Data Reconciliation for Wastewater Treatment Plant Simulation Studies—Planning for High-Quality Data and Typical Sources of Errors

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ABSTRACT: Model results are only as good as the data fed as input or used for calibration. Data reconciliation for wastewater treatment modeling is a demanding task, and standardized approaches are lacking. This paper suggests a procedure to obtain high-quality data sets for model-based studies. The proposed approach starts with the collection of existing historical data, followed by the planning of additional measurements for reliability checks, a data reconciliation step, and it ends with an intensive measuring campaign. With the suggested method, it should be possible to detect, isolate, and finally identify systematic measurement errors leading to verified and qualitative data sets.

To allow mass balances to be calculated or other reliability checks to be applied, few additional measurements must be introduced in addition to routine measurements. The intensive measurement campaign should be started only after all mass balances applied to the historical data are closed or the faults have been detected, isolated, and identified. In addition to the procedure itself, an overview of typical sources of errors is given. *Water Environ. Res.*, **82,** 426 (2010).

KEYWORDS: data quality, data reconciliation, fault detection, diagnosis, activated sludge model, modeling, measuring campaigns, sources of measuring errors.

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Introduction

In the last decade, wastewater treatment modeling has become a standard engineering tool for wastewater treatment plant (WWTP) design, process optimization, operator training, and developing control strategies (Rieger et al., 2008). However, model predictions can only be as good as the data fed as model input or otherwise used for calibration. Data reconciliation procedures include fault detection, fault isolation, fault identification (for definitions, see Isermann and Ballé, 1997), and preparation of a data set suitable for the modeling objective.

Data reconciliation for wastewater treatment modeling consumes time (and money), and the applied techniques are seldom straightforward and reliable. In this paper, the process of data collection and reconciliation is discussed, and a procedure is suggested regarding how to plan for and finally obtain reliable data sets for simulation studies in an efficient way.

Dependent on the objectives (e.g., steady-state versus dynamic simulations), a typical simulation study starts with the collection of historical data and may be complemented by an intensive measuring campaign. Typical reasons to pursue a dynamic simulation are, among others, blower sizing, evaluation of control concepts, and analyzing the effect of wet weather conditions. Historical data are used for steady-state calculations and provide information on the long-term behavior of the plant. Dynamic simulation studies often require high resolution data, which include daily and/or weekly variations for many compounds at different locations within the plant. The higher the resolution (temporal and spatial) and the longer the duration of the measuring campaign, the higher the costs will be. These additional data typically are obtained through one or more intensive measuring campaigns using classic sampling and laboratory analysis or online sensors. This paper presents a procedure to design these campaigns.

On the other hand, unreliable data will increase the required effort for data analysis. As a matter of fact, one-third or more of the time of a model-based study typically is directed at data reconciliation (Hauduc et al., 2009; Kurgan and Musilek, 2006). Working on existing data sets (often measured years ago) typically means guess work, as a result of missing information about instruments, settings, measuring location, and so on. To obtain such information, additional interviews with operators are essential, but time-consuming.

Furthermore, low data quality will limit the meaningfulness of the predictions. In the worst case, erroneous data will lead to faulty conclusions, which could lead to overly expensive decisions or could cause failing effluent license requirements. Therefore,

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and to decrease costs, well-designed measuring campaigns addressing data-quality issues are strongly recommended. The goal of this paper is not to provide overall advice on what to measure and how often, but to provide some hints on typical pitfalls.

In the experience of the authors, the standard way of planning simulation studies for WWTPs is to observe the processes of interest and set up a measuring campaign for specific compounds and key parameters related to these processes (e.g., NH_4, NO_3 for nitrification, solids retention time [SRT], mixed liquor suspended solids [MLSS]). However, to allow for a reliable and straightforward check of the data quality, the required measurements for the check itself (e.g., additional measurements to allow calculating a phosphorus mass balance) should be an integral part of the planned measuring campaigns.

The application of the proposed procedure should increase data quality and save money and manpower, which typically is spent for data reconciliation. Simulation results based on high-quality data allow more accurate design conclusions and prevent misuse of the models resulting from incorrect data. The paper describes how to plan for the required data quality.

Procedure

It is suggested to use mass balances with typical engineering numbers, such as influent or sludge compound ratios (e.g., biochemical oxygen demand [BOD]/chemical oxygen demand [COD] or volatile suspended solids [VSS]/total suspended solids [TSS]) or yields to check the reliability of existing historical data before starting an intensive measuring campaign or going directly to simulations. Although standard activated sludge models are based on the principles of mass balancing also, the data quality evaluation should start with model-independent checks (meaning that the model should not be used for mass balancing the data in a first step). Otherwise, one tries to detect errors in a data set by using a plant model, which should be calibrated on the same data. It should be clear that there is a strong dependency and subsequently a danger to squeeze the data to fit the model.

Another danger is to squeeze the model to fit erroneous data. During calibration of the plant model (consisting of several submodels, such as influent wastewater characterization, transport, and mixing model or aeration model), model parameters and reactor layout are changed to fit the measured values. If the database includes incorrect measurements, one will try to fit the model to erroneous data, and this will strongly increase the uncertainties of the predictions.

Organizational Priorities. It is important to maintain good communication with the plant operators. They know the weak points of the plant and have specific information, which is not available otherwise. Operators should be asked for special aspects, such as suspect sampling and recycle return locations, known errors in the databases (e.g., wrong units), or undocumented operational changes. Special emphasis should be given to collect physical plant data as built and not as designed.

Ideally, the intensive measuring campaign should be started after several weeks (ideally 2 to 3 SRTs) of stable operation, without major changes in flows, recycles, precipitant dosage, and so on. This is necessary to provide a well-defined starting point (initial conditions) for the model. However, this hardly can be reached in practice and makes it even more important to obtain access to information on all changes even before the period under evaluation.

Planning of High-Quality Data. Good data quality is essential for reliable simulation results and for the efficient operation of wastewater treatment systems. The planning of simulation studies should include a phase that is used to examine and analyze the existing data, close gaps in the data sets, and carry out some additional measurements for the model setup. Figure 1 proposes a concept to obtain and evaluate the database for dynamic simulation studies.

Phase 1—Collection of Existing Data. The first step is to collect existing data. This includes the following:

- Input data: Flowrates (daily average, diurnal flow, seasonal, event-based, etc.), influent and sidestream concentrations, additional information about wastewater characteristics, temperature, and so on.
- Physical data: Process scheme, number and volumes of tanks and lanes, hydraulic behavior (plug-flow to fully mixed), and so on.
- Operational settings: Includes all information on how the plant is operated, for example, constant or controlled return or internal sludge flowrates, controller set points (e.g., for dissolved oxygen, MLSS, and SRT), dosage of precipitants and digester supernatant, and so on.
- Performance data: Includes all information on the process behavior resulting from operational settings, input, and physical data, for example, effluent concentrations, reactor or sidestream concentrations, measured flowrates, MLSS and SRT (if not controlled), and so on.
- Additional information: Of interest is all information on "atypical" (e.g., intermittent industrial influence and special weekly or seasonal variations) or unusual (e.g., periodic shutdown of equipment for cleaning or maintenance and changes in operation) behavior. Also of interest are connecting systems (e.g., type and length of sewer system and effluent limits).

Phase 2—Data Analysis and Reconciliation. Examination of the available data will show gaps in historical measurements (e.g., for mass balancing), which must be closed for the next step. First reliability checks can be used to recognize potential problems and to plan additional experiments (e.g., check of autosamplers, flow measurements, or laboratory methods). However, the most powerful way to identify systematic errors is to use a combination of mass balances over different sections of the plant. For a listing of the most common sources of errors, see the Typical Sources of Measurement Errors section.

To make the best use of money and manpower, this phase should be used to detect, isolate, and identify systematic measurement errors (including quantification thereof) in the existing data and finally correct (or reconcile) the data set for use in the simulation study (Figure 2) (for definitions, see Isermann and Ballé, 1997). A few measurements in addition to the routine measurements will allow mass-balance checks (Barker and Dold, 1995; Meijer et al., 2002; Nowak et al., 1999). For example, the required measurements for phosphorus in the activated sludge to calculate a phosphorus mass balance over the biological stage of a WWTP are seldom available. Two additional measurements per week for 2 to 3 sludge ages will provide sufficient information to calculate the mass balance. The combination of overlapping mass balances for different compounds (e.g., phosphorus or iron) and boundaries allows

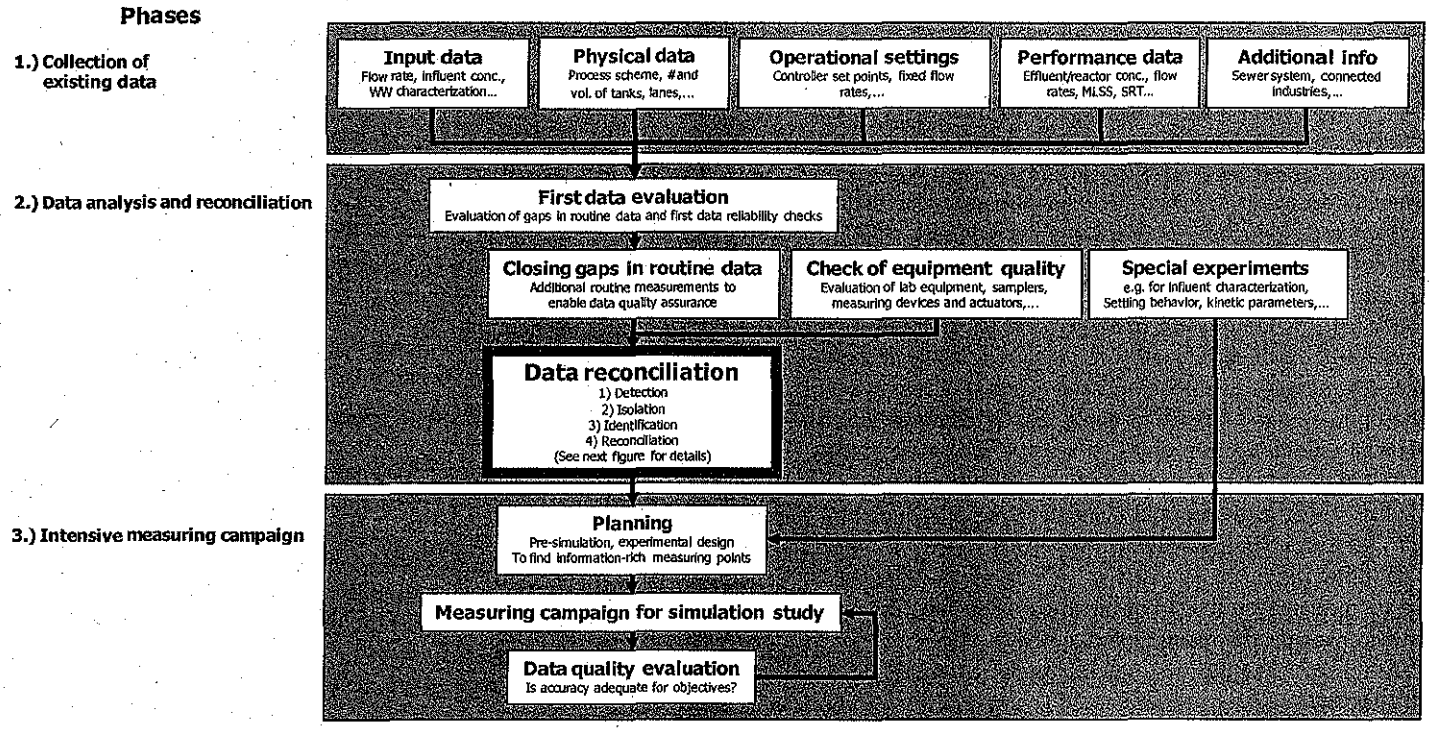

Figure 1—Concept of data collection, evaluation, and reconciliation for simulation studies.

systematic measurement errors to be identified efficiently (Meijer et al., 2002; Puig et al., 2008; Thomann, 2008).

In addition to mass balances, other reliability checks can be carried out. They are based mainly on engineering experience and give hints for detailed evaluations and, therefore, reduce efforts and costs. The following list is not complete, but provides an overview.

- Perhaps the most important check is a look at graphs with, for example, differences or specific ratios (e.g., influent COD/BOD, NH_4/TKN) over time. This is the easiest way to detect drifts, shifts, outliers, or special events.
- Comparison of calculated population equivalents with the connected population for different compounds, flows, or sludge production (see Metcalf & Eddy [2003] for population equivalent characterization for different countries).
- Comparison of measured sludge composition ratios with literature values (e.g., the ratios of single compounds to TSS or COD; $i_{P/TSS}$, $i_{N/TSS}$, and $i_{COD/TSS}$).
- Comparison of typical indices or other key numbers with literature values (e.g., kWh/m^3_{air}).
- Comparison of measured concentrations and other performance data with typical benchmark values for the same kind of plant (benchmarking, e.g., Lindtner et al., 2004).
- Check whether the rate of change in concentration is possible with respect to hydraulics (is mixing and diffusion sufficient to explain sudden change in concentration).

Even by using different overlapping mass balances and a whole set of reliability checks, it often is not possible to clearly relate a detected error to only one source. In such cases, validation experiments have to be carried out, and the data must be checked again by using the mass balances discussed above. The advantage of overlapping mass balances is that not all measurements have to be checked, but only those at locations where potential errors were detected and isolated (see Figure 2).

For special demands, in terms of prediction accuracy, additional experiments may be required to obtain values for the precision (spread) and trueness (bias) of laboratory equipment and analytical methods. Although this is no standard requirement, the authors suggest, at least, a visit to the plant laboratory and interview of the laboratory personnel. For dynamic simulation studies, special attention should be paid if online sensors are used, because they will provide the required high-frequency data. The accuracy and response time of the measuring devices should be checked during this phase (Rieger et al., 2003, 2005; Thomann et al., 2002). For special simulation objectives (e.g., to preconfigure a dissolved oxygen controller), it could be necessary to examine the response time of the actuators also.

Phase 2 also can be used for special experiments that would benefit model setup and calibration, for example, hydraulic behavior (e.g., using a tracer experiment), influent characterization, and measurement or estimation of kinetic and stoichiometric parameters.

The data-reconciliation step includes the following:

(1) Removal of gross errors (e.g., obvious measurement errors, such as soluble COD greater than total COD or identified outliers);
(2) Fixing of systematic errors (based on the detection methods listed above); and
(3) Calculation of the precision (which characterizes the random errors of the measurements and typically cannot be reduced, as it is largely dependent on the measuring principle).

The outcome of phase 2 is a reconciled historical data set, which can be used for modeling the plant's long-term behavior and helping to design the intensive measuring campaigns or other

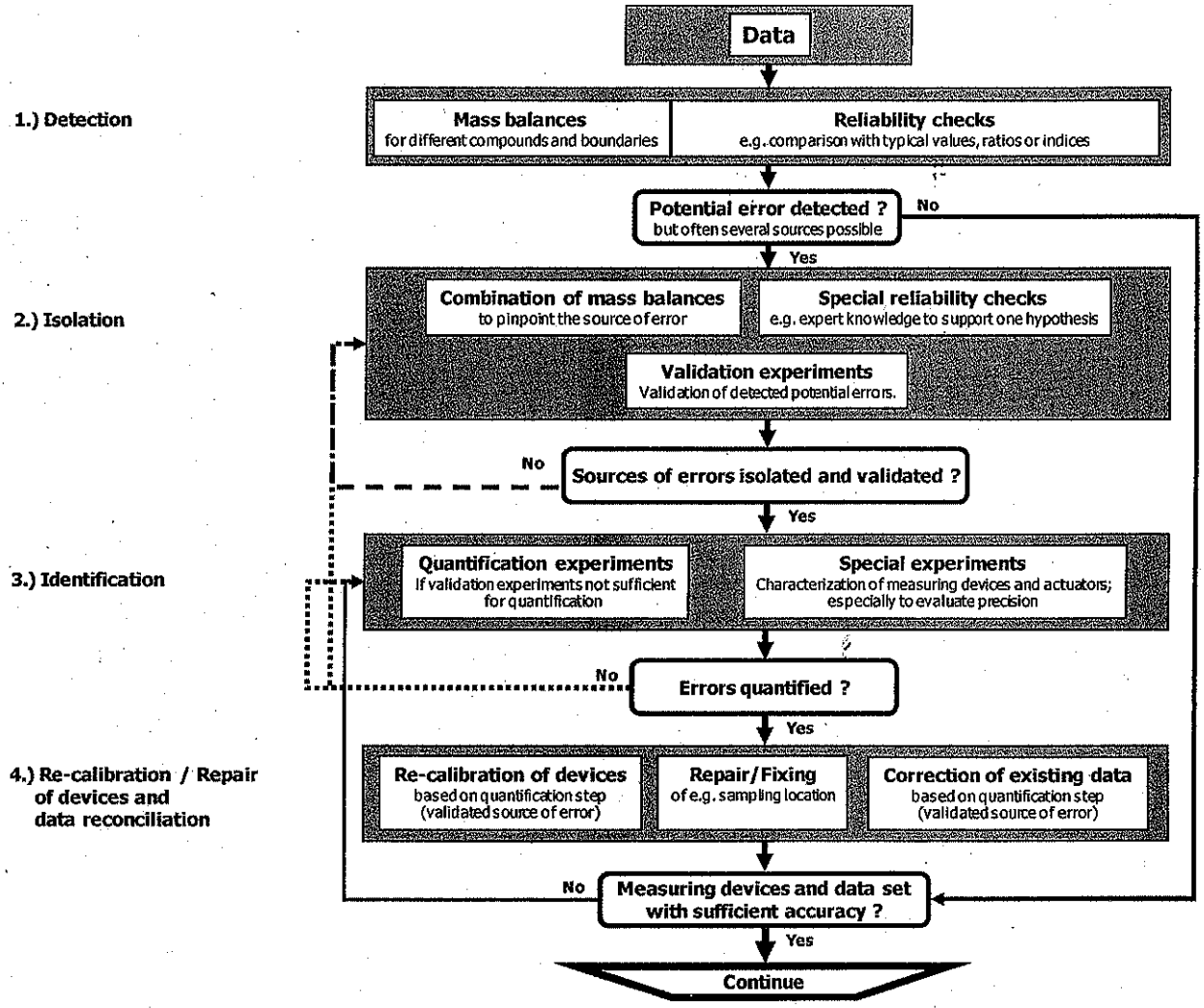

Figure 2—Data reconciliation procedure to detect, isolate, and identify errors, and reconcile data set.

short-term experiments and defining scenarios to be evaluated in the simulation study.

Phase 3—Intensive Measuring Campaign. The intensive measuring campaign for the simulation study should not start before the mass balances for the historical data are closed. Otherwise, the large effort for the intensive campaign presumably will lead to the same low-quality data with the same problems already detected for the historical data. For example, often the same autosamplers are used for routine and intensive measurements. If the sample is not representative for the total load, the same error will occur in the intensive data set. Even if the source of error is not identified by an experiment, the engineer should close the mass balances and decide where to assign the error. Otherwise, the model will propagate the error throughout the simulation. This often is not the best choice, because the error will affect plant performance predictions, because the model input, physical data, and operational settings are fixed in the model. If, for example, a phosphorus mass balance over the activated sludge part of a WWTP does not fit, in most of the cases, the wastage rate is erroneous (flow or concentration measurement). If in the model the wastage rate is fixed, the sludge age will be incorrect and therefore will call the whole simulation into question.

During the intensive measuring campaign, it is desirable to collect redundant information to enable data-quality evaluation and reconciliation on this data set also. One of the most reliable checks is a phosphorus (or iron, if used as precipitant) balance, where all inputs and outputs (in effluent, waste sludge, etc.) can be inferred from measurements.

Any other measuring campaign (e.g., for model validation, implementation of measures or success monitoring) also should be accompanied by additional measurements enabling data quality evaluation, but the measurement frequency can be reduced compared with the simulation data set.

Whereas the first part of this paper provides methods to evaluate existing data sets, the following part focuses on the measurement errors and also can be used to identify potential errors before the measurements start. This forward-looking approach would have the advantage that all required information is still available.

Typical Sources of Measurement Errors

Figure 3 shows the main influences on the quality of load data used (e.g., for simulation studies).

Flow Measurement. Special attention should be paid to the flow measurements. These are the most important measurements for WWTP operation and the simulation study, because each concentration must be multiplied by a flow to calculate the input load to the model. Beside the flow measurements, flow splitters

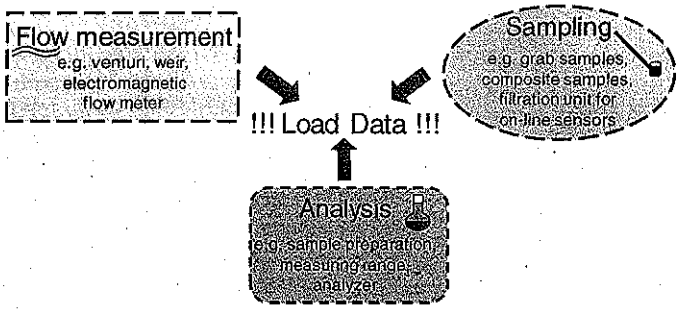

Figure 3—Influence on accuracy of load data.

can introduce significant errors into the model, if imbalances are not taken into account (Meijer et al., 2002). In addition to the flow in or out of the plant, internal flow measurements should be checked also. Often, the only available information is pump strokes or speed, which is inaccurate.

With older flow measuring devices, the flow often is calculated from the water level by a simple lookup table instead of using an exact hydraulic formula. It should be checked whether the range and the resulting accuracy are sufficient for the desired objective (e.g., test highest/lowest flows). Table 1 lists typical sources of errors of flow meters.

Sampling. Another important step to check is the sampling (Table 2). Autosampler (e.g., Haider and Haider, 1998) and filtration units of online sensors (e.g., van Griensven et al., 2000) often are one of the main sources of errors. For autosamplers, the settings for pump rate and pumping time should be chosen carefully to have a good compromise between a sufficiently high sampling frequency with suitable sampling time (to prevent sedimentation within the autosampler) during dry weather and a maximum possible volume for rain events. Special attention should be given to the location of the inlet hose. Placing it on the bottom can result in overestimation of the particulate compounds, and placing it too high can miss particulates.

Analysis. The analysis of a sample consists of sample storage, preparation, and finally the measurement using a specific analytical method. Mainly at small WWTPs, the laboratory conditions often allow only the use of test kits. In the author's experience, their accuracy is mostly sufficient (see also Thomann, 2003; Winkler et al., 2008), but should be checked with standard addition experiments on the matrix (laboratory-fortified matrix) or by dilution experiments (APHA et al., 2005). The use of control charts is recommended strongly (Montgomery, 2005). Table 3 shows typical sources of errors in the analysis of water samples.

Online Sensors. Online sensors provide the required high-frequency data, but should be checked regularly with reference measurements (Thomann et al., 2002). These sensors still have a high demand for maintenance, and, because they are exposed to harsh environmental conditions, their accuracy typically is lower, and the lower detection limit is higher than under standardized laboratory conditions. It should be kept in mind that the response time of such measuring systems (including the filtration unit) can introduce a significant modeling error, if not taken into account. The response time for ex situ nutrient sensors typically is between 15 and 30 minutes (Rieger et al., 2003). Old ultrafiltration units with long measuring intervals can lead to response times of more than 1 hour.

Table 4 presents potential sources of errors of online instruments.

Conclusions

The proposed procedure to obtain high-quality data for WWTP simulation studies starts with simple reliability tests, some additional measurements to enable mass balance calculations, and preliminary checks of the equipment used. Only when all preliminary tests are passed successfully and all mass balances can be closed within a certain range (typically 5 to 10%) should the intensive measuring campaign be started. This will reduce the efforts for data reconciliation and guarantee high-quality data as a basis for the simulation study.

Table 1—Potential sources of errors for flow measurements.

Measurement principle	Potential sources of errors	To be checked
General		Easy and reliable check by increase or decrease of water level in activated sludge or other tanks
Venturi or weir	Measurement of height	Calibration of ultra-sonic, echo-sonic, radar, bubbler • At least zero and maximum check • Check of temperature dependency
	Changing of cross-section	Cross-section cleanliness (algae or sediments) Leakages Cross-check dimension and installation with technical reference (physical check)
	Calculation of flow	Cross-check used formula with technical reference (for an independent check, there are special experiments, e.g., tracer experiments and mass balances)
	Miscellaneous	Signal transmission or conversion
Velocity and height	Measurement of height	See above
	Changing of cross-section	See above
	Measurement of velocity	Depending on measuring principle (e.g., doppler effect and transit time) In general, effect of particle concentration and flow profile
	Calculation of flow	See above
Electromagnetic flow meter	Air in pipe	Filling of pipe
	Changing of cross-section	Fouling in pipe
	In and outflow distances	Check distances (not long enough or not straight)
	Miscellaneous	Calibration, signal transmission, or conversion

Table 2—Potential sources of errors during sampling.

Type of sampling	Potential sources of errors	To be checked
General	Incorrect location	• Measured flow, process dynamics
	Insufficient homogeneity	• Mixing/dead zones, location in the cross-section
	Time	• Cross-check time stamp with SCADA system • Start/stop intervals
Autosampler	Kind of sampling	• Proportional to volume or time, fixed intervals
	Settings	• Check settings of pump rate and time. Most rain peaks should be included to prevent overestimation of loads.
	Cooling	• Always lower than 4°C (check for the smallest sampling interval resulting from the higher temperature emission of the distribution unit or sampling pump)
	Volume and pumping speed per single sampling event	• Unwanted sedimentation in pre-sampling vessel. • Proper flushing of the whole inlet hose. Undesired emptying of suction hose.
	Installation of inlet hose	• Hose length, unwanted bends, proper siphon
	Inlet hose	• Biofilm, sediments

Any other measuring campaign (e.g., for validation or to prove the success of an implementation) also should be accompanied by additional measurements enabling data quality evaluation and reconciliation, but their frequency can be reduced compared with the calibration data set.

The question could be raised why the proposed procedure focuses so much effort on historical data, whereas an intensive measuring campaign could be carried out by experienced laboratory staff with higher data quality. The reason is that the intensive data set can only be used to calibrate the model for a limited period. Relying only on one intensive measuring campaign often results in a forced calibration of the plant model. If no additional validation data sets are available, such models have limited (or unknown) predictive power, because the users are relying on one, necessarily limited, data set (sometimes not even reconciled). The authors suggest using reconciled historical data for the calibration of the long-term behavior of the plant, and these data also should form the basis to define the most critical conditions (e.g., limiting COD:N:P ratio and temperature versus critical loading) for an evaluation of different scenarios. Intensive campaigns also should be used to provide model-specific wastewater and sludge characterizations.

There remain unanswered questions about the required accuracy and benefits of the proposed approach in terms of cost reduction. The first part is strongly related to the objectives of the study. If two process schemes are compared, in most cases, even data from another plant can be used, because it is a relative comparison, and the errors will have the same or nearly the same

Table 3—Potential sources of errors during analysis.

Steps	Potential sources of errors	To be checked
Sample storage	Biological degradation, precipitation	• Best to measure directly after sampling • Cooling/freezing • Complete filling of bottle to prevent oxygen supply • Depending on the composition, prevent precipitation • Sufficient addition of inhibitor to prevent biodegradation
Sample preparation	Insufficient homogeneity	• Homogeneity
	Filtration	• Filter pore size • Content of unwanted compounds in the filter (COD, NO_3)
	Dilution	• Correct volumes (dilution as little as possible, frequent source of errors)
	Digestion/fractionation	• Suitability of digestion method
Analysis	Micropipettes	• Check of volume (with scale) • Cut tip for sludge measurements to prevent filter effect
	Laboratory scales	• Check with standard weights or • Check by supplier
	Photometer	• Maintenance—regular check by supplier recommended • Correct calibration factors (updates) • Cleanliness of optical system and cuvettes • Disturbance resulting from air bubbles
	Analysis	• Quality of reagents and standards (production and storage) • Calibration (check with standard solutions) • Matrix influence/cross sensitivities (check with standard addition/dilution experiments or reference measurements) • Measuring range • Cross-check with standard methods
	Data processing	• Check unit, dilution rate, typing errors • A well kept laboratory journal is strongly recommended

Table 4—Potential sources of errors of online sensors.

Steps	Potential sources of errors	To be checked
Filtration unit for online sensors	Inlet hose/filtrate outlet	• Biofilm or sediments. Check with measurements of influent/effluent of filtration unit.
	Installation of inlet hose/filtrate outlet	• Hoses too long, sharp bend, siphon
	Coordination with sensor	• Discontinuously working filtration devices should be triggered from the sensor.
	Membrane	• Clogging or biofilms growth
	Pump rate	• Pump rate not sufficient to reach low response time
Sensor/analyzer	Installation	• Location, gradients, flow velocity
	Condition	• Maintenance, cleaning system
	Clogging/biofilm/fouling	• Mainly a problem for in situ sensors • Check automatic cleaning system
	Air in measuring cell	• Check if incoming flow is high enough (particularly if several sensors are connected to one filtration unit) • Check for leakage • Check pump tubes
Analysis	Calibration standards	• Check age/expiration date • Check concentration of standard • Settings of the analyzer
	Reagents	• Check expiration date • Even original reagents from the supplier can be wrong
	Calibration	• Some methods require a calibration to the water matrix
	Matrix influence	• Check regularly with reference measurements
	Measuring range	• Check whether range is suitable for the measured variations • Check whether accuracy is sufficient over whole range
	Response time	• Check response time of the whole measurement system (can be more than 30 minutes)
Data transmission and processing	Amplifier	• Check filtering • Check delay • Check averaging • Check for interferences (e.g., radio) • Check noise profile
	Settings of sensor	• Check settings for output
	SCADA system	• Check incoming signal • Check data aggregation and filtering (actual versus processed value)

effect on both cases. If the goal is to predict the exact effluent concentrations, however, high-quality data is a prerequisite, which is also the answer to the second question. The value of a study is strongly limited if the data does not allow an accurate model prediction. In addition, experience shows that data reconciliation commonly consumes more than one-third of the time of a study. Designing a measuring campaign in a way that this task is more straightforward will lead to direct cost savings.

Another question is when to stop data reconciliation, recognize bad data, and move on? The main message the authors would like to convey is that one should "plan" the required data quality and make it an integral part of the measuring campaign design. If this is not possible, it is important that the engineer explicitly decides on where the error goes.

Credits

This paper is based partly on discussions in the International Water Association (London, United Kingdom) task group on Good Modelling Practice—Guidelines for Use of Activated Sludge Models. Peter A. Vanrolleghem holds the Canada Research Chair in Water Quality Modeling.

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