QUICS: Quantifying Uncertainty in Integrated Catchment Studies

D.6.7

A Framework for the application of uncertainty analysis

Lead Partner: TUD

Revision: 31/10/2017

Report Details

Title: A Framework for the application of uncertainty analysis

Deliverable Number: 6.7

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Dissemination Level: Public

Document History

Version	Date	Status	Submitted by	Checked by	Comment
v 0.1	13/05/2017	Structure	Franz Tscheikner-Gratl	Jeroen Langeveld, Simon Tait, Vasillis Bellos, Francois Clemens	Proposed structure and outline
v 0.2	14/05/2017	3.6.1	Mathieu Lepot	Franz Tscheikner-Gratl	Minimization of uncertainties in data collection
v 0.3	19/07/2017	Draft	Franz Tscheikner-Gratl	Jeroen Langeveld, Mathieu Lepot, Simon Tait, Alma Schellart, Elliot Gill	First draft
v 0.4	29/09/2017	Draft	Franz Tscheikner-Gratl	Jeroen Langeveld, Antonio Moreno Ródenas, Francois Clemens	Final draft without example
v 0.5	17/10/2017	4	Antonio Moreno-Rodenas	Franz Tscheikner-Gratl, Francois Clemens, Jeroen Langeveld	Example
v 0.6	20/10/2017	Final version	Franz Tscheikner-Gratl	James Shucksmith	

Acronyms and Abbreviations

AMALGAM	Multi-algorithm, genetically adaptive multi-objective method
ASM	Activated Sludge Model
BOD	Biochemical oxygen demand
COD	Chemical Oxygen Demand
CPU	Central processing unit
CSO	Combined Sewer Overflow

DO	Dissolved oxygen
EU	European Union
GLUE	Generalized Likelihood Uncertainty Estimation
GSA	Global sensitivity analysis
KALLISTO	Cost effective and integrative optimization of the urban wastewater system
KNMI	The Royal Netherlands Meteorological Institute
LH	Latin–Hypercube sampling
LSA	Local sensitivity analysis
MC	Monte Carlo sampling
NH_4	Ammonium
NO_3	Nitrate
NSE	Nash-Sutcliffe efficiency
OAT	‘‘One-factor-at-a-time’’ approaches
ODE	Ordinary Differential Equations
P	Phosphorus
PBIAS	Percent bias
PO_4	Phosphate
QUICS	Quantifying Uncertainty in Integrated Catchment Studies
RDM	Robust decision-making
RSR	Root mean square error observations standard deviation ratio
RTC	Real-time control
SA	Sensitivity analysis
SCEM-UA	Shuffled Complex Evolution Metropolis algorithm
SS	Suspended solids
TSS	Total suspended solids
UPA	Uncertainty propagation analysis
UV/VIS	Ultraviolet–visible spectroscopy
WFD	European Water Framework Directive
WWTP	Wastewater Treatment Plant

Acknowledgements

This project has received funding from the European Union’s Seventh Framework Programme for research, technological development and demonstration under grant agreement no 607000.

Executive Summary

This deliverable provides a framework for the application of uncertainty analysis in integrated urban water modelling. Its structure aims to provide a help for modellers by including the different uncertainties into a good modelling approach. Therefore, next to extensive literature for further information, a real world case study, which exemplary shows the approach, is included.

It is an implementation of existing frameworks for a global assessment of modelling uncertainties and uncertainty propagation analysis into a step-wise integrated urban water modelling approach, while expanding the scope of uncertainties incorporated. The idea is to see uncertainty analysis not as a standalone and separate process from the usual modelling workflow but as an integral part of it.

The process to construct and apply an integrated model can be subdivided into seven steps until a final report and assessment can be made. The assembled model and the sub-models applied need to be revised and if necessary refined with every step, creating a feedback loop for the model. Contemporaneously with this process, a thorough continuous documentation of the information, data, changes and assumptions applied during the process and the uncertainties of the beforementioned should be included to enable third parties to comprehend what has been done, what information the in- and output data can provide and how reliable are those results for further decision making. The treatment of uncertainties is incorporated here not as one step included in model analysis or calibration, but as a continuous work accompanying the entire integrated modelling process.

CONTENTS

1 Introduction

1.1 Background

The European Water Framework Directive (WFD (European Parliament and Council of the European Union, 2000)) has introduced a step change in water management in the European Union (EU), shifting the compliance focus from achieving water quality standards at individual locations to an approach on the scale of catchment systems. The WFD aims to achieve 'good ecological and chemical status' in inland and coastal waters through the implementation of "programs of measures" by EU member states against set timetables. Increasing wastewater treatment plant (WWTP) effluent quality standards and reducing intermittent wastewater discharges are suggested elements in the strategies by which these standards may be achieved.

Meeting the challenges of the WFD at an acceptable cost will require a sophisticated and holistic understanding and assessment of the water quality processes within a catchment, the ability to deploy models and assessment tools to achieve such a catchment wide overview is essential for informed decision making, efficient and effective management of the environment as well as delivering cost effective asset management and treatment strategies across the EU.

Until now deterministic integrated water quality models to predict water quality and treatment requirements across urban and rural catchment scales, have been the chosen method of assessment to deliver the WFD. Such models can simulate the interlinked dynamics of the catchment system, enable the assessment of a range of alternative responses (infrastructural/regulatory) and then allow the selection of the "best" response, i.e. the lowest "cost" or highest value response, although the impact of any response could be quite remote from the location of its implementation. Such an integrated modelling approach is increasingly seen as an essential technique for managing the impact on water quality from urban drainage and waste water systems, (mainly point sources) and diffuse pollution from rural areas (mainly associated with agricultural diffuse sources), on the environment and should lead to more cost effective and lower impact, both in terms of the achieved results for water quality and the consequences on the environment (e.g. fewer carbon emissions) when applying different solutions.

Significant asset investment and detailed water management strategies are based on the outputs of such modelling studies. However, there is an increasing concern that these deterministic models are being used improperly, leading to incorrect problem diagnosis and inefficient or possibly even adverse water quality and environmental management strategies. This is especially problematic for water infrastructure decisions, which are often very long lasting and extremely costly when over-sized, or when undersized and the performance of the asset is insufficient, resulting in a low quality of the receiving surface waters. The processes that impact on water quality in catchments include physical, chemical and biological processes with complex interactions that occur and propagate over a wide range of temporal and spatial scales. The modelling of these processes currently have a high level of uncertainty, which may be due to these processes not being fully understood, or because the chemical and physical transformations are dependent on parameters which are very difficult and expensive to quantify accurately, or have a high natural variability.

1.2 Partners Involved in Deliverable

Delft University of Technology, University of Sheffield and CH2M

1.3 Deliverable Objectives

The European project QUICS (Quantifying Uncertainty in Integrated Catchment Studies) contains 12 PhD candidates (Early Stage Researchers, ESR) and four postdoctoral researchers (Experienced Researchers, ER) in order to perform high quality research and collaborate with each other for developing and implementing uncertainty analysis tools for Integrated Catchment Modelling.

The objectives of QUICS Deliverable 6.7 are to provide:

- Definitions for the observable uncertainties in integrated catchment studies
- Linkage to scientific literature and further reading on the topic
- A framework for the practical application of uncertainty analysis in integrated catchment studies
- A practical example for the application of the proposed framework

2 Definitions

2.1 Integrated urban water modelling

Integrated modelling is founded on a set of interdependent science-based components (models, data, and assessment methods) for constructing an appropriate modelling system for a certain task (Laniak *et al.*, 2013). Integrated urban water modelling means by definition the joint modelling of two or more systems of the urban water system (see Figure 1), primarily the affected water bodies (HSGSim, 2008), by interweaving a sequence of sub models for the various elements of the system (Rauch *et al.*, 2002). In general the integrated urban water modelling can be characterized by three main features (Bach *et al.*, 2014):

- The modelling of a multitude of components and interactions between these components.
- The consideration of acute, chronic and delayed impacts of water quantity and quality processes over a long period (typically years) of simulation.
- The ability to see both local processes and the global perspective to broaden the scope for decision-making, policies or scientific knowledge.

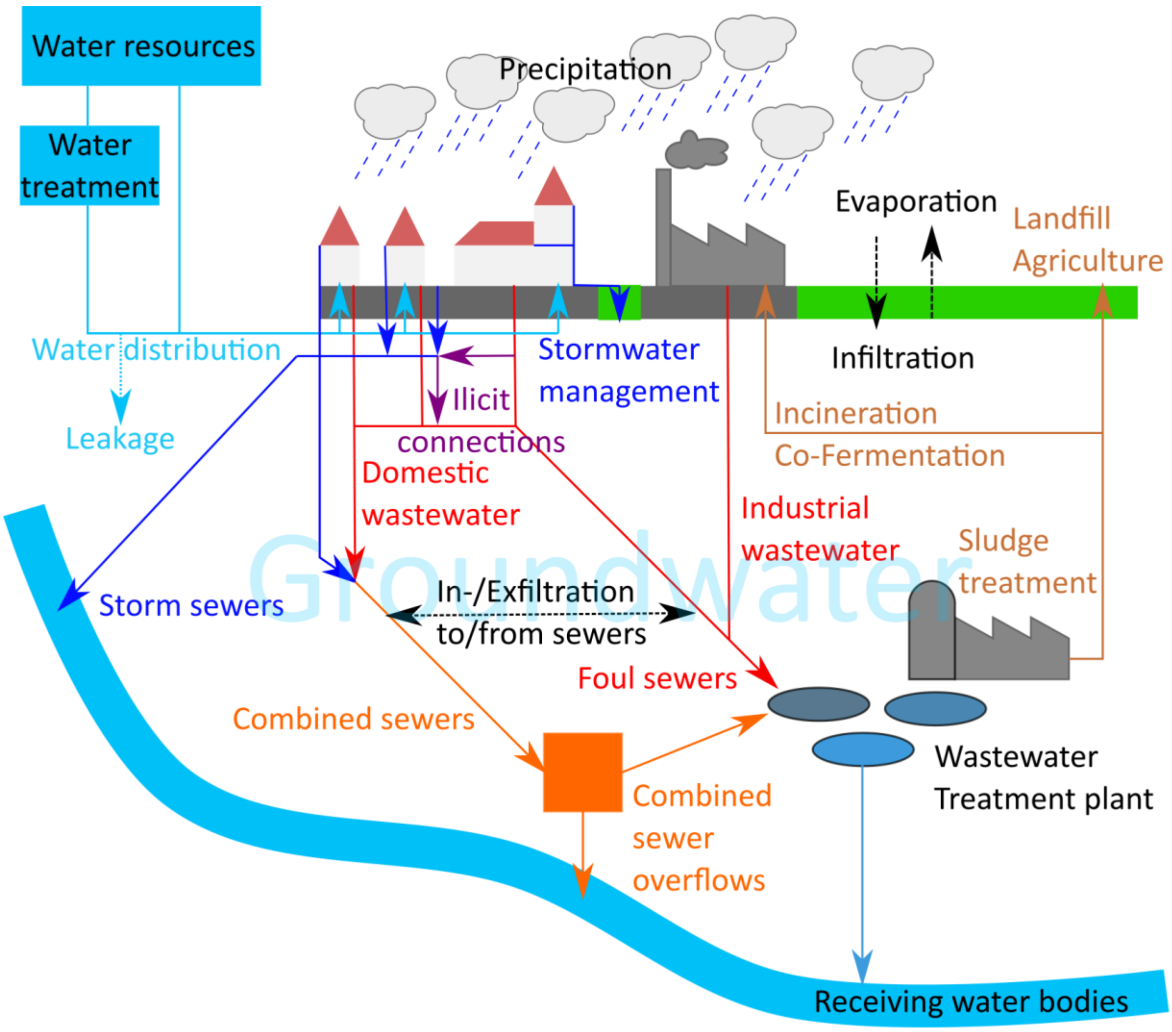

Figure 1: The urban water system

Integrated models are built to satisfy one or more of the following purposes (Brugnach and Pahl-Wostl, 2008; Kelly *et al.*, 2013):

- Prediction of a system's variable in a specified time period given knowledge of other system's variables in the same time period
- Forecasting of a system variable in future time periods, without knowledge of the values of other system variables in those periods
- Management and decision-making under uncertainty for selection between different options
- Social learning, which refers to the capacity of a society to communicate, learn from past behaviour, and perform collective action from this experience
- Developing system understanding and experimentation with different influences doing exploratory analysis

In the wide field of integrated environmental modelling those models can be classified into four groups with increasing complexity and a steadily broader scope – spatially as well as in terms of involved stakeholders (Bach *et al.*, 2014):

- Integrated Component-based Models represent the lowest level of integration and focus on the integration of components within the local urban water sub-system (e.g. the coupled modelling of different processes in a receiving water body).
- Integrated Urban Drainage Models or Integrated Water Supply Models are the second stage of integration, integrating sub-systems of either the urban drainage or water supply streams, particularly treatment and transport processes.
- The next level of integration is the linkage of these two models to an Integrated Urban Water Cycle Model.
- The final step of integration is then the implementation of further external influences, infrastructures and disciplines into an Integrated Urban Water System Model, which uses the interdisciplinary knowledge to assess water related problems.

Of course several steps in between these four groups with mixtures of implemented infrastructures and influences exist, depending on the posed problem or targeted concern, may it be in research or for day-to day operational decisions. An integrated assessment, which is still only a partial representation of reality, should cover all relevant issues to the stated problem (Rauch *et al.*, 2005). However, the integration of too many subsystems and processes irrelevant to the problem formulation can lead to unnecessary complexity (and errors) of the applied models. Furthermore, the decision on what is relevant for the actual question leaves room for subjective interpretation and differences of approach from the specialists that use integrated models, unless clear criteria are formulated. Due care is needed to ensure scale and concept consistency when linking components together (Voinov and Shugart, 2013).

2.2 Uncertainties

Models of integrated water systems do inherently include all aspects of uncertainty that occur due to the uncertainties inherent to the modelled subsystems (e.g. drainage system, wastewater treatment plant, receiving water system) and the linkage of these subsystems, however they also need to be acknowledged by their applicants. The diversity of uncertainty sources in these models (either for water quantity or quality) makes it non-trivial to deal with all of them in a rigorous way. Therefore, it is always important to provide a complete description of the existing and implemented uncertainties in any integrated model.

Walker *et al.* (2003), Refsgaard *et al.* (2007) and van der Keur *et al.* (2008) differentiate three dimensions of uncertainty:

- The location or source of uncertainty
- The type of uncertainty
- The nature of uncertainty

In the following sections a brief overview of the definitions from existing literature is given. These tend to be at times overlapping (e.g. mixing of input data uncertainty with model parameter uncertainty) in their definitions and also use different terminology. As an example can serve the usage of the term level (Walker *et al*., 2003) and type (Refsgaard *et al.*, 2007) for the same dimension of uncertainty. While level could also indicate the magnitude (to some extend also a connection could exist - see Figure 2) in this the less ambiguous term type is used. On the other hand, we keep the terms of location and source as exchangeable definitions, describing where the uncertainty manifests itself within the model complex. For definition of uncertainties apply the decision trees adapted as part of this deliverable, the reader is referred to Figure 4.

2.2.1 Location or source of uncertainty

Due to the fact that uncertainty can manifest itself in different locations within the model complex at an element in the process description of the integrated model, these locations can be used for differentiation, although the description of the model locations will vary according to the applied model (Walker *et al.*, 2003).

Deletic *et al.* (2012) distinguish three main sources of uncertainty:

- Model input uncertainties
- Calibration uncertainties
- Model structure uncertainties

Model input uncertainties concern the input data and selected model parameters (often from literature), that are required to apply a model to a problem. Model input data can be differentiated into input data that is needed for simulation (e.g. rainfall time series) and input data, that is needed to build the model (e.g. geometry of a sewer system, which may come from a system design drawing or GIS). While the first group of input data is mostly directly measured the second group is often estimated (although in theory should be measured) from existing data and depends therefore greatly on the quality of the data collection process. The uncertainties deriving from this data collection process can be large as well as the sensitivity of the model output to these uncertainties. Clemens (2001) showed that even often omitted network data (e.g. house connections, gully pots) can cause systematic errors when calibrating hydrodynamic models. The only possibility to minimize these uncertainties would be by detailed field inventories and subsequently keeping a consistent and up-to-date database to achieve the so-called “transparent infrastructure” (Tscheikner-Gratl, 2016). Uncertainties in measured input data can often be characterised as systematic uncertainties (e.g. insufficiently calibrated measurement equipment) or Gaussian distributed random uncertainties or a combination of these two effects. Input data as well as model parameter uncertainties are strongly related to calibration uncertainties (Kleidorfer, 2010). Uncertainties in input data can in parts be compensated during the calibration process by adaptation of the model parameters, if the spatial and temporal properties of the available data for calibration is the same as for the input data (Kleidorfer *et al.*, 2009a; Muschalla *et al.*, 2015). On the downside this compensation can lead to force fitting of model parameters (Vrugt *et al.*, 2008) and errors in the estimation of the relative importance of different uncertainty factors on the integrated model (Muthusamy *et al.*, 2017). If the model parameters are considered as reflecting reality, this representation is reduced when input and calibration data errors are considered (Dotto *et al.*, 2014).

Calibration uncertainties are related to the data used for calibration and their selection, and to the calibration methods (Leonhardt, 2015), depending on the model concept and even on the specific software applied. Deletic et al. (2012) trace their sources to measurement errors in both input and output data, the selection of appropriate calibration data, the applied calibration algorithms and objective functions used in the calibration process. Some model parameters cannot be taken from literature only, they have to be determined during model calibration. The choice of the measurement and model output data (e.g. the choice between using concentrations or loads to calibrate the empirical coefficients of a water quality model, or the choice between flow volume or water depth to calibrate parameters of a hydrodynamic sewer model) and the amount of data available for calibration (e.g. number of storm events, length of time series) can have a serious impact on the estimation of the calibrated model parameters. For example, Tscheikner-Gratl *et al.* (2016) showed the effect of different storm events and rain gauges used for calibration of the parameters subcatchment width (representing the flow time on the surface), imperviousness and pipe roughness for a hydrodynamic urban drainage model on the performance in terms of urban flooding. Achleitner (2008) compared three different quality indicators (Nash-Sutcliffe Efficiency, Index of agreement and Bias) and their influence on the calibration quality of parameters (maximum autotroph growth rate, autotroph decay coefficient and autotroph concentration in WWTP inflow) in a wastewater treatment plant model.

Model structure uncertainties, depend on how well the numerical model represents the systems and processes (Deletic *et al.*, 2012). They include uncertainties regarding the temporal and spatial resolution (for example using a 1D or 2D approach to simulate river mixing), the formulation and numerical solution of the posed problem and conceptualisation errors, such scale-issues or omitting key processes (Kreikenbaum *et al.*, 2004). It is difficult to assess these uncertainties when using only a single model approach, which may fail to sample adequately the relevant space of plausible models for one problem. It is prone to modelling bias and underestimation of predictive uncertainty (Refsgaard *et al.*, 2006).

The classification of Deletic *et al.* (2012) makes it difficult to include the model parameters into one of the classes for application in uncertainty analysis and documentation. While exact and fixed parameters can be included into the model structure, calibrated parameters can be seen as calibration uncertainties, and a priori selected parameters that may be difficult to identify by calibration and are selected to have a certain value range can be treated as model input. For example there are model parameters such as hydraulic roughness and also contributing area – which could be argued to fall either under input uncertainties, or, calibration uncertainties, e.g., you can estimate hydraulic roughness by looking at a river and comparing it with a library of river images with given roughness, or, you take the material and age of a sewer system into account and estimate hydraulic roughness and express this as ‘input uncertainty’ or you calibrate your model for hydraulic roughness, in which case it becomes a calibration uncertainty.

Furthermore, there is a relationship between model structure uncertainty and calibrated parameter uncertainty. A less sophisticated model with a limited number of parameters that does not simulate reality well may be calibrated with data obtained for both input and output under well-known conditions. In this case, model structure uncertainty will most likely dominate the result. In the case of a more complicated model with many parameters, the parameters may be manipulated to fit the calibration data beautifully, but the result may be dominated by parameter uncertainty (Walker *et al.*, 2003). It is however very difficult to isolate the value of the contribution of structure uncertainty in those cases, because it is then incorporated in the parameter uncertainty after calibration.

Therefore, to avoid ambiguity in definition the differentiation of uncertainty sources into 5 subgroups, as shown in Figure 4 and subsequently used in Table 1, containing these model parameters and the context (e.g. external circumstances at the boundaries of the system modelled), as done by Walker *et al.* (2003) and Refsgaard *et al.* (2007), is implemented into this deliverable (see Figure 4).

2.2.2 Type of uncertainty

Van der Keur *et al.* (2008) defined the types of uncertainty as a gradual transition from determinism (see Figure 2). They are distinguished by the knowledge about the possible outcomes of a model and the probability of the occurrence of these outcomes (Brown, 2004).

Starting point is the ideal of determinism, where all outcomes are known with absolute certainty and therefore no uncertainty exists (Refsgaard *et al.*, 2007). It bases on the concept, that if all underlying physical, chemical and biological processes can be identified and described, so that a full and exact understanding is possible (Harremoës and Madsen, 1999). This, of course, is a state, which does not exist in reality. The next step contains uncertainties, which can be grasped and handled statistically. All the possible outcomes are known and the probabilities of these outcomes can be described statistically. When the probabilities cease to be describable by statistical means but the possible outcomes are estimable we have scenario uncertainties. When not all probabilities of the outcomes and not even all of the outcomes themselves are estimable, then qualitative uncertainty takes place. Recognised ignorance occurs when there is an awareness of lack of knowledge on a certain issue (van der Keur *et al.*, 2008). If this cannot be resolved by further research, indeterminacy takes place, where some possible outcomes are deemed unknowable (Brown, 2004). Finally, total ignorance describes a state of complete unawareness of missing knowledge (van der Keur *et al.*, 2008). We separate deep uncertainties from the more tractable uncertainties encountered in statistics and scenario analysis with known probabilities (Cox, 2012). In practice, it is not uncommon to have to address different uncertainty types simultaneously in the modelling and decision making processes. For example, some uncertainties are represented by probability distributions when sufficient data is available, while others are better represented by fuzzy sets to capture linguistic expert knowledge (Fu *et al.*, 2011).

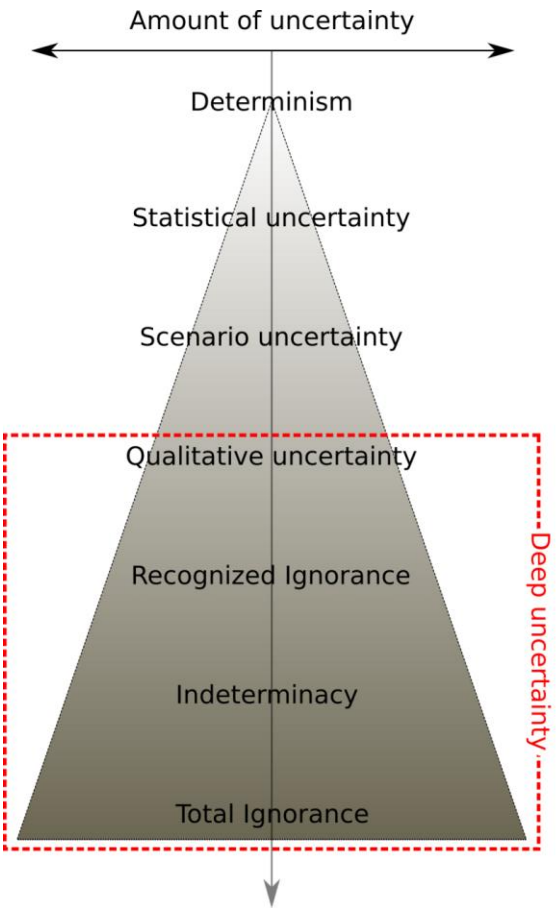

Figure 2: Types of uncertainties adapted from van der Keur et al. (2008)

2.2.3 Nature of uncertainty

An important feature of the nature of uncertainty is the distinction between epistemic and variability uncertainty (Walker *et al.*, 2003). While epistemic uncertainty describes the uncertainty due to lack of knowledge, which may be reduced by more research and empirical efforts, variability or aleatory or stochastic uncertainty represents the inherent variability of the examined system (e.g. short-term climate variability). The fundamental difference between these two uncertainties is the fact that epistemic uncertainty can be reduced, for example statistical uncertainty by collecting more data (however, also the opposite can happen depending on the data), while variability uncertainty cannot be reduced (van der Keur *et al.*, 2008). Therefore, also a discrimination into reducible and irreducible nature of uncertainty could be applied (Belia *et al.*, 2009). However, a lot of times uncertainty on a certain event includes both epistemic and stochastic parts (Refsgaard *et al.*, 2007), so it seems more applicable to keep this differentiation for this deliverable. Still the differentiation between epistemic and variability is difficult and could also be dependent on the scale of observation.

For example, uncertainty about climate change could be reduced if we collect more data on carbon outputs, reflection from sea ice, methane outputs and so on. As a result more sophisticated models to try and understand it better can be developed – so the uncertainty can be defined as epistemic. About the dependency on the scale of the observation, rainfall has a variability which is dependent on spatial and temporal scales, e.g. to work out average rainfall on a 10 km^2 area, you could collect data from a single rain gauge in this area, but there is an uncertainty as to how representative this data is for the whole 10km^2 area, so you can collect more data to reduce this uncertainty, defining it as an epistemic uncertainty. You could collect data from 3 rain gauges within the same 10km^2 area, which means you have more confidence in the average rainfall value. However, due to the inherent variability of rainfall, you can move these 3 gauges around to different places within the 10 km^2, or add more gauges, and you would keep getting slightly different area average values, due to the inherent variability of rainfall, hence it won't ever become a deterministic input – it stays a variability uncertainty. Examples for this can be found in Tscheikner-Gratl *et al.* (2016) and Muthusamy *et al.* (2017).

Warmink *et al.* (2010) discriminate a third nature of uncertainty called ambiguity, which is the simultaneous presence of multiple equally valid frames of knowledge (Dewulf *et al.*, 2005). For example the different involved parties and stakeholders in an environmental impact study (from environmental activists to project manager) can have very different views on the model boundaries, which are all in themselves absolutely valid. Before deciding on a frame and boundaries thinking about other possible frames from different viewpoints should be included in an integrated modelling process. Therefore, this further discrimination is necessary and included into this deliverable, because ambiguity is neither stochastic, nor is it fully reducible by more information.

3 Application of uncertainty analysis

3.1 Framework

The framework proposed here (see Figure 3) is an implementation of the framework for a global assessment of modelling uncertainties (Deletic *et al.*, 2012; Refsgaard *et al.*, 2007) and uncertainty propagation analysis (Heuvelink *et al.*, 2017) into integrated urban water modelling using the outlines proposed by HSGSim (2008), Belia *et al.* (2009), Muschalla *et al.* (2009) and Bach *et al.* (2014) while broadening the framework by Deletic *et al.* (2012), which focussed on statistical descriptions of uncertainty, through incorporating a wider definition of uncertainty The idea is to see uncertainty analysis not as a standalone and separate process from the usual modelling workflow but as an integral part of it (Sriwastava and Moreno-Rodenas, 2017).

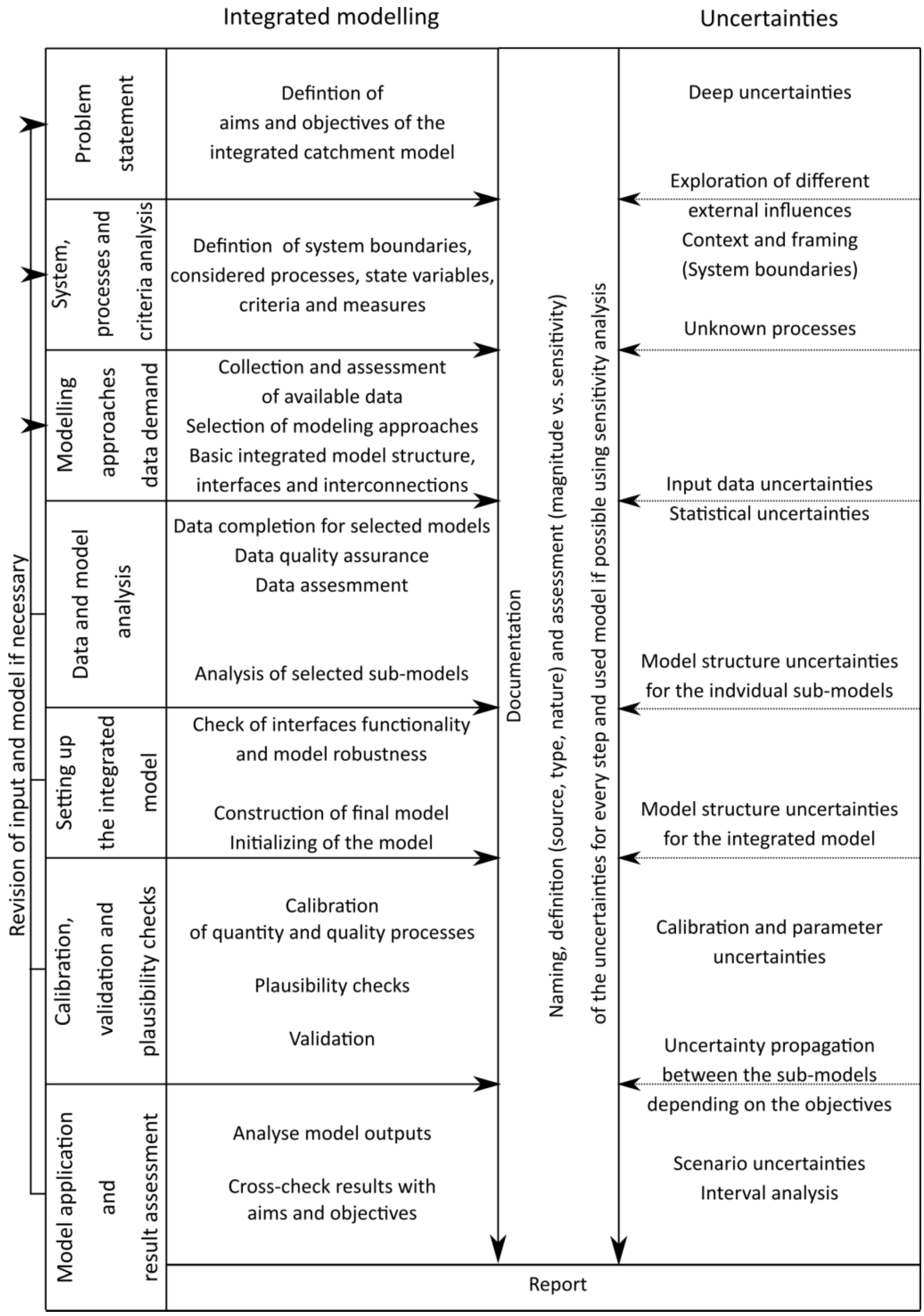

Figure 3: Framework for uncertainties in integrated urban water models

The process to construct and apply an integrated model can be subdivided into seven steps until a final report and assessment can be made (see Figure 3). The used model and sub-models need to be revised and if necessary refined with every step, creating a feedback loop for the model. Contemporaneously with this process, a thorough continuous documentation of the information, data, changes and assumptions used during the process and the uncertainties of the before mentioned should be included to enable other people to comprehend what has been done and what every bit of data means (Tscheikner-Gratl, 2016). The treatment of uncertainties should therefore not be seen as one step included in model analysis or calibration, but rather as a continuous work accompanying the entire integrated modelling process.

3.2 Documentation and classification of uncertainties

The documentation of an integrated model simulation study must comprise of a detailed list of the objectives of the study, selected modelling approaches (including explanatory statements), software packages used (including version number), all the relevant operation and process data of the system analysed, final simulation models, list of used parameter sets (with an explanation if the selected parameter values differ significantly from the usual parameter ranges), relevant results of data evaluation (e.g. mass balance) and calibration and validation results (Muschalla *et al.*, 2009), assumptions made and the estimated uncertainties following the framework shown in Figure 3. Every step of this framework has to be described to enable reproduction of the modelling approach and the final simulation results. In terms of the uncertainty assessment of the modelling approach it is advisable to take the time and define for every step of the framework the inputs and define them in terms of source, type and nature of uncertainty (use Table 1 and Figure 4).

Table 1: Uncertainty matrix for definition and examples for uncertainties adapted from Walker et al. (2003), Refsgaard et al. (2007) and Warmink et al. (2010)

Description of input	Source					Type				Nature		
	Context	Model input	Parameter	Calibration	Model structure	Determinism	Statistical	Scenario	Deep uncertainty	Epistemic	Stochastic	Ambiguity
Climate change scenarios	X							X			X	
Infiltration parameters			X				X				X	
Rainfall data		X					X				X	
Car parking in urban catchment , which increase the friction (drag force) in surface flooding	X								X	X		
Geographical data of urban drainage manholes and of other subsystems that should be taken into account with different scales		X				X				X		

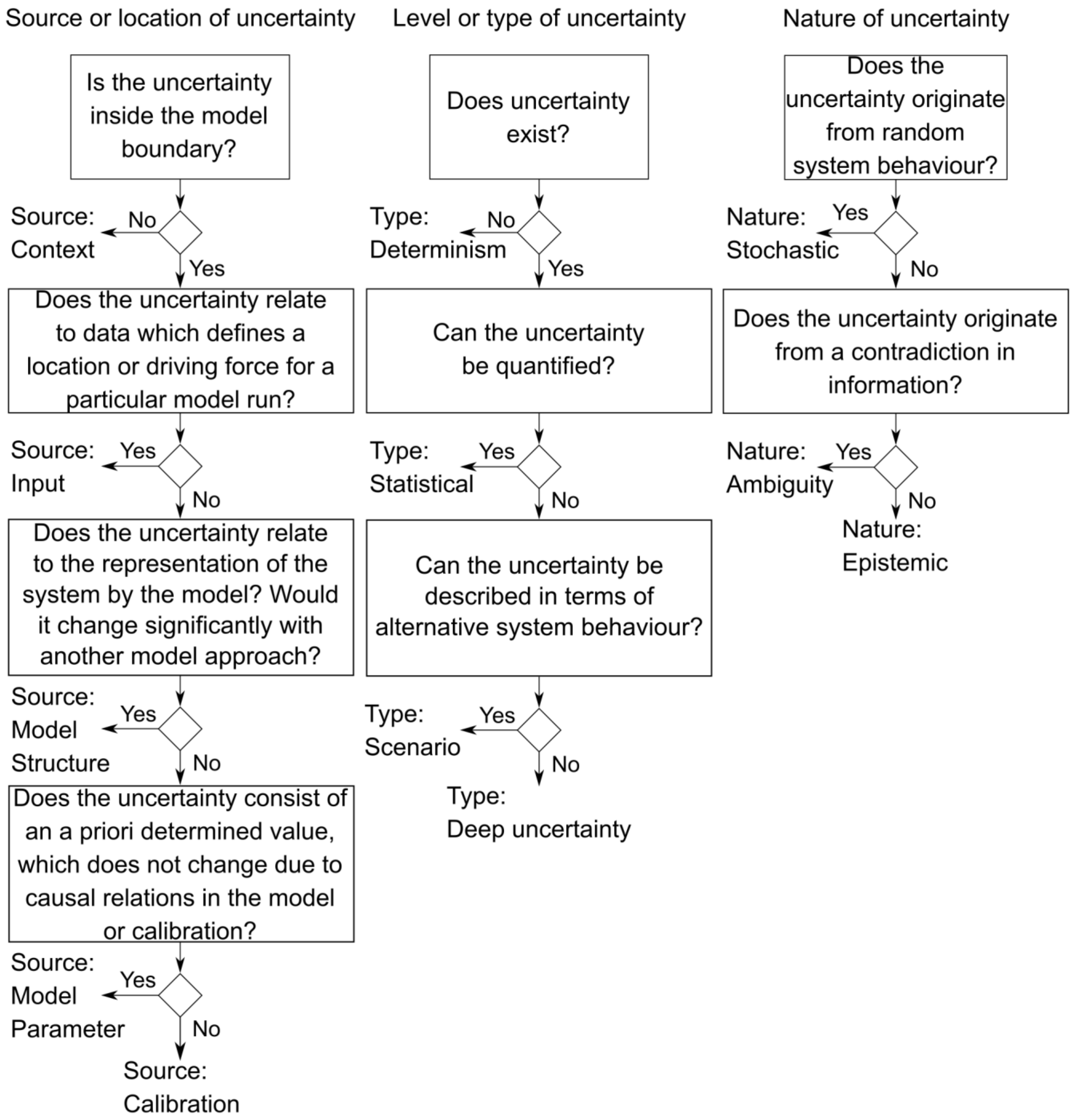

Figure 4: Decision trees for defining uncertainties, adapted from Warmink et al. (2010)

Thereby, it is not the most important task to mark all the boxes, but to assess what the modeller knows about his data, inputs and models. In addition, it is important that thought is given to “deep uncertainties” (as in Figure 2), assessing what is not known or definable for the chosen integrated model and its boundaries. In filling in the matrix, one should be aware that the type and nature of the uncertainty that occurs at any location can manifest itself in various forms simultaneously (Walker *et al.*, 2003). So, even a more pragmatic approach by defining uncertainty only by their treatment in the modelling process either into statistical, scenario or deep uncertainties (i.e. not considered) can be sufficient if it is done by an extensive data, inputs and models assessment.

Because models, in most cases, can have a high number of inputs it is, although in theory necessary, not possible in practice to treat all inputs as uncertain, due to constraints in time and resources allocated to the modelling process. To decide, which inputs contribute most to the uncertainty in model output, two factors have to be considered (Heuvelink *et al.*, 2017):

- The magnitude of uncertainty about the model input
- The sensitivity of the model output to changes in the input

Both factors are either based on expert judgement and/or deterministic sensitivity analyses and depend highly on the aim of the modelling activity. Expert elicitation can be used to estimate the level of uncertainty in model inputs and parameters even when field data is limited (Schellart *et al.*, 2010). The decision about which of the input will be considered further can be aided by using a priority table, where the magnitude of uncertainty and the sensitivity of each input is ranked (Heuvelink *et al.*, 2017), in addition to an graphical assessment (see Figure 5). The input is depicted as a data point in the area of the two decision factors and the distance to the point of no uncertainty (0,0). Substantial contribution to output uncertainty occurs when both factors are higher than a certain threshold. The definition of these thresholds will influence the assessment of uncertainty greatly and should therefore be taken with care. Furthermore, if the two factors are based on expert knowledge alone, an evaluation of these assumptions has to be made and if necessary adjustments and recalculations. It must be taken care that these assumptions derive from really comparable cases, due to the differences in perception of the magnitude of uncertainty and sensitivity depending on the goal of the modelling approach. That is also true for the following examples in Figure 5:

- High magnitude of uncertainty and low sensitivity (1):
  For example: the dry weather flow, when modelling urban flooding. The model output may not be very sensitive to this input but (depending on the input data quality) the magnitude of uncertainty may be quite high.
- High magnitude of uncertainty and high sensitivity (2):
  For example: water quality parameter (e.g. BOD, P) concentrations of CSO into receiving water bodies, when modelling dissolved oxygen concentration in rivers. The model output may be very sensitive to these concentrations (depending on the volumes) and they may be very uncertain, when for example few measurement values were used or none at all but literature values.
- Low magnitude of uncertainty and high sensitivity (3):
  For example: the height of weir crests, when modelling CSO volumes. The model output may be very sensitive to these values but the uncertainty in most cases is very low and restricted to geodetic measurement errors.
- Low magnitude of uncertainty and low sensitivity (4):
  For example: pump characteristics of wastewater pumps, when modelling urban flooding. The sensitivity of the model output may be in cases very low, depending on the pump locations in the network, and can be quite certain due to sufficient data.

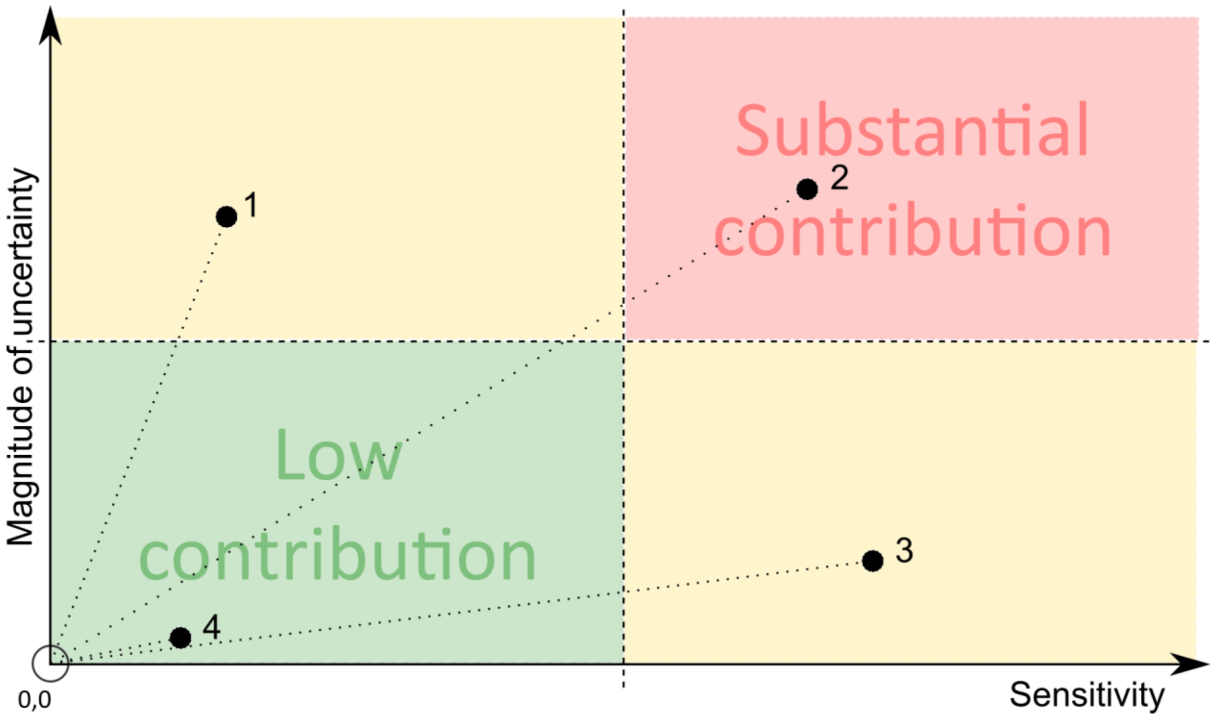

Figure 5: Graphical assessment of contribution to the uncertainty in the model output

3.2.1 Sensitivity analysis

Sensitivity analysis (SA) can be defined as the investigation of the response function that links the variation in the model outputs to changes in the input variables or/and parameters, which allows the determination of the relative contributions of different uncertainty sources to the variation in outputs using qualitative or quantitative approaches under a given set of assumptions and objectives (Song *et al.*, 2015). So, sensitivity analysis assesses the sensitivity of the model outcome to changes in the model input, highlighting the input which has a high impact on the model result. The result enhances the understanding of the model and further delivers information about parameter boundaries for calibration. For sensitivity analysis no measurement data is necessary but could be helpful to limit the parameter space (Camhy *et al.*, 2013). An important factor for choosing sensitivity analysis is the available time and computational budget of the project. Depending on these factors, the method and the parameters, the graphical assessment in Figure 5 can be used for preselection in case that not enough budget is available to assess all parameters. Although a maximisation of the assessed parameters for the computational budget is recommendable, care has to be taken that the amount of simulations does not drop below a certain level (depending on the method and the parameter space (Vanrolleghem *et al.*, 2015)) in order to keep the results reliable.

The Sensitivity Analysis (SA) methods can be classified into three categories (Saltelli *et al.*, 2006), which can be seen as complementary (Sun *et al.*, 2012):

- Local sensitivity analysis (LSA)
- Global sensitivity analysis (GSA)
- Screening methods

A local sensitivity analysis evaluates sensitivity at one point in the parameter hyperspace. This point may be defined by default values or a crude manual model calibration. Typical choices are published “default” values or values gained through preliminary analysis (Kleidorfer, 2010). Sensitivities are usually defined by computing partial derivatives of the output functions with respect to the parameters. A sensitivity index can be calculated for a small change of the parameter value, while the other input parameters are held constant (van Griensven *et al.*, 2006) and therefore are also called ‘‘one-factor-at-a-time’’ (OAT) approaches (Saltelli *et al.*, 2006). Local sensitivity analysis is based on a linearization of the model and use for other models than strictly linear ones can be problematic (Saltelli *et al.*, 2006). Its main advantage is that local sensitivity analysis is computationally relatively inexpensive (Kleidorfer, 2010) and specific methods for local sensitivity analysis for computationally expensive urban hydrodynamic systems exist (Clemens, 2001). The use of a local SA method to draw conclusions on the relative impacts of uncertain model parameters on model prediction should be avoided unless the uncertainty of the model parameters is small (Sun *et al.*, 2012).

Integrated modelling consists mainly of non-linear dynamic models; hence local sensitivity analysis can only deliver a rough estimation of sensitivity. Contrary to local sensitivity analysis, Global sensitivity analysis (GSA) methods assess how the model outputs are influenced by the variation of the model factors over their entire variation range (Vanrolleghem *et al.*, 2015). This is already similar to methods used for uncertainty analysis and if parameter distributions are chosen according to known uncertainties this can be interpreted as analysis of sensitivity of model result in respect to uncertainties of model parameters (Kleidorfer, 2010). Essential to this method is the sampling strategy, often Monte Carlo (MC) or Latin–Hypercube (LH) sampling (van Griensven *et al.*, 2006; Fu *et al.*, 2009). The robustness of GSA can be significantly increased by using multiple methods, multiple objectives and testing convergence (Vanrolleghem *et al.*, 2015).

Screening methods (e.g. Campolongo *et al.* (2007)) are model simplifications. The objective of this setting is to identify the factor or the subset of input factors that can be fixed at any given value over their range of uncertainty without reducing significantly the output variance and therefore without significant loss of information in the model. It gives a good overview with respect to importance and interactions/non-linearity (Gamerith *et al.*, 2013). It can also be used to prove or falsify prior assumptions in the model (Saltelli *et al.*, 2006). This screening process can be used as a first step before applying a GSA, when the number of input factors involved in the model is too high to afford a computationally expensive quantitative analysis (Sun *et al.*, 2012). However, care must be taken that no factors are excluded, that in the end turn out to be important (Vanrolleghem *et al.*, 2015).

3.3 Problem statement

The foundation of any modelling and decision making approach is the definition of a problem statement (Hoppe, 2006). A problem statement contains objectives or project goals, context, questions to be answered and a targeted concern. The purpose of the problem statement is to provide the information needed to guide the subsequent steps

(Laniak *et al.*, 2013). Also it should answer the question if and why modelling is required for this particular study (Refsgaard *et al.*, 2007). Furthermore, the question about the tolerance boundaries of uncertainty in the model should be addressed, which is still seldom done in modelling practice. This can vary significantly, depending on the overall problem statement and the objectives connected to it.

Usually, the problem statement derives from known deficits, often due to legal requirements, of an observed system or the need to optimisation of an existing (Muschalla *et al.*, 2009). Although the knowledge about the modelled system increases during the modelling process, this gain of knowledge is seldom the driving force in practice (but rather in science), but often external motivation on the operator of a system is triggering the process (e.g. by public opinion or legislative changes). Often integrated models are used to demonstrate that a system will comply with a regulation. A first step is therefore the translation of this motivation from more abstract and qualitative formulations to a concise problem formulation.

Muschalla *et al.* (2009) suggest a deficit analysis to help with this formulation process. The first step is therefore the determination of the current state from available data, which is then in the next step compared to a target condition. These target conditions can be classified into water quantity (e.g. flooding, storage volume) or quality requirements (e.g. river water quality). Often they can be quantified by application of legal requirements (HSGSim, 2008). Another possibility is the targeting of monetary values (e.g. pumping costs) if the motivation is of an economical nature. To define the target conditions and the expected accuracy of modelling results (which can vary from case to case), the involved actors and their goals have to be thought of. Refsgaard *et al.* (2007) define four types of actors, which is extended to five in this deliverable, which could be involved in the problem definition process:

- The water manager, representing the organisation or person that owns the problem and commissions the study
- The modeller, which conducts the modelling study. He could be of the same organisation as the water manager or an external expert
- The reviewer, which adds external expertise to the study by reviewing the work
- The stakeholders/public, which can be either a competent authority, interest groups and general public
- The regulator with legal powers, which should be independent from the other four types

Because the necessary effort (e.g. expressed as monetary and social costs) increases with increased requirements, it is important to reach a consensus between the involved parties on the level of confidence and effort required to achieve each project goal, because a correlation between increased effort and increased complexity of the modelling objective can be surmised (Belia *et al.*, 2009).

3.3.1 Deep uncertainties

The modeller has to consider, that the overall uncertainty might be larger than the quantifiable uncertainty. Non-quantifiable or deep uncertainties (as defined in Figure 2) may in some case be more serious than the quantifiable uncertainties (Willems, 2008). Deep uncertainties are hard to incorporate into any modelling study. However, when thinking about the problem statement and defining the goals of the modelling approach it is good to think about the things one cannot know, or know but cannot incorporate. Nevertheless, the realisation that we may be completely ignorant to case-effect relationships (Harremoës and Madsen, 1999) may be beneficial in concentrating on the aim and the possible outcome of the modelling process. However, the definition of total ignorance and indeterminacy implies that implementation is nearly impossible (or more of a philosophical matter) and therefore we will focus on qualitative uncertainty and recognized and reducible ignorance. The nature of this ignorance allows it to be reduced by further research, if wanted.

How to treat these uncertainties depends on the aim of the modelling approach. If the idea is to design a system for longer periods the implementation of these uncertainties can be useful to accomplish the aim of a fault-tolerant, survivable, and resilient one (Cox, 2012). The same applies if the goal is exploratory for understanding the system behaviour for different influences as well as showing these influences to other stakeholders. If it is used for showing that present regulations are met it is less important to treat these uncertainties. Nevertheless, this decision should be documented and based on good arguments (e.g. by using an uncertainty matrix as shown in Table 1).

For these levels of uncertainty the uncertainty matrix (Table 1) can be used for definition, while for magnitude assessment expert elicitation, extended external review and discussion with stakeholder involvement and if available numeric and literature values can be applied (Refsgaard *et al.*, 2007). Furthermore it is possible to identify context scenarios, in contrast to a traditional scenario planning, to cover a wide range of scenarios to explore the deeply uncertain scenario space, even if it does not cover all of it (Urich and Rauch, 2014). These context scenarios can be developed from qualitative guidance (e.g. strong, medium, low increase of area) and narrative perceptions (for examples of narratives see e.g. Ashley and Tait (2012)). Together with more certain scenarios at the level of scenario uncertainty, they could be implemented in scenario analysis. Depending on the available resources (time and computational) as many scenarios as practical would have to be modelled to cover as much as possible of the uncertainty scenario space. The results can then be involved into a robust decision-making (RDM) approach (Lempert *et al.*, 2006).

3.4 System and processes analysis and definition of criteria

After the definition of the objectives and the deficits, the reasons for these deficits and the involved processes and criteria together with possible optimization potentials have to be identified (HSGSim, 2008). This requires a more detailed system and significant process analysis, which correlates directly with the definition of relevant criteria (Muschalla *et al.*, 2009). These relevant criteria can be derived from the aforementioned project goals. For water quality it can be either emission or immission based evaluation (Benedetti *et al.*, 2010), for quantity flooding and CSO volumes, number and return periods of events. If the criteria are not representing fixed legislative values, they can be however updated if necessary during the process. Finally, for both quality and quantity, costs can be used for evaluation.

In general, integrated modelling should cover the full urban water system (see Figure 1). Depending on the scope and objectives of planning, it is permissible to exclude or neglect single sub-systems, components, interfaces or processes within or between sub-systems, which do not contribute to the solving of the stated problem (Schmitt and Huber, 2006). However, the utmost care has to be taken when deciding these system boundaries in order to cover all the significant processes. It is very important to be aware, that omitting of processes introduces an unknown magnitude of model structure uncertainty. Therefore, these decisions have to be a well-documented, well-discussed and well-argumentized choice. Furthermore, the setting of the system boundaries is a continuous process influenced by the system and process analysis. The final goal is to set the system constraints as narrowly as possible, which can be achieved by starting with a full integrated model and then reducing it by eliminating parts of the model which are not significantly influential (Meirlaen and Vanrolleghem, 2002). This model reduction, driven by sensitivity analysis, with minimal deterioration of the accuracy of the model output is also a way to develop a fast, less computationally expensive, model (Vanrolleghem *et al.*, 2005a).

For example, for a quantitative estimation of the hydraulic performance of a combined sewer system only flow volume will be considered, excluding water supply systems, water quality aspects as well as groundwater, if no high infiltration is expected. For water quality modelling of receiving water bodies other system boundaries are necessary, including wastewater treatment plants and depending on the detail of the evaluation either standard wastewater parameters, such as suspended solids (SS), Chemical Oxygen Demand (COD) and nitrogen, or specific trace pollutants (Schmitt and Huber, 2006).

3.4.1 Context and framing uncertainties

Context can be defined as the conditions and circumstances which are the base of the selection of the system boundaries, as well as the framing and formulation of problems within these boundaries (Walker *et al.*, 2003) and occurs mainly in the problem definition phase. Context includes the boundary conditions as regulatory conditions and other external factors such as the impacts of future economic, environmental, political, social and technological developments (van der Keur *et al.*, 2008), if these aspects are not explicitly included in the modelling study. This context could fall within the past, the present, or the future (Walker *et al.*, 2003), while for practitioners mainly the future (and to a smaller extent the present) is of interest, for researchers the past can also be of interest.

Framing includes differences in societal views of different actors on an issue, i.e. different definitions or recognition of the main problems, different view on what's at stake, difference on which goals should be achieved at what price (Newig *et al.*, 2005). Simultaneous presence of multiple equally valid frames of knowledge, the so-called ambiguity (Dewulf *et al.*, 2005), often occurs in multi-actor projects, which is true for most integrated catchment studies. Care should be taken that these different frames are made explicit in the documentation and therefore the implementation into uncertainty assessment transparent. For example, the different involved parties and stakeholders in an environmental impact study (from environmental activists to project manager) can have very different views on the model boundaries, which are all absolutely valid in themselves. Before deciding on a frame and boundaries, considering other possible frames from different viewpoints (and maybe estimating them in the wake of stakeholder involvement) and documenting those viewpoints and frames can be beneficial for the modelling process but mainly for the communication and justification of model results at the end of the process.

These two sources of uncertainty can be implemented into a scenario analysis, if they are not statistically graspable, which is mostly the case, either if the possible outcomes are known as scenario uncertainties and if not as deep uncertainties.

3.5 Modelling approaches and data demand

In general the modelling approaches adopted should be flexible to fit the identified problem (Harremoës and Madsen, 1999). After reducing the system boundaries to enable a manageable (in terms of complexity and computational effort) model concept, the model approaches for the different integrated processes should be selected. Hereby, it is not the most complex model that is preferred, but, following Ockham’s razor, the least complex that answers the asked question reliably, in a comprehensible and verifiable way (Rauch *et al.*, 2002). This also includes the knowledge of the limitations of the applied models and sub-models, which will include models for diverse processes such as rainfall runoff relationship, hydraulic transport/routing, pollutant transport/routing and pollutant transformation processes (Achleitner, 2008). Also between the subsystems, the level of complexity has to be consistent, depending on the problem statement. For some applications and scales the estimation with coarse models of CSO volumes, multiplied by a fixed concentration, as input for a detailed river model, taking several water quality processes into account, can be acceptable, while for others a detailed river water quality model makes no sense if the input from wastewater treatment plants and urban runoff is estimated by more rough models (Rauch *et al.*, 1998). On the other hand, it can be unnecessary effort to use a very detailed model as input for a simple one, for example a very detailed sewer model for water quality for estimating input into a very simple river water quality model (Schellart *et al.*, 2010). Essential is that the selection of the models is a conscious decision, also considering the uncertainties implied, and not dictated by availability and commodity. Potential mismatches of models could lead to waste of computational resources, while not improving the accuracy of the model output.

Beyond the modelling approaches, an adequate amount of data is essential to define the model setup and to identify the model parameters (Muschalla *et al.*, 2009). Different level of model integration also demands different amount and quality of data for modelling and decision-making (Eggimann *et al.*, 2017). Normally, the data for the subsystems will be available with different quality and on different (temporal and spatial) scales. The required quality of the data is determined by the selected modelling approaches and by the defined processes respectively. The more detailed the modelling approach to describe the physical interrelationships is, the higher the data requirements are (Muschalla *et al.*, 2009).

The selection of modelling approaches is an iterative process (HSGSim, 2008). The modelling approaches and the available data always need to be evaluated and compared with the selected objectives and evaluation criteria. If a discrepancy arises, three solutions are possible:

- Conduction of additional measuring campaigns to close the data gap (Muschalla *et al.*, 2009) or the usage of historical data collection and reconstruction tools (Benedetti *et al.*, 2008).
- Usage of alternative model approaches which allow modelling with the available restrictions or the development of new models based on them.
- Limitation of the project objectives and reconsideration what objectives can be reached given the restrictions on data and if these objectives suffice for the agreed problem statement.

The decision between these three solutions is often an economic one, although an objective beneficial cost-benefit ratio is still missing (Eggimann *et al.*, 2017), as well dictated by time constraints given by project timeframes. Higher complexity in modelling approaches requires larger and more costly monitoring campaigns (Freni *et al.*, 2009). One possibility is the restriction of the objectives to the achievable results for the available data, if this does not inhibit the solving of the stated problem too much. If other models or the expertise to develop new ones exist, suitable for the objectives, this would be the next possibility. Finally, if no other possibility is left a data demand has to be defined and data collection has to be carried through. Sometimes the use of data reconstruction tools (Benedetti *et al.*, 2008) or the adoption of literature-derived parameter values (Freni *et al.*, 2009) could be applicable, however good quality measurement data is preferable.

3.6 Data and model analysis

Based on the estimated input and calibration data demand a quality assurance strategy for the data has to be applied. This strategy should include the available data (geographical data and historical and/or ongoing measurements) as well as necessary additional measurements. The planning of measurements and the model setup is a mutually dependent process. While measuring is necessary for the model setup, the model itself can be used to design the monitoring (Kleidorfer *et al.*, 2009b).

Data validation should be based on criteria derived from available information about the data themselves, the sensors used, the environment and the context of the measurement process or a combination of these elements (Bertrand-Krajewski *et al.*, 2003). Furthermore, it also depends on the focus of the study as well as the required spatial and temporal scale for approaching the problem statement. It should be taken into account that due to data validation the amount of available validated data can be significantly less than the amount of measured data (Langeveld *et al.*, 2013b).

Preliminary simulations should be performed using the sub-models and the integrated model under development. The primary objectives of this analysis are the identification of unstable simulation runs as well as wrongly set parameter value definitions as well as problems in the model structure. Useful indicators can be implausible loads and concentrations in the receiving water (e.g. by comparing to literature values (Brombach *et al.*, 2005)) or surcharged nodes at high points in the sewer system and so on (Muschalla *et al.*, 2009). Furthermore, a sensitivity analysis of selected input data and parameters regarding the sub-models should be carried out to make sure that all the sensitive data was included.

An important point for all these data and modelling approaches is the data management. All of the available, measured or estimated data as well as all of the sub-models should be stored in the project database. Preferably, versioning should be used to enable assessment of the model evolutions. This can be included into data management schemes of operating companies (Tscheikner-Gratl, 2016).

3.6.1 Minimization of uncertainties in data collection

This section will briefly present the main sources of uncertainties (in data) and how to reduce them. It is crucial to validate data and to evaluate uncertainties and representativity of measurements carried out (Bertrand-Krajewski *et al.*, 2003). Uncertainty is defined here as the dispersion of the measured values around the true one. The values are measured by a data acquisition system, containing at least one sensor, one transmitter and one data logger i.e. from the value of interest until the final file where the data are stored. Two main sources may lead to large uncertainties: bias and noise.

Bias consists of systematic errors, i.e. over or under estimations (sometimes both for the same sensor, with different behaviour along the measuring range). Bias can be decreased with a smart positioning of the probe and the accurate calibration of the entire data acquisition system. The correct positioning does respect standard methods (mostly defined in standards, guidelines or codes of practice) and common sense: e.g. a rain gauge should not be placed too close to a building, a water level sensor should not be placed in a hydraulic jump or in a layer of sediment. Even if those affirmations seem trivial, basic mistakes such as the ones described still happen relatively often.

All sensors and analytical methods shall be calibrated with specific certified standard devices, solutions or procedures (Bertrand-Krajewski *et al.*, 2003). Calibration enables the correction of the data acquisition errors, aging, drifts, and so on. Standard methods for sensor or sensor and transmitter calibration are well documented and easily accessible. Bias can also originate from data logging systems: e.g. tension falls along the cable, mistakes and bugs in the software, logger time drift. That’s why a calibration of the full data acquisition is required, i.e. from the standard value (solution, pressure, etc.) to the value record in the final file. The dispersion of the measured values around the corrected values (i.e. after applying the calibration correction) can be influenced by several factors: the design and the realization of the data acquisition system, the environment, the selection of the sampling location and the presence of (sometimes hidden) smoothing algorithms within the data acquisition system. In order to start a detailed check of the system, those algorithms should be disabled and the access to raw data should be guaranteed.

A wrong choice of equipment (some types are known to be noisy), the wrong choice of the location (close from powerful antenna, high-power electricity cables) and the wrong cables (non-shielded cables or shielded cables not connected to the earth) may lead to noisy, random values i.e. non-systematic uncertainty. Also, the relation between process variability, accuracy and sampling frequency should be considered. For example, a measurement with high frequency but low accuracy can still produce only noisy data. Discussions with experienced people, a general scientific culture and a deep observational sense will help to reduce those sources of uncertainties. Another key to reduce uncertainty is the selection of the necessary quality and purchase of accurate equipment for this task. For example, the usage of tipping bucket rain gauges (Chvíla *et al.*, 2005) or electronic weight systems (Sevruk and Chvíla, 2005) for precipitation measurements can lead to different measurement errors, although errors induced by wind-induced loss and spray water can be comparable (Hoppe, 2006).

3.7 Setting up the integrated model

The first step of linkage covers the aspects of model robustness and verification of the interfaces' functionality (Muschalla *et al.*, 2009) and compatibility (Bach *et al.*, 2014). The main challenges of linkage in terms of data transfer are (HSGSim, 2008; Bach *et al.*, 2014):

- variables have different definitions or change their meaning from one component to another, or simply do not exist in all sub-models
- conversion processes (especially chemical processes in particular, where the chemical mass balance cannot be easily solved) at the interfaces are tedious and error-prone including problems with data units
- differences in temporal or spatial discretization between the sub-models

These issues also primarily relate to water quality rather than quantity. One challenge is the linking between different water quality models, which usually have different sets of state variables (Benedetti *et al.*, 2013). This can be approached for example by using a continuity-based model interface (Vanrolleghem *et al.*, 2005b). Blöschl and Sivapalan (1995) distinguish between a process, observation and modelling scale. Under the best scenario, those scales should match, but this is not always the case, and transformations based on downscaling and upscaling techniques might be necessary to obtain the required match between scales (Cristiano *et al.*, 2017).

Integration of sub-models is a simulation as well as a software or computational hardware requirements question. Sub-models either run for the entire time-period before information is conveyed on to the next component (sequential) or models are run alongside each other (parallel) (Bach *et al.*, 2014). The parallel simulation of subsystems is not vital for an integrated modelling (Achleitner *et al.*, 2007), as long as no feed- back fluxes occur (e.g. for real time control). However, in order to minimise calculation time, the possibility of parallel calculation of models should be exploited as far as possible, as long as it does not interfere with model performance. It also is an important part in the application of parallel computing (i.e. multi-core computing) to exploit all of the available computing resources provided by modern CPUs (Burger *et al.*, 2016). The linkage of the sub-models can in terms of software either be implemented in a common language (Burger *et al.*, 2016) or by establishing interfaces (e.g. open software interfaces (Gregersen *et al.*, 2007)) between the sub-models.

3.7.1 Model structure uncertainties

When describing a system there are three major dimensions in which the system has to be conceptualised for a model (Kelly *et al.*, 2013):

- Space
- Time
- Structure

Spatial resolutions in models range from non-spatial models over lumped spatial models, compartmental spatial models, grid, cell or element based spatial models to continuous space models. Different spatial scale results also in different outcomes for the same model. For example a build-up/wash-off model physically-based at the scale of elementary surfaces, is actually a black-box model at the catchment-scale (Bonhomme and Petrucci, 2017). Or different levels of detail in the representation of urban sub-catchments can lead to substantial differences in the shape of the hydrograph for a rainfall runoff model (Tscheikner-Gratl *et al.*, 2016).

Similar to the treatment of space, temporal resolution can increase from mere steady state models over discrete and dynamic models to continuous ones. A good example is the usage of rainfall data with different temporal (and spatial) resolution as input for hydrological models (Cecinati *et al.*, 2017; Muthusamy *et al.*, 2017), which can have a high impact on the results. For hydrodynamic models of urban drainage systems these different scales, in terms of temporal resolution of rainfall input data (Notaro *et al.*, 2013) or spatial distribution of rainfall measurements (Notaro *et al.*, 2013; Rico-Ramirez *et al.*, 2015; Tscheikner-Gratl *et al.*, 2016) can have a high impact when forecasting urban flooding. For integrated models, the entire model may not employ a single spatial or temporal scale or resolution, which creates additional problems in integration. In terms of structure we can distinguish between individual-based and aggregated models (Kelly *et al.*, 2013).

Model structure uncertainties are difficult to assess and distinguish from other sources of uncertainty. Model sensitivity is highly dependent on the adequate selection of model parameters and processes, adequate process formulation and the adequate choice of the spatial and temporal resolution of the model (Del Giudice *et al.*, 2015). Often, when a model structure lacks a certain component or when the different sub-models are unbalanced in their complexity, errors can be compensated by calibration on the cost of introducing another ‘error’ in the parameter estimates (Cierkens *et al.*, 2012).

Neumann and Gujer (2008) propose model structure extension to correctly estimate the influence of model structure uncertainty, but it was difficult to apply. Del Giudice et al. (2015) proposed a process to estimate the effect of structural errors, by analysing a system with increasingly complex model structures while describing their output bias. However this can only partially quantify the effects of the different error sources and not distinguish all of it, but using different models for comparison gives a good first impression and can better represent the system under investigation (Deletic *et al.*, 2012). If different models end up with very different estimates for the same scenario and similar parameterization, it may be a safe assumption that the structural uncertainty related to the estimate is large. However, it is again crucial to make sure that the variables presented in the model are equal or reasonably comparable (Uusitalo *et al.*, 2015).

Dotto et al. (2011), for example, compared an empirical regression model to a process-based build-up/wash-off model for storm water pollutant prediction, finding that these models poorly represent reality and have a high level of uncertainty. Refsgaard et al. (2006) compared five alternative conceptual models by five different consultants for the same problem in water resource modelling, which differed substantially from each other. This also shows the connection between the model structure uncertainty and framing ambiguity, where different stakeholders can have very different views and therefore approaches and models for the same problem.

3.8 Calibration, validation and plausibility checks

As the complexity of the models grows, so does the difficulty in assessing their accuracy (Fletcher *et al.*, 2013). This is also true for the difficulty in calibrating and validating of integrated models. Calibration can be defined as the (mostly iterative) adjustment of any model parameter to improve the fit to measured data (Belia *et al.*, 2009). For this purpose, simultaneous measurements of precipitation, discharge, and concentration need to be available at different locations in the system considered to deliver sufficient measurement data for the calibration process (Muschalla *et al.*, 2009). One of the problems of calibration using this measurement data is a possible limitation of the model representability to the boundaries of the applied data, when those data series often do not include extreme events (Harremoës and Madsen, 1999). Furthermore it requires a substantial amount of data and in consequence computational effort in order to allow calibration and validation (Langeveld *et al.*, 2013b). Missing data on important input, for example, precipitation can render a data set useless for calibration of integrated models (Benedetti *et al.*, 2013).

Bach *et al.* (2014) defined three possible approaches for calibration of integrated models, with descending quality:

- Calibration of the entire integrated model at once
- Gradually calibrating the sub-models of the integrated model
- Calibrating the sub-models before integrating them into the integrated model

Gradual calibration means that upstream sub-models parameters are calibrated first and then kept constant during the calibration of downstream parameters, so errors elicited by upstream models can be compensated by downstream models. Analogously, water quantity modules were calibrated first and then kept constant during the calibration of the quality modules (Freni *et al.*, 2009). In all the steps the calibration is performed first only for the hydrology and hydraulics and second for the quality processes, where the hydraulics are independent from the quality processes but not the other way round (Muschalla *et al.*, 2009).

It is possible to use multiple of these steps in combination, for example starting with calibrating the sub-models before integrating and then a calibration of the whole system with a special focus on the targets of modelling. Calibrating the sub-models alone tends to deliver different results than the calibration of the integrated model. However, aimed at identifying systematic errors in the model performance the calibration of the sub-models can deliver important insights (Langeveld *et al.*, 2013b). Therefore integrated models need adjustments and re-calibration after the components are put together (Voinov and Cerco, 2010), as far as it is applicable. This usage of calibration to deal with issues such as data transfer between models and time and space mismatch between models distorts our model results to a certain amount, and leads to the consequence that the modular design of our integrated models has less advantage because for every application a new calibration is necessary. However, due to the fact that not all sub-models can be calibrated (missing measurements e.g. for run-off models) and every sub-model will always be influenced by the calibration of the ‘upstream’ models used as input, distortion is unavoidable in practice with linked models and could only be avoided by building an integrated model from scratch.

Validation can be defined as testing of the model performance against independent data that have not been used for calibration in order to assess the accuracy and credibility of the model simulations for situations comparable to those intended in the goals of the modelling approach (Refsgaard *et al.*, 2007). A wide range of statistical measures and visual techniques can be used to assess goodness-of-fit to validate a used model (Bellocchi *et al.*, 2010).

If no calibration and validation can be conducted or a proper parameter estimation is not possible (e.g. due to missing data) only qualitative statements can be derived from integrated models. Then at least a plausibility check of the parameter set and of the simulation results has to be carried out (Muschalla *et al.*, 2009). However, from the perspective of accuracy it is often better to apply a simplified calibrated model than uncalibrated models (van Daal-Rombouts *et al.*, 2016).

So essentially in practice a five step general procedure can be applied (Bennett *et al.*, 2013):

- Revisit, reassess and implement the models aim for the process
- Check the used data for calibration and/or validation for sufficiency and quality
- Visual performance analysis and plausibility check
- Select a performance criteria depending on the aim of the modelling for calibration and/or validation

- Application of the calibration and validation process and refinements of the model if necessary

3.8.1 Calibration and parameter uncertainties

Defining calibration uncertainties can be difficult, especially differentiating them from parameter and model input parameters. As can be seen in Figure 4, the differentiation from parameter is made if the uncertainty consists of an a priori determined value, which does not change due to causal relations in the model or calibration. So calibration uncertainties can be uncertainties that are caused by or influence the calibration process while uncertainty in the parameter estimates is directly related to the amount and quality of the available information (Der Kiureghian and Ditlevsen, 2009). Either the data used for calibration, in terms of quality as well as the pre-selection of data, or the methods used for calibration, both the algorithm and the objective functions (Deletic *et al.*, 2012).

To address the uncertainty from considering the data quality does not differ significantly from model input data uncertainty. Choosing the data for calibration is another problem. Special attention has to be paid to temporal and spatial availability of calibration data. It was shown that – as worst case – a model could seem to be calibrated sufficiently on few single events or on few measurement sites, but completely fails in predicting outside the calibration period (Kleidorfer, 2010). So, the selection of sufficient length, amount and variability (both temporal and spatial) of calibration data, depending on the model target is of paramount importance.

In general, calibration is an optimisation problem that can either be solved by trial and error approaches or by using an adequate optimisation technique using suitable quality indicators (Muschalla *et al.*, 2009). Bennett *et al.* (2013) gives a good overview of the different quantitative performance indicators and quantitative testing methods for performance characterization of environmental models in overall, which not all may make sense for all applications in calibration. The selection of one method depends on the goal of calibration (volume, peaks, etc.). In general quantitative testing methods can be subdivided into 7 categories (Bennett *et al.*, 2013):

- Methods for direct comparison of models (e.g. comparison of mean and variance)
- Metrics that compare real and modelled values concurrently (e.g. information mean square error)
- Key residual criteria (e.g. root mean square error)
- Residual methods that use data transformations (e.g. Square-Root Transformed Root Mean Square Error)
- Correlation and model efficiency performance measures (e.g. Nash-Sutcliffe Model Efficiency or Relative Absolute Error)
- Metrics based on model parameters (e.g. Bayesian Information Criterion)
- Transformation methods (e.g. Empirical Orthogonal Functions)

Moriasi *et al.* (2007) recommend a combination of graphical techniques and dimensionless error index statistics for model evaluation. In addition to hydrographs and percent exceedance probability curves, the correlation and model efficiency performance measures Nash-Sutcliffe efficiency (NSE), Percent bias (PBIAS) and root mean square error observations standard deviation ratio (RSR) were recommended.

To avoid trial and error approaches a variety of search algorithms can be applied to calibrate various environmental models. These can be subdivided into local, global, and hybrid search techniques. A good overview is given by Matott *et al.* (2009). The calibration performance itself may in some applications be not very sensitive to the choice of optimization algorithm and objective function, but the parameters obtained may be significantly different. As parameters represent processes, the choice of the calibration algorithm and objective function may be critical in interpreting the model results (Kouchi *et al.*, 2017). To limit the uncertainty the usage of different performance indicators (e.g. one sensitive for volume and one for peaks) and algorithms, if computationally viable, is encouraged. Also the usage of different objective functions in a multi-objective framework could be thought of (Wöhling *et al.*, 2008).

3.8.2 Uncertainty propagation

For the uncertainty propagation analysis (UPA) one QUICS deliverable exists (Heuvelink *et al.*, 2017), therefore only an small overview of the methodology is represented here. For further details see Heuvelink *et al.* (2017). For each dataset and sub-model used in the integrated model the steps presented in Figure 6 are needed to perform a Monte Carlo UPA.

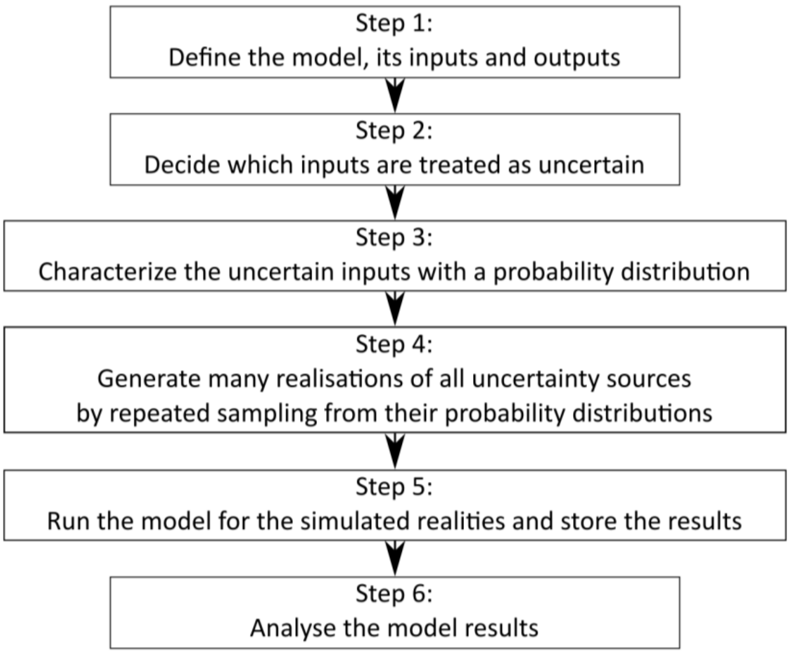

Figure 6: Flowchart of uncertainty propagation analysis (adapted from Heuvelink et al. (2017))

The objective of an uncertainty propagation analysis (UPA) is to analyse how uncertainties in model input data, parameters and structure propagate to model outputs. Application of UPA in integrated urban water modelling requires that the uncertainty propagation is analysed for each of the sub-models used in the integrated model. The most common approach to uncertainty propagation analysis makes use of Monte Carlo (MC) stochastic simulation. In short, the MC method consists of two main steps. First, many sets of possible uncertain inputs are generated from their joint probability distribution using a pseudo- random number generator. Second, the model is run for each of the simulated input sets. This creates a sample of model outputs that can be used to derive statistical properties of the model output. In particular, the spread in the model outputs characterises how uncertainty about the model inputs have propagated to the model output. Some of these steps (especially step 1 and 2) can be taken from the documentation following the proposed framework (see Figure 3).

3.9 Approaches for statistical uncertainties

In general, two groups of approaches exist that typically are applied to this type of uncertainty (statistical):

- Forward modelling
- Inverse modelling

The selection of the method depends on the problem statement, data availability and computational expense for running the model. For forward modelling, influences on the model results deriving from uncertainties of the input (data, parameter or context) are estimated either using error propagation equations or Monte Carlo based methods. Inverse modelling is mainly used to estimate model parameters and their distribution (e.g. calibration). Model results are compared to measurement data to thereby estimate uncertainties. Often both methods are used in combination (see Figure 7). The first step would then be the usage of a reference or calibration period with available measurements to estimate uncertainties and then apply the estimated findings on a forecast period (without available measurement data) using forward modelling.

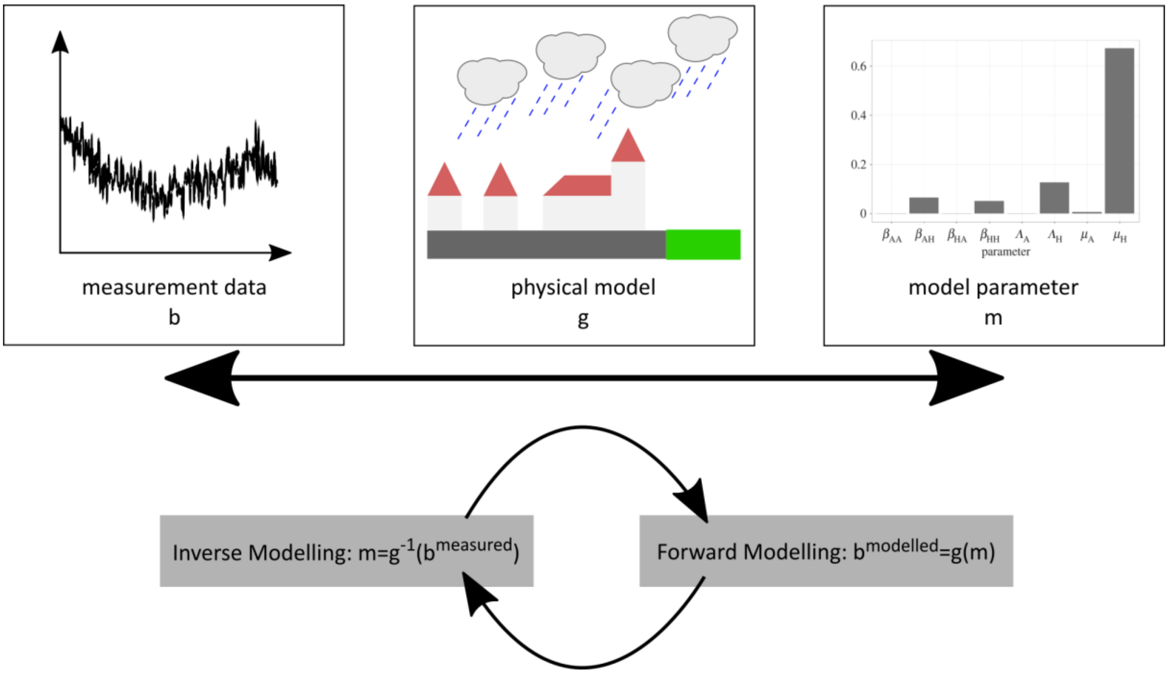

Figure 7: Scheme of combined application of forward and inverse modelling

For forward uncertainty propagation, different approaches are possible which can be mainly divided into two groups which are (analytical) uncertainty propagation equations or (probabilistic) Monte Carlo sampling based methods. Please refer to e.g. Kuczera and Parent (1998), Bertrand-Krajewski *et al.* (2002), McCarthy *et al.* (2008), Thorndahl *et al.* (2008), Thorndahl and Willems (2008) and Kleidorfer *et al.* (2009b) for more information. Uncertainty can be propagated analytically through simple, linear or nearly linear models. The sub-models used and the integrated model itself however are seldom linear and an application of the analytical uncertainty propagation can lead to inaccuracies. This is discussed in another QUICS deliverable (Sriwastava and Moreno-Rodenas, 2017). The limiting factor of the Monte-Carlo analysis is the computational time required to adequately sample the parameter space, which for high dimensional problems will be considerable. Random sampling provides no guarantee that the higher likelihood parameter space is adequately sampled, which makes it difficult to identify a priori the required number of samples and therefore estimate the necessary computational budget (Hutton *et al.*, 2011).

The inverse problem attempts to infer the values of the model parameters that are consistent with the observed data and prior information on the parameters. In water infrastructure system models the model structure is not exact, has a non-linear response and the observed data is limited in time, space and representativeness, and subject to error. As a result, the inverse problem may be ill-posed in the absence of prior information (Renard *et al.*, 2010) with many plausible combinations of parameters producing model simulations consistent with the observed data and their uncertainties. Vanrolleghem *et al.* (2011) propose a step-wise procedure for statistical uncertainty assessment by inverse modelling:

- Preparing the calibration problem by defining objectives, calibration data and methods
- Parameter estimation for example by using either a Bayesian, optimisation or trial and error approach
- Diagnostic testing of hypotheses either using residuals analysis or singular value decomposition
- Model validation and estimation of prediction intervals

Dotto *et al.* (2012) compared some of the most common methods used for assessing urban drainage model parameter uncertainties:

- Generalized Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992)
- Shuffled Complex Evolution Metropolis algorithm (SCEM-UA) applied in combination with GLUE (Blasone *et al.*, 2008)
- A multi-algorithm, genetically adaptive multi-objective method (AMALGAM) (Vrugt and Robinson, 2007)
- Classical Bayesian approach based on a Markov Chain Monte Carlo method and the Metropolis Hastings sampler

The four investigated methods provides similar results in terms of model performances (Wöhling *et al.*, 2008; Dotto *et al.*, 2012). Vanrolleghem *et al.* (2011) recommend the usage of the Bayesian paradigm for the inverse problem. However, the identification of the most appropriate method for the specific problem is always a trade-off between the need for a strong theory-based description of uncertainty, simplicity and computational efficiency (Dotto *et al.*, 2012). If enough capacity is available the application and comparison of different method is encouraged. Furthermore, there exist multiple software packages combining several optimization approaches (e.g. Houska et al. (2015)).

3.10 Scenario uncertainties

Scenario uncertainties must be considered if probabilities cease to be describable by statistical means but possible outcomes are known. These uncertainties stem mainly from the context (e.g. urban development, climate change) or ambiguities between different stakeholders in the planning process. The role of scenarios in planning is to help policy and decision-makers recognise, consider and reflect on uncertainties they are likely to face in the future. While no scenario provides an accurate description of what will happen in the future, they serve to identify and describe possible or preferred futures as part of the planning process. Therefore, a minimum requirement for any modelling approach is at least to apply interval analysis by using a median scenario, a worst- and a best- case scenario. One of those scenarios often includes the business-as-usual scenario. The mitigation measures to be analysed should be implemented in those simulation scenarios. The scenarios are then assessed regarding the defined criteria and objectives. The different scenarios are compared with a reference scenario (mostly a scenario without mitigation) based on the defined criteria either as an absolute and/or a relative assessment of the scenarios (Muschalla *et al.*, 2009).

Three main categories of scenario studies can be distinguished (Börjeson *et al.*, 2006):

- Predictive scenarios, which attempt to predict what is going to happen in the future. They can be further subdivided into forecasts, that are conditioned by what will happen if the most likely development unfolds and what-if scenarios, which investigate what could happen on the condition of some specified near-future events of great importance for future development.
- Explorative scenarios, which explore situations or developments that are regarded as possible to happen, usually from a variety of perspectives. They can be further subdivided into external scenarios, which focus only on factors beyond the control of the relevant actors and strategic scenarios, which incorporate policy measures at the hand of the intended scenario user to cope with the issue at stake.
- Normative scenarios, which aim to define solutions to reach a specific target. They can be further subdivided into preserving scenarios, where the task is to find out how a certain target can be efficiently met and back-casting, where the result is typically several target-fulfilling images of the future, which present a solution to a problem, together with a discussion of what changes would be needed in order to reach these targets.

Predictive forecasts are normally short-term scenarios of the existing system structure. An example for forecasts can be probabilistic forecasts (Laio and Tamea, 2006) of continuous hydrological variables (e.g. discharge). Predictive What-if scenarios are typically short-term scenarios, which allow the comparison of different system structures or one system structure using varying different external influences. An example can be different construction measures in an urban drainage system to reduce combined sewer overflow volume in the next year (HSGSim, 2008). Explorative external scenarios focus mainly on the external influences on a system over a longer period, for example the impacts of climate change and urbanisation on the performance of a combined sewer system (Semadeni-Davies *et al.*, 2008). Explorative strategic scenarios include an internal response to the long term external influences of the external scenarios, for example adaptation and rehabilitation of combined sewer systems (Tscheikner-Gratl *et al.*, 2014) or the adaptation of the urban water management in general (Urich and Rauch, 2014) to a changing environment. Normative preserving scenarios are setting goals for a distant future and explore ways towards these goals. An example is regional planning, where the starting point for a new plan is often a group of targets concerning environmental, social, economic and cultural factors (Börjeson *et al.*, 2006). Back-casting sets a desired state in a distant future and tries to explore pathways to this desired state. For example a gradually change of an existing city to a new more ecological and inhabitant friendly state at a new location is set as a goal and the pathways of gradually adapting the urban water infrastructure (while maintaining their functionality) during the relocation process is explored (Zischg *et al.*, 2017).

3.11 Model application, result assessment and reporting

The final step of integrated modelling is the application and assessment of the model. If the level of uncertainty in the final assessment is outside of the tolerable range, as defined in the problem statement, a revision of the modelling process will be necessary. It is advisable to start with the most influential input in terms of uncertainty as defined in Figure 5.

The final integrated product will need to be evaluated in the light of the study's objectives. The modelling outcomes should be discussed with a wide, multidisciplinary, group of project participants. Such a participatory approach to project evaluation can ensure whether the model is truly an output of an integrative effort that project participants can identify with (Kragt *et al.*, 2013). In addition, it is important for the modeller to seek and share experience by professional exchange with other modeller colleagues.

An often overlooked but important part of integrated modelling is the reporting of the results to the decision makers. It is important to communicate our results to the decision makers in an appropriate way for the aspired audience. A scientific audience requires a different report than a political decision maker or an internal technical specialist, which will present the model results to a decision maker within a water utility. Communicating the uncertainties in our models has to be part of this reporting, not only in order to show the uncertainties of the model and the data but also to strengthen the confidence of the decision makers in the model by showing that uncertainties have been accounted for. Further, it is good to show and also discuss how much uncertainty we are willing to accept for our problem. To find an optimum of uncertainty is difficult to achieve, while too few uncertainty leads to “safe” solutions which tend to be costly and not innovative while accepting too much uncertainty may lead to non-applicable solutions (Geldof, 1997).

4 Example for the application of the framework

As an example a theoretical exercise based on the results of the KALLISTO project (Benedetti *et al.*, 2012b), which encompassed the assembly of the integrated model and decision support based on this model without the herein described uncertainty analysis, is shown.

4.1 Problem statement

The river De Dommel (see Figure 8) is a relatively small river located in the southern part of the Netherlands and the northern region of Belgium. The section of interest encompasses roughly 120 km of river tributaries. The river flow at the end of the section fluctuates between 5-40 m^3/s during dry and storm conditions. This river system receives discharges of several urban areas by 200 combined sewer overflows (CSOs) and through a wastewater treatment plant (WWTP) representing a population equivalent of 750,000 (located at the city of Eindhoven). Due to the intense urbanization in the area, the river is confronted with water quality issues, which threaten its ecological status. Dissolved oxygen content suffers strong fluctuations after rainfall events with medium and high intensities. This impact is suspected to derive mainly from CSOs at overloaded urban drainage systems and a low DO concentration in the WWTP effluent during wet weather flow conditions.

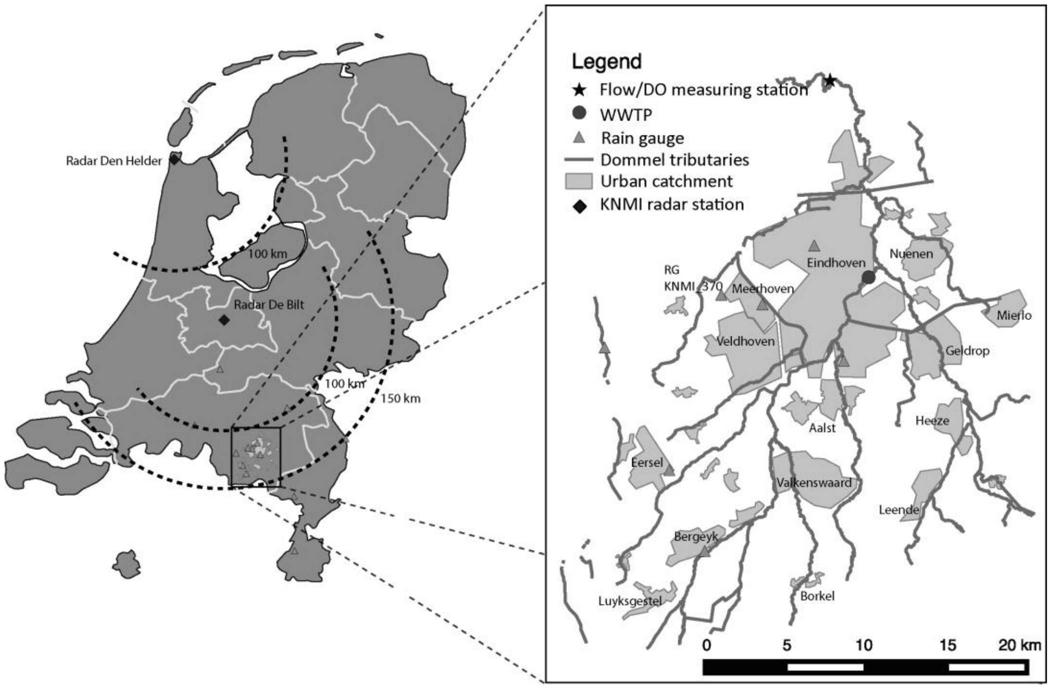

Figure 8: Geographical boundaries of the De Dommel catchment

The Waterboard de Dommel envisioned a series of substantial investments in a plan to improve the ecological status in the river. An integrated river water quality model was developed as a decision support tool to efficiently direct resources and estimate the effect of the selected measures.

Therefore, a modelling study was carried out with the following objectives:

- Simulation of the water quality status expressed by environmental metrics based on dissolved oxygen (DO) and ammonium dynamics (NH_4).
- Assessing and evaluating of the effects of different corrective structural and operational changes on the water quality status.
- Establishing of a knowledge repository, which includes information about the status of the physical system.

In view of conciseness, we will focus only on the first objective in this deliverable. A relevant point in the uncertainty analysis process is the definition of an acceptable uncertainty level. If the model predictive uncertainty is too large, there is no guarantee that the decisions are well supported by the model results. The water quality status of the system is evaluated through the use of intensity-duration-frequency tables (FWR, 2012). The acceptable levels for this case study are shown in Table 2.

Table 2: Intensity-duration-frequency levels for the De Dommel river

		NH_4 critical (mg/l)			DO critical (mg/l)			DO basic (mg/l)		
Duration		**1-5 h**	**6-24 h**	**>24 h**	**1-5 h**	**6-24 h**	**>24 h**	**1-5 h**	**6-24 h**	**>24 h**
Tolerated Frequency per year	12	1.5	0.7	0.3	5.5	6	7	3	3.5	4
	4	2	1.2	0.5	4	5.5	6	2.5	3	3.5
	1	2.5	1.5	0.7	3	4.5	5.5	2	2.5	3
	0.2	4.5	3	1.5	1.5	2	3	1	1.5	2

Occurrence frequencies in the simulated time series are compared with the tolerated ones. From this comparison, a classification into 5 condition states derives:

- Class 1 simulated frequency less than 0.5 tunes the tolerated one
- Class 2 simulated frequency less than 1 time the tolerated
- Class 3 simulated frequency more than 1 time the tolerated
- Class 4 simulated frequency more than 1.2 times the tolerated
- Class 5 simulated frequency more than 2 times the tolerated frequency

Due to the uncertainty analysis the results of the modelling approach will deliver a more detailed view on these environmental criteria classes. Uncertainty level required by the model is therefore specified as a level of dispersion of the water quality status class. This results in probabilities of occurrence for all five classes, which can be compared for different future measures as well as the status quo. These dispersion has to be presented and discussed with the decision maker or authority and then limits have to derive from this process.

The geographical boundaries were selected to be the area of the river De Dommel between the border of Belgium and the Netherlands up to 20 km downstream of the city of Eindhoven as seen in Figure 8. The proposed case study is affected by a series of inherent uncertainties, which should be identified and taken into account during the modelling process:

Uncertainties due to boundary conditions:

An appropriate identification of the influxes of external masses should be carefully performed and will be a source of inherent (or deep) uncertainty. For example:

- Pollution loads from upstream sections (beyond the Belgium border) were not considered in the study and they were estimated from monitoring data, based on monthly grab samples.
- Connections of many small surface bodies were neglected when possible to minimize the added complexity.
- The implementation of external influences (e.g. the water level at diversion structures).

Uncertainties due to extrapolation of system structure:

The model structure was developed and calibrated based on the current physical status. In order to test alternative measures, they are virtually implemented in the model and its effect modelled. This is considered structural extrapolation since the model structure is changed in the process (e.g. adding new control rules, changing physically based parameters as sewer capacity, infiltration etc.).

Deep uncertainties:

Investments on the water system present long payoff periods (10-30 years). Thus, the modelled conditions should be representative of worst expected conditions. Such conditions can only be approximated, for many aspects are unforeseeable. Those include:

- Change of environmental criteria and legislation
- Dominating technology change (e.g. adoption of decentralised wastewater treatment strategies)
- Change in urbanisation structure or land usage (industrial-agriculture development)
- Change in climatological conditions

4.2 System and processes analysis

The water system of the De Dommel is representative for a lowland river area, although drainage in certain sections is dominated by gravity due to mild sloped terrain. The flow velocity of the river is relatively slow with significant flow-depth regulatory structures in the river section and a significant diffusive flow propagation behaviour. The urban areas, consisting of around 30 contributing subcatchments (in 10 municipalities), are scattered in an area of roughly 25x25 km and all drain to a centralized WWTP located in the lower part of the catchment in the middle of Eindhoven. The WWTP effluent can provide up to 50% of the base-flow in summer conditions during dry weather and up to 90% at certain times during wet weather in the river section near the WWTP, due to the higher response time of the WWTP with respect to the river. The city of Eindhoven represents the largest contributing area (generating a spatial clustering factor). A high in-sewer retention volume characterizes urban drainage structures with transport affected by backwater effects.

The main subsystems considered in the model design are listed below:

Urban drainage processes:

- Rainfall-runoff, accounting for wetting losses and infiltration dynamics
- Sewer transport of storm and wastewater effluents on combined-separative systems
- Production of urban wastewater
- Combined sewer overflow discharges

Wastewater transport system:

- Collection and transport of effluent towards the treatment facilities.

Wastewater treatment processes:

- Primary settling tanks
- Biologically activated sludge reactors
- Secondary clarifiers
- Nutrient removal
- By-pass storm settling tank

Rural hydrology:

- Hydrological base-flow contribution
- Rural baseflow water quality characteristics

River dynamics:

- Flow propagation and pollutant transport
- Organic matter degradation
- Nitrification-denitrification
- BOD-COD sedimentation
- Sediment dissolved oxygen consumption
- Macrophyte dynamics

The description and selection of the relevant processes is key in the model structural design. Only certain processes can be described by the model equations, due to the lack of data at certain processes and due to the ignorance of certain system elements. Some of those elements, which limit the description of the correct processes, are assigned to structural uncertainties and ignorance influencing the formulation of problems within the system boundaries.

Context uncertainties due to process ignorance:

- Inability to model water quality dynamics at the rural hydrology baseflow (lack of data).
- River microstructure characteristics (depth variability, lateral flows).
- Effect of annex water surface storage (ponds, small connected channels etc.).
- Inaccuracy to describe real control characteristics (pump/element failure, WWTP maintenance patterns).
- Sediment patterns (flooding sediment wash-off, river dredging and cleaning operations).

The sensitivity of the model to and the level of influence of these uncertainties could be determined by explorative scenario analysis. This would extend the scope for this study and the necessary effort beyond reasonable measures and was therefore omitted.

4.3 Modelling approaches and data demand

The modelling platform should integrate all relevant subsystems defined before (river, urban drainage and water treatment works). Real time control loops are proposed as corrective measures. Therefore, the modelling study should account for the subsystem interaction at simulation time. Urban water drainage systems were modelled using lumped conceptual models. This simplifies the model complexity and reduces significantly the necessary computational requirements for running the simulation. It should be verified, that the loss in accuracy of this simplified representation has no significant effect on the performance of the sub-models located downstream. The urban drainage model requires the following input data:

- Rainfall input at each contributing area
- Evaporation dynamics
- Water infiltration in/out the sewer system – groundwater connection
- Residential wastewater production patterns
- Industrial wastewater production patterns
- Inhabitant density (Tourist seasonality)
- Control inputs (pumping operational rules)

The WWTP was modelled by a fully detailed Biokinetic model (ASM2d (Henze *et al.*, 1999)), a secondary settler, aeration and a Phosphate removal unit model. This structure requires as inputs:

- The characteristics of the influent water quality (influent synthetic generator (Langeveld *et al.*, 2017))
- Atmospheric temperature
- Control characteristics
- Maintenance logs

The river was conceptualised by a simplified model. This is based on discretising the model in fully mixed tank-in-series in which the biochemical processes of relevance are computed. This requires as input:

- Discharge at CSO flows and water quality characteristics (from the urban drainage subsystem)
- WWTP effluent and water quality characteristics (from the WWTP sub-model)
- Rural hydrological base-flow and water quality characteristics
- Water temperature
- Solar radiation
- Diversion and control structures operational logs
- Inputs for water quality at the upstream boundary

4.4 Data and model analysis

An extensive dataset was collected about the system. Table 3 shows the most relevant measured variables.

Table 3: Description of measured variables adapted from Langeveld *et al.* (2013)

Type of measurement	Monitoring frequency (min^{-1})	Remarks
Rainfall	10	1 automatic weighting rain gauge KNMI
	5	8 Rain gauges Waterboard de Dommel and the municipality of Eindhoven
	5	C-Band corrected radar KNMI
Water level	1	Water level sensors in all pumping stations and control structures
	1	Water level sensors at 26 CSOs at the Municipality of Eindhoven
	1	Water level sensors at 200 CSO of the system
Flow	1	Flow monitoring at all pumping stations and control structures at the river De Dommel
	1	WWTP influent separated by 3 regional drainage systems
Water quality	2	UV/VIS at WWTP influent
	1	NH_4 at WWTP influent
	1	PO_4 at WWTP primary clarifier effluent
	2	UV/VIS at WWTP primary clarifier effluent
	1	NH_4, NO_3 and PO_4 at WWTP effluent
	1	DO at the WWTP aeration tank
	1	DO at 6 locations in the River De Dommel
	1	NH_4 at 1 location in the River De Dommel
	Individual sampling	Samples of water quality at several CSO (BOD, COD, NH_4, NO_3, PO_4, TSS). Campaign at individual storm events.

These data were provided by the Water Board de Dommel and by the municipality of Eindhoven. Data quality was categorized based on visual observations and expert knowledge on the system's behaviour. Details on the data availability and associated quality can be found at Langeveld *et al.* (2013). The sub-models were individually tested to characterise their limits of applicability and to validate the proposed assumptions (Moreno-Rodenas *et al.*, 2017a). Special attention should be paid to the settings of the model solver. A pre-screening of the sub-model dynamics at the individual and integrated model was performed to minimise the errors due to time discretization and solver errors. An example of this process (for WWTP modelling) can be found at Benedetti *et al.* (2012a).

Uncertainties associated to this section can be identified as:

- Model structural uncertainties (conceptualisation at each sub-model)
- Selection of ODE solver and solver settings
- Statistical uncertainties due to sensor errors
- Errors due to spatial-temporal sampling characteristics

4.5 Setting up the integrated model

A key factor in the process of linking sub-models is the definition of the appropriate transformations between model state-variables. Since sub-models often produce outputs at different "related" state variables (e.g. transformation of organic matter content at the WWTP effluent to fractionated chemical and biological oxygen demand in the river (COD-BOD)). It is of importance to verify the effect of the sub-model linkage, which presents different space-time characteristic patters.

Uncertainties associated to the sub-model integration can be identified as:

- State-variable transformations at the sub-model boundary
- Spatiotemporal scales of the different subsystems

4.6 Documentation of uncertainties

Before applying calibration and uncertainty propagation techniques we will show here the documentation of uncertainties, which was an on-going process during the aforementioned steps. The list of identified main uncertainty sources, founding on the uncertainty matrix, and the prioritization of relevant sources will lay the foundation of the assessed uncertainties in the following steps.

Table 4 presents the sources of uncertainties, which were identified in the model design process. This follows the classification scheme proposed in the uncertainty analysis framework. The identified uncertainty sources are classified by its degree of uncertainty and the expected model sensitivity, presented in Figure 9.

In this manner, a pre-screening of uncertainties can be done, selecting those inputs, which should be carefully addressed. This follows the iterative nature described in the uncertainty analysis framework in which uncertainty sources are initially identified and classified based on expert knowledge.

Table 4: List of identified main uncertainty sources

System	ID	Uncertainty sources	Source					Type				Nature		
			Context	Model Input	Parameter	Calibration	Model structure	Determinism	Statistical	Scenario	Deep Uncertainty	Epistemic	Stochastic	Ambiguity
River	1	Temperature River (measurement)		■					■				■	
	2	Luminosity River (measurement)		■					■				■	
	3	River upstream Pollution		■					■				■	
	4	Baseflow hydrology					■		■			■		
	5	Pollution load rural catchment					■		■			■		
	6	River diversion/retention structures levels					■	■				■		
	7	River geometry		■					■			■		
	8	River energy losses/roughness		■					■			■		
	9	Sediment evolution (unaccounted dredging and transport)					■				■	■		
	10	Errors at measured water quality data		■					■				■	
Urban drainage	11	Rainfall Data measurement errors		■					■				■	
	12	Rainfall data input characteristics (time-space resolution)					■		■				■	
	13	Soil characteristics for infiltration			■				■				■	
	14	Water infiltration in the sewer				■			■				■	
	15	Evaporation potential		■					■				■	
	16	Daily/seasonal pattern urban pollution load		■					■				■	
	17	Population density	■							■		■		
	18	Urban drainage CSO pollution mean concentration			■				■				■	
	19	Pumping capacity-activation levels	■							■		■		
	20	Georeference of main CSO structures					■	■				■		
	21	CSO weir geometry					■	■				■		
	22	Layout of connected draining areas					■			■		■		
	23	Transport line to WWTP capacity				■				■		■		
Waste-water treatment plant	24	WWTP reactor conditions				■			■				■	
	25	Temperature WWTP		■					■				■	
	26	Control WWTP			■			■				■		
	27	Water treatment chemical addition			■			■				■		
Integrated Model	28	Model extrapolation to simulate corrective measures	■							■		■		
	29	Climatological scenarios	■							■		■		
	30	Urban to WWTP link state-variable transformations					■	■				■		
	31	WWTP to River link state-variable transformations					■	■				■		
	32	Changes of environmental criteria and legislation	■								■	■		
	33	Technological changes	■								■	■		
	34	Change in urbanisation structure	■								■	■		
	35	Change in land usage (agriculture-industrial)	■								■	■		
	36	Solver settings				■		■				■		

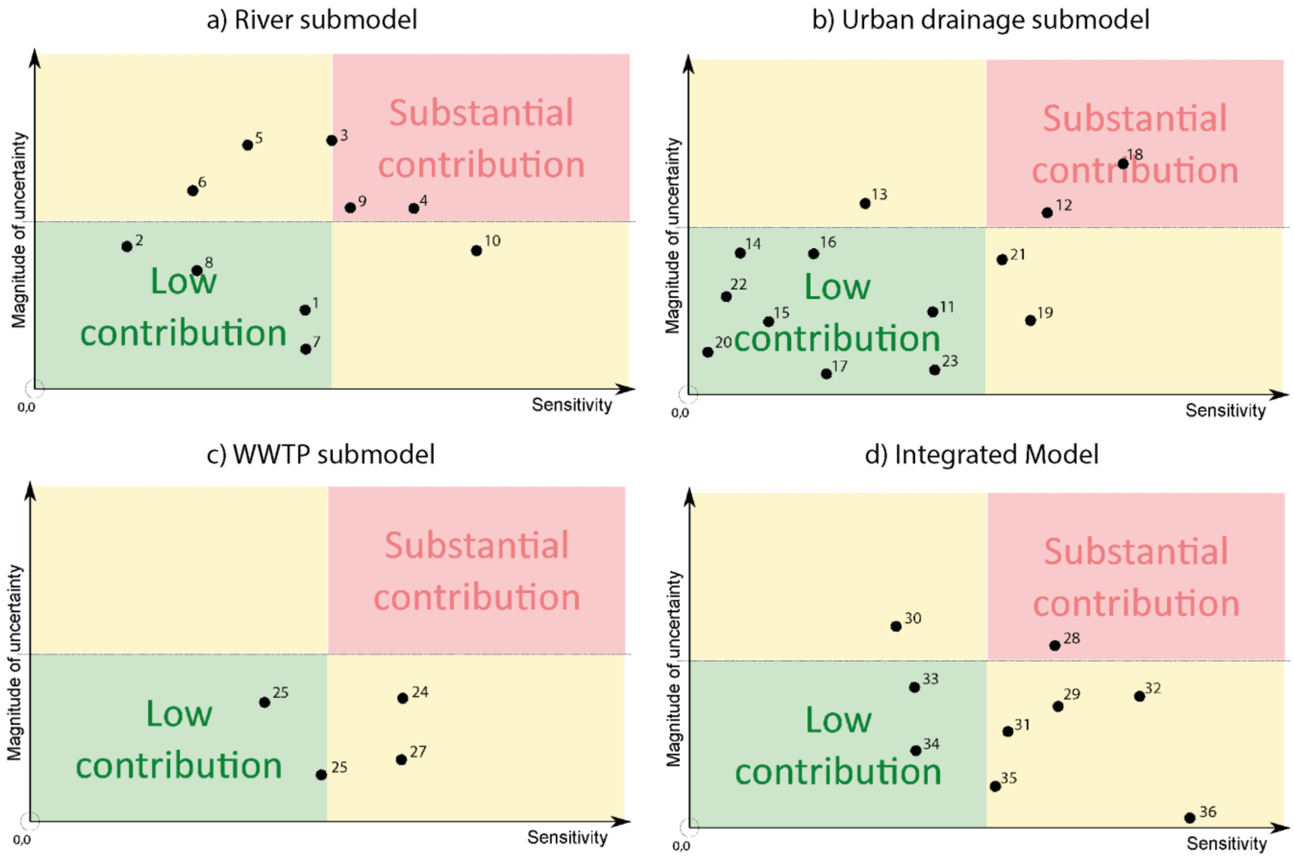

Figure 9: Elicited uncertainty source prioritization graphical panels

Those sources considered highly relevant (large uncertainty and high model sensitivity) are further studied in the process. This generates a feedback loop in which first an initial model structure is proposed, uncertainty sources are propagated-studied and this directs efforts for model refinement or monitoring data acquisition.

Here we present some of the most relevant uncertainty sources (extracted from the red-yellow sections in Figure 9). The numeration can be found at Table 4. We provide also with a discussion on the process followed to quantify or minimise their effect as a feedback loop in the model design and operation process.

- River upstream pollution load (3): Water quality dynamics beyond the Belgium border were not included in the model platform. Thus, constant pollutant concentration loads were assumed. This simplified description was expected to present high uncertainties and a significant contribution to the system dynamics. To ascertain the effect of this assumption, the Waterboard de Dommel carried out a dedicated measurement campaign. This verified that the boundary pollutant input had very little effect on the downstream sections of the system and therefore the sensitivity of the model is significantly lower than initially expected. The new measurement dataset also rendered a reduction on the uncertainty level. Figure 10 presents an updated uncertainty source graphical prioritization after the evaluation.

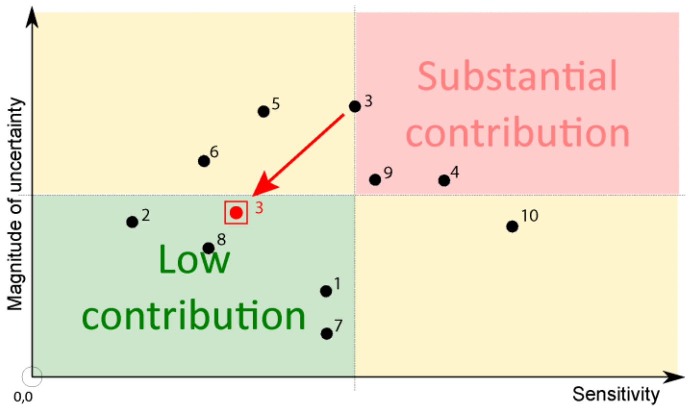

Figure 10: Updated uncertainty source prioritization graphical panel for the river sub-model after the dedicated monitoring study of the upstream boundary pollution load (3)

- Sediment evolution (dredging and transport) (9): The river Dommel sediment bed represents a significant source oxygen demand. This effect was modelled through a constant oxygen demand rate based on onsite measurements, and by modelling the sedimentation of BOD matter in the river and its latter degradation. However, this model structure assumed that the physical layout of the sediment bed remains constant. Nevertheless, it is known that the river authorities have performed dredging activities to clean the riverbed and this is likely to happen in the future. This creates two effects: Firstly, during the activity period, strong oxygen depletion processes occur in the river (which will not be represented by the model), and secondly it will create a non-stationary process between before-after cleaning. This can be accounted for by varying the constant sediment oxygen demand parameter.
- Base-flow hydrology (4): The effect of baseflow hydrology uncertainties was taking into account through the use of a constant multiplier factor of the modelled hydrology input. This dominates the river volume (therefore dilution), which has an important effect in pollutant transformation and transport rates.
- Errors at measured water quality data (10): Conditions for monitoring stations in the river section are not ideal and this can generate significant errors in the measured dataset. This can affect the calibration phase. Thus, a dedicated quality control was performed in the data set to identify reliable time series.
- Pollution load rural catchment (5): The contribution from rural areas to river flow can become significant in some conditions. No monitoring data addressed this issue. Therefore, possible values for this pollution were represented using elicited parametric ranges.
- Urban drainage CSO mean pollutant concentration vectors (18): Uncertainties due to the CSO water quality input were assessed by propagation forward their effect based on feasible ranges extracted from monitoring datasets. More information can be found in Moreno Ródenas *et al.* (2017b).
- Rainfall data input characteristics (space-time resolution) (12): A dedicated study was performed to identify the optimal description of the temporal and spatial characteristics at urban rainfall inputs. This was performed by using 2

rain gauge networks (KNMI and de Dommel Waterboard) and a C-Band radar. This aimed to minimise and characterise the effect of uncertainties contained in the rainfall estimated input to CSO and dissolved oxygen dynamics. Further details can be found at Moreno Ródenas *et al.* (2016).

- WWTP reactor conditions (24): The internal state variables at bioactive reactors in the WWTP model can have a significant effect in the model performance. Concentration rates at reactors can take several weeks-months to reach stable levels. Therefore, initial conditions for the WWTP were always extracted from a burn-in simulation period.
- Model extrapolation to simulate corrective measures (28): This source of uncertainty is not directly quantifiable since no monitoring data is present when using an extrapolated model structure. However, this effect should be acknowledged and communicated.
- Changes of environmental criteria and legislation (32): Conclusions from the decision-making process based on modelling results are affected by the selected environmental criteria.
- Solver settings (36): A series of pre-test were performed to extract optimal solver settings, which minimise simulation times but respect the required output accuracy.

4.7 Model calibration

Calibration of the individual sub-models was performed based on:

- Urban drainage: Calibration using detailed hydrodynamic modelling outputs as ground-truth. Validation using year-accumulated discharged volumes. Details can be found in Langeveld *et al.* (2013a).
- WWTP: The calibration was performed following the BIOMATH calibration protocol (Vanrolleghem *et al.*, 2003).
- The river model was calibrated using flow and dissolved oxygen data in a section of the catchment. The outputs of WWTP and CSO (inputs of the river sub-model) were derived from the monitoring database during 8 months. The calibration phase consisted in a parametric inference in which 4 geometrical parameters for flow and 8 parameters for the water quality process description. (Moreno-Rodenas *et al.*, 2017a).

  Figure 11 presents the uncertainty quantification at the inference process for the flow propagation at the river De Dommel (assuming a normally distributed error process). Figure 12 presents the posterior probability distributions for the inferred parameters at flow dynamics.

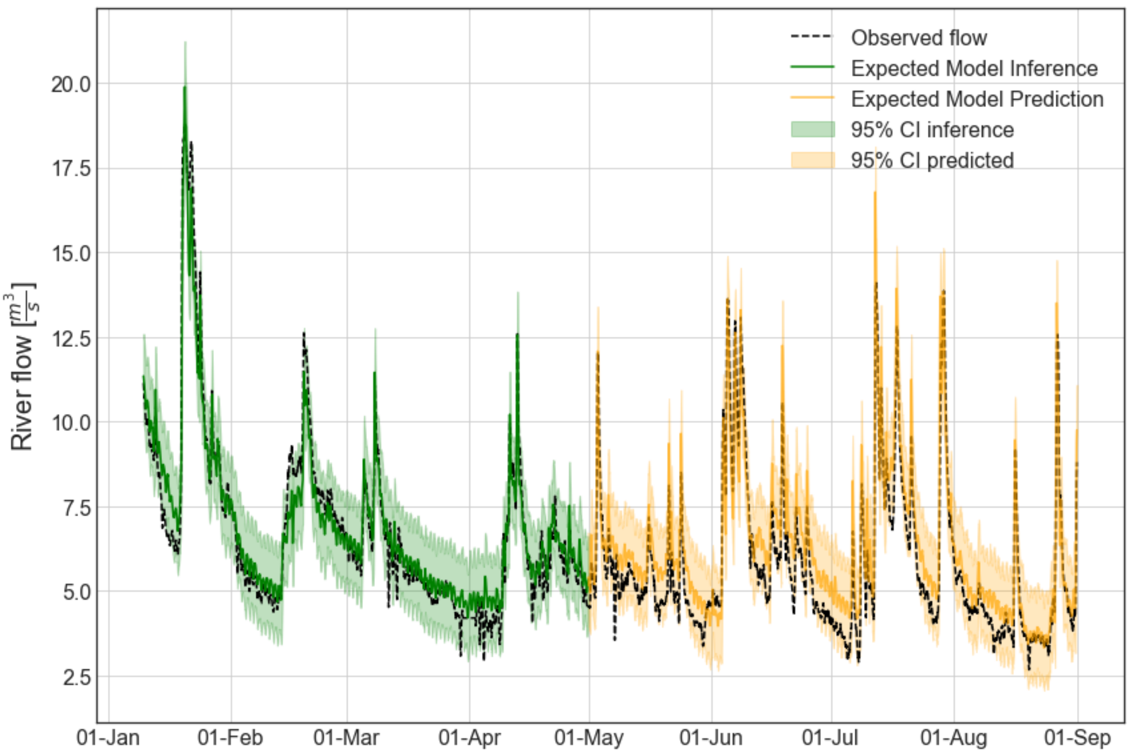

*Figure 11**:** Flow river model inferred with 95% confidence intervals vs monitoring data. In green, the calibration phase and in orange the prediction phase vs monitoring (validation)*

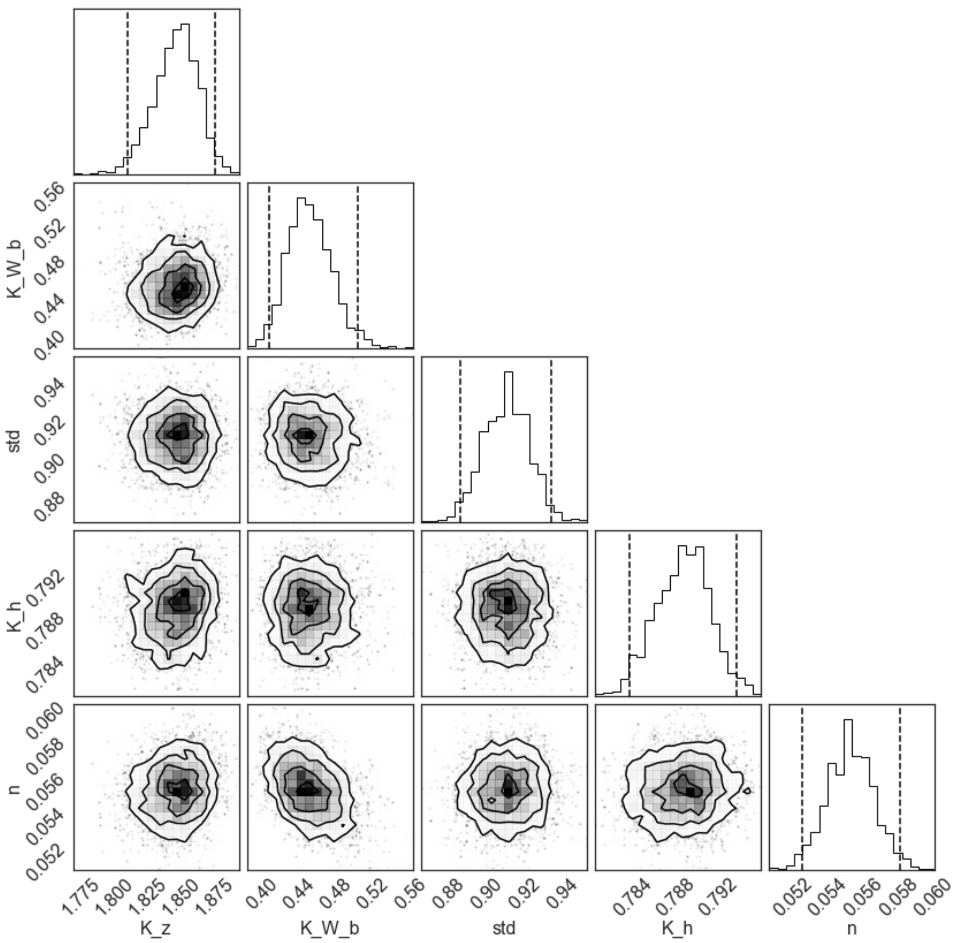

*Figure 12**:** Posterior probability density function for the 5 parameters inferred from flow data*

The performance of the integrated model was validated against modelling data during 3 years. The process of partial sub-model inference helps identifying structural model errors while at the same time the effect of upstream sub-model errors is minimized. However, measurement data uncertainties and erroneous description of the error process can influence parametric inferred (or calibrated) values. Additionally, highly parameterised models can provide enough flexibility to fit the process to the data under erroneous parameter values. This degenerates in a black-box model structure, which provided that it is used for extrapolation purposes (virtual corrective alternative testing) can lead to erroneous conclusions.

4.8 Uncertainty propagation

The time series (in orange) in Figure 11 represents a forward propagation of the uncertainties contained in the flow modelling process at the river model. This was part of the preliminary study to evaluate the effect of river geometrical description (sediment dynamics) and the effect of rural hydrology, and the uncertainties produced at the flow propagation model structure (which corresponds to uncertainty sources (4) and (9)).

In Moreno Ródenas *et al.* (2017b) the uncertainties contained in the CSO water quality input were propagated through the river water quality (see Figure 13). This attended to the study dedicated to evaluate the uncertainty source (18).

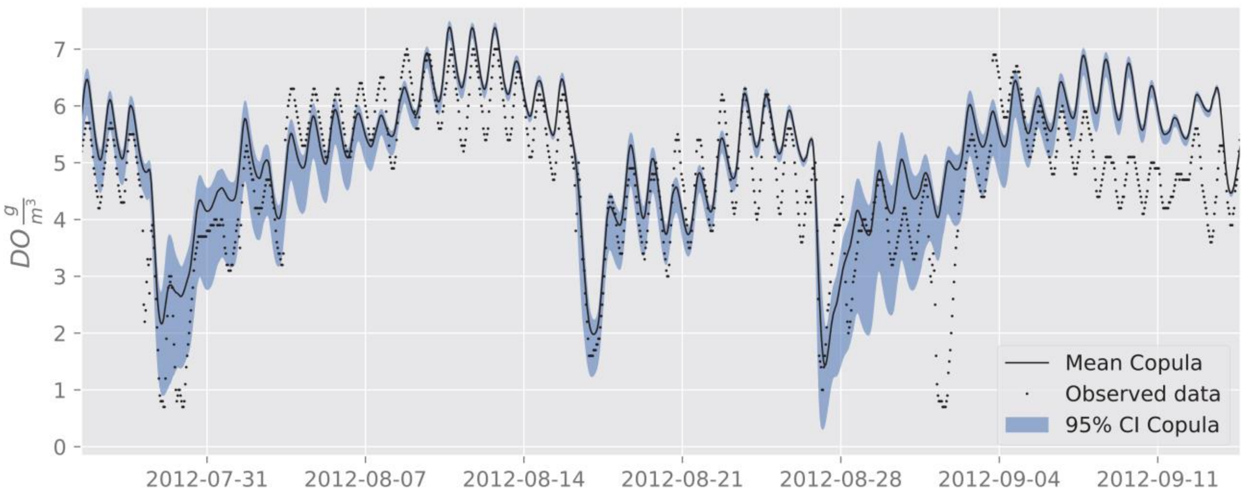

Figure 13: River dissolved oxygen forward uncertainty propagation due to errors in the CSO water quality input

4.9 Model application

The model structure described was used to study the effect of implementing a real-time control system (RTC), which actuates on selected variables at the urban drainage and WWTP subsystem (see Figure 14). The uncertainty analysis described on this document was carried out to discriminate between different sources and improve the model structure. Further details of this application can be found at Langeveld *et al.* (2013a).

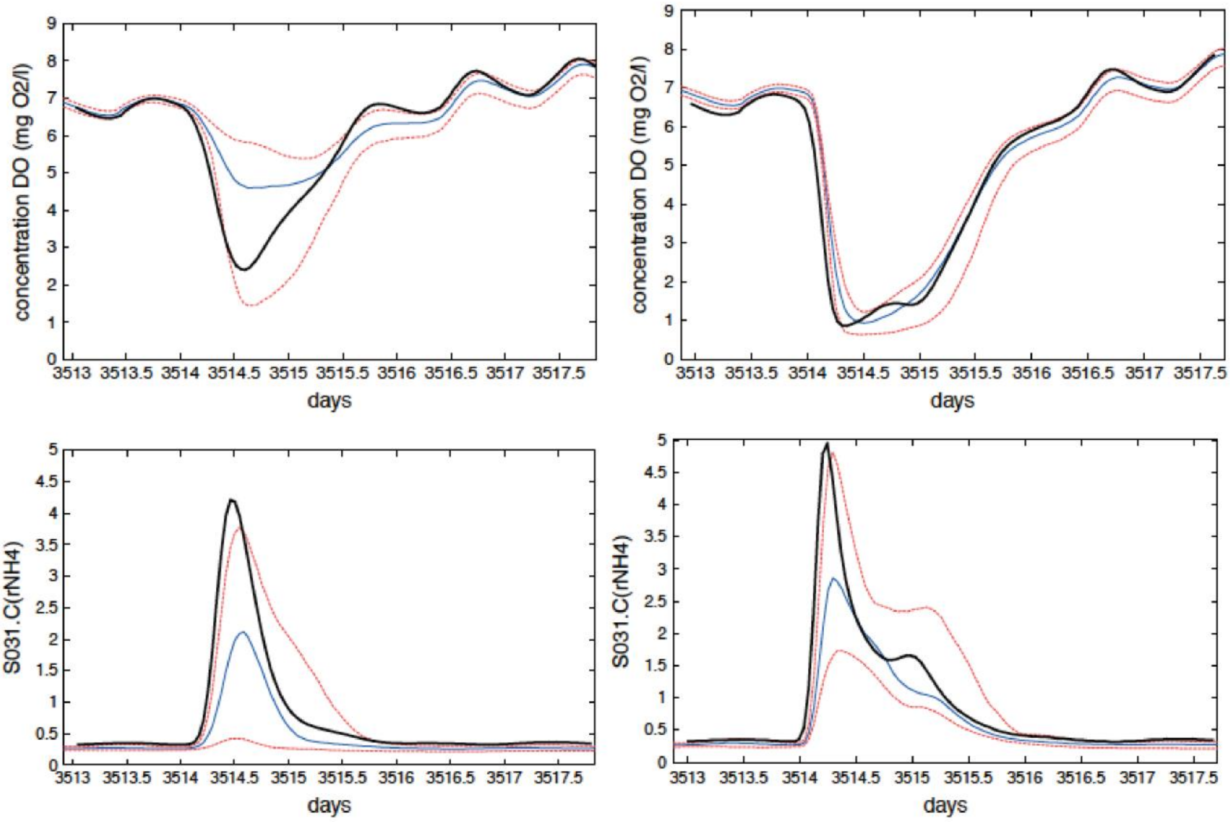

Figure 14: Global sensitivity analysis of DO and NH_4 concentrations at different sections in the river by the use of a RTC system (adapted from Langeveld et al. (2013a))

The accuracy of model outputs for the RTC application in the De Dommel catchment proved sufficient to evaluate its effect in the system's dynamics. This study concluded that RTC can improve the receiving water quality on the current system, yet it was insufficient to meet the desired water quality criteria established by the authorities. This example is based on the results of the KALLISTO project (Benedetti *et al.*, 2012b), which encompassed the assembly of the integrated model and decision support based on this model without the herein described uncertainty analysis. Therefore, this example should be taken as a theoretical exercise. Further information can be found in the work of van Daal-Rombouts *et al.* (2016) and van Daal *et al.* (2017).

Nevertheless, it seems important to highlight that this process did not only focus on a quantification of the output model uncertainty, which although necessary for its communication to the user, is of little use for the modeller. Rather, the uncertainty framework appoints the modeller to perform an inline uncertainty assessment in the model development phase. This feedback loop served to gain detailed information in the physical processes involved and in the performance of the individual sub-models. Which were used to direct further model structural improvements and guide efforts for monitoring data acquisition.

5 Conclusion

The application of uncertainty analysis in planning practice depends on the available data, computational resources and an equilibrium between effort, in terms of labour and costs, and the expected benefit. A basic uncertainty analysis of the model however should be part of any planning process. The framework established in this deliverable covers the bandwidth between these minimal requirements and more sophisticated methods, which are advisable for models assigned to more complex planning endeavours. The treatment of uncertainties is incorporated here not as one step included in model analysis or calibration, but as a continuous work accompanying the entire integrated modelling process. This deliverable, in concert with other outcomes of the QUICS project, provides information and references for modellers in integrated catchment studies.

Four main points sum up the content and intent of this deliverable and for these points this deliverable also wants to provide a discussion contribution:

- Uncertainty analysis should be a process performed in parallel to the modelling exercise rather than being a small part of it. It is a continuous work accompanying the entire integrated modelling process. The same applies to documentation of the modelling steps and the uncertainties connected. When uncertainties are approached in this manner, it gets much easier to rehearse and justify the simplifications, assumptions and finally decisions made.
- Linking together different models is a difficult task and requires proper handling. The important issue is not the scale of a model, but the integration of different models developed at different scales. It is often at these interfaces that the modelling approach radically changes. This also intertwines with the question of calibration of integrated models. Due to the fact that not all sub-models can be calibrated and every sub-model will always be influenced by the calibration of the ‘upstream’ models used as input, distortion is unavoidable in practice with linked models and could only be avoided by building an integrated model from scratch.
- Although not all uncertainties are graspable for every modelling effort and some still for none, the choice of omitting them in the modelling process should be a conscious choice. Even if it is not completely voluntarily but rather forced by limitations in budget, time, information or computational budget implementing these uncertainties into the modelling process and knowing (and documenting) the reasons why they were not considered can bring benefit to all involved parties as well as following projects.
- An often overlooked but important part of integrated modelling is the reporting of the results to the decision makers. It is important to communicate our results to the decision makers in an appropriate way for the aspired audience. This will be an ongoing discussion on how uncertainty can be included into the decision process, especially about how much uncertainty are the decision makers willing to accept for different goals as well as in future regulations.

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