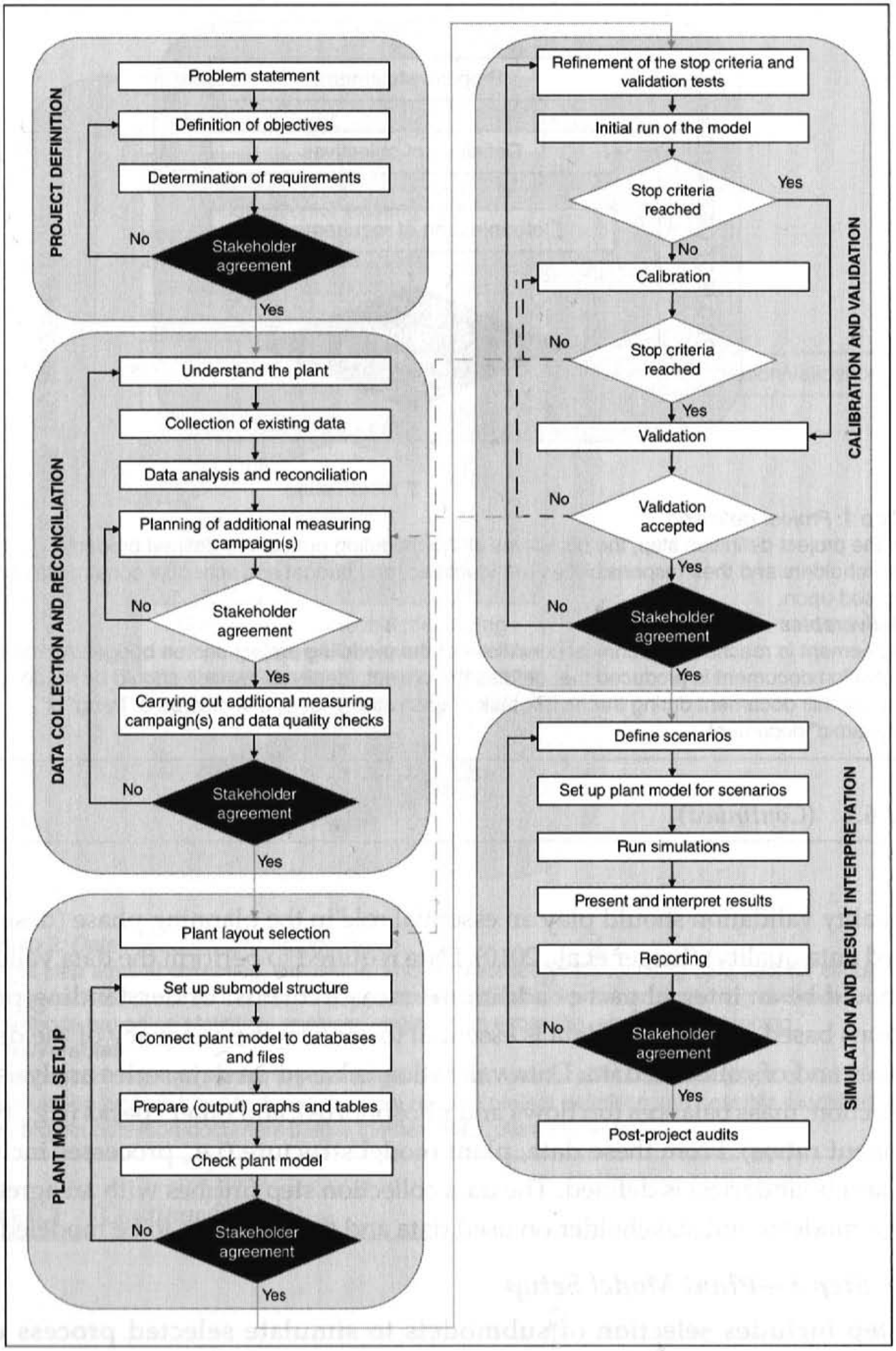
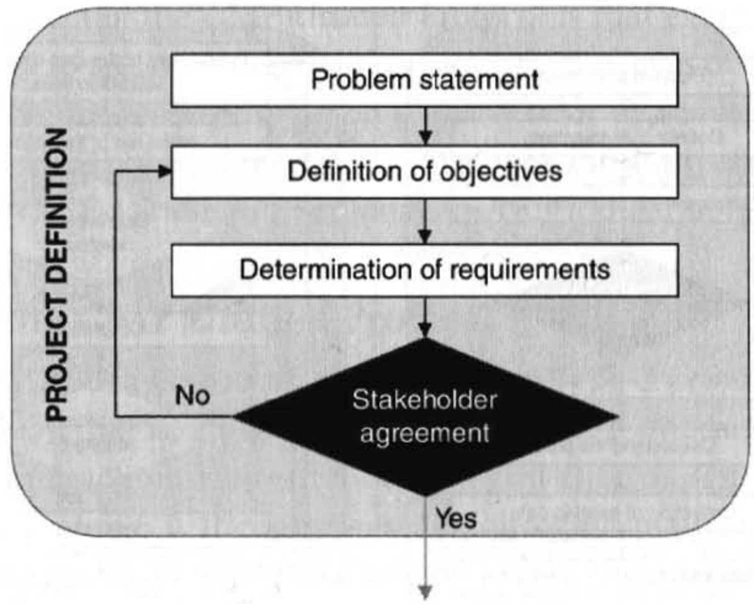


FIGURE 6.1 Proposed GMP unified protocol.



Step 1: Project definition

In the project definition step, the objectives of the modeling project are defined properly, stakeholders and their responsibilities are identified, and budget and schedule constraints agreed upon.

Deliverables

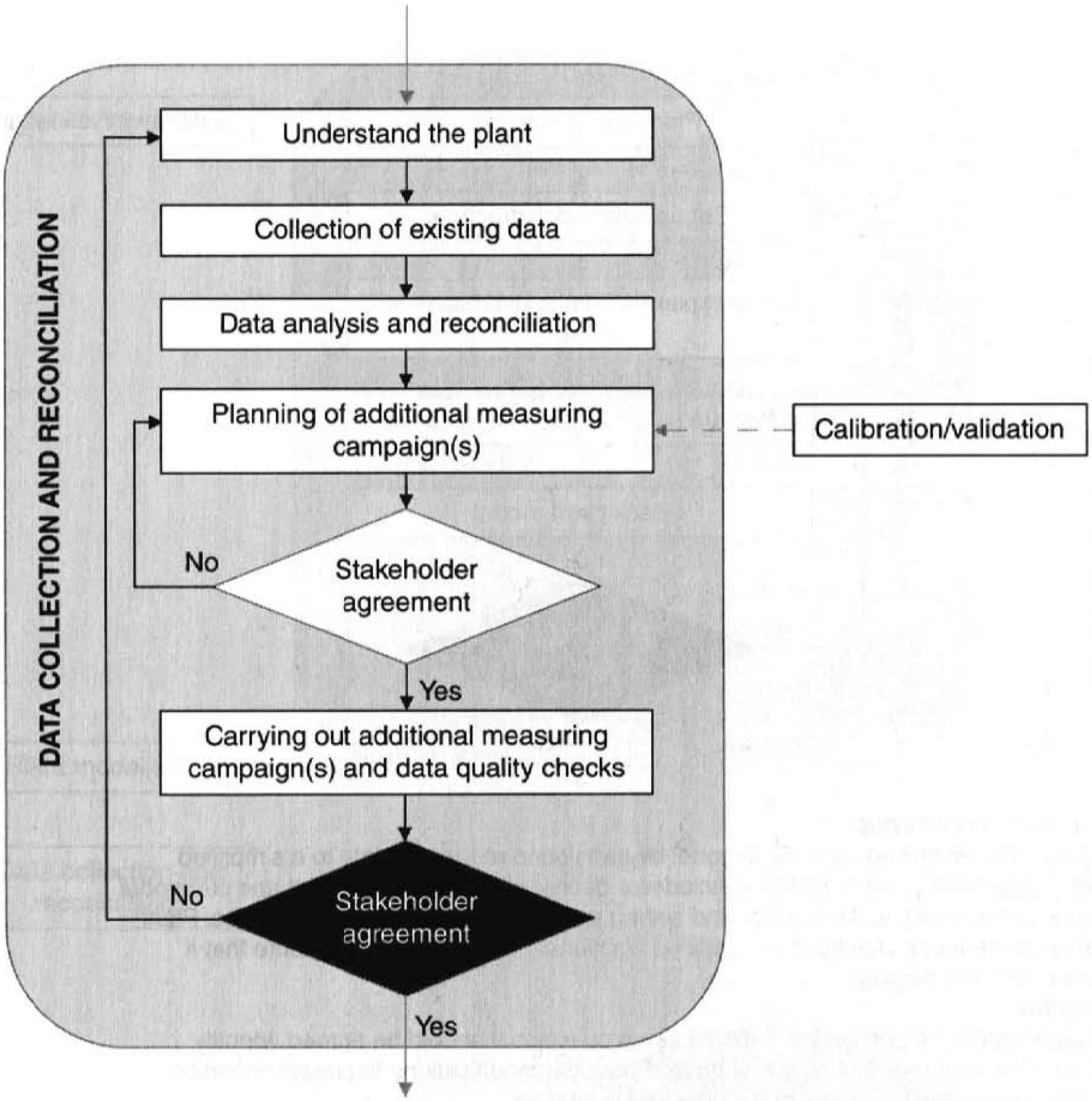
Agreement is reached on technical conditions of the modeling project and on budget. A project definition document is produced that defines the project. Ideally, allowance should be made to modify this document during the review task of each step, that is, it should be a "living" or "dynamic" document.

FIGURE **6.1** (*Continued*)

data quality validation should play an essential role in the planning phase (design the required data quality) (Rieger et al., 2010). Data required to perform the data validation step should be an integral part of additional measurements. Understanding process conditions based on collected data is essential to confirm the adequacy of the defined objectives and of collected data. Data validation is based on data series analysis, outlier detection, mass balances (on flows and phosphorus), and other checks (e.g., typical component ratios). From these data, plant model structure (i.e., processes included, flows, and boundaries) is defined. The data collection step finishes with an agreement between modeler and stakeholder on used data and the processes to be modeled.

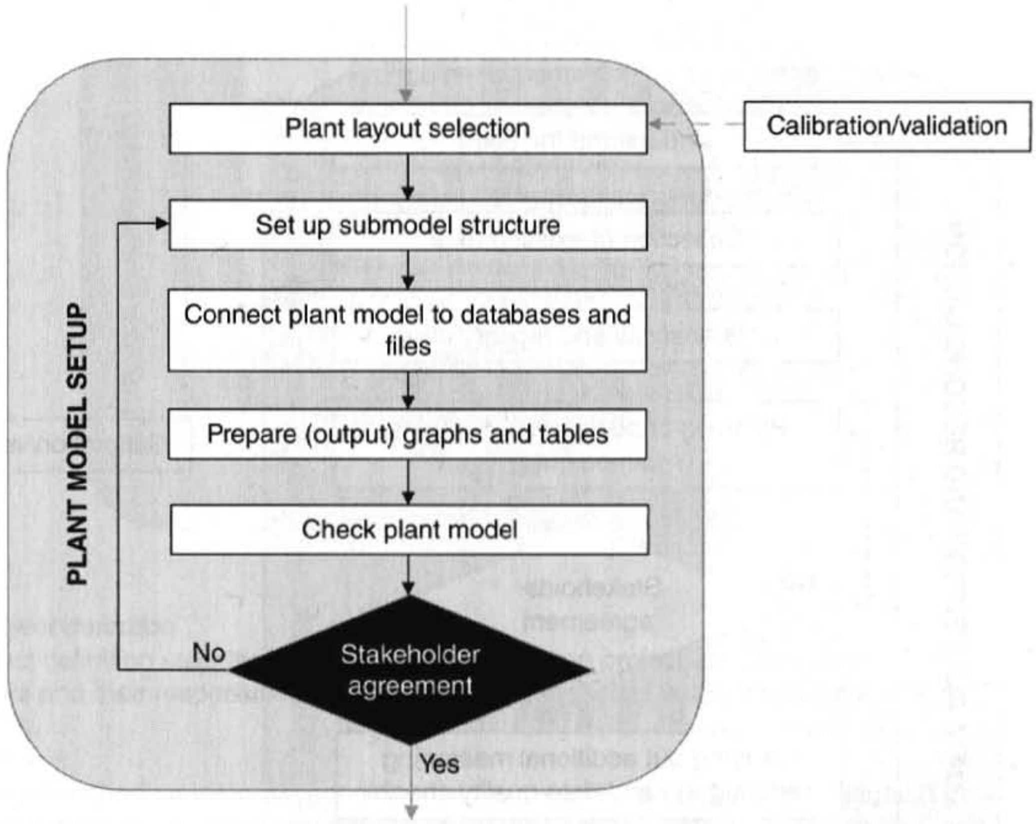
3.2.3 Step 3—Plant Model Setup

This step includes selection of submodels to simulate selected process units. A number of physical and operational values are set at this stage, such as tank



Step 2: Data collection and reconciliation
This step aims at collecting, assessing, and—if necessary—reconciling data sets for simulation projects. A stepwise procedure to analyze collected data is provided, including dedicated methods based on statistical analysis, engineering expertise, and mass balancing.
Deliverables
Reconciled data sets, which are the single data sources for all subsequent steps of the simulation project. Identify deviations from original project definition and possible modifications to project definition document before the next step: plant model setup.

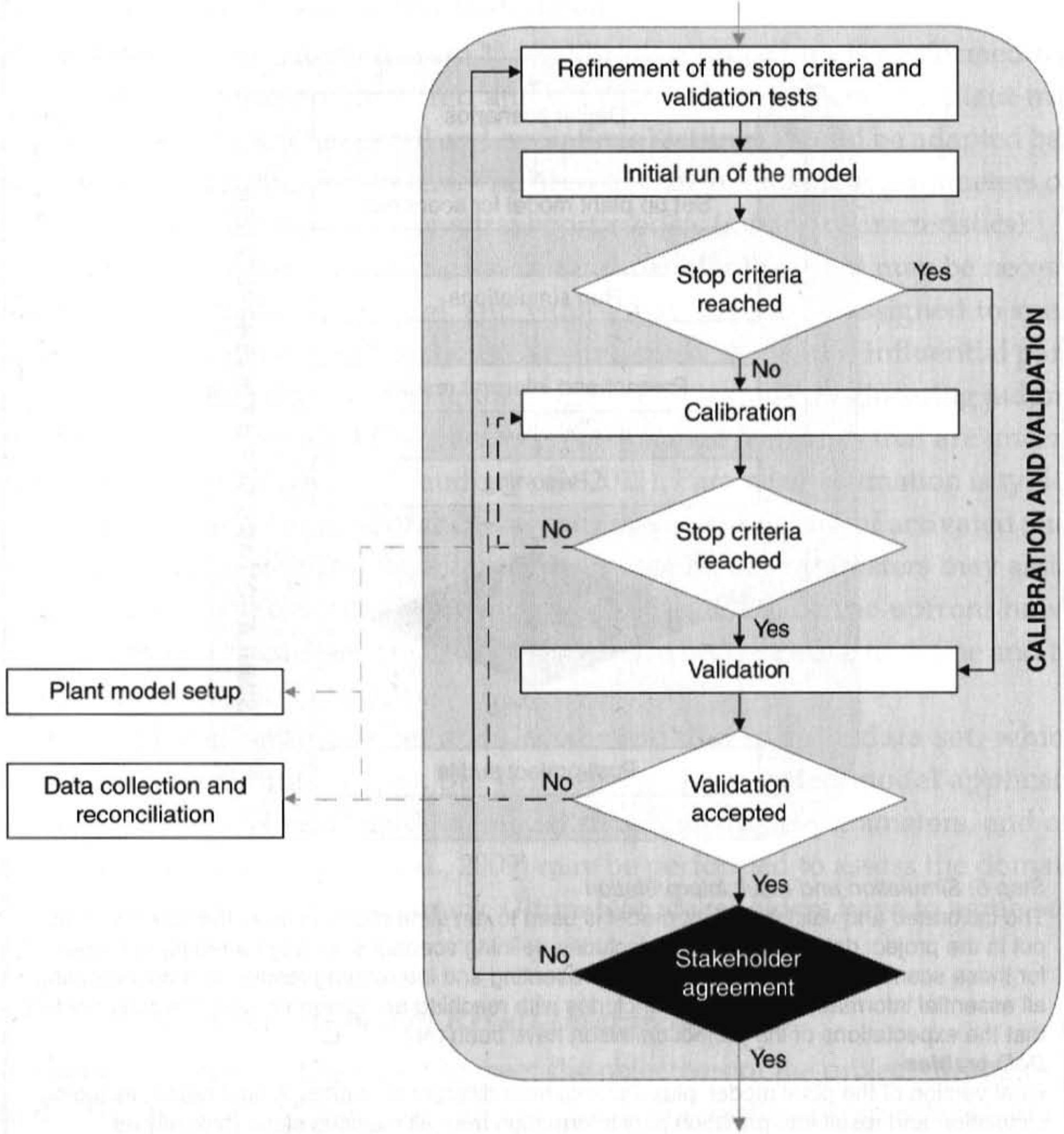
Figure 6.1 *(Continued)*



Step 3: Plant model setup
This step involves setting up a plant model by translating real world data to a simplified mathematical description of reality. It includes a decision on the model layout, the submodel structure, connections to databases, and setting up model output graphs and tables. Plant model set up requires checks of the general functionality of the model to ensure that it produces sensible outputs.
Deliverables
Base plant model. Report on plant model setup on which it should be agreed. Identify deviations from original project definition and possible modifications to project definition document before the next step: calibration and validation.

FIGURE 6.1 (*Continued*)

volumes, flows, controller setpoints, and so on. A preliminary selection of average influent data with a set of wastewater characteristics (often defaults) is used during first implementation in the simulator. A number of initial test runs allow for functionality tests and for checking mass balances, thereby better defining boundaries and critical conditions. The functional model is tested for sensible outputs, and stakeholders should agree on model adequacy.



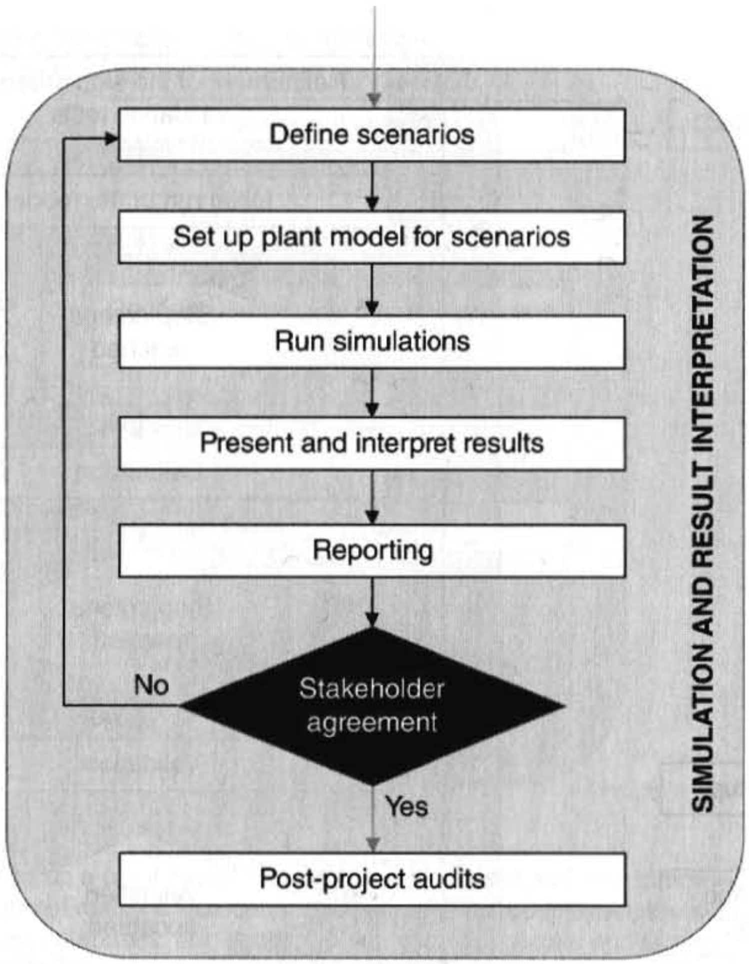
Step 4: Calibration and validation

Model calibration is the process of modifying input parameters until simulation results match an observed set of data. The process is completed when simulated results are close to experimental ones, within a previously defined acceptable margin of error. Validation tests are performed to ensure the use of the plant model with the level of confidence required to meet modeling objectives.

Deliverables

Calibrated and validated parameter sets. Report on calibration and validation on which there is agreement. Identify deviations from original project definition and possible modifications to project definition document before the next step: Simulation and result interpretation.

FIGURE 6.1 *(Continued)*



Step 5: Simulation and result interpretation
The calibrated and validated plant model is used to run simulations to meet the objective laid out in the project definition. This step includes defining scenarios, setting up the plant model for these scenarios, running simulations, presenting and interpreting results, and documenting all essential information. This step concludes with reaching an agreement with the stakeholders that the expectations of the project definition have been met.
Deliverables
Final version of the plant model, plus variants from different scenarios. A final report, including simulation and result interpretation plus information from all previous steps (typically as appendices). Agreement between stakeholders and modeler that the objectives of the project definition have been fulfilled.

Figure 6.1 *(Continued)*

3.2.4 *Step 4—Calibration and Validation*

Having defined stop criteria in Step 1, a calibration procedure is performed to get to an agreement between measured and simulated values. First, the plant model should be set up in required detail and operational settings should be adapted before changing any biokinetic parameters. The need to change biokinetic parameters often points to erroneous data or to wrong transport models (mixing characteristics).

For atypical conditions (e.g., significant industrial influent), it may be necessary to recalibrate the biokinetic model, and values may have to be assigned to specific parameters. Sensitivity analyses should be conducted to identify influential parameters (i.e., parameters that have a significant effect on results). Engineering judgment should be exercised to select few parameters to change (i.e., ones that are uncertain and have wide typical ranges) (Hauduc et al., 2011). Parameter estimation is typically carried out manually because of the over-parameterized nature of activated sludge models. However, automatic algorithms to estimate model parameters may assist in speeding up the process (see Chapter 5). It is important to define upfront how the calibration should be carried out. Good practice is to set up a table to define and track all parameter changes.

The resulting parameter set should be validated using a data set, which is independent of calibration data, but still reflects the targeted model application. Uncertainty analysis (based on data, model structure, model parameters, and other sources of uncertainty) (Belia et al., 2009) may be performed to assess the domain of validity of the model and its accuracy. Ultimately, stakeholders have to agree on the model accuracy that is reached.

3.2.5 *Step 5—Simulation and Result Interpretation*

The validated plant model is used to meet the objectives of the project through simulations. This typically requires definition of scenarios, setting up specific plant models, and, finally, running a set of simulations. If the original objectives cannot be met, the reasons have to be justified and discussed with the client.

All important aspects of the modeling project, including significant decisions, results, interpretation, and conclusions, have to be documented in a final report. The report should allow the client to assess the study's quality, to compare the results with similar studies from other facilities or other studies for the same facility (e.g., non-modeling studies), and to provide required information for future simulations (i.e., for reuse of the model). Finally, simulation results are presented to the client for discussion. Agreement should be sought as to whether the objectives of the project have been met.

4.0 BENEFITS AND POTENTIAL RISKS OF MODELING AND SIMULATION PROTOCOLS

4.1 Introduction

Modeling and simulation protocols can improve the quality of the results and may reduce the required effort. In addition to a direct positive effect on the simulation study, there are several additional benefits such as improved data quality for operation and design. The following are some of the main benefits of using modeling and simulation protocols:

- As a standardization process, protocols lead to better comparable, reproducible, and transferable results; comparison of simulation projects is, indeed, facilitated by use of standard procedures.
- Protocols give guidance to clearly define requirements and limitations of the obtained model and what can be reached at the beginning of the project and, therefore, help prevent misconceptions.
- Checking the quality of a project against standard procedures should lead to improved quality assurance/quality control (Shaw et al., 2011).
- Inexperienced modelers and clients are guided throughout the project.

4.2 Benefits of Using Standardized Modeling and Simulation Protocols

The benefits of using modeling and simulation protocols can be structured into the following categories: benefits for modelers, benefits for WRRFs, benefits for regulatory bodies, and general benefits:

- Benefits for modelers—a GMP survey (Hauduc et al., 2009) found through a questionnaire that the majority of model users have never received organized training in process modeling. A standardized protocol can lead modelers through all steps of a simulation project and, therefore, reduce engineer training time through one consistent source of information. A standardized procedure might highlight typical pitfalls and, therefore, save time and improve model quality. Intensive data analysis and quality checks reduce the time it takes to produce and use a high quality model, which, in turn, reduces reworking requirements. A comprehensive and consistent report format standardizes and, therefore, speeds up model documentation and communication with the client.

- Benefits to WRRFs—following a standardized protocol allows a client to check the quality of the modeler's work against standard procedures. This should lead to improved quality assurance/quality control by the client and increased confidence in the model. Detailed documentation will increase transferability of the modeling study and of the model itself so that it may be used for future applications (even by another modeler).
- Benefits to regulatory bodies—having a state-of-the-art procedure for carrying out simulation studies provides a quality measure to evaluate whether a simulation study followed good modeling practice, even for nonmodelers.
- General benefits—guidance for the interaction between modeler and clients helps define responsibilities and set clear objectives. Quality simulation projects will provide additional benefits in terms of highlighting existing (often undetected) facility problems and data inconsistencies.

4.3 Potential Risks of Standardization

One of the disadvantages of using standardized protocols is that it may block innovative and more cost-effective solutions. Therefore, a structure common to all modeling projects should be suggested, although the modeler should feel free to decide on the best methods and models available for the project's specific objectives.

Another potential problem relates to the danger of strictly following a protocol without taking into account the defined objectives and case characteristics; that is, unnecessary complex (and expensive) steps should be avoided if possible.

Modeling and simulation protocols should lead to a continuous increase in efficiency of simulation projects. Therefore, the goal should be to regularly reassess the suggested methods and to add improvements if they are commonly accepted and standardized. More simulation projects will lead to more experience with parameter values (or typical ranges), and the models will further improve in terms of completeness and applicability. Newly developed technologies might require new models, and a state-of-the-art modeling and simulation protocol should not exclude better-suited models.

TABLE 6.1 Information on protocol steps by chapter.

GMP unified protocol step	Linked chapter in MOP 31
Step 1—project definition	Chapter 7 Project Definition
Step 2—data collection and reconciliation	Chapter 8 Building a Facility Model Section 2 Data Collection Section 3 Data Reconciliation
Step 3—plant model setup	Chapter 8 Building a Facility Model Section 4 Facility Model Setup
Step 4—calibration and validation	Chapter 8 Building a Facility Model Section 5 Calibration and Validation
Step 5—Simulation and result interpretation (including documentation)	Chapter 8 Building a Facility Model Section 6 Quality Assurance/Quality Control Chapter 9 Using Models for Design

5.0 LINK BETWEEN GOOD MODELING PRACTICE UNIFIED PROTOCOL AND MANUAL OF PRACTICE 31

This manual suggests following the five steps of the GMP Unified Protocol. Table 6.1 shows chapters in which the reader can find more information on a specific protocol step.

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Preface

Over the past 20 years, mathematical modeling of wastewater treatment processes has become the default tool for process design in many engineering firms throughout the world and is beginning to be used at operating facilities to help make day-to-day operating decisions. Increased computer processing power and user-friendly simulation software make it possible to model many of the complexities of a water resource recovery facility (WRRF) using personal computers. These simulators can be used to develop mass-balance models of the plant, linking several unit processes together and modeling their interactions. In addition, they can be used to carry out dynamic simulations to investigate diurnal and other transient behavior of a WRRF, such as the effect of wet weather.

With an increased use of process models through user-friendly simulators, there has been widespread acknowledgment in the industry that good training and expert guidance is needed to ensure that these models are developed, used, and documented correctly. This manual provides a broad range of information to help process engineers, operators, regulators, and owners understand general modeling concepts, terminology unique to computer modeling, and practical guidance and ideas on how to use process models for design and operation of small, medium, and large WRRFs. The modeling approach presented in this manual is consistent with the unified protocol proposed by the International Water Association task group on good modeling practice.

This publication was produced under the direction of Andrew R. Shaw, P.E., *Chair,* and Bruce R. Johnson, P.E., BCEE, *Vice-Chair.*

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