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DEVELOPMENT AND APPLICATION OF SOFTWARE SENSORS AND REVERSE MODELS FOR URBAN DRAINAGE SYSTEMS

Model-based approaches for gaining more information from measurement data

DISSERTATION

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Zusammenfassung

Der Betrieb von technischen Anlagen zur Siedlungsentwässerung verfolgt heute zwei wesentliche Ziele: i) die Minimierung von negativen Auswirkungen auf die Umwelt, insbesondere auf die Wasserressourcen, und ii) den Schutz öffentlichen und privaten Eigentums durch die Vermeidung von Überflutungen bei Starkregenereignissen. Darüber hinaus müssen diese Anlagen nach wirtschaftlichen Grundsätzen, d. h. möglichst kosteneffizient betrieben werden.

Um einen optimalen Betrieb zu ermöglichen sind viele Kanalsysteme bzw. einzelne Bauwerke mit automatischen Messsensoren ausgestattet. Die Messdaten werden meist in kurzen Zeitschritten von wenigen Minuten aufgezeichnet, sofort übertragen und zentral erfasst. Dies ermöglicht neben einer späteren (*Offline-*) Auswertung der Daten auch eine sofortige (*Online-* oder *Echtzeit-*) Analyse der aktuellen Situation im Kanalsystem. Neben der Interpretation durch geschultes Personal können die Daten auch automatisiert weiterverarbeitet werden. Dies erfolgt mit Hilfe von mathematischen Algorithmen und Modellen. Ziel einer solchen Analyse ist entweder die automatische Echtzeitsteuerung des Systems oder die Gewinnung zusätzlicher Informationen und Daten. In letzterem Fall bezeichnet man die Algorithmen und Modelle als *softwarebasierte Sensoren*. Obwohl die grundlegenden Methoden schon vor einigen Jahrzehnten entwickelt wurden ist der Einsatz von softwarebasierten Sensoren und Echtzeit-Modellen bisher auf wenige große Kanalsysteme beschränkt.

Die vorliegende Arbeit stellt Methoden vor, mit denen neue Informationen und Daten über die Situation im System aus hydraulischen Messdaten gewonnen werden können. Die Verfahren basieren auf konzeptionellen mathematischen Modellen und können online oder offline angewandt werden. Dabei werden die Unsicherheiten in Messdaten und Modellparametern berücksichtigt. Die folgenden grundlegenden Methoden können unterschieden werden: Bei der *Rückwärts-Modellierung* (*reverse modelling*) eines Systems werden die Eingangsdaten auf Basis von gemessenen Ausgangsdaten ermittelt. Der Begriff *rückwärts* bezieht sich hier auf die Richtung des Wasserflusses und die übliche Formulierung hydrologischer Modelle. Die zweite Methode ist die automatische *Modellnachführung* (*model updating*). Dabei wird ein Online-Modell laufend auf Basis von Online-Messdaten angepasst, um die Simulationsergebnisse zu verbessern.

Bei den unterschiedlichen Anwendungen der *Rückwärts-Modellierung* konnten einige grundlegende Probleme dieser Methode sowie generelle Ansätze zu deren Lösung identifiziert werden. Ein wesentlicher Teil aller Lösungsansätze ist die Berücksichtigung von Unsicherheiten in den Messdaten, da hochfrequente Schwankungen und Messfehler durch *Rückwärts-Modelle* verstärkt werden. Darüber hinaus müssen die Ansätze physikalisch plausible Ergebnisse gewährleisten.

In der ersten Anwendung wird *Rückwärts-Modellierung* eingesetzt, um Niederschlagsintensitäten aus Abflussmessungen im Kanal zu berechnen. Der so ermittelte Niederschlag entspricht dem Netto-Gebietsniederschlag über dem angeschlossenen Einzugsgebiet. Je nach Art der Anwendung - offline oder online - können unterschiedliche Methoden eingesetzt werden. In Bezug auf die Genauigkeit und die Unsicherheits-Bandbreite können mit der Methode für Offline-Anwendungen deutlich bessere Ergebnisse erzielt werden. Diese Methode wurde zur Analyse der Unsicherheiten des Netto-Gebietsniederschlags eingesetzt. Die Ergebnisse wurden mit jenen eines Fehlermodells für Niederschlagsdaten verglichen. Mit einer Kombination aus Rückwärts-Modell und Fehlermodell können plausible Werte für Lücken in Niederschlagsdaten geschätzt werden. Die Methode für Online-Anwendungen wurde in einem Modell zur Abschätzung von Mischwasserentlastungsfrachten in verschiedenen Teileinzugsgebieten eines Kanalsystems eingesetzt.

In der zweiten Anwendung wird *Rückwärts-Modellierung* zur Ermittlung des Zuflusses in das Becken eines Mischwasserentlastungsbauwerks eingesetzt. Aufgrund der unvermeidbaren Unsicherheiten in Messdaten ist auch hier die Anwendung deterministischer Methoden mit Einschränkungen bzw. Problemen verbunden. Diesen kann mit dem *Bayesian Geostatistical Approach*, ein Bayessches Schätzverfahren aus der Geostatistik, begegnet werden. Der Zufluss wird dabei mit Hilfe eines *Vorwärts-Modells* des Speicherbauwerks auf Basis von Messdaten des Wasserstandes sowie der Ausflüsse ermittelt. Eine realistische Lösung wird dabei durch Regularisierung gewährleistet. Mit einem einfachen, linearen Vorwärts-Modell kann das Verfahren auch in Echtzeit eingesetzt werden.

Für ein Niederschlags-Abfluss Modell zur Abschätzung der Mischwasserentlastungsmengen wurde eine Methode zur automatischen Modellnachführung entwickelt. Dabei werden Messdaten verwendet, die lediglich Informationen über das Auftreten der Entlastung liefern. Anhand dieser binären Daten in Form einer Zeitreihe von “ja/nein”-Werten wird die Verteilung des Modellparameters *Abflusswirksame Fläche* laufend angepasst. Dazu wurde das Konzept des *Bayesschen updating* für die Verwendung von binären Messdaten angepasst. Bei entsprechender Qualität der binären Daten kann so die Online-Abschätzung der Entlastungsvolumina verbessert werden.

Alle vorgestellten Methoden basieren auf Messdaten, die mit relativ einfachen Sensoren gewonnen werden können. Die Methoden können daher zu einem vermehrten Einsatz von softwarebasierten Sensoren in der Siedlungsentwässerung beitragen. Außerdem ermöglichen sie die Gewinnung neuer Informationen auf Basis von Messeinrichtungen und Daten, die in vielen Kanalsystemen bereits vorhanden sind.

Abstract

The operation of urban drainage systems aims to pursue two important targets: i) minimizing negative impacts on the environment, and ii) avoiding damage to public and private property. In addition, most activities to achieve those requirements must be carried out under the principle of economic efficiency.

To support the operation, many sewer networks are equipped with online sensors, i. e. devices connected to networks for automatic transmission and acquisition of measurement data. The performance of measurements and transmission of data in short time intervals (of a few minutes) allows to assess the states of the entire drainage system or certain parts not only in retrospect (referred to as *offline*), but also in real-time (*online*). Apart from the direct assessment of the data by a responsible person, it can be processed automatically by mathematical algorithms or models to support the operation of the system directly, or to obtain information beyond that provided by the sensors themselves. If the data is processed with the aim of deriving new information, the techniques are referred to as *software sensors*. Although many basic methodologies were developed a couple of decades ago, software sensor techniques and online models have so far only been implemented in large sewer networks.

The present work introduces methodologies and their application to derive new information from hydraulic measurements in sewer networks. The developed software sensors are based on conceptual models and estimate different quantities of interest either online or offline. All approaches consider uncertainties in both, data and model parameters. Among the presented approaches and applications, two basic methodologies can be differentiated: The first one is referred to as *reverse modelling*, which denotes the estimation of system inputs from measured outputs. The term *reverse* thus refers to the direction of water flow and the common formulation and use of hydrological models. The second methodology is referred to as *model updating*, i. e. the sequential assimilation of the model to new measurements from the real system, in order to improve the estimation of model outputs in real time.

Based on different applications of reverse modelling, some common basic problems and general methodologies to address them have been identified. The consideration of measurements uncertainties is an essential part of the methodologies, as errors might be amplified when propagated through reverse models. Furthermore, specific techniques must be used to ensure physically meaningful and thus useful results.

In the first application, reverse modelling is used to estimate rainfall intensities from flow measurements in the sewer system. Estimated rainfall intensities represent net areal precipitation on the corresponding urban catchment area. Different techniques can be applied, whether rainfall is estimated online or offline. The technique for

offline applications, which considers one or several entire events, clearly outperforms the technique for use in real time in terms of accuracy and uncertainty. The offline technique is applied to estimate rainfall uncertainties and results are compared to those of a rainfall error model. A combination of both, reverse model and error model can be used to fill gaps in time series of measured rainfall. The real time technique is applied in an online model to estimate combined sewer overflow in several sub-catchments of a sewer network.

The second application of reverse modelling deals with the estimation of inflow to combined sewer overflow and storage structures in sewer systems. A technique denoted *Bayesian Geostatistical Approach* is employed to encounter theses problems. The inflow hydrograph is estimated based on measurements of water level and outflow, and a forward routing model. A realistic solution is obtained by imposing specific regularization constraints. The use of specific forward models allows the application in real time, although the estimation is computationally rather demanding.

Model updating is applied to a conceptual model to simulate combined sewer overflow in real time. Data which can be obtained with simple (real) sensors, providing a binary time series on overflow occurrence in terms of "yes/no" is used to update the distribution of a model parameter. The basic concept of sequential Bayesian updating has been adapted to the specific requirements of binary information. If the binary data is of good quality, the updating can improve the online estimation of overflow volumes.

The presented methodologies and applications are based on data which can be obtained with simple devices. They might thus contribute to a more widespread use of software sensors in urban drainage. The methods can be used to gain more information from real sensors and data which are already available in many sewer systems.

Acknowledgements

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I would like to thank Prof. Wolfgang Rauch, head of the unit, for his advice and guidance during the supervision of this work. Furthermore, I appreciate a lot that he always supported the presentation of different stages and results of this work at various national and international conferences, which provided the possibility to enable contacts to colleagues from all over the world.

A considerable part of this work results from a six month stay at the urban hydrology group of the Laboratoire de Génie Civil et d'Ingénierie Environnementale at the Institut National des Sciences Appliquées de Lyon. I would like to express my thanks to Prof. Jean-Luc Bertrand-Krajewski for enabling this stay and the profound and valuable discussions about my work. Furthermore, he provided me access to the data base from OTHU monitoring sites, which is also a base for some of my publications.

My thanks go to Prof. Karsten Arnbjerg-Nielsen from the Technical University of Denmark for agreeing to evaluate this thesis as a referee and coming to Innsbruck as examiner.

As most urban drainage research, this work relies on a lot of field data collected by operators. I want to thank the team of the Abwasserverband Zirl und Umgebung for providing various data, the easy access to their facilities and the support for our measurement campaigns.

It would not have been possible to do this work all on my own. I would thus like to thank all colleagues from the Unit of Environmental Engineering in Innsbruck. In particular I would like to mention and thank Stefan Fach and Carolina Kinzel (Engelhard) for the support during the measurement campaigns, Gregor Burger for support in applications of CityDrain3, and Manfred Kleidorfer for his advice on all uncertainty issues.

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I would also like to thank my family, who always supported my education, which is the main basis for this work. They have always been open for my goals and provide me a place where I know I am always welcome.

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Contents

List of Figures

List of Papers

The following publications are a core part of this thesis. They are attached in the appendix[1] and in the text referred to by the following numbers (e. g. as **Paper 2**)

1. A software-based sensor for combined sewer overflows
   Leonhardt, G., Fach, S., Engelhard, C., Kinzel, H., Rauch, W.
   Water Science and Technology (2012) 66(7): 1475-1482
   doi: 10.2166/wst.2012.331

2. Comparison of two model based approaches for areal rainfall estimation in urban hydrology
   Leonhardt, G., Sun, S., Rauch, W., Bertrand-Krajewski, J.-L.
   Journal of Hydrology (2014) 511: 880-890
   doi: 10.1016/j.jhydrol.2014.02.048

3. Estimating Areal Rainfall and Accompanied Uncertainty by Combining Two Model-Based Approaches
   Sun, S., **Leonhardt, G.**, Bertrand-Krajewski, J.-L., Rauch, W.
   Submitted to the 13th *International Conference on Urban Drainage*, Sarawak, Malaysia, September 2014

4. Estimating inflow to a CSO structure with storage tank in real time - evaluation of different approaches
   Leonhardt, G., D'Oria, M., Kleidorfer, M., Rauch, W.
   Submitted to *Water Science and Technology*

5. Using "cheap data" for model updating in online simulation
   Leonhardt, G., Kleidorfer, M., Rauch, W.
   Submitted to *Journal of Hydrology*

[1]Papers are only included in the printed version

1 Introduction

The core objectives of urban drainage systems can be summarized as follows:

1. Sanitation in urban areas
2. Prevention of pluvial flooding in urban areas
3. Protection of the environment, in particular water resources

Nowadays, this is not only achieved by appropriate design of the infrastructure, but also by its operation. In particular with regard to the second and third objective, the operation of a sewer system can be an important issue. Successful operation of a sewer system requires reliable and meaningful data. This data can either be interpreted and assessed by the operating staff, as a basis for actions to control the system, or be processed automatically by systems for real time control. Furthermore, an analysis of the data in retrospect can provide valuable information for future operation or optimisation.

To provide data in real time, online sensors and systems for data transmission must be installed, including central processing, storage and visualisation of the data. However, most measurement devices require constant supervision and maintenance, and specific sensors might be costly. Furthermore, some data might be difficult to obtain, if no suitable online sensors for the desired quantity are available. As sewer systems must be operated under the principle of economic efficiency, all approaches and methodologies to facilitate the data acquisition can support the achievement of the overall objectives mentioned above.

1.1 Software sensors and online models in urban drainage

A real (physical) sensor is a device to directly measure a quantity of interest in a system, e. g. the discharge in a sewer conduit. For many quantities in environmental systems, a direct measurement is either laborious, expensive, difficult, or even impossible. The concept of a *software sensor* is to replace the direct measurement by an algorithm to calculate the desired quantity from other data, which can be measured more easily with real sensors. In more complex systems, a suitable algorithm usually corresponds to a mathematical model of the system.

As illustrated in Fig. 1.1, a model used as software sensor should thus provide additional information about the system. Furthermore, it should consider all available measurements to provide the best possible estimate of the quantity of interest. An estimation of the associated uncertainties would also be desirable. This requires the consideration of as many sources of uncertainty as possible in the model.

A software sensor can be used online or offline. *Online* software sensors provide the quantity of interest (almost) immediately, and can thus be used to control the system. *Offline* use refers to the application of the model in retrospect. The online application of a model constrains the available data, as only current and past measurements are available in the moment of calculation. This might also limit the available mathematical methods.

Within urban water management, wastewater treatment is probably the field with the longest tradition and most frequent use of software sensors (Olsson et al., 1989; Vanrolleghem, 2000). With the exception of a few earlier examples (e.g. Carstensen et al., 1996; Rauch and Harremoës, 1999), online model applications in urban drainage, mostly with a focus on real time control purposes, have only been published more recently (e.g Löwe et al., 2012; Breinholt et al., 2011).

1.2 Scope and structure of the dissertation

This dissertation explores the application of urban drainage models as software sensors. New methodologies for their application in urban catchments and sewer systems, and specific sub-systems, as combined sewer overflow (CSO) and storage structures, are introduced. They address both, online and offline applications. There is of course no sharp boundary between offline software sensors and common model applications. However, *software sensor* is used here as umbrella term for both, online and offline models, also to distinguish them from other model applications (e.g. system design).

Fig. 1.2 gives an overview of the developed software sensors. They are applied to estimate areal rainfall, inflow to storage structures, and combined sewer overflow

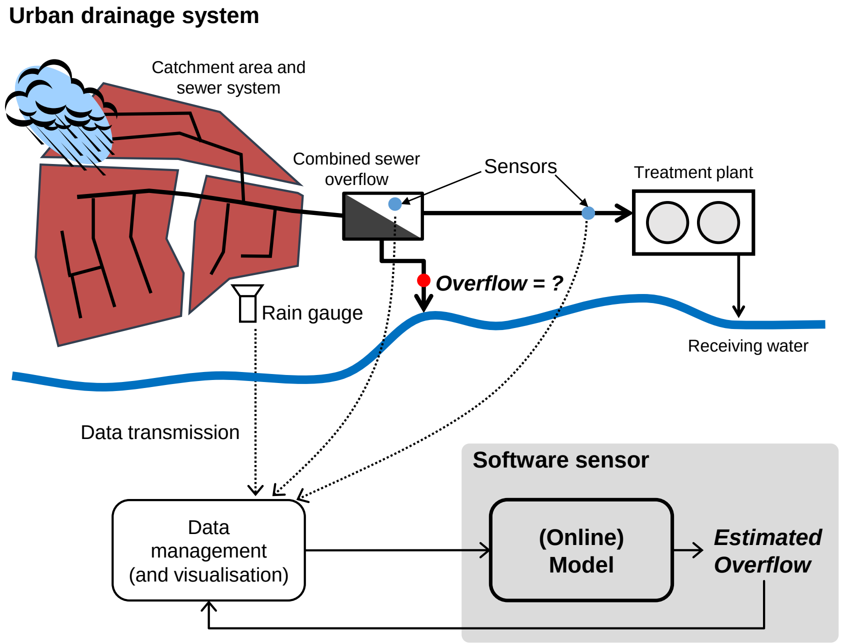

Figure 1.1: The concept of a software sensor for an urban drainage system: based on data from real sensors (which is transmitted to a central management unit), a mathematical model provides additional information on system states (in this case overflow discharge).

discharge. Apart from the application mode (online or offline), they are distinguished with respect to the basic methodology:

Reverse modelling refers to the application of models to estimate system input based on measurements of system output. This implies that the direction of the flow of information is opposite to the direction of water flow. This is in contrast to the common use of urban drainage models.

Model updating aims to improve the agreement between model estimates and real system states, using measurements from the modelled system (other than inputs). This is achieved by updating (i. e. "correcting") model states, parameters, inputs or outputs.

Reverse modelling could initially be considered as a rather intuitive approach to obtain additional information from measurements. Simple model equations which can easily be reformulated let it appear even more attractive. However, in the case of many hydrological systems and models, respectively, reverse modelling involves a couple of problems and challenges to be overcome. Specific approaches are required to ensure physically meaningful and thus useful results. The number of publications on reverse modelling in urban drainage and comparable fields in hydrology is rather small. Due to the mentioned challenges, a couple of experiments might have not been successful. In the available literature, the problems are not always explicitly addressed, which makes it difficult to draw conclusions for further applications. This dissertation aims to provide a systematic overview on methodologies, possible applications and also limits of reverse modelling in the field or urban hydrology.

Model updating methodologies are widely applied to improve online model forecasts in hydrology. Some methods are equally applied in urban drainage, usually within the scope of real time control. The known applications are so far limited to larger sewer system. Among the reasons which avoid the application of online model updating in practise are the requirements for online data, as e. g. flow measurements. Such data might not be available, and suitable devices are costly. The methodology presented in this dissertation focuses on the use measurement data which can be obtained with lower effort and simple devices.

Methodology	Application mode	
	Online	**Offline**
Reverse modelling	Areal rainfall, inflow to storage structures, CSO discharge (deterministic)	
	Paper 1 **Paper 4**	**Paper 2** **Paper 3** **Paper 4**
Model updating	CSO discharge **Paper 5**	

Figure 1.2: Application of software sensors presented in this dissertation.

Fig. 1.2 also lists the scientific articles where methodologies and applications of software sensors have been or are to be published. These five papers present the methodologies and results in detail, and are thus an integral part of the dissertation. They are included in the dissertation as appendices[1] and referred to in the text as **Paper 1**, **Paper 2** etc.

The work for research projects related to the topic of the dissertation resulted in further publications, which are listed below (Sec. 1.3). Whereas the five main papers listed in Fig. 1.2 deal with hydraulic aspects, these publications also address water quality issues.

The following three chapters provide a common introduction and overview on the topic of the dissertation. Chapter 2 outlines the methodological basis. It provides an overview on measurement techniques (Sec. 2.1), general modelling approaches

[1]Papers are only included in the printed version

(Sec. 2.2), and concepts and methodologies to deal with uncertainties (Sec. 2.3). This is followed by an overview on software sensors in urban water management and urban drainage (Chapter 3). Finally, the case studies for the application of the developed methods are briefly introduced (Chapter 4).

Chapter 5 provides a systematic common description of the methods of reverse modelling, followed by a summary and common discussion of the results of the corresponding papers.

Chapter 6 introduces the methods for model updating and provides a summary of the developed approach for the use of "low-cost" data.

A brief discussion of water quality issues with regard to software sensors is included in Chapter 7. Chapter 8 provides a common discussion, conclusions on the overall topic, as well as an outlook on possible future research.

1.3 List of further publications related to the subject of the dissertation

- **Leonhardt, G.**, Kinzel, H., Fach, S., Engelhard, C., Rauch, W. (2011): Online-Ermittlung von Mischwasserentlastungsfrachten mit einer Kombination von Standardmessdaten und Modellierung (Online-estimation of combined sewer overflow emission loads by combining standard measurements and modelling). In: Haberl, R., Ertl, T. (Eds.): *Kanalmanagement 2011*, *Wiener Mitteilungen* 223: L1 - L18; Universität für Bodenkultur.
- Engelhard, C., Fach, S., **Leonhardt, G.**, Rauch, W. (2011): Lessons learned from a measurement campaign in an alpine catchment with highly distributed rainfall. In: *Proceedings of the 12th International Conference on Urban Drainage*. September 11-15, 2011, Porto Alegre, Brazil; IWA Publishing, London.
- [2]**Leonhardt, G.**, Fach, S., Engelhard, C., Kinzel, H., Rauch, W. (2011): A software-based sensor for combined sewer overflows. In: *Proceedings of the 12th International Conference on Urban Drainage*. September 11-15, 2011, Porto Alegre - Brazil; IWA Publishing, London.
- Rauch, W., Schöpf, M., Mair, M., Kinzel, H., **Leonhardt, G.**, Kleidorfer, M. (2011): Uncertainty in online predictions of urban drainage models. In: *Proceedings of the 12th International Conference on Urban Drainage*. September 11-15, 2011, Porto Alegre, Brazil; IWA Publishing, London.

[2] Although this publication has the same title as **Paper 1**, it presents additional results, in particular on water quality

- Kleidorfer, M., **Leonhardt, G.**, Rauch, W. (2012): Identifiability analysis in conceptual sewer modelling. In: *Water Science and Technology* 66 (7): 1467-1474.
- **Leonhardt, G.**, Kleidorfer, M., Gruber, G., Pressl, A., Ertl, T., Muschalla, D., Rauch, W. (2013): Fallbeispiel Schwechat: Identifikation von Auswirkungen der Siedlungsentwässerung im Gewässer (Case study Schwechat: Identification of effects of urban drainage in the receiving water body). In: *Aqua & Gas, Fachzeitschrift für Gas, Wasser und Abwasser* 93/10: 40-44.
- Gamerith, V., **Leonhardt, G.**, Hofer, T., Engelhard, C., Kleidorfer, M., Rauch, W. (2013): Integrated assessment of receiving water quality based on validated high resolution data and water quality modelling. In: *Proceedings of the 8th International Conference on Sustainable Techniques and Strategies in Urban Water Management (NOVATECH)*, June 23-25, Lyon, France; GRAIE.
- Burger, G., Urich, C., **Leonhardt G.**, Bach, P., Kleidorfer, M., Rauch, W.: Design and Implementation of CityDrain3, a Multi-Core Capable Integrated Urban Drainage Modelling Toolkit. *Submitted manuscript.*

2 Data, measurements and modelling in urban drainage

This chapter provides an introduction to the basics for mathematical modelling of urban drainage systems, which are also prerequisites for the application of software sensors. In the first part (Sec. 2.1), measurement techniques (using real sensors) for the most important quantities are introduced. Modelling approaches and important concepts for time-dynamic models are discussed in the second part (Sec. 2.2). The third part (Sec. 2.3) presents methods and concepts to handle different uncertainties in modelling.

2.1 Data and measurements

Modelling requires data, either for development and formulation of models, or for their application, comprising model inputs and data for model calibration and evaluation. In general, the required data can be categorized as follows:

1. Data about the system, e. g. the size and land use of the catchment area, the layout of the sewer network and other structures, or rules and algorithms for the operation of the system. The requirements on such data are strongly related to the level of detail of the model. Some of this data is represented as model parameters (e. g. the effective impervious catchment area).
2. Data about system states and inputs, e. g. rainfall, flow or pollutant concentrations. For the application in time-dynamic models, this data is required in the form of time series.

Although both groups of data can be considered as equally important, the issue of data about the system is, with few exceptions as Lei (1996); Hoppe (2006) or Tscheikner-Gratl et al. (2013), rarely discussed in the literature. With regard to the application of software sensors, this section provides a short summary on measurements of input forcings and system states in urban drainage. Whereas some standard measurement methods and related problems are briefly discussed in common textbooks as Butler and Davies (2004) or Gujer (2008), Bertrand-Krajewski et al. (2008) published a book dedicated to metrology (in French). Data requirements for modelling are e. g. discussed in Vanrolleghem et al. (1999).

2.1.1 Rainfall and hydraulic data

One of the most important quantities in urban drainage is rainfall (precipitation), as it constitutes the main driving force for many processes. Other important quantities are discharge and water levels at different locations in sewer systems, which provide information about the response of the catchment to rainfall, but also about dry weather flow. Furthermore, operational data, e. g. the operation periods of a pump, and other data providing reduced information with regard to dynamics, e. g. the time of occurrence of overflow, can be used in modelling.

2.1.1.1 Rainfall

Rainfall can be measured with rain gauges, which perform point measurements, or indirect methods. Modern rain gauges are either tipping bucket gauges or based on weighing of the volume of water collected in a bucket. New devices are based on optical detection of raindrops and their size. Tipping bucket gauges are considered as less accurate in case of high rainfall intensities (e.g. La Barbera et al., 2002; Sevruk et al., 2009) and cannot measure precipitation in solid form, but they are still widely used (Einfalt et al., 2002; Sevruk, 2002), probably due to their simple setup and data recording (only the time of a tilt must be recorded). As rainfall shows a high variability in time with respect to the time of concentration of typical urban catchments, short recording time steps of a few minutes are required for modelling. From the literature review on rain gauge measurement errors in Hoppe (2006), an uncertainty in the range of 10 to 15% can be assumed, whereas the total rainfall is assumed to be underestimated (Rauch et al., 2002b).

Rainfall, in particular during storm events with high intensities, is also highly variable in space. For design of urban drainage systems, this issue is addressed by an *areal reduction factor* (ARF) to avoid overestimation of runoff when using data from a single rain gauge or design storms derived from the latter (e.g. Butler and Davies, 2004). Einfalt et al. (1998) analysed rainfall data in a large urban catchment together with synoptic situations. They propose different ARFs for different synoptic situations. Vaes et al. (2005) propose areal rainfall *correction* coefficients rather than ARFs. Their investigations are based on a spatial rainfall generator and show that for small catchments and low intensities the derived factors might account for an increase rather than a decrease in rain intensity.

For more sophisticated modelling purposes, indirect methods are used to overcome the limited representativeness of point measurements and their interpolation. The most common indirect estimation method is the use of radar, where rainfall intensities are estimated from measurements of reflectivity in a three dimensional section of the atmosphere, which depends on the distribution of the rain drop size. The drop size distribution also influences the rainfall intensity on the ground. Thus, a relationship between reflectivity and rainfall intensity can be established (Einfalt et al., 2004). The concept to estimate rainfall intensities from radar was first introduced by Marshall et al. (1947), who also proposed a relationship between reflectivity and rainfall intensity (Marshall and Palmer, 1948). Probably one of the first references on assessment of rainfall radar data in the field of urban hydrology is by Austin and Austin (1974). The first applications for modelling, both in the context of real time control, can be found in Bachoc et al. (1984) and Verworn (1991). Einfalt et al. (2004) give an overview on the use of radar in urban hydrology, which also includes short term rainfall forecasts.

Other indirect rainfall estimation methods use sensors on satellites or, more recently, mobile phone telecommunication networks. Satellite-based methods are based on sensors for different ranges of the electromagnetic spectrum, as visible light, infrared, and microwave, whereby also active microwave techniques (i. e. radar) are used (Stephens and Kummerow, 2007; Kidd and Levizzani, 2011). However, applications targeted to urban drainage modelling are not known. A rather new technique uses the attenuation of signals in networks for mobile telecommunication (Messer et al., 2006; Leijnse et al., 2007; Fenicia et al., 2012; Overeem et al., 2011). Fencl et al. (2013) investigated the suitability of the technique for urban drainage modelling based on synthetic rainfall and could achieve a considerable improvement of model results.

The spatial and temporal resolution of rainfall data for modelling has probably been discussed by hydrologists all times, and thus also with a focus on urban hydrology (e.g. Schilling, 1984; Einfalt et al., 1998; Rauch et al., 1998; Schilling, 1991). Due to the short times of concentrations, a high resolution with respect to time is generally important. Schilling (1991) highlights the relationship between the size of the catchment and the time step required for adequate representation of peak flow with a model. He proposes simple relationships to estimate the required time step from model-related catchment characteristics (e. g. time of concentration or storage constant). The required spatial resolution depends on the spatial differentiation of the model and its purpose. Measurement errors might be compensated for in model calibration, and their effect depends again on the model application (see e.g. Rauch et al., 1998).

2.1.1.2 Water level and discharge

Water levels are frequently measured in sewer systems, as the sensors are rather simple. The data is either used directly, e. g. in storage tanks to calculate stored volume or overflow discharge at a weir, or for the measurement of other quantities, e. g. in-sewer discharge (see below). Commonly used sensors are ultrasonic devices (measuring the distance from the sensor downwards), or pressure sensors, installed at the invert. Apart from the sensor's accuracy, uncertainties are introduced by waves, sediments (for pressures sensors), floating solids and big differences in air temperature (for ultrasonic devices). Bertrand-Krajewski and Bardin (2002) and Bertrand-Krajewski et al. (2003) assume a standard uncertainty of 5 mm for in-sewer water level measurements using a pressure sensor.

A direct measurement of discharge is only possible in case of pressurized flows, using a magnetic flow meter. In case of free surface flows, measurements of both, water level and flow velocity are needed to calculate the discharge. Velocity measurements might be replaced by rating curves or the *Manning-Strickler-Formula*, but this introduces additional uncertainties due to hysteresis-effects. Relative uncertainties in runoff data are reported in ranges from 10 to 20% (Bertrand-Krajewski and Bardin, 2002; Bertrand-Krajewski et al., 2003; Hoppe, 2006; Harmel et al., 2006).

2.1.1.3 Other data about hydraulic conditions

Apart from the quantities mentioned above, other information on the hydraulic conditions in a sewer system might be useful for modelling, if it is available as time series. This might be operation data of pumps (e.g. Carstensen et al., 1998), or data providing binary information, i. e. in terms of "yes/no". Examples are the duration and occurrence of overflow (Rasmussen et al., 2008), or the exceedance of a certain water level in a storage facility. Data in binary form can be obtained with simple sensors, as on-off switches or temperature sensors (which are useful in case of a significant difference between water and air temperature).

2.1.2 Water quality data

2.1.2.1 Parameters of interest

Different water quality parameters are of interest because of their harmful effect when emitted into the natural environment. Further substances are of importance for the treatment process, or because they impede the operation of urban drainage systems or harm the facilities (e.g. by clogging or corrosion). From a modelling point of view pollutants can be divided in *solutes* and *particulate material*. However, certain substances can be occur in both forms. Furthermore, their behaviour can be *conservative* or *non-conservative*, i. e. subject to conversion (e.g. biochemical degradation) or chemical reaction.

As water quality problems are manifold, a list of parameters and substances could never be exhaustive. More detailed discussions can be found in textbooks as Gujer (2007) or Butler and Davies (2004). The following list thus provides an overview on important parameters of interest with regard to the entire urban drainage system and the surrounding environment.

- Physical parameters, as temperature, pH or electric conductivity
- Total suspended solids (TSS)
- Organic matter, expressed as cumulated parameters, e. g. biochemical oxygen demand (BOD_n), chemical oxygen demand (COD), total organic carbon (TOC), or dissolved organic carbon (DOC)
- Nitrogen (N), in different compounds or as cumulate parameter, e. g. Ammonia (NH_4-N), Nitrate (NO_3-N), or total Nitrogen (N_{tot})
- Phosphorus (P)
- Heavy metals, e. g. Copper (Cu), Cadmium (Cd), Lead (Pb), or Zinc (Zn)
- *Micropollutants*

Whereas suspended solids, organic matter and nutrients are considered as “classical” parameters, heavy metals and *micropollutants* came into focus more recently. Micropollutants is an generic term for a large variety of substances occurring in comparably low concentrations, originating from pharmaceuticals, personal care products, pesticides, herbicides and many other products. Government authorities published lists of priority substances to be considered in monitoring and quality assessment, as e. g. the European Directive on environmental quality standards in the field of water policy (2008/105/EC) as amendment to the European water framework directive (2000/60/EC) or its corresponding Austrian regulation (BGBl. II Nr. 96/2006). Examples for the large number of publications dealing with aspects of micropollutants in urban drainage are Engelhard (2006); Eriksson et al. (2007); Vezzaro (2011); Rieckermann et al. (2011) or Gasperi et al. (2013).

2.1.2.2 Water quality measurements

Sampling The simplest approach to measure water quality is sampling followed by laboratory analysis of the samples. Samples might be taken as grab samples or composite samples, usually using automatic samplers. Whereas composite samples are suitable to determine total loads or mean concentrations, grab samples can provide a discrete picture of a pollutograph. In the context of dynamic modelling, the advantage of sampling is the possibility to measure various water quality parameters in the lab. However, sampling in short time intervals can only be performed for limited periods, and the data is not available in real time. In addition, various sources of uncertainties exist, as the representativeness of the sample, its modification during storage, and the analysis in the laboratory. Uncertainties related to sampling in urban drainage are e. g. discussed in Bertrand-Krajewski and Bardin (2002); Rossi et al. (2010) or Ort et al. (2010, 2011).

Online monitoring Some water quality parameters can be measured with sensors, which allow a monitoring in real time. Due to the rough conditions in sewers, sensors are often installed in a bypass flume (e.g. Gruber et al., 2004; Bertrand-Krajewski et al., 2007). The use of sensors for physical parameters is usually straightforward. Ammonia in higher concentration ranges, as in domestic waste water, can be measured using ion selective electrodes, whereas lower concentrations require automatic analysers. A focus of research in the field of online monitoring is on classical waste water parameters as TSS and COD. These parameters are measured indirectly, using turbidimeters or spectrophotometers. Both types of instruments measure the absorbance of light, either in one or two specific ranges of wavelength, or over a large spectrum. A calibration model is thus needed, relating turbidity or the absorbance and the pollutant (TSS, COD). Those models are derived based on samples, and thus further uncertainties are introduced. The issue of sensor calibration is intensively discussed e. g. in Langergraber et al. (2003); Bertrand-Krajewski (2004); Rieger et al. (2006); Torres and Bertrand-Krajewski (2008). Lepot et al. (2013) compare different types of sensors for measurement of TSS and COD.

2.2 Urban drainage modelling

2.2.1 A short history of model applications in urban drainage

The initial objectives of urban drainage were sanitation and the prevention of pluvial flooding in urban areas. Since the early days of public urban drainage infrastructure, engineers responsible for design have been using simplified mathematical descriptions of rainfall-runoff processes, which can be considered as *models.* Butler and Davies (2004) mention Mulvaney (1851) and Kuichling (1889) as the first ones to introduce the rational method for the estimation of peak discharge from (measured) rainfall. In a contemporary context, modelling in urban drainage usually refers to the use of mathematical methods describing, at least partly, the dynamics of the processes of interest.

In the meanwhile, the objectives of urban drainage are much more manifold. Since about 50 years, the protection of water resources is of equal importance as the initial objectives. More recently, also socio-economic aspects are considered in planning and adaptation of urban water systems (Brown et al., 2010). The widening of the objectives led to an approach referred to as *integrated assessment* and consequently *integrated modelling* of urban drainage systems. Integrated modelling stands for common consideration of two ore more (physical) sub-systems of the *integrated urban water system*, including their interactions (Rauch et al., 2002a). These sub-systems include, but are not limited to urban catchments, sewer system, wastewater treatment facilities, receiving water and groundwater. The issue of *integrated urban drainage modelling* has been discussed intensively by the scientific community (e.g. Lijklema et al., 1993; Rauch et al., 2005; Muschalla et al., 2009), and has in the meanwhile been further developed to *integrated urban water system modelling* (Bach et al., 2014), seeking to consider the entire urban water cycle and interactions with non-physical systems.

As a consequence of new objectives in urban drainage, the field of model applications increased considerably. Apart from infrastructure design as one of the initial purposes, models are used for the assessment of impacts on the environment, performance assessment of systems under present and possible future conditions or more complex planning issues, e. g. in combination with urban development (Arnbjerg-Nielsen et al., 2013; Zhou et al., 2013; Kleidorfer et al., 2014; Mikovits et al., 2014).

The new fields of applications require the use of dynamic models. Whereas e.g. knowledge of the maximum peak flow in a sewer conduit is sufficient to determine the pipe diameter, the assessment of ecological impacts in a receiving water might require the exact occurrence and dynamics of combined sewer overflow. Furthermore, water quality became an important focus of modelling.

The objective of receiving water protection and the integrated approach also initiated changes in the operation of sewer systems. Thus, systems for online monitoring and automatic data transmission were installed. The concept of *real time control* was introduced in the 1960s (Schilling et al., 1996) as an approach to improve the efficiency of urban drainage systems, also with regard to the new objectives. Real time control is often based on results of prior model simulations or online models.

2.2.2 Formal definition and classification of models for urban drainage systems

A model is often referred to as a description of a *system*. A suitable definition of this term can be found in Reichert (2009, p.4): "*[...] a system is a part of the natural or man-made environment, separated from the rest of the world by well defined system boundaries.*" Environmental systems are rather complex, and models can therefore only be simplified and abstract representations of the real system, addressing certain aspects which are of importance to the modeller. The formulation of a model should be inferred from observations of input and output from the represented system (Reichert, 2009). With regard to biophysical systems, the aspects considered in a model are also referred to as *processes*.

An entire urban drainage system, even that of a small community, is a rather complex environment. For modelling purposes, it is divided into many sub-systems, whereas the level of subdivision primarily depends on the problem to be studied. Consequently, an urban drainage model consists of several sub-models. Each sub-model might represent one or more processes. However, the distinction between *processes* and *sub-systems* is not always made as rigorously as the definitions given above. As an example, the components of a rainfall-runoff model are often referred to as *rainfall loss model* and *routing model*. The first part describes the *process* of runoff formation, and the second part the *process* of runoff concentration, whereas both sub-models together can represent the *(sub-)system* impervious catchment area (which cannot be further subdivided in physical systems).

As a consequence of the subjective choice of certain aspects by a modeller, which should be made with regard to the application, there is no general objective quality criteria to judge models. An assessment should thus always be made with respect to the current problem and application (e.g. Bertrand-Krajewski, 2007; Reichert, 2009).

Mathematical models can be distinguished with regard to different properties, as the level of detail or the mathematical structure. However, not all distinctions listed below are completely strict. Furthermore, for some common model types different terms are used. The following overview is thus not exhaustive.

A **mechanistic** model aims to describe the causal relationships of a system, whereas a **phenomenological** model represents the systems behaviour in terms of the relationship between input and output (Reichert, 2009). In the field of urban drainage, phenomenological models are also referred to as **conceptual** models, and individual model variables might still have a certain physical meaning. The term *conceptual model* is thus used throughout this work. The most popular mechanistic model used in urban drainage are the hydrodynamic flow routing equations, whereas surface runoff is usually represented with conceptual models. If the relationship between system input and output is purely derived from data, models are also referred to as **data driven**, as e. g. artificial neural networks or statistical models.

With a **deterministic** model, a certain input always produces the same output. In contrast, a **stochastic** model contains random elements, and the user is usually interested in the statistical distribution of outputs. Stochastic models are mainly motivated by two facts: i) certain parts of environmental systems are considered to behave stochastically, and ii) to capture different sources of uncertainty in the entire modelling procedure (Beven, 2009).

Other terms for the types of models introduced so far are **white box** (deterministic and mechanistic) and **black box** (purely data driven, statistical) models. **Grey box** models attempt to combine features of both types of models, i.e. a deterministic part based on states and parameters with a physical meaning, and a stochastic part, which allows to use specific statistical methods for parameter estimation (Harremoës and Madsen, 1999; Bechmann et al., 1999).

With respect to the spatial representation of the system, **lumped** and **distributed** models can be be distinguished. In urban drainage, lumped models are always conceptual (phenomenological) models, and spatial refinement mostly involves the use of more detailed (mechanistic) models.

Furthermore, models differ in their capability to represent the **dynamics** of a system. Models for the estimation of temporal mean values are mainly used for water quality issues.

2.2.2.1 General representation of a model

A general representation suitable for the urban drainage model applications discussed in the present dissertation is the *state space* representation (e.g. Reichert, 2009; Beven, 2009). The model $\boldsymbol{M}$ describes the variation of state variables $x_j(t)$ with respect to time t as a function of model inputs $\mathbf{u}(t)$ and parameters θ. The vector of model states $\mathbf{x_{t_i}}$ at a certain time t_i is assumed to be directly dependent only on the previous state $\mathbf{x_{t_{i-1}}}$, the vector of inputs $\mathbf{u_{t_i}}$(since t_{i-1}) and the model parameters:

$$\mathbf{x_{t_i}} = \boldsymbol{M}(\mathbf{x_{t_{i-1}}}, \mathbf{u_{t_i}}, \theta) \tag{2.1}$$

A model output y representing a quantity which can be measured in the real system is related to the states by a function $\boldsymbol{h}_t$, also referred to as *measurement operator* :

$$\mathbf{y_{t_i}} = \boldsymbol{h}_{t_i}(\mathbf{x_{t_i}}) \tag{2.2}$$

A schematic representation of a state space model is shown in Fig. 2.1. In the case of many urban drainage models, the function $\boldsymbol{h}_t$ is both, rather simple and constant with respect to time, i. e. the output often corresponds to a model state. Measurable outputs y and not necessarily measurable states x are thus not always distinguished in mathematical model formulations.

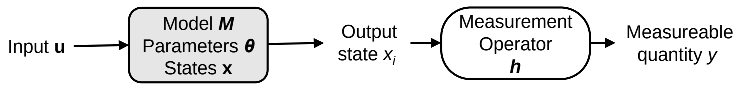

Figure 2.1: Graphical representation of a state-space model.

2.2.3 Modelling concepts for urban drainage systems

The following section introduces the most important modelling concepts used in urban drainage and provides a more detailed description of the approaches used within this dissertation. The description is structured according to the flow direction, from rainfall to the receiving water.

Mathematical models of urban drainage systems are built to represent mass fluxes within and between the different sub-systems. The most important flux is that of water, which is the transport media for all pollutants. The most important external driving forces and system inputs, respectively, are rainfall and domestic and industrial waste water. Rainfall input clearly outreaches waste water with respect to temporal variability. Thus, the basis of most models is the description of water flow, and pollutant transport is usually added as an extension. Fig. 2.2 shows the urban drainage system and a possible division into sub-systems for modelling.

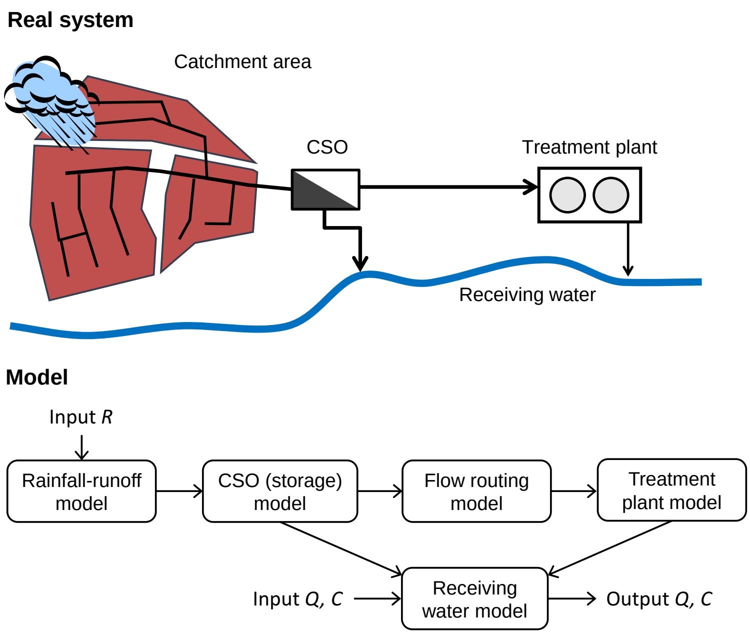

Figure 2.2: A simple integrated urban drainage system and its possible subdivision for modelling.

2.2.3.1 Rainfall-runoff models

Rainfall-runoff models are used to simulate the response of a catchment to rainfall, and are applied in both, lumped and distributed models. Depending on the level of detail in the spatial representation, these models are used to describe the catchment area of a single manhole or gully, or an entire city district or village, including the sewer system. A rainfall-runoff model comprises the description of two main phenomena:

Runoff formation: the transformation of rainfall to surface runoff on the catchment's surface

Runoff concentration: the transport of surface runoff to the outlet of the catchment

Models for runoff formation account for different *rainfall losses* i. e. the fact that not all rainfall results in surface runoff. The input to a loss model is gross rainfall r, its output is net rainfall r_{net}. Rainfall losses include wetting of the surface, infiltration on permeable surfaces, storage in depressions and evaporation. Although most of those losses vary during a rainfall event, rather simple model concepts are widely used. A common model concept assumes two types of losses, the *initial loss* and the *permanent loss*, as shown in Eq. 2.3. The *initial loss* L_i (in [L]) is a threshold value and represents the amount of rainfall to be exceeded before surface runoff starts. To account for possible different preconditions at the beginning of an event, the available initial loss can be modelled as a function of time by assuming a certain evaporation rate during dry periods. The *permanent loss* L_p (in [L/T]) accounts roughly for permeable areas and infiltration. L_p is mostly calculated as a fraction p of the actual rainfall intensity as $L_p = pr(t)$, but could also be a certain rainfall depth or varying with time.

$$r_{net}(t) = \begin{cases} 0 & \text{if } L_i \geq \int_{t=0}^{t} r \cdot dt \\ r(t) - L_p & \text{if } (L_i + L_p) < \int_{t=0}^{t} r \cdot dt \end{cases} \tag{2.3}$$

The dimensionless *runoff coefficient* ψ is another common concept to account for losses during an event. It is a simple reduction factor applied to the catchment area A, and the resulting quantity is referred to as *effective impervious catchment area* A_e (Eq. 2.4).

$$A \cdot \psi = A_e \tag{2.4}$$

With regard to the amount of surface runoff $R(t) = r(t)A$, the runoff coefficient and a permanent loss $L_p = pr(t)$ have the same effect, where $p = 1 - \psi$. If large permeable areas are considered, more complex loss models are used, as the infiltration capacity generally decreases with rainfall duration (Chow et al., 1988). It should be mentioned that some authors report that the identifiability of loss model parameters from measured data is limited (Arnbjerg-Nielsen and Harremoës, 1996b; Kleidorfer et al., 2009; Dotto et al., 2012).

Runoff concentration models are used to represent the transformation of net rainfall to a runoff hydrograph at the outlet of the catchment. As main modelling concepts, the *kinematic wave* and *transfer functions* can be distinguished. The *kinematic wave* is an approximation of the *Saint-Venant Equations*, neglecting acceleration and pressure force terms. With regard to the focus of this dissertation (in particular **Paper 2**), the transfer functions are discussed in more detail.

Transfer functions are based on the idea that the transformation of net rainfall on a catchment's surface to a runoff hydrograph at its outlet can be modelled as a linear system. The transfer function describes the system's response to *unit net rainfall* input and is thus a hypothetical hydrograph. Furthermore, the system is assumed to be time invariant. From linearity and time invariance the principles of superposition and proportionality can be deduced. That is, the catchment's response to any arbitrary rainfall input can be calculated by superposition and scaling of transfer functions (Chow et al., 1988; Rauch et al., 2002b).

In mathematical terms, the superposition is referred to as *convolution* of the net hyetograph with the transfer function $g(\tau)$ (in [L^2/T]). In discrete time, the convolution integral can be written as follows (Chow et al., 1988; Rauch et al., 2002b):

$$Q_{t_k} = \sum_{i=1}^{k} r_{net,t_i} \cdot g_{\tau=t_{k-i+1}} \tag{2.5}$$

$r_{net,t_i}$is the rainfall depth (in [L]) during the time step from $t_{i-1}(= t_i - \Delta t)$ to t_i, and Q_{t_k} is the flow at the catchment's outlet (in [L^3/T]) at time $t_k = t_1 + k\Delta t$. Note that $g(\tau)$ accounts for the catchment area (A_e).

The transfer function $g(\tau)$ can by derived with different approaches:

The unit hydrograph is a transfer function derived from measured data of rainfall and flow by inverse estimation methods.

The linear reservoir model is a basic model concept relating inflow to and outflow from a storage.

The time area method (also referred as isochrones method) is a model concept considering the flow travel time from different sub-areas to the catchment's outlet.

It should be mentioned that all rainfall-runoff models presented here are based on the assumption that rainfall input represents *areal precipitation*, i. e. rainfall is assumed to be uniformly distributed over the entire catchment area.

Time-area method The time-area method is based on the simple concept that runoff from rainfall reaches the catchment's outlet within a certain time period. The catchment area is divided into a finite number of N sub-areas, separated by isochrones (lines of equal *flow travel time* to the catchment's outlet). Rainfall runoff from a specific sub-area is assumed to reach the outlet within the same time interval Δt. If the sub-areas are all of the same size, the area A_n of one-sub area is computed from the effective impervious catchment area A_e as follows:

$$A_n = \frac{A_e}{N} \tag{2.6}$$

Based on the concept mentioned above, flow at the catchment's outlet Q_{t_i} as mean value for a discrete time step (from $t_{i-1}(= t_i - \Delta t)$ to t_i) is computed from the rainfall depth r_t (in [L]) as follows:

$$Q_{t_i} = \frac{1}{\Delta t} \sum_{j=0}^{N-1} A_n r_{t_{i-j}} \tag{2.7}$$

The corresponding discrete transfer function g is a moving-average operator with window size N:

$$g_n = \frac{A_e}{N\Delta t} = \frac{A_n}{\Delta t} \text{ where } n = 1, 2, \ldots, N \tag{2.8}$$

The product of the number of sub-areas and the time step is referred to as *time of concentration* $t_c = N\Delta t$ and corresponds to the maximum flow travel time in the catchment.

Linear reservoir model The linear reservoir model is the simplest application of the *general hydrologic system model (Chow et al., 1988)* and based on the following two equations:

$$\frac{dV}{dt} = R(t) - Q(t) \tag{2.9}$$

$$Q(t) = \frac{1}{K} \cdot V(t) \tag{2.10}$$

The *equation of continuity* (Eq. 2.9) relates inflow (from rainfall) $R(t) = r_{net}(t)A_e$, outflow $Q(t)$ and storage $V(t)$. The *storage equation* (Eq. 2.10) describes the linear behaviour by relating outflow and storage by a constant K in [T].

Building the derivative of Eq. 2.10 with respect to time

$$\frac{dQ}{dt} = \frac{1}{K} \cdot \frac{dV}{dt} \tag{2.11}$$

and inserting Eq. 2.9 gives

$$\frac{dQ}{dt} = \frac{1}{K} \cdot (R(t) - Q(t)) \tag{2.12}$$

Eq. 2.12 can be solved recursively after discretization. Alternatively, an analytical solution can be found, which yields the following transfer function g (Chow et al., 1988; Rauch et al., 2002b):

$$g(\tau) = \begin{cases} A_e \left(1 - e^{-\frac{\tau}{K}}\right) & \text{for } \tau \leq \Delta t \\ A_e \left(1 - e^{-\frac{\tau}{K}}\right) e^{-\frac{\tau - \Delta t}{K}} & \text{for } \tau > \Delta t \end{cases} \tag{2.13}$$

Note that Eq. 2.13 must be convoluted with rainfall r instead of surface runoff R. However, the application of the following discrete recursive solution for each time step Δt, derived from the analytical solutions, is often preferred:

$$Q_{t_i} = R_{t_i} \left(1 - e^{-\frac{\Delta t}{K}}\right) + Q_{t_{i-1}} e^{-\frac{\Delta t}{K}} \tag{2.14}$$

With the substitutions $e^{-\frac{\Delta t}{K}} = C_1$ and $1 - e^{-\frac{\Delta t}{K}} = 1 - C_1 = C_2$, equation Eq. 2.14 can be written as follows:

$$Q_{t_i} = R_{t_i} C_2 + Q_{t_{i-1}} C_1 \tag{2.15}$$

Discrete transfer functions of a linear reservoir and the time-area method are shown in Fig. 2.3. Despite the simple shape (in particular in case of the time-area method), their superposition based on a real hyetograph results in a realistic representation of a runoff hydrograph.

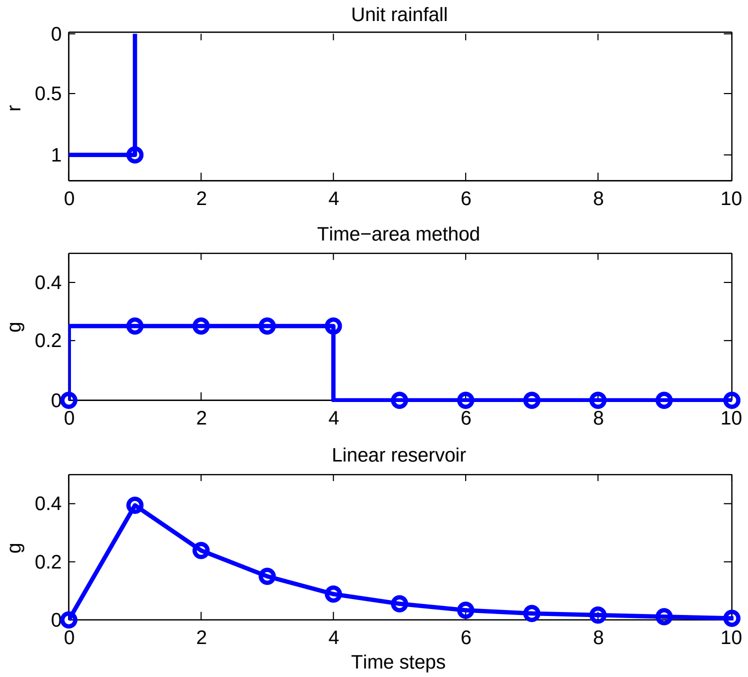

Figure 2.3: Unit rainfall input and discrete transfer functions for the time-area method with $N = 4$ and equal sub-areas, and a linear reservoir with $K = 2\Delta t$.

Applications of the linear reservoir concept For rainfall-runoff models of real catchments, the linear reservoir as presented above is often used as a module in more complex models. These complex models consist of several linear reservoirs connected in series or in parallel (or both).

Linear reservoirs in series are used to model a time delay and stronger attenuation of the runoff hydrograph.

Linear reservoirs in parallel are used to model different runoff components with different response times, e.g. from impervious and pervious catchment areas. The two reservoirs typically represent fast (Q_f) and slow (Q_s) reacting flow, respectively. Each of the parallel reservoirs itself can be replaced by reservoirs in series. Total rainfall runoff R is distributed among the two reservoirs by a factor α as follows:

$$R_f = R\alpha \tag{2.16}$$

$$R_s = R(1 - \alpha) \tag{2.17}$$

From R_f and R_s, the flows Q_f and Q_s are computed with equation Eq. 2.14 (or the application in series). Total flow Q_{tot} is the sum of Q_f and Q_s.

2.2.3.2 Flow routing models

Mechanistic flow routing models for sewer systems are based on the one or two-dimensional *Saint-Venant Equations*. Apart from the full *dynamic wave* equation of motion, approximations as the *diffusive* or *kinematic* wave equation can be used.

Conceptual flow routing models are either based on storage equations or assume a simple translation, i. e. a displacement in time without any attenuation of the runoff peak. Common methods to model both, translation and attenuation are series of (linear) reservoirs or the *Muskingum* routing scheme (Chow et al., 1988).

2.2.3.3 Models for storage and overflow structures

Storage and overflow structures are usually characterized by rather complex hydraulic conditions. However, detailed mechanistic models applying computational fluid dynamics are only used for detailed problems (e.g. Fach et al., 2009; Isel et al., 2013). Commonly used conceptual models are again based on simple storage equations. If the geometry of the storage volume and thus the *level-storage relation*, i. e. the relation between water level h and stored volume $V = f(h)$ is known, the *level-pool routing* equation (Butler and Davies, 2004) can be applied. It relates inflow Q_{IN}, outflow Q_{OUT} and stored volume as follows:

$$\frac{dV}{dt} = Q_{IN}(t) - Q_{OUT}(t) \tag{2.18}$$

If outflows are known from independent measurements Eq. 2.18 can be solved straightforward. However, e. g. in the case of a CSO structure, outflows as spill flow discharge Q_E (to the receiving water) and outflow Q_{TP} through throttle valves (to the interceptor or treatment plant), can be computed by applying the Bernoulli equation and a suitable reduction coefficient, i. e. an overflow formula and Torricelli's law, respectively. They are thus dependent on the water level ($Q_E = f(h)$, $Q_{TP} = f(h)$).

Standard procedures to solve the problem are the derivation of a *storage-outflow* relationship or the *Runge-Kutta* method (Chow et al., 1988; Butler and Davies, 2004). In urban drainage modelling, the problem is often further simplified by assuming an ideal or regulated throttle outflow and unlimited overflow. The water level and the level-storage relation can thus be omitted, and the following model, as presented e. g in Achleitner (2006) can be formulated. As model parameters, the maximum storage volume V_{max} and the maximum throttle outflow $Q_{TP,max}$ are introduced and defined beforehand. All discrete flows Q_{t_i} are considered as mean values for the time step t_{i-1} to t_i. For the calculation, a virtual volume $V^{'}$ is introduced:

$$V^{'}_{t_i} = (Q_{IN,t_i} - Q_{TP,max})\,\Delta t + V_{t_{i-1}} \tag{2.19}$$

Based on $V^{'}_t$, three cases for the calculation of V_t, $Q_{TP,t}$ and $Q_{E,t}$ are defined:

- $V^{'}_{t_i} < 0$ (no overflow, no storage)

$$\begin{aligned} V_{t_i} &= 0 \\ Q_{TP,t_i} &= \frac{V_{t_{i-1}}}{\Delta t} + Q_{IN,t_i} \\ Q_{E,t_i} &= 0 \end{aligned} \tag{2.20}$$

- $V^{'}_{t_i} > V_{max}$ (maximal storage volume exceeded, overflow)

$$\begin{aligned} V_{t_i} &= V_{max} \\ Q_{TP,t_i} &= Q_{TP,max} \\ Q_{E,t_i} &= Q_{IN,t_i} - Q_{TP,max} - \frac{V_{max} - V_{t_{i-1}}}{\Delta t} \end{aligned} \tag{2.20a}$$

- $0 \leq V^{'}_{t_i} \leq V_{max}$ (filling or emptying of storage volume)

$$\begin{aligned} V_{t_i} &= (Q_{IN,t_i} - Q_{TP,t_i})\,\Delta t + V_{t_{i-1}} \\ Q_{TP,t} &= Q_{TP,max} \\ Q_{E,t} &= 0 \end{aligned} \tag{2.20b}$$

When applying conceptual storage models (e. g. Eq. 2.20 to Eq. 2.20b), it might be necessary to account for storage volume in the sewer system by increasing V with respect to the geometric value.

2.2.3.4 Water quality models

As main motivations to consider water quality in urban drainage models the following issues can be mentioned:

- Estimation of emissions of pollutants to the natural environment, in particular receiving waters
- Estimation of pollutants loads in the inflow to treatment facilities
- Assessment of the treatment processes
- Assessment of the effects in receiving waters.

As the waste water discharge during dry weather can be measured rather easily, the wet weather discharge is the main focus of quality modelling in catchments and sewer systems, aiming to quantify pollutant loads discharged with stormwater. Important processes involve thus the mobilisation and transport of pollutants. In contrast, models of treatment facilities and receiving waters focus on conversion (degradation) of substances and thus biochemical processes.

Water quality modelling concepts for catchments and sewer systems

Pollutant sources Quality models for catchments and sewer systems aim to represent the accumulation of substances in the catchment and the sewer system, and their erosion and transport during storm events. The underlying processes are extremely complex, heterogeneous and often considered as stochastic. The common models are rather conceptual and often of a simple mathematical structure. A comprehensive overview on stormwater quality models is given by Métadier (2011).

The simplest models are not fully dynamic, i. e. the output is not a pollutograph, but a single mean pollutant concentration or load for an entire event. The simplest approach is the *site mean concentration*, derived from measurements. Models for *event mean concentration (EMC)* or *event load (EL)* consider the relationship between the mean concentration (or load) of a specific substance during an event and one or more aggregated input variables, e.g. total event rainfall, maximum rainfall intensity or total runoff volume. The relationship is derived from measurements, usually by means of regression analysis. An overview on EL models as well as investigations with respect to the data for parameter estimation can be found in Sun and Bertrand-Krajewski (2012) or Mourad et al. (2005a,b).

The simplest dynamic model also relates input forcing I_t and pollutant concentration or load P_t per time step with a simple empirical formula (Butler and Davies, 2004):

$$P_t = a_1 I_t^{a_2} \tag{2.21}$$

The constants a_1 and a_2 have to be calibrated based on measurements. Note that the model assumes infinite availability of the pollutant.

A more complex concept, developed for fine solid particles and first introduced by Sartor and Boyd (1972), considers accumulation during dry periods and the amount of pollutants available for washoff. It consists of the build-up and the washoff equation:

$$\frac{dM_s}{dt} = k_1 \left(M_0 - M(t) \right) \tag{2.22}$$

$$P(t) = -\frac{dM_s}{dt} = k_2 r(t)^{k_3} M_S(t) \tag{2.23}$$

In Eq. 2.22 and Eq. 2.23, M_S is the actual and M_0 the initial mass of solids on the surface, typically in in g/m^2. $P(t)$ is the washoff rate, typically in $g/(m^2 \Delta t)$. The constants k_1 to k_3 and the initial mass M_0 are again parameters to be estimated based on measurements. The build-up equation (Eq. 2.22) is sometimes also simplified to a linear relationship (Butler and Davies, 2004). Bertrand-Krajewski et al. (1993) review different build-up and washoff formulas.

Pollutant transport A mechanistic description of transport for solutes is provided by the *advection-dispersion equation*, where a term representing *reaction* (e.g. degradation) might be included. Analogous to flow routing, different conceptual models are available, as e.g. the *cascade of stirred tank reactors*. The results of a routing equation serve as boundary condition for the transport equation (Rauch et al., 2002b). Transport of particulate material is a more complex process, as sediments in sewers are often cohesive. A review of different sediment transport formulas is provided by Bertrand-Krajewski et al. (1993). A comprehensive overview on various aspects of transport modelling can be found in dedicated textbooks as e. g. Gujer 2008.

In conceptual models storage structures are usually assumed to be ideally mixed. The settling of particulate materials in CSO structures and storage tanks can be considered by the introduction of a settling coefficient to reduce the concentrations in the spill flow volume and increase those in the remaining volume.

Water quality modelling in treatment plants and receiving waters The main focus of models of treatment plants and receiving waters is usually on conversion processes, i. e. the physical and biochemical processes resulting in degradation and conversion of organic matter and nutrients. A very common model concept to represent activated sludge processes in treatment plants is referred to as *ASM - Activated Sludge Model*, whereof four generations have been published so far (Henze et al., 2000). They are based on an exhaustive and rather detailed description of processes and state variables. A review of all generations of ASM and other deterministic model concepts can be found in Gernaey et al. (2004). A common empirical model for clarifiers is introduced by Takács et al. (1991). The same modelling approach as used in the ASM models has been transferred and adapted to river water quality problems. The concept is referred to as *RWQM1 - River Water Quality Model No. 1* and described in full detail in Reichert et al. (2001b); Shanahan et al. (2001); Reichert et al. (2001a); Vanrolleghem et al. (2001) and Vanrolleghem et al. (2001).

It should be mentioned that conversion models are also applied to sewers, as e. g. shown in Hvitved-Jacobsen et al. (2002) and Huisman et al. (2004a,b). However, the focus of those applications is on dry weather conditions and not on storm events.

2.3 Uncertainties in modelling

Probably the first and simplest way and a rather lumped approach to account for uncertainty are safety factors, as used in engineering design (Beven, 2009; Harremoës and Madsen, 1999). Over the last decades, rather analytic approaches have been developed in research areas related to environmental modelling and thus also urban drainage modelling. The application of appropriate techniques to consider, analyse and quantify uncertainty has thus become “state of the art” in scientific model applications.

Basically, there are two reasons why uncertainties are immanent to environmental modelling:

- Uncertainties in data, related to the measurement process and to their representativeness or information content

- The limited understanding of the real systems and processes and their simplified description by the models used

As a result of all uncertainties associated with the modelling process, model parameters might not be identifiable during calibration, and a model might have a poor predictive performance. A concept to categorize uncertainties in the context of modelling in urban drainage has been proposed by Deletic et al. (2012). It is strongly related to model calibration and defines three main groups of uncertainties, which are of course interlinked:

Model input uncertainties comprise uncertainties in the input data as such, and uncertainties in (calibrated) model parameters.

Calibration uncertainties are related to the data used for calibration and their selection, and to the calibration methods.

Model structure uncertainties are caused by the simplifications of the real systems, the mathematical structure of the equations, and their possible numerical solution.

Although assigned to the first group, uncertainties in model parameters are influenced by all three groups.

2.3.1 Estimation and quantification of uncertainties in measured data

Uncertainties in measurements are caused by systematic and random effects. Both should be accounted for when data is analysed and used for modelling. Measurement uncertainties are described by probability distributions of random variables, whereof measurements are single realisations. A formal concept to describe uncertainty in measurements is provided by the *Guide to the Expression of Uncertainty in Measurement* (GUM, Joint Committee for Guides in Metrology (JCGM) (2010), also published by ISO (2008)). The uncertainty of a measured quantity X should be reported as *standard uncertainty* $u(x)$, which corresponds to the standard deviation σ_x associated with each single measurement. According to the GUM, $u(x)$ accounts for random errors after the elimination of all systematic effects.

As most measurements in urban drainage cannot be repeated (e. g. a rainfall measurement), their uncertainty cannot be derived by statistical analysis from a large number of repetitions, but must be deduced from other information (e. g. known uncertainties of basic measurements, specifications of the measurement devices, preliminary tests) referred to as *a priori* distributions. In the case of symmetric (Gaussian) a priori distributions and a linear relationship between a measured quantity $Y = f(X_1, X_2, \ldots, X_N)$ and input quantities X_i with known standard uncertainty $u(x_i)$, the combined standard uncertainty $u_c(y)$ is calculated using the *law of propagation of uncertainties* (LPU):

$$u_c^2(y) = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i)u(x_j)r(x_i, x_j) \tag{2.24}$$

where $r(x_i, x_j)$ is the correlation coefficient. If the input quantities are uncorrelated (i. e. $r(x_i, x_j) = 0$), the second term diminishes. If the hypothesis for the distributions and the relationship $Y = f(X_1, X_2, \ldots, X_N)$ mentioned above are not true, the combined standard uncertainty $u_c(y)$ can be estimated with the Monte Carlo method (also referred to as *law of propagation of distributions* LPD).

In addition to the standard uncertainty $u(x)$, the GUM introduces the expanded uncertainty $U(x)$, which covers a large fraction of the distribution and is obtained by multiplication with a *coverage factor* k:

$$U(x) = k \cdot u(x) \tag{2.25}$$

Typical values are $k = 2$ or $k = 3$. The ratio ${}^{u(x)}/_{|x|}$ is referred to as *relative standard uncertainty.*

Although the GUM states that systematic effects must be removed beforehand, the Monte Carlo method can be applied to propagate both, random and systematic errors, which might be more suitable in the context of modelling (Deletic et al., 2012). This corresponds to the formulation of *error models* for measured data.

2.3.2 Estimation and quantification of uncertainties in modelling

Almost all urban drainage models contain parameters which need to be determined during calibration based on measurements of model input and output. This is referred to as an inverse problem, which can be addressed by different methodologies (see e.g. Beven, 2009; Reichert, 2009; Menke, 2012).

The general approach to model calibration is as follows:

- Selection of a suitable calibration data set, i. e. model input and measurements of model output
- Selection of an objective function to quantify the agreement between model outputs and corresponding measurements
- Variation of model parameter values in order to minimize the objective function value

Traditionally, the aim of model calibration was to identify a set of *optimal* parameters. This was often tried to achieve manually, or using optimisation algorithms. However, today there is broad consensus (among researchers) that for many environmental models optimal parameter sets are inexistent, which is referred to as the *equifinality* concept (Beven and Binley, 1992; Beven, 2006). Therefore calibration should focus on the estimation of model parameter uncertainties, considering as many sources of modelling uncertainties (see above) as possible. Dotto et al. (2010b) and Deletic et al. (2012) outline an approach referred to as *Global Assessment of Modelling Uncertainties*. Apart from a careful selection of data sets, calibration algorithms and objective functions, the derivation of probability distributions of model parameters is the core of the uncertainty assessment, which must include the consideration of all data uncertainties. The model should then be applied to another data set, again propagating all uncertainties. The analysis of residuals between model output and measurements is part of the assessment of the predictive uncertainty. Uncertainties of model structure can however only be evaluated by comparison of different models.

Different methods are capable to consider uncertainties in model calibration, including approaches based on *frequentist* and *Bayesian* statistics. Frequentist approaches are based on statistical estimators and tests and include techniques as regression analysis. The Bayesian approach has become very popular in hydrology and urban drainage modelling and is often considered as more powerful to estimate model parameters and assess uncertainties (Gallagher and Doherty, 2007; Deletic et al., 2009).

In Bayesian approaches, model parameters are considered as random variables, and their distributions are inferred from the data, according to Bayes formula. This requires the formulation of a *likelihood function* and *prior distributions* of the model parameters. The likelihood function describes the probability of a certain model output given model input and parameters. It is also a measure for the agreement between model outputs and measurements. Prior distributions express a priori information about the parameters. *Posterior parameter distributions* are then inferred using Bayes formula as follows (Kleidorfer, 2009):

$$P(\theta|\mathbf{Y}) = \frac{P(\mathbf{Y}|\theta) \cdot P(\theta)}{P(\mathbf{Y})} \tag{2.26}$$

In Eq. 2.26, $P(\theta)$ represents the prior distribution of model parameters θ, $P(\mathbf{Y}|\theta)$ the likelihood function, $P(\mathbf{Y})$ the distribution of the data, and $P(\theta|\mathbf{Y})$ the desired posterior distribution of model parameters. The solution is usually obtained by numerical techniques based on Monte Carlo simulations.

The approach can also be considered as a learning strategy (Beven, 2009), which is even more evident in the Bayesian methods used for model updating (see Chapter 6). In particular the choice of the prior distributions, but also that of the likelihood function might introduce subjective belief to the inference process, which makes the Bayesian approach both, attractive to modellers and subject to discussion (Reichert, 2009; Beven, 2009).

Techniques for Bayesian inference used in environmental modelling can be distinguished with regard to the employed likelihood function:

Formal methods use a formal likelihood function, i.e. a mathematical description of the expected errors in model output in closed form. The assumed error structure should of course be met by the calibrated model. However, this is not always the case in environmental modelling. Commonly used techniques to obtain solutions are Markov-Chain Monte Carlo (MCMC) sampling, e. g. the Metropolis algorithm (Kuczera and Parent, 1998) or the differential evolution adaptive Metropolis (DREAM) algorithm (Vrugt et al., 2008).

Informal methods (also referred to as *pseudo-Bayesian* methods) use an informal likelihood measure to express the belief in a certain model result (given certain parameter values), thus no formal model for the error structure is required (Beven and Binley, 1992; Dotto et al., 2012). Informal methods have become popular due to the introduction of the technique referred to as *Generalized Likelihood Uncertainty Estimation* (GLUE) by Beven and Binley (1992). GLUE has also been subject to vivid and critical discussion, e. g. with contributions from Mantovan and Todini (2006) or Vrugt et al. (2009).

Nevertheless, both types of Bayesian methods have been applied frequently in hydrologic and urban drainage modelling. Comparisons of formal and informal methods based on urban drainage models can be found in Freni et al. (2009) or Dotto et al.

(2012), who could achieve comparable results with both approaches.

Formal Bayesian approaches are considered more suitable to separately account for different sources of uncertainty in model calibration (in place of lumping uncertainty into parameters and model output). This is achieved by the introduction of error models for different data, and joint estimation of the parameters of the error models and the model of the investigated system. Kavetski et al. (2006a,b) introduced and applied a framework for *Bayesian total error analysis* (BATEA) in hydrological modelling. As examples, Vrugt et al. (2008); Kleidorfer et al. (2009) or Sun and Bertrand-Krajewski (2013) explicitly account for and estimate uncertainty in input data, i. e. rainfall, in rainfall-runoff modelling, and Dotto et al. (2014) account for uncertainty in all measured data in stormwater quantity and quality modelling.

2.3.2.1 Implementation of the GLUE-methodology

As the GLUE-methodology is used in model calibration for **Paper 1** and is the basis for the updating algorithm in **Paper 5**, a brief outline is given here:

1. Selection of model parameters to be inferred and definition of prior distributions, e. g. uniform distribution within the physical limits of parameters.
2. Selection of an objective function to assign a single performance value to each model result.
3. Selection of a weighting function to assign a likelihood (a value between one and zero) to each model result and parameter set, respectively, and to discriminate between *behavioural* and *non-behavioural* results. This requires the definition of limits for acceptance. Non-behavioural results are assigned a likelihood of zero. Certain objective functions, e. g. the Nash-Sutcliffe-efficiency (Nash and Sutcliffe, 1970) do not require a weighting function.
4. Performance of a Monte Carlo simulation with parameter sets sampled from the prior distribution.
5. Assignment of a likelihood to all model results and parameter samples, respectively.
6. Derivation of posterior parameter distributions from the likelihood surface by scaling to unity, division of the parameter ranges in a discrete number of small intervals, and summarizing the likelihoods of all parameter samples in each interval (Kleidorfer, 2009).

As concluded by Freni et al. (2008) and Freni and Mannina (2010) for urban drainage models, results can be sensitive to choices made in steps 1 to 3.

2.3.2.2 Other methods related to model calibration and uncertainty

Stochastic models (forward uncertainty propagation) Apart from calibration, uncertainties can be considered by a stochastic representation of input forcings or parameter values, as e. g. applied by Willems and Berlamont (2002) or Rossi et al. (2005). Although this approach does not infer model uncertainties from the data, it can be a suitable method e. g. for design purposes. The choice of distributions should of course be based on sound knowledge and all available data and information.

Sensitivity analysis Sensitivity analysis (SA) investigates the sensitivity of model outputs to changes in model parameters or inputs (together also referred to as *factors*), aiming to identify those which contribute considerably to uncertainty in output (Saltelli and Annoni, 2010). It is thus not a method for full uncertainty assessment, but it can provide valuable information to the modeller and be applied for preliminary analysis. As it can be performed without measurements of model output it can be attractive for model applications in the absence of such data, e. g. assessment of possible future scenarios. With regard to the parameter space considered, *local* and *global* sensitivity analysis can be distinguished.

Local sensitivity analysis investigates the effect of factors on model output at a specific point in the parameter space. As it is based on partial derivatives of model output with respect to each factor, it is also referred to as "one at a time" (OAT) analysis (Saltelli and Annoni, 2010).

Global sensitivity analysis investigates a considerable part of the parameter space, which should be based on some knowledge of parameter distributions (and is therefore called *regional* sensitivity analysis by some authors) (Reichert, 2009).

Applications of (global) sensitivity analysis in urban drainage modelling have been published by Arnbjerg-Nielsen and Harremoës (1996a); Willems (2008); Vezzaro and Mikkelsen (2012) or Gamerith et al. (2013b).

Identifiability analysis Information on the identifiability of model parameters is provided be the methods for uncertainty analysis. As they are mostly based on Monte Carlo simulations, the application to models with many parameters can be computationally very demanding. Brun et al. (2001) proposed a methodology tailored to models with a large number of parameters, referred to as *"overparameterized with respect to given sets of observations"*. Identifiability analysis is used to determine how clearly model parameters can be inferred from the available data. Reichert and Vanrolleghem (2001) applied the method introduced by Brun et al. (2001) to a river water quality model. Kleidorfer et al. (2012) applied identifiability analysis to a semi-distributed urban drainage model to evaluate different measurement layouts with respect to the number of measurement sites.

3 Software sensors and online models in urban drainage

This chapter provides a general introduction to the subject of online models and the concept of software sensors. It includes general definitions and explanations, as well as a review on their application in urban drainage. The following chapters introduce the case studies (Chapter 4) and present the methodologies applied in this dissertation (Chapter 5 and Chapter 6), including reviews of the specific literature from urban drainage and other fields of their application.

3.1 Introduction

Online models (or *real time* models) are operated synchronously to the real system, i. e. a process is represented by the model at the same time as it occurs in reality (Ellis et al., 2004, p. 110). This requires the connection of the model to online sensors measuring inputs or states in the real system. However, as states are not measured continuously, but only in discrete time intervals, real time models usually provide their results with a short time delay after the availability of the measurement values. Due to the short time intervals required to capture the dynamics in urban drainage systems (usually 1 - 15 min), the online application of a model constrains the time available for computation (in particular if the model results are used for control purposes). Furthermore, it constrains the available data, as only past measurements are available (see Fig. 3.1). This is an important issue in some numerical model implementations. In contrast to online or real time modelling, *offline* modelling refers to the application of a model in retrospect, i. e. without a direct connection to the real system, and no constraints with respect to the available data.

Software sensors (also referred to as *software-based* or *soft sensors*) are models or algorithms to estimate a (primary) system state of interest, using measurements of other (secondary) system states. Usually, the secondary system variables can be measured more easily with real sensors than the primary variable. Software sensors are thus models of different type used to provide additional information on system states (Dürrenmatt and Gujer, 2012; Haimi et al., 2013). Although software sensors are particularly attractive for online application, they can also be used for off-line-diagnosis.

Apart from the application as software sensors, the probably most common application of online models is for control purposes. *Model(-based) predictive control* (MPC) uses model simulations (in addition to online measurements) in real time control. *Real time control* (RTC) means that devices in the system, (e.g. pumps, valves, generally referred to as *regulators* or *actuators*) are operated based on information from the system and nearly synchronously to the process (Schütze et al., 2004). A model might also be used to predict future system states, i.e. to provide a flow prediction based on rainfall forecasts (e.g. Löwe et al., 2012).

The application of online models requires automatic sensors and data transmission systems, as well as central data management. These systems are referred to as *supervisory control and data acquisition* (SCADA) systems, and are usually available to the operating staff of modern sewer systems. The data should preferably be checked automatically before it is used in online models (e.g. Branisavljević et al., 2010; Campisano et al., 2013).

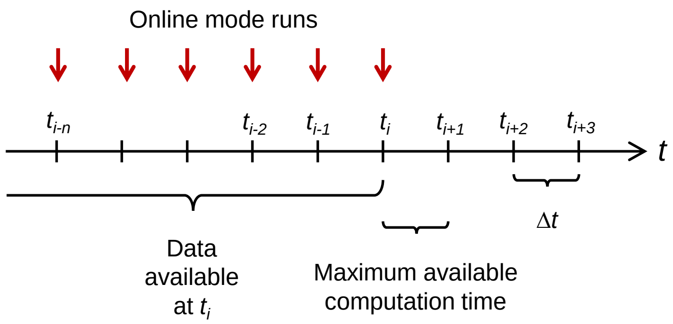

Figure 3.1: Data availability and maximum available computation time for online model simulations based on measurements performed in time intervals Δt.

3.2 Software sensors and online models in urban water management

The first applications of software sensors in urban water management can be found in wastewater treatment, dating back to the 1980s (see e. g. Holmberg and Ranta 1982 or the review by Olsson et al. 1989). They were based on either deterministic or black-box models. To address the issues of uncertainties and physical interpretation of states, several applications of grey-box models (based on stochastic differential equations) as software sensors for treatment plants (Carstensen et al., 1993, 1994) were developed in the 1990s, and the methodology was also applied to urban drainage systems in Denmark. This was also related to the increased use of online monitoring devices in sewer systems (Carstensen et al., 1996). In treatment plant operation software sensors based on different types of models are still frequently used (Vanrolleghem (2000); Zyngier et al. (2001); Dürrenmatt and Gujer (2012); Cecil and Kozlowska (2010); Haimi et al. (2013)). However, due to different system characteristics regarding dynamics, input forcing (e. g. spatially distributed rainfall), definition of system boundaries, and different levels of detail in processes descriptions, the methods applied in wastewater treatment can obviously not be easily transferred to sewer systems.

A grey-box model used as software sensor for a storage sewer equipped with several level measurements is described in detail in Carstensen and Harremoës (1997, 1999). It is based on a simple water balance model, overflow formulas and pump models, which relate the different measurements to each other. During parameter estimation, considerable violations of some assumptions were identified and the models were adapted accordingly. This included the formulation of new overflow relations and specific error models.

In Carstensen et al. (1998) water level measurements and pump operation data are used for a software sensor measuring inflow to a treatment plant. Data from this software sensor is then used to calibrate but also to update a rainfall-runoff model for inflow prediction. A deterministically used regression-model and an extension of the latter by an autoregressive error model (referred to as grey-box model) performed equally well and better than a mechanistic model for inflow prediction.

A software sensor based on flow and level measurements for detection of backwater to be used in RTC is briefly introduced in Carstensen et al. (1996). Bechmann et al. (1999) use a grey-box model to estimate fluxes of COD and TSS from a sewer system as a function of flow.

Apart from software sensors based on models of larger (sub-)systems, specific methods to facilitate the measurement of certain quantities have been proposed. Dürrenmatt et al. (2013) compare dynamic time warping and cross correlation (as already introduced by Beck et al., 1969; Beck, 1981) to estimate the flow velocity in sewers from measurements of natural tracers (e. g. temperature). Both methods could also be applied online. Online applications of deterministic models for RTC and MPC, respectively, can be found in Rauch and Harremoës (1999); Puig et al. (2009) or Meirlaen et al. (2002).

4 Case studies

4.1 Zirl, Austria

The sanitary unit (*Abwasserverband*) Zirl in the province of Tyrol, Austria, is responsible for collection and treatment of storm- and wastewater from 14 rural communities. The drained area covers the bottom and some hillsides of a large alpine valley. It is divided in 17 sub-catchments, whereof nine sub-catchments are drained by combined sewer systems. Combined sewer overflow (CSO) structures are situated at the outlets of the combined sewer sub-catchments, upstream of the discharge points into the interceptor. Fig. 4.1 gives an overview on the catchment area with a focus on the combined sewers sub-catchments.

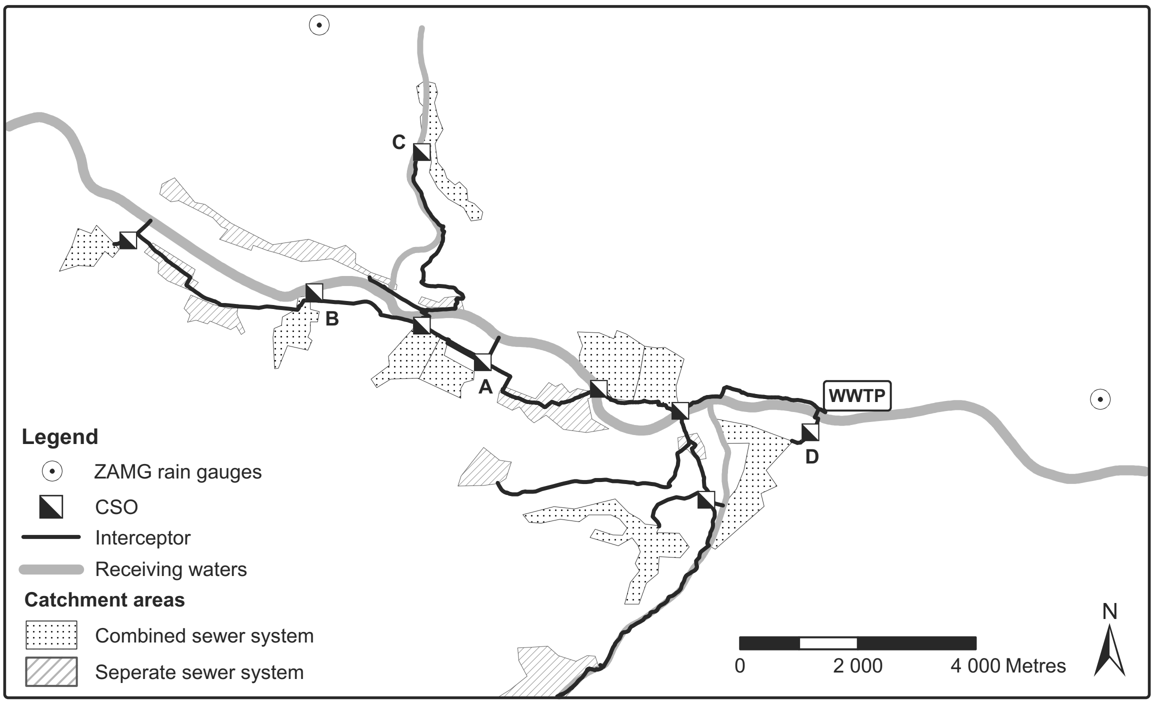

Figure 4.1: Map of the main drainage area of the sanitary unit Zirl, Austria.

Three tipping bucket rain gauges and one weighing gauge were installed at the CSO structures marked with A, B, C and D in Fig. 4.1. Additional rainfall data is available from two official weather stations of the *Austrian Central Institute for Meteorology and Geodynamics* (*ZAMG*) located a few kilometres to the north and east of the sub-catchments, respectively (see Fig. 4.1).

About 90 sensors to measure flows and water levels are installed in the entire sewer system, mainly in CSO structures and pumping stations. The sensors are connected to the SCADA system of the operator and data is available in two-minute time steps. Fig. 4.2 shows the detailed layout of the CSO structure C and the location of sensors. Outflow to the interceptor and treatment plant, respectively, is measured with a magnetic flow meter, whereas ultrasonic sensors are used to measure water levels. The excess flow is computed from the water level at the overflow weir by a simple overflow relation, coded directly in the device. The water level data from the tank has a rather poor resolution of about 2.5 cm due to a conversion to relative depth as integer values prior to data transmission. The level-storage relation and the uncertainty range in the calculated volume, resulting from the resolution of the data and imprecisions in the geometry, are shown in Fig. 4.2.

A similar sensor setup can also be found in some of the other CSO structures, whereas others are equipped with water level sensors only. Three of the CSO structures are connected to and thus influenced by pumping stations.

The data used for modelling was checked and validated manually. Characteristic dry weather profiles to be used in different models were derived from flow measurements. They differ with respect to weekdays and seasons. The online model introduced in **Paper 1** represents the entire case study. **Paper 4** and **Paper 5** are based on sub-catchment and CSO structure C, respectively.

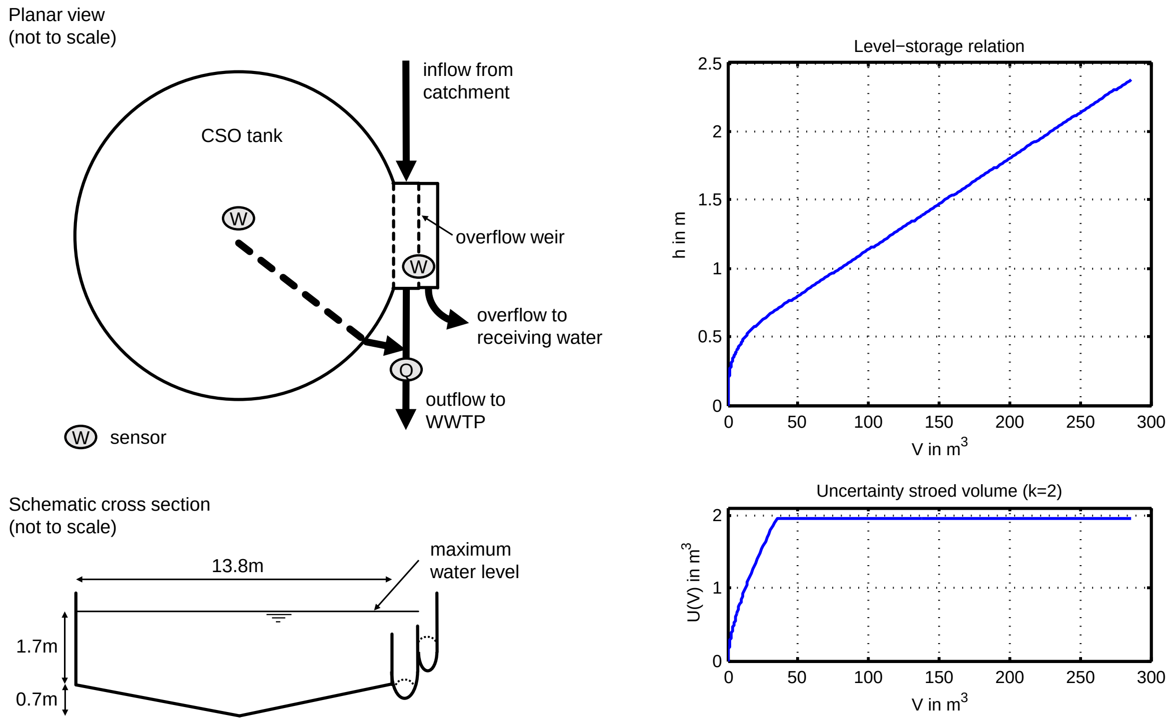

Figure 4.2: CSO structure C; left: layout and location of the sensors for water level (W) and flow (Q); right: level-storage relation and uncertainty in calculated stored volume.

4.2 Chassieu catchment, Grand Lyon, France

The Chassieu catchment, located in the East of Lyon, France, is used as case study in **Paper 2** and **Paper 3**. The catchment covers a mainly industrial area of 185 ha drained by a separate sewer system, whereof the storm sewer is used as monitoring site. The impervious fraction of the area is about 72 %. The catchment is one of the experimental sites of the OTHU project (Observatoire de Terrain en Hydrologie Urbaine - Field Observatory for Urban Water Management, see `www.othu.org`).

Rainfall is measured using a 0.2 mm tipping bucket gauge. Catchment runoff is computed from measurements of water level and mean flow velocity and available in two-minute time steps. Relative standard uncertainties in flow measurements approximately range from 15 to 25 % (Leonhardt et al., 2014). Although it is a storm sewer, a certain amount of dry weather flow is constantly measured. More details on the site and the data (including long term turbidity measurements) can e. g. be found in Bertrand-Krajewski et al. (2007) or Métadier and Bertrand-Krajewski (2012).

5 Reverse Modelling

5.1 Introduction to *reverse modelling*

Usual, physically based conceptual models in hydrology are formulated analogously to the direction of water flow. Models are used to estimate outflow(s) from a system of interest, based on data on inflow(s) to that system (e.g. rainfall-runoff models are used to estimate runoff from a catchment based on measured rainfall input). *Reverse modelling* refers to the application of models opposite to the direction of water flow, and thus opposite to their common use. This form of application is sometimes also referred to as *inverse modelling* (as in **Paper 1**). However, to avoid confusion with the problem of model parameter estimation (which is also referred to as *inverse problem*), the term "reverse modelling" is used. For clear distinction in the present text, commonly formulated models are referred to as *forward models*. Fig. 5.1 illustrates the terminology outlined above.

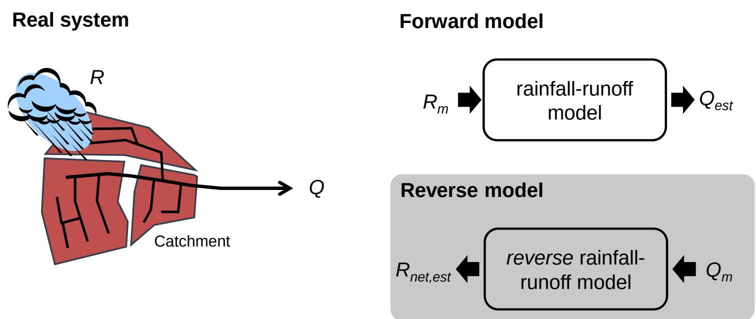

Figure 5.1: An urban catchment and its representation by a *forward* model and a *reverse* model; measured inputs and estimated outputs are marked with subscripts *m* and *est*, respectively.

5.1.1 Motivation

Reverse modelling targets to estimate unknown system input from known system output. It becomes attractive if measurements of system input are difficult, troublesome or not reliable, but a sufficient mathematical description of the system and reliable measurements of its output are available. However, it is important to keep in mind that estimated inputs are always conditional on the applied model and the underlying process description. Furthermore, a unique relationship is assumed, at least within the expected ranges of input and output.

5.1.2 Basic methodologies

Reverse modelling can be implemented based on two different strategies:

1. Reformulation of the forward model's equations
2. Estimation of forward model input based on measurements of output

Both strategies are visualized in Fig. 5.2,

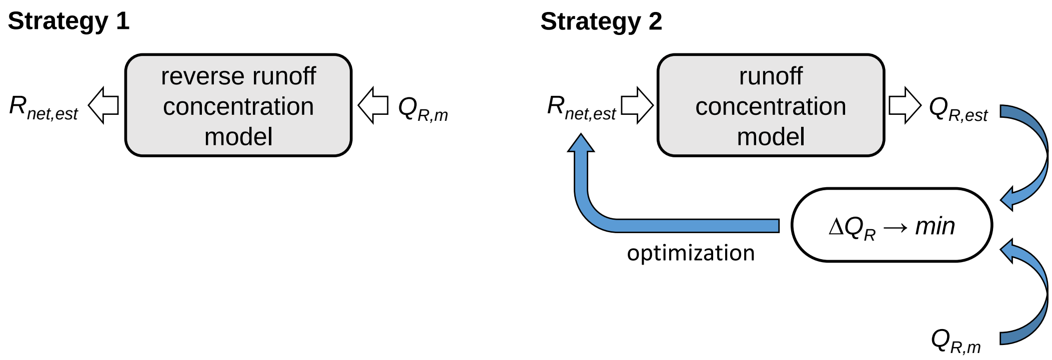

Figure 5.2: The basic strategies for reverse modelling in the case of a rainfall-runoff model (measured inputs and estimated outputs are marked with subscripts m and est, respectively).

Although both strategies are conceptually different, they share some challenges to be overcome. Those challenges are related to the mathematical structure of most forward models, formulated as a single or more differential equations, which are solved by integration. This implies that the solution to the reverse model is found by differentiation. When the reverse model is based on the first strategy, the derivatives are calculated from measured data, and measurement noise and other fast dynamics (high frequency variations) are amplified. Consequently the solutions show spurious oscillations and physically meaningful results are not ensured. When applying the second strategy, this property manifests itself by over-fitting or non-uniqueness of the solutions, caused by data uncertainties and the simplified representation of real processes by the models used. It is thus necessary to discuss reverse modelling in the context of uncertainties in both, data and models.

The property mentioned above can be demonstrated by reformulation of the linear reservoir equation (Eq. 2.12)

$$\frac{dQ}{dt} = \frac{1}{K} \cdot (R(t) - Q(t)) \tag{5.1}$$

which can be rearranged to

$$R(t) = K \cdot \frac{dQ}{dt} + Q(t). \tag{5.2}$$

Another point of departure for the illustration of the problems is the *low-pass filter property* of many routing models in analogy to the real processes. This applies for example to a catchment, which transforms rainfall varying at high frequency to a runoff hydrograph which varies more smoothly. This property is perfectly reproduced by model concepts for runoff concentration, and has been mentioned in different contexts by Schilling (1991) or Sun and Bertrand-Krajewski (2013). The same property applies to open channel or reservoir routing. As a consequence, reverse model formulations amplify high frequency variations.

5.2 Examples of reverse model applications in hydrology

In the following section, examples of reverse modelling from literature, which are relevant for urban drainage systems, are summarized. With regard to the applications presented in this dissertation, examples of reverse rainfall-runoff-modelling and reverse routing are distinguished.

5.2.1 Reverse rainfall-runoff modelling

To the best of the author's knowledge, the only application of a reverse rainfall-runoff model in an urban catchment is published in the Master thesis by Marceau (1997), who tested the methodology in the context of a real time control system. The main problem is the estimation of negative rainfall intensities, which is addressed by filtering of flow data. The use of catchment runoff as a measure for areal precipitation in urban catchments is mentioned in the abstract of the Ph.D. thesis by Blanchet (1993, full text not accessible).

Furthermore, the topic has been addressed in a few publications in catchment hydrology. Hino and Hasebe (1981) estimated effective precipitation from daily runoff data applying system identification methods (filtering) and representing the hydrological system by autoregressive models for two catchments in Japan. The methodology includes the separation of total runoff into surface runoff, interflow and baseflow. In a qualitative comparison the general shape of the estimated hyetographs shows good agreement with the measurements. Although the total depth is estimated rather well, at least a small rainfall depth was estimated for every day. The adaptation and application of the method to hourly data from specific events is shown in Hino and Hasebe (1984). Their results indicate a similar performance in the estimation of hyetographs as for daily data. Furthermore, an approach based on the formulation of the catchment's response (or the response of a subsystem as e. g. surface runoff) to rainfall as a system of linear equations was published in Hino (1986). Rainfall intensities are estimated from hourly runoff data using smoothed least squares and linear programming. In contrast to the previous publications negative rainfall intensities were estimated for the falling limb of the hydrograph. This problem was only tackled by strong smoothing of the solution (see also **Paper 2**).

An approach starting from the same point of departure, the analysis of streamflow data, is presented by Kirchner (2009). Assuming the catchment to act as a simple non-linear storage, the storage-flow relationship is estimated from hourly flow data of certain periods, when evapotranspiration can be neglected (a similar method to estimate the storage constant of a reservoir model is mentioned in Rauch et al., 2002b). Finally, the relationship is used to estimate hourly rainfall intensities. Timing, shape and general magnitude of the estimated hyetographs for two catchments in the UK show good agreement with the measurements. It should be mentioned that the streamflow hydrographs shown in Kirchner (2009) have a very "typical" shape (steep rises and curved falling limbs) which is rarely observed in urban catchments.

Ranzi et al. (2003) use a calibrated hydrological model to estimate areal precipitation in small and medium alpine catchments in northern Italy and compare the results to data derived from a gauge network. The estimates of total event rainfall from the reverse model show the same tendency as areal precipitation derived from gauge data, and differences are comparable to the estimated uncertainties for both methods.

5.2.2 Reverse routing

Reverse routing refers to the estimation of inflow to a system based on measurements of outflow or change in storage. Examples in the literature with a certain relevance for urban drainage deal with reverse flow routing in open channels and reverse level-pool routing in reservoirs.

5.2.2.1 Reverse flow routing

Reverse flow routing is applied to estimate the upstream inflow to an open channel reach. Koussis et al. (2012) investigated different methods and numerical parameters for reverse flow routing using the *Muskingum* scheme based on synthetic data. The amplification of measurement errors is tackled by either low-pass filtering or optimisation. The performance is similar to an application of the *Saint-Venant Equations* for reverse routing in Bruen and Dooge (2007). The same basic problem was investigated by D'Oria and Tanda (2012) based on more realistic data (non-prismatic channels with varying friction). To overcome the shortcomings of reverse calculation based on reformulated models, the estimation of the inflow to the forward model is proposed (the application of strategy 2 - see Sec. 5.1). The *Bayesian Geostatistical Approach* (BGA, see Sec. 5.4.2) is introduced and proposed as suitable method to estimate model input, i.e. inflow to the channel reach where only outflow is measured.

Similar methods are also be applied to pollutant transport (e.g. Boano et al., 2005; El Badia et al., 2005). Another problem of reverse flow estimation, in the literature referred to as *open channel inverse problem*, is the estimation of channel flow from multiple water level measurements (see e.g. Roux and Dartus, 2008; Durand et al., 2014).

5.2.2.2 Reverse level-pool routing

Reverse level-pool routing addresses the problem to estimate reservoir inflow from measurements of water level. The basic problems in reverse level-pool routing are the same as in reverse flow routing, i. e. numerical stability and the amplification of measurement errors. The method can be applied to storage structures in sewer systems.

The choice of the discretization scheme can be an important issue in the solution of the forward problem in case of storage-dependent outflow and is thus discussed in literature (e.g. Fiorentini and Orlandini, 2013). Zoppou (1999) investigates different numerical schemes for reverse level-pool routing based on a synthetic and a real case. The use of a centred explicit scheme is recommended, as implicit schemes require filtering of the solution to remove oscillations. As in the case of reverse flow routing, the problem can also be addressed by estimating the inflow using the forward model. D'Oria et al. (2012) compare the reverse formulation of the level-pool routing equation to the use of the forward model (strategy 2 - see Sec. 5.1, using the BGA) to estimate inflow to flood retention reservoirs. The latter methodology outperforms the reformulated model in terms of stability in different synthetic cases and a real case, both with movable outflow gates.

5.3 Reverse rainfall-runoff models as software sensors

Reverse rainfall runoff-models can be applied to estimate areal precipitation for the represented catchment area. In urban catchments rainfall runoff reaching the catchments outlet via the sewer system can be considered as the response of the effective impervious area to net rainfall. If the effective impervious area and other model parameters are known (usually from calibration), net areal rainfall can be calculated with a reverse rainfall-runoff model. The result is basically a quantity which is used in modelling. Depending on the homogeneity of the catchment with regard to the spatial distribution of the area effectively drained by the sewer system, the estimated quantity might be more or less representative for the real areal precipitation. However, with regard to the difficulties in measuring areal rainfall (see Sec. 2.1.1.1), the estimated rainfall is still a useful result. In the case of dry weather flow (sanitary flow or parasite water) in the sewer system, runoff from rainfall must be separated from the total flow. This introduces additional uncertainties.

Possible applications are mentioned and demonstrated in **Paper 1**, **Paper 2**, and **Paper 3**: provision of input to other models, assessment of other measurements and filling of gaps in gauge data or calibration of indirect measurements. A reverse model might also be used to estimate the amount of initial rainfall loss in combination with measurements.

Reverse rainfall-runoff modelling (in combination with reverse level-pool routing) has been applied in an online model to simulate CSO discharge, as presented in **Paper 1**. In **Paper 2**, the reverse model is applied offline with a focus on the propagation of uncertainties and the comparison to the estimation of rainfall errors based on rain gauge data. **Paper 3** presents a methodology to combine an offline reverse model and an error model to fill gaps in measured data from rain gauges. All presented applications are based on calibrated models.

In analogy to the direct models based on superposition and a time-invariant transfer function, the operation underlying the reverse model is referred to as *deconvolution*. Another application of deconvolution is the estimation of unit hydrographs from measurements of rainfall and flow (Chow et al., 1988).

5.3.1 Reverse formulation of rainfall-runoff models (strategy 1)

5.3.1.1 Time-area method

The reverse formulation for the case of sub-areas of equal size is obtained by re-arrangement of the forward model (Eq. 2.7):

$$r_{t_i} = \frac{Q_{t_i}}{A_n}\Delta t - \sum_{j=1}^{N-1} r_{t_{i-j}} \tag{5.3}$$

As the rainfall depth r_{t_i} in Eq. 5.3 depends on the rainfall estimates from previous time steps, errors (and corrections) thereof are propagated to subsequent time steps. Eq. 5.3 can also be expressed in terms of runoff Q_t as follows:

$$r_{t_i} = \begin{cases} \frac{Q_{t_i}}{A_n}\Delta t & \text{if } i = 1 \\ \frac{Q_{t_i}}{A_n}\Delta t - \frac{Q_{t_{i-1}}}{A_n}\Delta t & \text{if } 1 < i \leq N \\ \sum\limits_{j=0}^{\lfloor t/N \rfloor} \frac{Q_{t_{i-jN}}}{A_N}\Delta t - \sum\limits_{j=0}^{\lfloor t/N \rfloor} \frac{Q_{t_{i-jN-1}}}{A_N}\Delta t & \text{if } i > N \end{cases} \tag{5.4}$$

Similar equations can be derived for the case of sub-areas of different sizes. Note that this formulation is based on differences between measured runoff from consecutive time steps and thus sensitive to uncertainties. Furthermore, the number of summands is increasing with t in cases for $t_i > N\Delta t$ in Eq. 5.4. However, in contrast to Eq. 5.3, the formulation in Eq. 5.4 does not propagate corrections or errors in r_t.

In contrast to Eq. 5.4, Eq. 5.3 requires only data from the limited period ranging from t_{i-N-1} to t_i, which might be of interest in practical implementation. The formulation in Eq. 5.3 is used in the application in **Paper 1**. If there is no time delay between rainfall and measured runoff, it can be used in real time, as the calculation of r_t

requires only data from current and past time steps. If, however, the flow measurement is located further downstream and the effect of rainfall r_{t_i} is only measured at $t_i + n\Delta t$ (and translation must thus be considered in the model), rainfall can only be estimated with a delay of n time steps.

5.3.1.2 Linear reservoir model

The reverse formulation of the linear reservoir equation, expressing R in terms of Q, obtained by rearranging Eq. 2.12, has already been introduced. Rainfall intensities are obtained from division by the effective impervious catchment area A_e:

$$r(t) = \frac{R(t)}{A_e} \tag{5.5}$$

Simple discretization For a numerical solution of Eq. 5.2, the derivative $\frac{dQ}{dt}$ can be replaced by $\frac{\Delta Q}{\Delta t}$. If Q_{t_i} and R_{t_i} refer to the time step from $t_i - \Delta t$ to t_i, $\Delta Q = Q_{t_i} - Q_{t_{i-1}}$. Eq. 5.2 can be thus be discretized as follows:

$$R_{t_i} = K \cdot \frac{Q_{t_i} - Q_{t_{i-1}}}{\Delta t} + Q_{t_i} \tag{5.6}$$

Reverse linear reservoir based on the discretization of the analytical solution The reverse model can also be derived from Eq. 2.14 and Eq. 2.15, respectively:

$$R_{t_i} = \frac{Q_{t_i} - Q_{t_{i-1}} C_1}{C_2} \tag{5.7}$$

In the discrete case, the rainfall depth r_{t_i}in the time step from $t_i - \Delta t$ to t_i is obtained as follows:

$$r_{t_i} = \frac{R_{t_i}}{A_e} \Delta t \tag{5.8}$$

The rainfall depth can be easily converted to a mean intensity for each time step.

For reverse linear reservoirs in series Eq. 5.7 is applied repeatedly and rainfall intensities are finally calculated using Eq. 5.8. Numerically, the outflow from a cascade of reservoirs in series responds immediately to rainfall r_{t_i} with a rather small runoff signal Q_{t_i}. An online estimation of r_{t_i} would thus be theoretically possible. However, in case of a longer cascade the uncertainty of measured runoff might constitute a practical limit.

A reverse model of parallel reservoirs cannot be formulated by rearranging the equations, as the ratio between the outflows Q_f and Q_s varies with time. However, the reverse model can be formulated according to strategy 2 (see Sec. 5.3.2).

5.3.1.3 Physical constraints and consideration of uncertainties

As already mentioned, reverse models are rather sensitive to uncertainties in input data, and also unavoidable simplifications and imperfections of the (direct) model can yield results which are physically not meaningful, i. e. negative rainfall intensities. In a straightforward approach, such values could be corrected to $r_t = 0$. However, this violates the mass balance and the correction might be propagated to following time steps (e. g in Eq. 5.3). With a focus on online application, the following approaches to tackle these problems have been identified:

1. Filtering of input data
2. Propagation of uncertainties

A rationale for filtering is the reduction or removal of high frequency variations and thus to avoid their amplification. However, on time scales and time steps typical for urban drainage systems, the filters are also smoothing the runoff peaks considerably. Furthermore, an online model requires the use of *causal* filters, i. e. only data from the current and past time steps is used to calculate the filtered value. Many causal filters introduce a delay to the filtered time series (Olsson and Newell, 1999). This effect is visualized in Fig. 5.3.

Furthermore, filtering can "shape" the time series in order to be more consistent with the forward model, i. e. the transfer function g. This is most effective if the transfer function, scaled to unity, is used as filter. This corresponds to a convolution of the flow time series with the transfer function. In the case of the time-area method with equal sub-areas, this is equivalent to a moving average filter with constant weights.

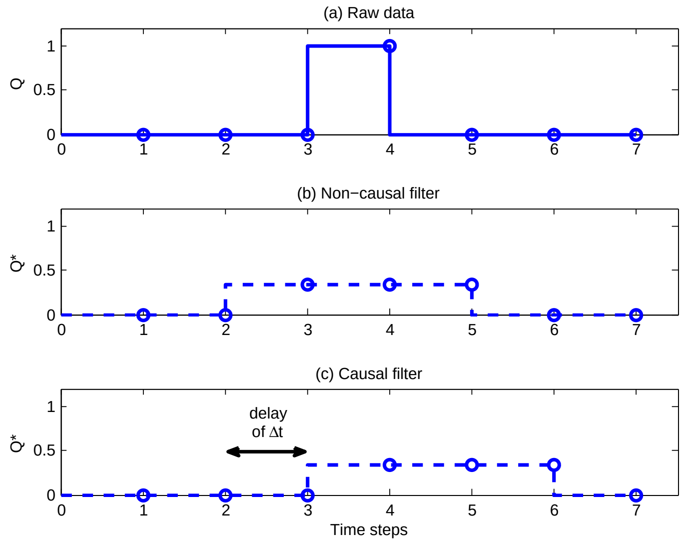

Figure 5.3: A discrete flow pulse (a) and the effect of applying a *non-causal* (b) and a *causal* (c) moving average filter with window size $w = 3$.

Propagation of uncertainties in flow data and model parameters through the reverse model accounts for both sources, but does not avoid implausible results. However, such results can either be corrected or discarded. In addition, an uncertainty range for the estimated rainfall is provided. Due to the constraints, Monte Carlo simulation is usually more suitable than analytical propagation. In principle, filtering and uncertainty propagation can be combined, but interpretation of the resulting uncertainties would be difficult.

5.3.2 Reverse rainfall-runoff modelling based on strategy 2

A forward rainfall-runoff model based on a linear transfer function g can be written as a system of linear equations as follows:

$$\mathbf{M}\mathbf{r} = \mathbf{q} \tag{5.9}$$

In Eq. 5.9, $\mathbf{r}$=$(r_1, r_2, \ldots, r_m)^{\mathrm{T}}$ is the vector of rainfall inputs (in [L]), $\mathbf{q}$=$(q_1, q_2, \ldots, q_m)^{\mathrm{T}}$

the vector of flows (in [L^3/T]) and $\mathbf{M}$ the $m \times m$ *model* matrix structured as follows:

$$\mathbf{M} = \begin{pmatrix} g_1 & 0 & 0 & & \cdots & & 0 \\ g_2 & g_1 & 0 & & & & \\ g_3 & g_2 & g_1 & & & & \vdots \\ \vdots & & & \ddots & & & \\ g_{m-2} & & & & g_1 & 0 & 0 \\ g_{m-1} & g_{m-2} & & & g_2 & g_1 & 0 \\ g_m & g_{m-1} & g_{m-2} & \cdots & g_3 & g_2 & g_1 \end{pmatrix} \tag{5.10}$$

The columns of $\mathbf{M}$ below the main diagonal are built from the *discrete transfer function* according to the model concept which is used. Depending on the length of g, $\mathbf{M}$ is a lower triangular or a lower triangular band matrix. To calculate rainfall $\mathbf{r}$ from runoff $\mathbf{q}$, the system of equations (Eq. 5.9) can be solved for $\mathbf{r}$ as follows:

$$\mathbf{r} = \mathbf{M}^{-1}\mathbf{q} \tag{5.11}$$

However, the solution of Eq. 5.11 is not necessarily physically meaningful, as it might e. g. contain negative rainfall. This expresses the imperfect representation of real system by the model, as well as uncertainties in the runoff measurements. The estimation of positive rainfall can be ensured by imposing the physical constraint $r_i \geq 0$. As a consequence of the constraint, mass conservation is no longer ensured. To overcome this problem, a mass balance equation is added to the system:

$$\left(\sum_{i=1}^{m} g_i \quad \sum_{i=1}^{m-1} g_i \quad \sum_{i=11}^{m-2} g_i \quad \ldots \quad \sum_{i=1}^{3} g_i \quad \sum_{i=1}^{2} g_i \quad g_1 \right) \mathbf{r} = \sum_{i=1}^{m} q_i \tag{5.12}$$

Consequently, $\mathbf{M}$ in Eq. 5.9 is extended to an $(m+1) \times m$ matrix $\hat{\mathbf{M}}$, and $\mathbf{q}$ becomes a vector $\hat{\mathbf{q}}$ of length $m+1$:

$$\hat{\mathbf{M}} = \begin{pmatrix} g_1 & 0 & 0 & & \cdots & & 0 \\ g_2 & g_1 & 0 & & & & \\ g_3 & g_2 & g_1 & & & & \vdots \\ \vdots & & & \ddots & & & \\ g_{m-2} & & & & g_1 & 0 & 0 \\ g_{m-1} & g_{m-2} & & & g_2 & g_1 & 0 \\ g_m & g_{m-1} & g_{m-2} & \cdots & g_3 & g_2 & g_1 \\ \sum_{i=1}^{m} g_i & \sum_{i=1}^{m-1} g_i & \sum_{i=11}^{m-2} g_i & \cdots & \sum_{i=1}^{3} g_i & \sum_{i=1}^{2} g_i & g_1 \end{pmatrix} \tag{5.13}$$

$$\hat{\mathbf{q}} = \left(q_1, q_2, \ldots, q_m, \sum_{1}^{m} q_i\right)^{\mathrm{T}} \tag{5.14}$$

The system $\mathbf{r} = \hat{\mathbf{M}}^{-1}\hat{\mathbf{q}}$ can then be solved with an algorithm for non-negative least-squares constraints problems.

Eq. 5.13 is applied in **Paper 2** and **Paper 3**, using the transfer function of two linear reservoirs in series. Due to the required mass balance equation, the approach cannot be applied online, but only to an entire event. That is, the hydrograph must include all runoff from rainfall.

Application to parallel linear reservoirs In the case of parallel reservoirs, equation Eq. 5.9 is extended as follows:

$$\mathbf{M_f}\mathbf{r}\alpha + \mathbf{M_s}\mathbf{r}(1-\alpha) = \mathbf{q} \tag{5.15}$$

$\mathbf{M_f}$ and $\mathbf{M_s}$ represent the two reservoirs and therefore are of the same dimensions. Applying the distributive law, Eq. 5.15 can be rearranged:

$$(\mathbf{M_f}\alpha + \mathbf{M_s}(1-\alpha))\mathbf{r} = \mathbf{q} \tag{5.16}$$

Rainfall $\mathbf{r}$ can then be computed as above, replacing $\mathbf{M}$ in Eq. 5.11 by $(\mathbf{M_f}\alpha+\mathbf{M_s}(1-\alpha))$.

5.3.2.1 Consideration of uncertainties

In contrast to the sequential solution based on the reformulated model, the second strategy ensures physically plausible results and mass conservation. Nevertheless, amplification of high frequency variations cannot by avoided. Thus, the propagation of uncertainties in flow measurements and model parameters is highly recommended. Due to the constraint $r_i \geq 0$, the Monte Carlo method must be employed. The issue of uncertainties is exhaustively discussed in **Paper 2**.

5.3.3 Application results and discussion

5.3.3.1 Synthetic data

The basic problem to be tackled in reverse rainfall-runoff modelling - the amplification of high-frequency variations - is illustrated based on synthetic data in Fig. 5.4. The flow data has been generated with the forward model, based on the linear reservoir equation. When the simulated flow is used as input to the reverse model, the assumed rainfall is perfectly reproduced. As this is not realistic, uncertainty was introduced to model measurement errors of the flow data and an imperfect reverse model. The uncertainty in runoff is represented by independent normally distributed random errors with constant variance, which corresponds to 5 % of the peak flow. A random flow sample was drawn and used as input to the reverse model (Fig. 5.4, plot b). The hyetograph estimated with solution strategy 1 shows slightly stronger oscillations then the result from strategy 2, but in general they are rather similar (Fig. 5.4, plot c and d).

For further evaluation, Monte Carlo simulations with 50 000 flow samples were performed to propagate input uncertainties through the model. The results for both strategies are shown in Fig. 5.5. Estimated hyetographs are evaluated with respect to mass conservation, and also indirectly, that is they are used as input to the forward model. This allows an assessment of the simulated runoff.

Mass conservation is evaluated using the relative mass balance error E_V, which is calculated as follows:

$$E_V = \frac{V_R - V_Q}{V_Q} \tag{5.17}$$

where $V_R = A_e \sum_t r_t$ is the total rainfall volume and $V_Q = \sum_t Q_t \Delta t$ the total runoff volume.

For the indirect assessment, any common measure of model performance, e. g. the sum of squared errors or the Nash-Sutcliffe Efficiency (Nash and Sutcliffe, 1970), can be used.

Whereas the maximum uncertainty, i. e the maximum width of the 95 % coverage range (at the rainfall peak), is the same for both strategies, strategy 2 results in smaller uncertainty ranges before and after the peak. However, the median of all estimates with strategy 1 agrees better with the measurement than that obtained with strategy 2. Significant differences are revealed by the indirect assessment using the forward model. Rainfall estimates obtained with strategy 2 do not only result in a smaller uncertainty in simulated runoff for a larger part of the hydrograph, but also in a significantly better representation of the shape. These differences between the strategies become also evident in Fig. 5.6, which shows histograms of mass balance error and the performance measure used for assessment of simulated flow.

It can thus be concluded that strategy 2 outperforms strategy 1 in terms of mass conservation, uncertainty in rainfall estimates and also with regard to the indirect evaluation. However, as a drawback it can only be applied offline, i. e. to an entire event. As an alternative, strategy 1 can be combined with filtering of input data.

Fig. 5.7 shows results for the synthetic event using strategy 1 in combination with filtering of flow data, using a moving average filter. As the method is of interest in online applications, the filter was implemented as a casual filter. The oscillations in each single estimate and thus the uncertainty range estimated with the Monte Carlo method are clearly reduced. Consequently, the uncertainty in simulated runoff and the mass balance errors are considerably smaller. Thus, at first glance filtering improves both, mass conservation and runoff simulation. However, the peaks (of both estimated rainfall and simulated flow) are smoothed and shifted with respect to the measurement. This effect correlates with the filter parameter, which in an online application must be chosen in advance.

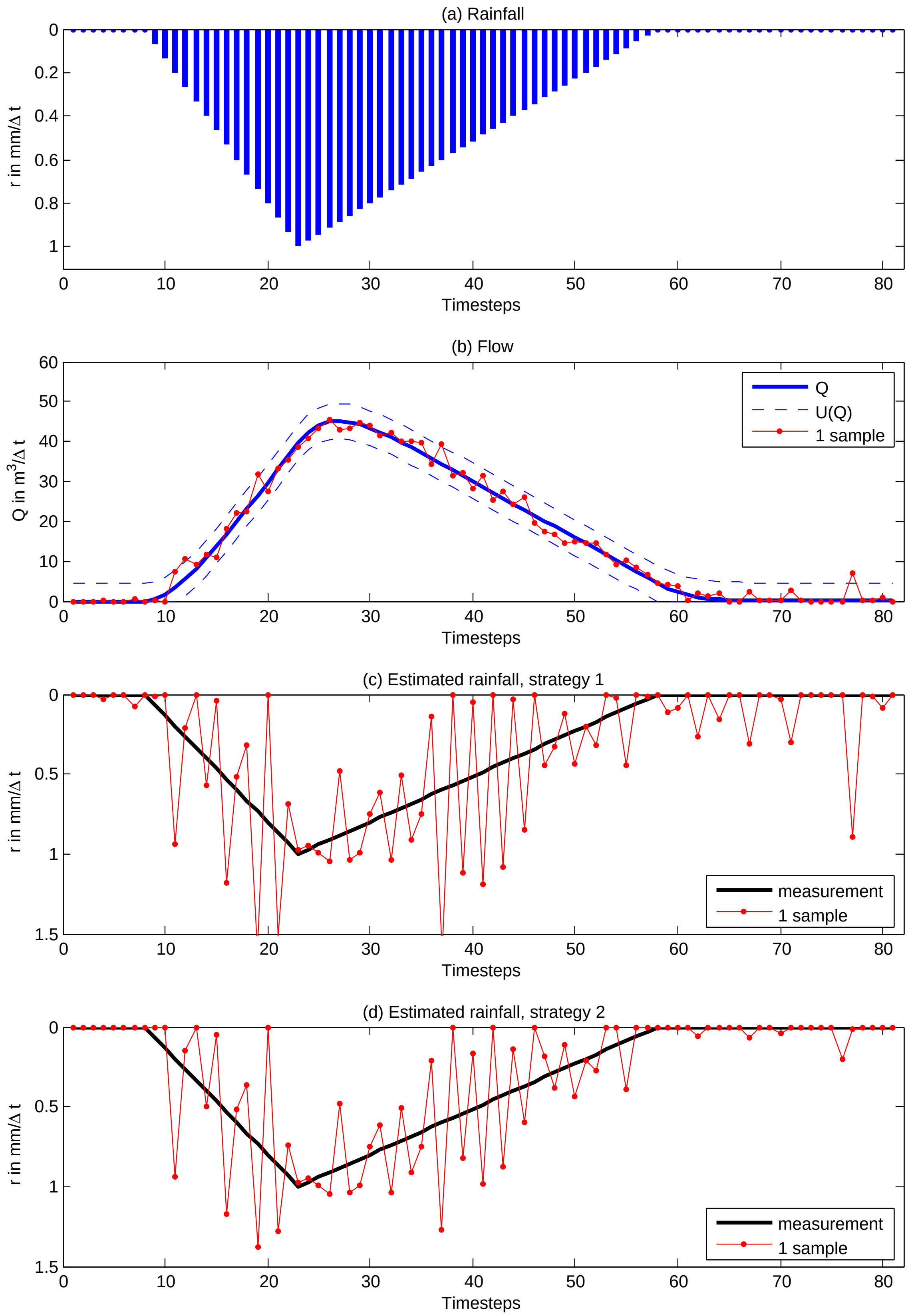

Figure 5.4: Reverse rainfall-runoff model: comparison of solution strategies for a synthetic rainfall event based on a single sample of flow data.

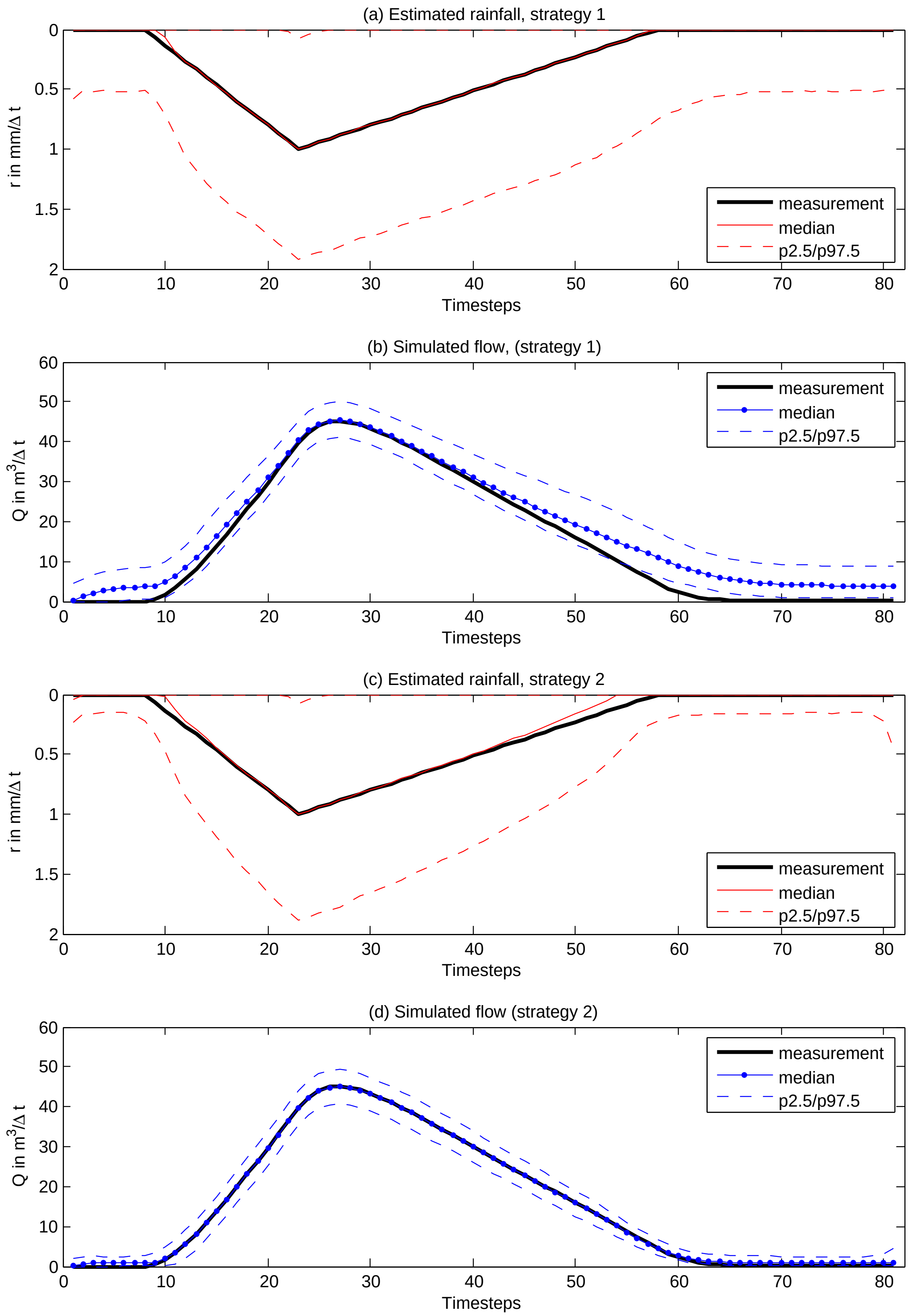

Figure 5.5: Reverse rainfall-runoff model: comparison of solution strategies for a synthetic rainfall event based on Monte Carlo simulation to consider uncertainties.

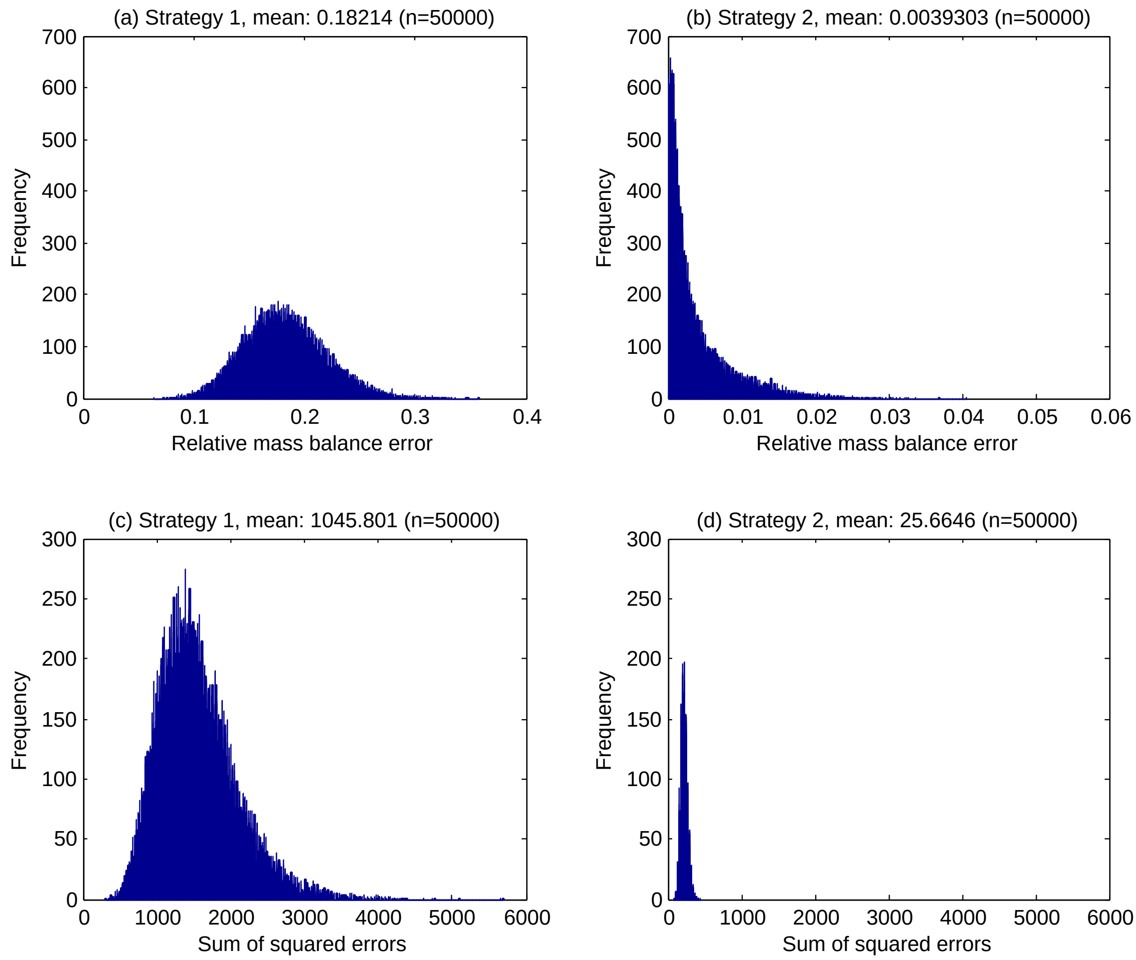

Figure 5.6: Distributions of relative mass balance errors ((a) and (b), mind the different ranges of the x-axes) and the performance measures for the simulation of flow ((c) and (d), sum of squared errors).

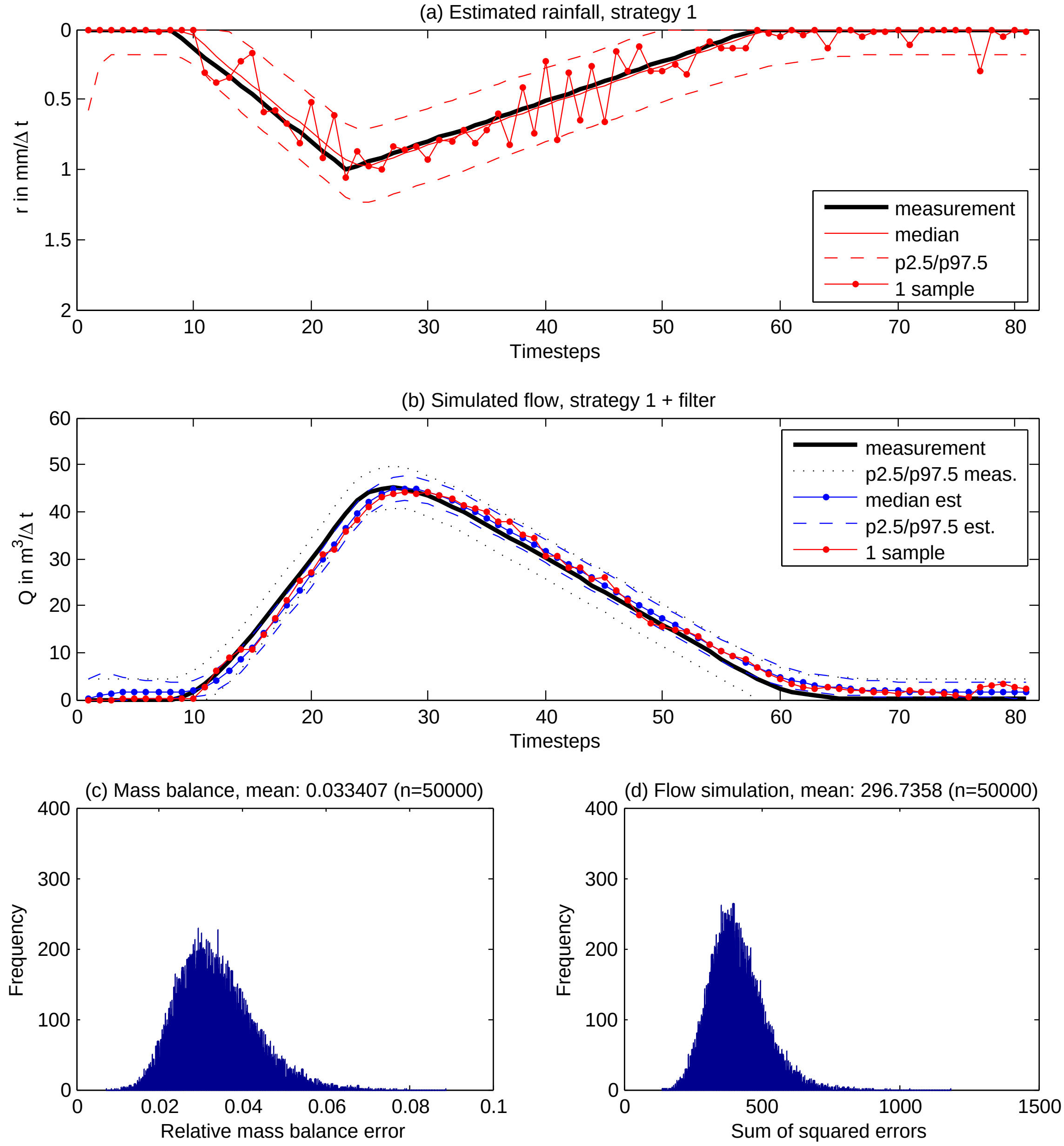

Figure 5.7: Reverse rainfall-runoff model: solution strategy 1 combined with filtering (moving average filter, $w = 3$) for a synthetic rainfall event.

5.3.3.2 Application to real case studies

An application of a reverse model based on strategy 1 is used in **Paper 1**, which presents an online model to simulate CSO discharge in several sub-catchments of the case study Zirl, Austria (Sec. 4.1). The reverse rainfall-runoff model is combined with a reverse level-pool routing model to estimate total catchment runoff, and the estimation of dry weather flow. Filtering is applied to limit mass balance errors and avoid extreme rainfall intensities. The methods were implemented in specific modules for the software *CityDrain3* (Burger et al., 2010; Burger et al., submitted). The focus of **Paper 1** is the simulation of CSO discharge using estimated rainfall in neighbouring sub-catchments. Fig. 5.8 shows measured and estimated rainfall for different sub-catchments, and Tab. 5.1 lists total depth and maximum intensities as well as the mass balance errors associated with the reverse rainfall runoff model. Whereas the estimated total depth can be considered to be in a realistic range, the estimated maximum intensities are too low, which is the effect of filtering. Nevertheless, the performance of the online model to simulate CSO discharge is similar, whether estimated rainfall or rain gauge measurements are used. However, in both cases a detailed estimation of overflow discharge remains difficult.

Table 5.1: Estimated and measured rainfall and relative mass balance errors for different sub-catchments of the case study Zirl (see Fig. 4.1).

Sub-catchment/Gauge	E_V (-)	**Total rainfall** in mm		**Maximum intensity** in mm/h	
		estimated	measured	estimated	measured
A	0.014	214.73	218.53	4.68	120.00*
B	0.032	157.14	264.40	5.64	86.64*
C	0.118	262.02	285.02	57.48	63.84*
D			275.22		53.40*
ZAMG east			107.6		87.00**
ZAMG north			144.1		65.40**

*from 5 min data, **from 10 min data

The issue of uncertainties in the case of an offline rainfall estimation based on strategy 2 is intensively discussed in **Paper 2**. The reverse model is applied to a storm sewer catchment (Chassieu catchment, Grand Lyon, France, Sec. 4.2) based on long-term flow measurements in short time steps. A sound calibration of the direct model using rain gauge measurements was performed beforehand. Uncertainties in input data, i.e. flow measurements, and model parameters were propagated through the model by Monte Carlo simulation to estimate rainfall uncertainties. As in the synthetic example presented above, uncertainties are in the same order of magnitude as the

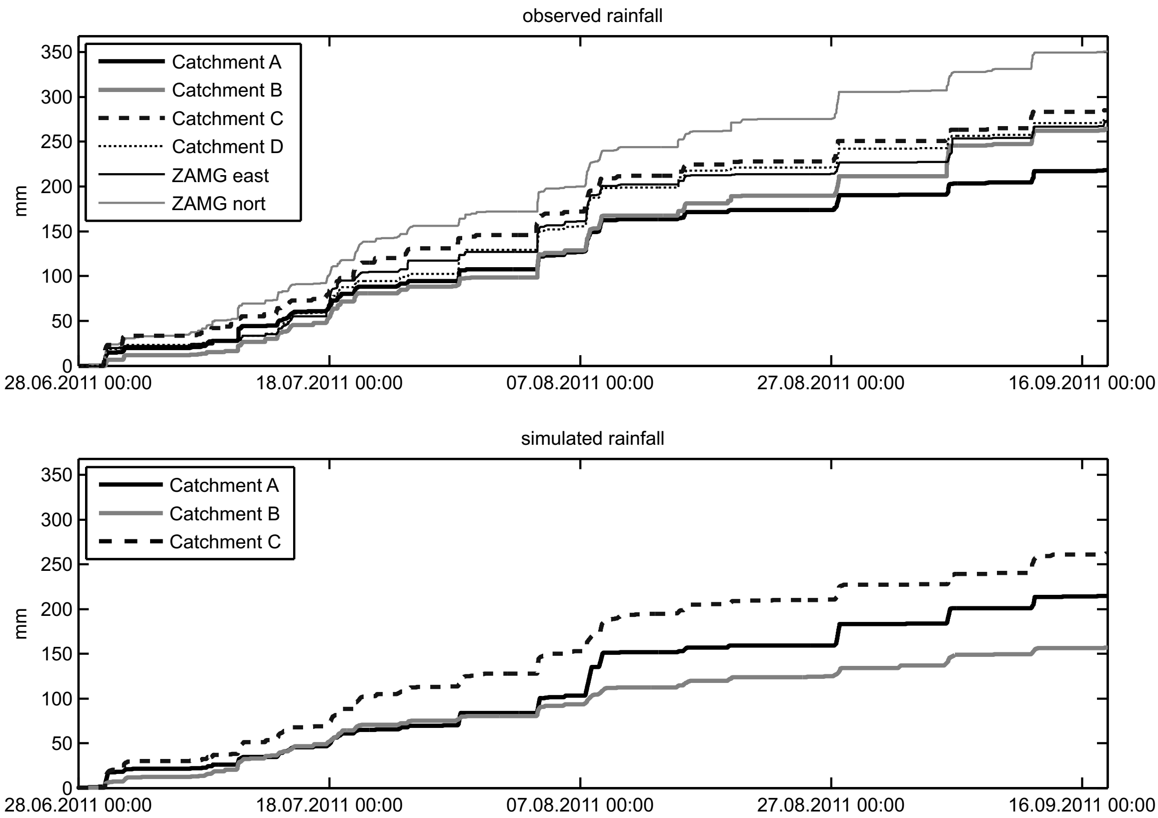

Figure 5.8: Estimated and measured rainfall in different sub-catchments of the case study Zirl (see Fig. 4.1).

rainfall, but the median of all single results can be considered as a realistic estimate of areal rainfall when compared to the gauge data. Rainfall uncertainties represent uncorrelated random uncertainties. Interestingly, there is little difference in the maximum uncertainty in estimated rainfall, whether only measurement uncertainties or both measurement and parameter uncertainties are considered. The consideration of both uncertainties increases only the average width of the uncertainty range.

Furthermore, **Paper 2** compares the reverse model to an error model, which is used to estimate errors of rain gauge measurements, based on gauge data and flow measurements using a Bayesian approach. The estimated rainfall errors are considerably smaller than the uncertainty range of estimated rainfall (using the reverse model). However, they are based on additional data and constraint by the error model structure and the assumed prior distribution of error model parameters.

Fig. 5.9 compares results of both strategies applied to the data used in **Paper 2**, i. e. a real event. In both cases, uncertainties in flow measurements and model parameters are considered. In addition to the uncertainty ranges and the median values, deterministic estimates (obtained with the Maximum Likelihood-values of model parameters) with both strategies are shown. The uncertainty range of rainfall estimates from strategy 1 is extremely large, and the deterministic result shows strong oscillations. Only the median of the results (strategy 1) is comparable to the measurement and the corresponding result from strategy 2. As shown in Fig. 5.9 (d), the deterministic result from strategy 1 overestimates measured total rainfall by 100 %. Thus, in case strategy 1 is applied without filtering of input data, only the median of a Monte Carlo simulation can be considered as plausible result, whereas the uncertainty range is clearly overestimated.

Paper 3 presents a method to fill gaps in measured rainfall data, which combines the reverse model based on strategy 2 and the rainfall error model (as presented in **Paper 2**). Rainfall for the entire event or considered period is estimated with the reverse model by Monte Carlo simulation (an application to the gap period only has proven less suitable in preliminary tests). The estimated rainfall distribution is then used as a prior distribution for the error model in the gap period. The error model is applied for the entire event or period, i. e. to available gauge data and the gap period.

5.3.3.3 Common discussion

The results presented above show that in offline applications of reverse rainfall-runoff models, strategy 2 should be preferred to strategy 1, as it assures small mass balance errors and physically meaningful results. Although the deterministic estimate in the case of the real event can be considered as plausible, uncertainties of input data and possibly model parameters should be propagated to provide an uncertainty range of estimated rainfall. The median can be considered as a reliable estimate of net areal rainfall. The result can also be used as prior information for further estimations.

In an online application, propagation of uncertainties yields extremely large uncertainty ranges of estimated rainfall. In the presented real case, only the median can be considered as plausible. Alternatively, input data can be filtered. However, the choice of filter parameters is a compromise between the loss of information and the prevention of unrealistic oscillations. Furthermore, a full online application, i. e. the estimation of r_{t_i} based on Q_{t_i}, is limited to cases where the catchment's reaction to rainfall is immediately observed at the flow measurement site. This applies to small catchments with a flow measurement directly at the outlet. In those cases the reverse model does not need to consider translation, but only runoff concentration.

In both cases, the reverse low-pass filter effect is visualized by the large uncertainty ranges of estimated rainfall. Uncertainty propagation should thus be considered as an essential part of the methodologies. However, the reverse model can serve as a software sensor to estimate net areal precipitation, which can only be measured approximately by other means.

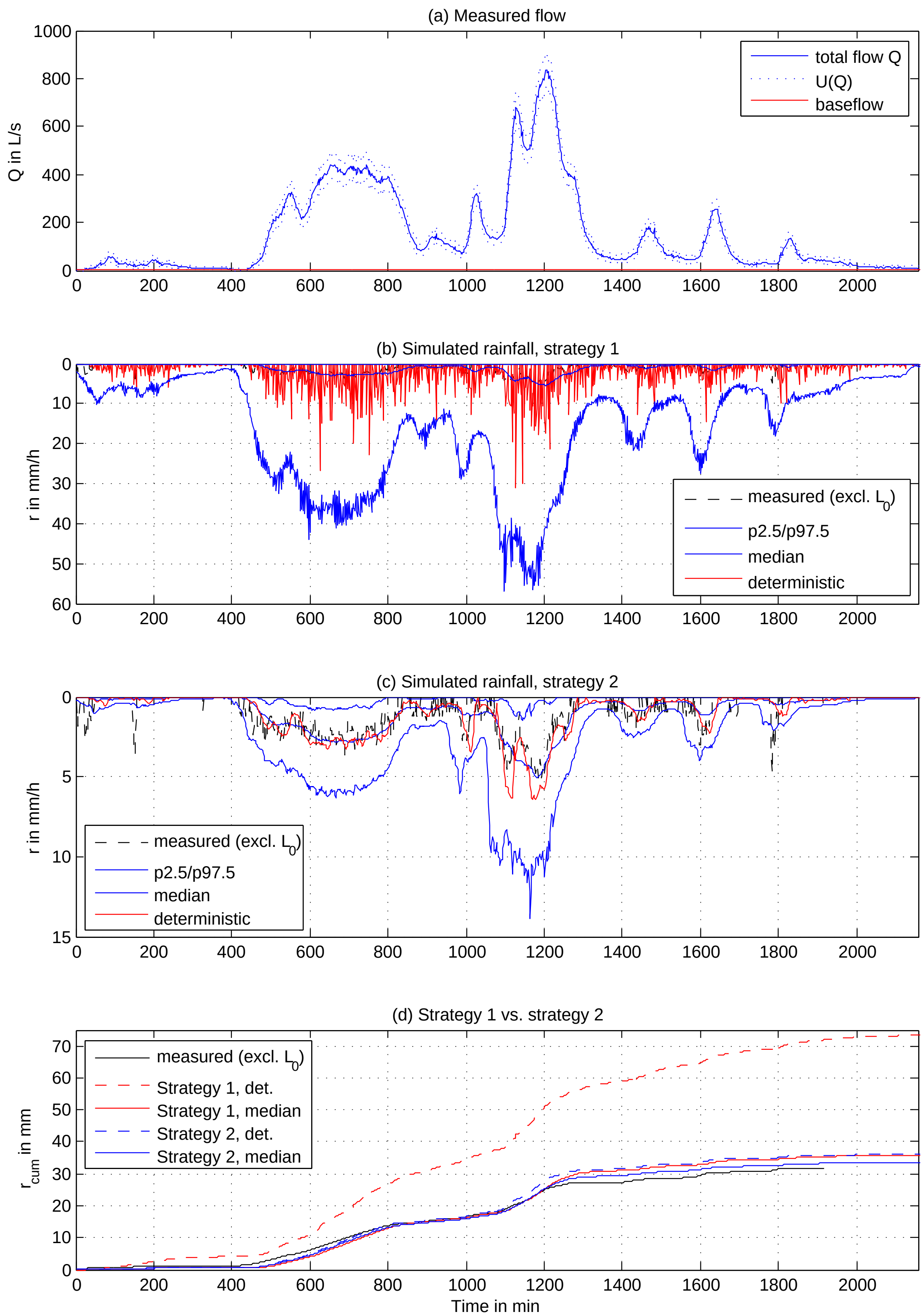

Figure 5.9: Results of the application of reverse rainfall-runoff models based on both strategies for a real event (see main text for details).

5.4 A software sensor based on reverse level-pool routing

Reverse level-pool routing can be applied to estimate inflow to storage structures from measurements of water level together with known level-storage and level-outflow relationships or measurements of the latter. Thus, a model of a storage structure can be used as software sensor for inflow, which possibly corresponds to the total flow from a (sub-)catchment and is thus an important quantity. A further requirement is that the basic assumption of a horizontal water level are met and thus hydrodynamic effects inside the storage tank can be neglected. Both basic strategies can be used to implement a reverse model for a storage structure.

5.4.1 Solution strategy 1

The formulation of a reverse level-pool-routing model in discrete time is preferably derived from the discretization of the level-pool-routing equation (Eq. 2.18). For application to a CSO structure, the total outflow Q_{OUT} is replaced by the sum of outflow to the treatment plant Q_{TP} and excess flow to the receiving water Q_E. As the choice of the discretization scheme can be an important issue in forward model applications, different schemes can be considered to address the problems occurring in the reverse model case. Zoppou (1999) compared the three following schemes:

- Scheme 1
$$\frac{V_{t_i} - V_{t_{i-1}}}{\Delta t} = Q_{IN,t_i} - Q_{E,t_i} - Q_{TP,t_i} \tag{5.18}$$
- Scheme 2
$$\frac{V_{t_{i+1}} - V_{t_{i-1}}}{2\Delta t} = Q_{IN,t_i} - Q_{E,t_i} - Q_{TP,t_i} \tag{5.19}$$
- Scheme 3
$$\frac{V_{t_i} - V_{t_{i-1}}}{\Delta t} = \frac{Q_{IN,t_{i-1}} + Q_{IN,t_i} - (Q_{E,t_{i-1}} + Q_{E,t_i}) - (Q_{TP,t_{i-1}} + Q_{TP,t_i})}{2} \tag{5.20}$$

Scheme 3 (Eq. 5.20) is a common discretization for the solution of the forward problem. The three schemes are rearranged to solve the reverse problem, i.e. to calculate Q_{in}:

- Scheme 1
$$Q_{IN,t_i} = Q_{E,t_i} - Q_{TP,t_i} + \frac{V_{t_i} - V_{t_{i-1}}}{\Delta t} \tag{5.21}$$

- Scheme 2

$$Q_{IN,t_i} = Q_{E,t_i} - Q_{TP,t_i} + \frac{V_{t_{i+1}} - V_{t_{i-1}}}{2\Delta t} \tag{5.22}$$

- Scheme 3

$$Q_{IN,t_i} = 2\frac{V_{t_i} - V_{t_{i-1}}}{\Delta t} + (Q_{E,t_{i-1}} + Q_{E,t_i}) + (Q_{TP,t_{i-1}} + Q_{TP,t_i}) - Q_{IN,t_{i-1}} \tag{5.23}$$

Note that scheme 2 (Eq. 5.22) is not suitable for online application, as it requires the knowledge of $V_{t_{i+1}}$ to calculate Q_{IN,t_i}.

The problem of oscillations can be tackled by filtering of input data. Although flow data usually shows more smoothness than rainfall, the same consequences as discussed for reverse rainfall-runoff models, i. e. the loss of information, must be considered. scheme 1 (Eq. 5.21) has been used in **Paper 4** together with a causal moving average filter applied to measured data.

5.4.2 Solution strategy 2

In contrast to rainfall, time series of flow show at least some autocorrelation (smoothness). This enables the use of specific estimation methods when applying solution strategy 2. The use of regularization constraints avoids over-fitting and non-uniqueness of the solution, by forcing smoother results.

D'Oria et al. (2012) demonstrated the suitability of the *Bayesian Geostatistical Approach* (BGA) for reverse level-pool routing in a flood retention reservoir. It is a Bayesian approach for inverse parameter estimation, developed for highly-parametrized problems in subsurface hydraulics (Kitanidis, 1995; Fienen et al., 2008, 2013). In the case of reverse routing, the inflow values are considered as model parameters, which are to be estimated using the forward model and measurements of water level and possibly outflow.

The BGA is implemented in the software *bgaPEST,* which is freely available from U.S. Geological Survey (2013). The following short summary is based on detailed descriptions which can be found in the *bgaPEST* documentation (Fienen et al., 2013) as well as in D'Oria and Tanda (2012) and D'Oria et al. (2012).

The BGA attempts to balance smoothness and over-fitting of the estimated parameters, i. e. the inflow hydrograph. According to Bayes theory, the parameters are considered as a vector of random variables, whereof statistical properties can be defined. Among these properties, the structure of the covariance model is chosen by the modeller as prior information in terms of Bayes formula. Thus, no prior assumption on the shape of the parameter vector is required, which enables flexibility and enforces only limited smoothness to the estimated parameter vector. Nevertheless, the covariance model acts as a regularization constraint. The covariance matrix is modelled using geostatistical functions and tools (e. g. *variograms*), which describe the variation among parameters as a function of their distance (which is in this case their time lag). During the estimation process, the parameters of the covariance model are inferred from the data. They are referred to as *structural parameters* and are likewise treated as random variables.

Another structural parameter is the *epistemic uncertainty* σ_R, which defines the covariance of the likelihood function. The latter is represented by a Gaussian distribution. Furthermore, σ_R describes the residuals between model output and measured data. The epistemic uncertainty thus accounts for uncertainties in measured data and due to model simplifications, but also from other sources. It can be estimated together with the other structural parameters, or chosen by the modeller (see **Paper 4**).

The structural parameters and the model parameters are estimated in repeated consecutive iterations. The model parameters (inflow values) are estimated based on the Jacobian matrix of the model, which describes the sensitivity of model outputs to changes in model parameters. In case of a linear model, the Jacobian matrix is constant and can be calculated beforehand. Otherwise, this matrix is approximated in the vicinity of the current parameter values by a finite difference method, which in the case of n parameters requires $n + 1$ model runs. This can require considerable computing time.

As a result, the method provides the parameters with the maximum posterior probability and their covariance. As the likelihood function and all prior probabilities are represented by Gaussian distributions, the same applies for the posterior distributions.

bgaPEST is used to realize a software sensor for inflow to a CSO storage tank. **Paper 4** presents its offline and online application. In both applications, the level-pool-routing equation discretized as in Eq. 5.21 is used as forward model. In the offline application, inflow is estimated for an entire event. In the online application, inflow is repeatedly estimated for a period $T = n\Delta t$ ranging from t_{i-n} to the current time t_i. This procedure is illustrated in Fig. 5.10. At time t_i, one estimate for Q_{IN,t_i} is available. In the course of an online simulation, the inflow for a certain time t is thus estimated n times. The result of an online simulation is an array of piecewise inflow estimates. As they cover a certain range, envelope curves are computed for visualisation.

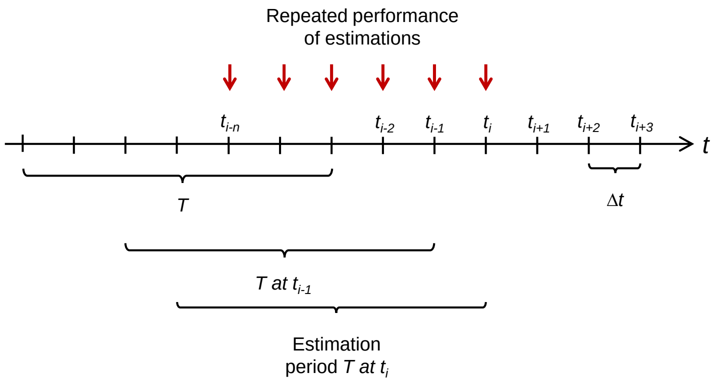

Figure 5.10: Estimation period T in the online application of the BGA for reverse estimation of inflow to a CSO structure.

5.4.3 Summary and discussion of results

5.4.3.1 Comparison of discretization schemes for solution strategy 1

The three discretization schemes were used to calculate CSO inflow for catchment C in Zirl, Austria (see Fig. 4.2). Measurement data from an overflow event used for demonstrations is shown in Fig. 5.11. The calculated inflows are illustrated in Fig. 5.12. Results obtained with schemes 1 (Eq. 5.21) and 2 (Eq. 5.22) show oscillations and negative inflow values for periods when the stored volume decreases. In case of scheme 2, the oscillations are less frequent and their amplitude is lower. However, this scheme is, as mentioned, limited to offline applications. The significant negative spike at $t = 12.5$h is caused by the simplified representation of the model, which does not consider the storage volume in the sewer. This volume is emptied prior to the offline tank (see Fig. 4.2). Zoppou (1999) proposes a specific moving average filter to be applied to the result from scheme 3 (Eq. 5.23), but its application to the presented data did not remove a sufficient part of the strong oscillations. It can thus not be considered as useful for this application. The uncertainty ranges in Fig. 5.12 (c) are obtained by propagating uncertainties in measured data through Eq. 5.21 and Eq. 5.22. Uncertainty in stored volume is dominated by the resolution of the water level data (see Sec. 4.1 and Fig. 4.2). A standard uncertainty of 10 % is assumed for the measured outflows. They uncertainty ranges in the calculated inflow underline the numerical advantages of scheme 2 (Eq. 5.22) with regard to the amplification of errors.

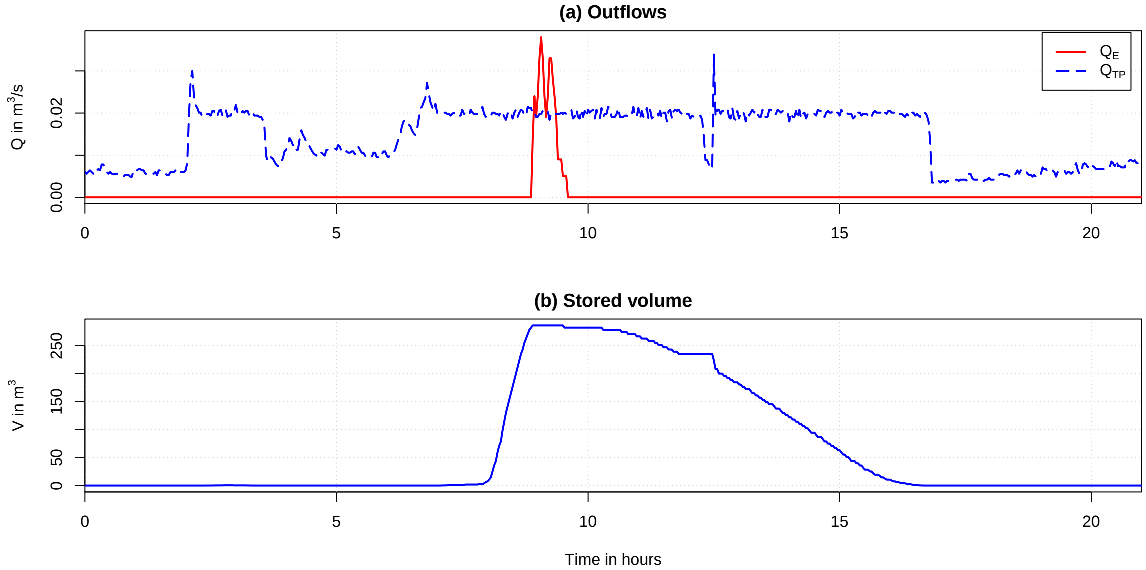

Figure 5.11: Measurements from an overflow event at CSO structure C in the case study Zirl, Austria.

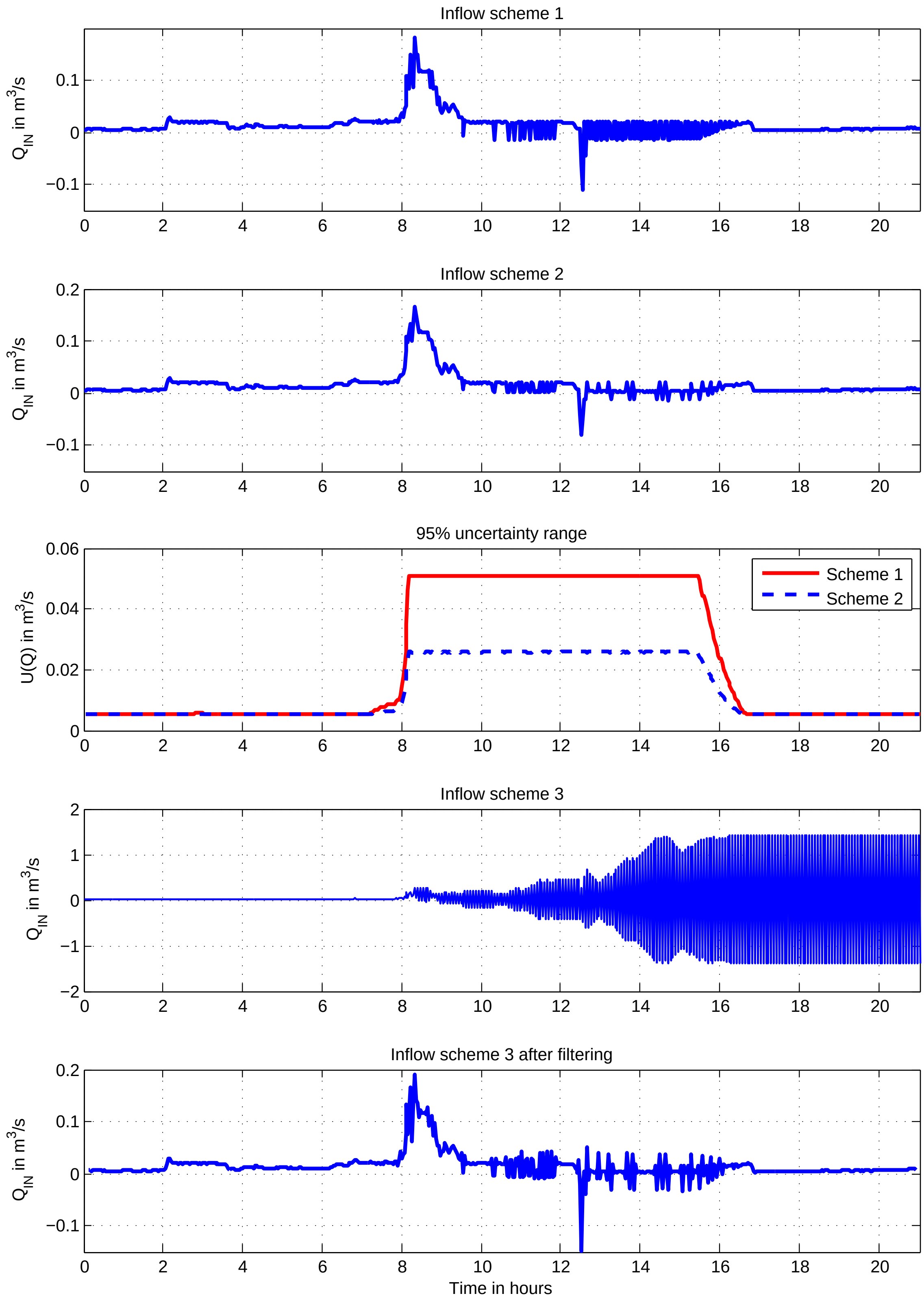

Figure 5.12: Inflow to CSO structure C calculated from the data in Fig. 5.11 using the three discretization schemes (Eq. 5.21, Eq. 5.22, and Eq. 5.23) and 95 % uncertainty ranges for schemes 1 and 2.

5.4.3.2 Offline and online application of the BGA (strategy 2)

In both, the online and the offline application, the BGA provides an estimate of the inflow hydrograph which is physically meaningful and free of oscillations. Fig. 5.13 shows results for the event in Fig. 5.11. For the online case, the upper and lower bounds of the range of all piecewise estimates are plotted. The offline estimate and the range of the online results show a very good agreement. In the online case, the maximum 95 % credibility range of estimated inflow is larger, in particular for periods of $V > 0$ (see also Fig. 5.14).

The use of the linear forward model (Eq. 5.21) enables a real online application of solution strategy 2. As the model allows to calculate the Jacobian matrix in advance, the Bayesian estimation of inflow can be sped up considerably. Furthermore, the computation time is determined by the estimation period T (see Fig. 5.10). Finally, the possible time step for an online application depends of course on the implementation of the code and the available computing resources. In the presented case a choice of $T = 100\,\text{min}$ allows an application in time steps of three to five minutes (see **Paper 4**).

The choice of the estimation period T is also important regarding the reliability of the method. Measurement errors or model simplifications can cause failure of the estimation if T is too short. Fig. 5.14 shows the widths of ranges of inflow estimates and maximum 95% credibility ranges for different estimation periods. Considerable differences occur only after $t = 12.5$h and are related to model simplifications (as the negative spike in the deterministic result).

5.4.3.3 Comparison of both solution strategies

Paper 4 and the examples presented above demonstrate the use of a reverse level-pool routing model as a software sensor for total catchment runoff and inflow to a CSO storage tank, respectively. Both strategies can be applied online and offline. Solution strategy 1 is easy to implement and computationally fast, and can thus be applied in real time without constraints. However, physically meaningful results are not always ensured and filtering of input data is required.

In both, the online and the offline application, solution strategy 2 outperforms the use of strategy 1, as it is more powerful to ensure physically meaningful and plausible results. However, so far the online application is limited to rather simple forward models, which might not be suitable for all CSO structures. A further advantage of

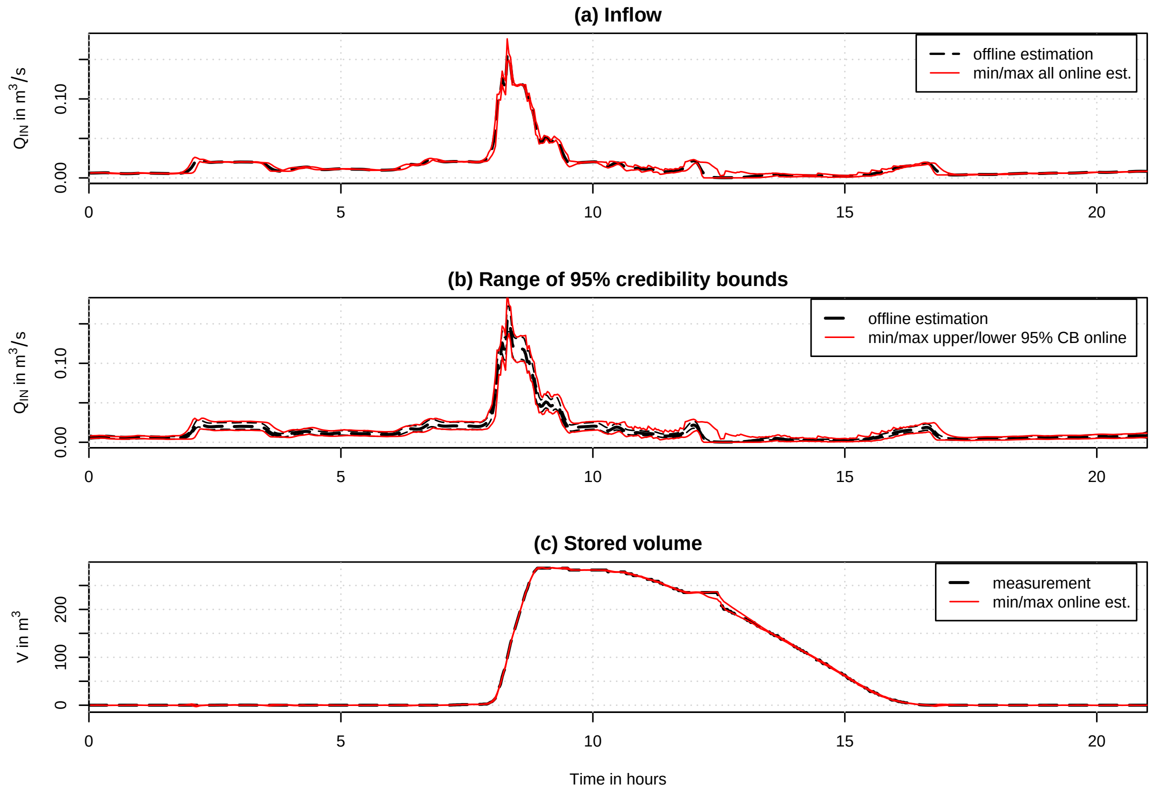

Figure 5.13: Estimation of inflow from the data in Fig. 5.11 with the BGA - upper and lower limit of all online estimations for $T = 100\,\mathrm{min}$ and result of the offline estimation: (a) estimated inflow, (b) (maximum) 95 % credibility range, and (c) stored volume calculated from estimated inflow.

strategy 2 (and the BGA, respectively) in offline cases is its applicability to various forward models. It could thus also be used for other reverse model applications. Although not all of the assumptions of the underlying theory are fulfilled completely (e. g. normally distributed errors), it has proven rather robust in the presented case study.

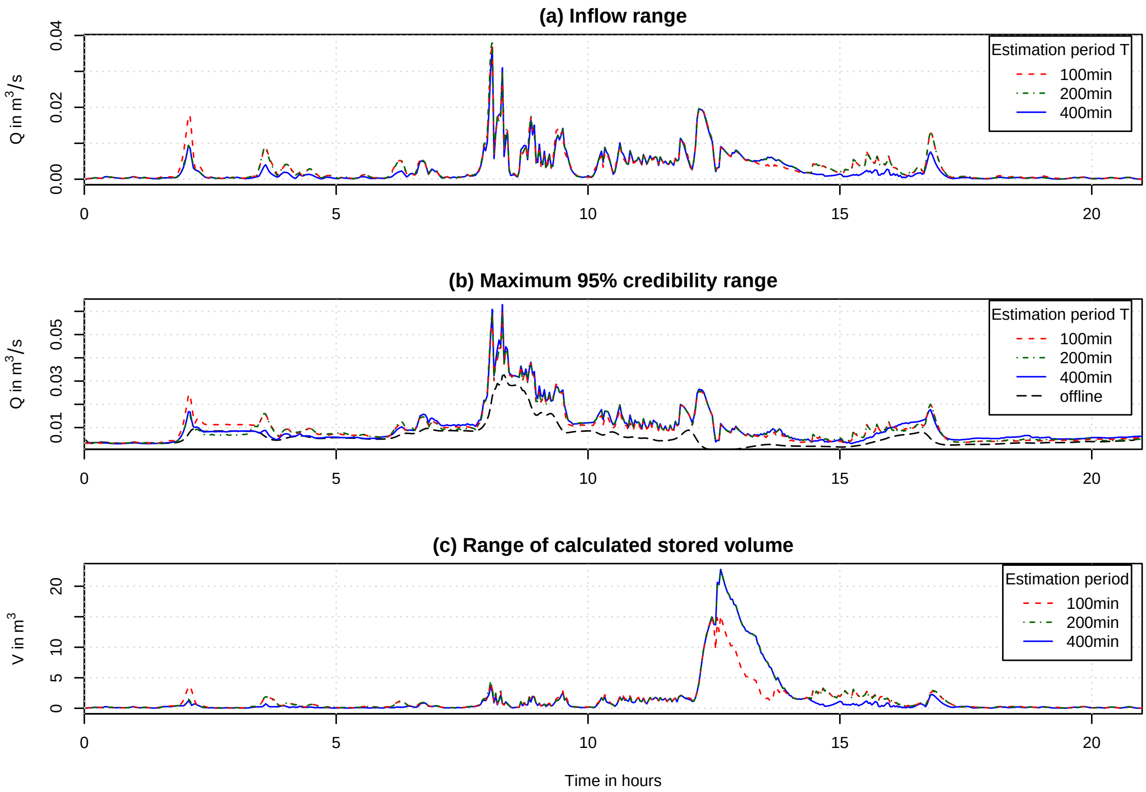

Figure 5.14: Estimation of inflow from the data in Fig. 5.11 with the BGA - online application with different estimation periods T: (a) ranges of estimated inflows, (b) maximum 95% credibility ranges, and (c) ranges of stored volume calculated from estimated inflow.

6 Model updating

6.1 The problem of model updating and classical approaches

If a model is operated to estimate system states or outputs in real time, and online measurements from the real system are available, it would be desirable to benefit from measured data to improve the model's estimations. Furthermore, uncertainties in both, model estimates and measurements should be considered. The corresponding methodologies are referred to as *model updating* or *(real time data) assimilation*. For this purpose, the general state-space representation of a model (see Eq. 2.1 and Eq. 2.2) is extended by error terms w and v as follows:

$$\mathbf{x_{t_i}} = \boldsymbol{M}(\mathbf{x_{t_{i-1}}}, \mathbf{u_{t_i,t_{i-1}}}, \theta) + w_{t_i} \tag{6.1}$$

$$\mathbf{y_{t_i}} = \boldsymbol{h}_{t_i}(\mathbf{x_{t_i}}) + v_{t_i} \tag{6.2}$$

The information from measurements can in principle be used to update model *inputs*, *states*, *parameters* or *outputs*.

Most updating methodologies have their roots in system identification (electrical engineering) and originally aimed to update model states. The basic problem of updating a (directly observable) state x using a measurement y can be illustrated according to Beven (2009) as follows:

$$x^{\star} = x + W(y - x) \tag{6.3}$$

where $x^\star$ is the updated state and W a weighting coefficient to be determined. If the best estimate is assumed to be the least square solution, W can be calculated as follows:

$$W = \frac{\sigma_x^2}{\sigma_x^2 - \sigma_y^2} \tag{6.4}$$

However, in reality σ_x^2 and σ_y^2 are usually unknown and must be estimated. In an online application, the estimate must be performed *recursively*, i. e. step by step, as new measurements become available. The problem can be addressed by repeated application of Bayes formula (Eq. 2.26). Model updating is thus also referred to as *sequential Bayesian updating*.

The *Kalman filter* (Kalman, 1960) was the first solution to the problem of recursive state estimation. It considers uncertainties of measurements and the model, whereof only initial estimates are required. However, its application is limited to linear models and Gaussian distributions of errors (e.g. Beven, 2009; Ridler et al., 2014). The approach has thus been further developed to overcome these limitations.

The *extended Kalman filter* linearises the model around the estimated current state (Welch and Bishop, 2006; Moradkhani et al., 2005). The *ensemble Kalman filter* (Evensen, 1994, 2003) is based on Monte Carlo approximation of the distribution of states and applicable to highly non-linear models. Methods referred to as *particle filter* or *sequential Monte Carlo* method tend to overcome all limitations of the aforementioned methods by the approximation and propagation of all distributions by Monte Carlo simulation. The methods have thus no requirements with regard to error distributions (Gordon et al., 1993; Arulampalam et al., 2002). Elaborated sampling strategies were developed to increase the numerical stability (Arulampalam et al., 2002; Ridler et al., 2014).

Variational methods for model updating have been developed and applied in weather forecasting and oceanography and are not commonly used in hydrology. A comprehensive review on updating methodologies and applications in hydrological modelling (in particular flood forecasting) is given by Liu et al. (2012), whereas a more didactic presentation can be found in Beven (2009).

The particle filter is also applied in hydrological modelling for sequential updating of model parameters or common updating of parameters and states (e.g. Moradkhani et al., 2005; Smith et al., 2008). If parameters are updated they are assumed to be time-varying, which is in contrast to the common approaches to parameter estimation. Another approach which can be applied to complex online models for longer prediction horizons is *error updating*. It is implemented by updating the state of a forecast-error model. This approach reduces the number of states to be updated, but it does not improve the model as such (Liu et al., 2012; Beven, 2009).

According to the common terminology (e.g. Moradkhani et al., 2005), *filtering* refers to the estimation of the current state x_{t_i} based on current input u_{t_i} and the current observation y_{t_i}. The sequential estimation of past states $x_{t_1}, x_{t_2}, \ldots, x_{t_{i-1}}$ is referred to as *smoothing*, and a *forecast* tends to estimate a future state $x_{t_{i+1}}$. With regard to the interdependency of states in hydrological modelling, the combination of smoothing and filtering appears to be a reasonable approach to improve the model estimations.

6.1.1 Model updating applications in urban drainage

In contrast to the field of online modelling in catchment hydrology, the literature on model updating in urban drainage is less extensive. Puig et al. (2009) briefly mention the application of recursive parameter estimation in real time. This issue has been investigated and published in more detail recently in Danish case studies of RTC based on model predictions. The use of grey-box models for online rainfall-runoff simulation is described by Breinholt et al. (2011) and Thordarson et al. (2012), who compare different elaborated error representations and evaluate the uncertainty of flow predictions. Löwe et al. (2014a) investigate the uncertainty of forecasts of runoff volumes rather than flows and the prediction of overflow risk. They conclude that a detailed consideration of rainfall uncertainty is important. Vezzaro et al. (2013) briefly describe a deterministic approach based on repeated Bayesian parameter estimation of the model in real time, and compare it to the updating of grey-box models for two example events. The use of different rainfall forecasts based on radar and rain gauges as input to grey-box models with various structures for real time forecasting is investigated in Löwe et al. (2014b). They conclude that it is also important to account for spatial variability in the model.

Deterministic updating of model states is applied by Borup et al. (2011) to a distributed hydrodynamic model considering impervious areas and sewer infiltration. Based on a semi-synthetic case and a lumped rainfall-runoff model, Borup et al. (2013) demonstrate that a time displacement of rainfall data reduces the accuracy of a forecast more than a rainfall bias, when model states are updated based on flow measurements. A simple deterministic possibility to update a hydrodynamic model based on water level measurements was investigated by Hansen et al. (2011). They conclude that good knowledge of the level-flow relationship is crucial to avoid the introduction of instabilities.

6.2 Model updating for online estimation of CSO discharge

The most suitable data to update a rainfall-runoff model in real time are flow measurements, or water level measurements where a level-flow relationship is available. Preferably, those measurements are performed in the sewer system upstream of any storage structure or pumping station. In those cases, the measurement operator $\boldsymbol{h}$ in the observation equation (Eq. 6.2) is equal to unity. However, such flow measurements are rarely installed in small and medium size sewer systems. Yet, simple measurement devices can provide information about system states.

Paper 5 presents a methodology to update a conceptual rainfall-runoff model which can be used for online estimation of CSO discharge. The methodology is designed for application in smaller and medium size sewer systems where only simple measurement devices are available. Catchment C in the case study Zirl, Austria (see Sec. 4.1) is used for demonstration.

Simple measurement devices can provide binary information on model states. In **Paper 5** data from the water level sensor in the CSO storage tank is used to indicate the occurrence of overflow. Due to the coarse resolution of the water level data (see Sec. 4.1), only binary data on overflow occurrence in terms of "yes/no" can be derived. The transformation of water level data to a binary time series based on a threshold value is visualized in Fig. 6.1 (see Sec. 2.1.1.3 for further possibilities to obtain binary data). However, the information in such binary data is limited, as the overflow dynamics remain unknown.

Nevertheless it has been demonstrated that binary data can be used in model calibration (Rasmussen et al., 2008; Thorndahl et al., 2008). For comparison of model states to binary measurement data, the measurement operator $\boldsymbol{h}$ in Eq. 6.2 must convert the estimated model state into binary form. Furthermore, specific objective functions to compare simulation results and measurements must be formulated. As an example,

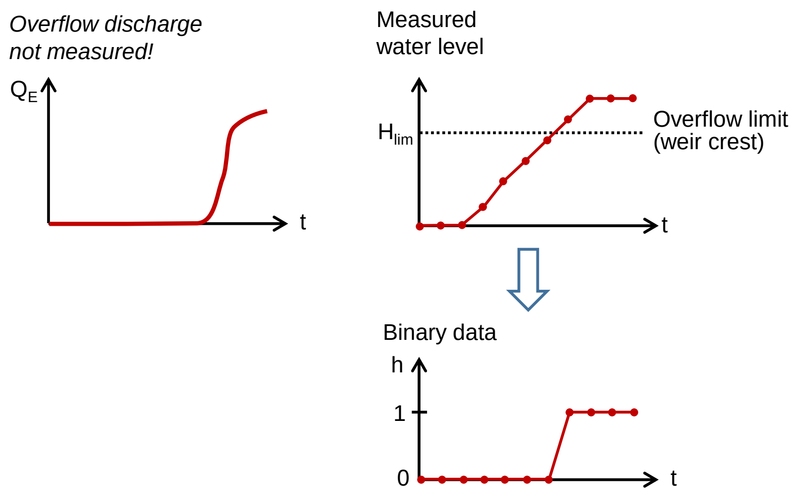

Figure 6.1: Derivation of a binary time series indicating overflow occurrence from water level data with a coarse resolution.

overflow time and duration can be compared as follows:

$$E = \frac{\sum_{i=1}^{n} |q_{E_i} - h_i|}{n} \tag{6.5}$$

In Eq. 6.5, q_E and h represent the binary model result and measurement data, respectively, and n is the length of the time series.

Fig. 6.2 shows results from an event-based offline calibration using binary data on overflow occurrence. Parameter distributions were inferred with the GLUE methodology using Eq. 6.5 as objective function. In particular the model parameter *effective impervious catchment area* could be clearly identified, and the 95 % coverage range of simulated overflow discharge includes the measurements.

In **Paper 5**, binary data on overflow occurrence (derived from the water level data with coarse resolution), is used to update the rainfall-runoff model during online simulation. The independent measurement of overflow discharge is used for evaluation of the results.

A specific algorithm has been developed: Based on rainfall measurements, the updating is activated only during rainfall events. The algorithm combines smoothing and filtering, i. e. it estimates past and present states. This is achieved by updating the distribution of the parameters *effective impervious area* A_e using the GLUE methodology (which includes Monte Carlo simulations - see section Sec. 2.3.2.1). The period considered for updating ranges from the beginning of the event to the current

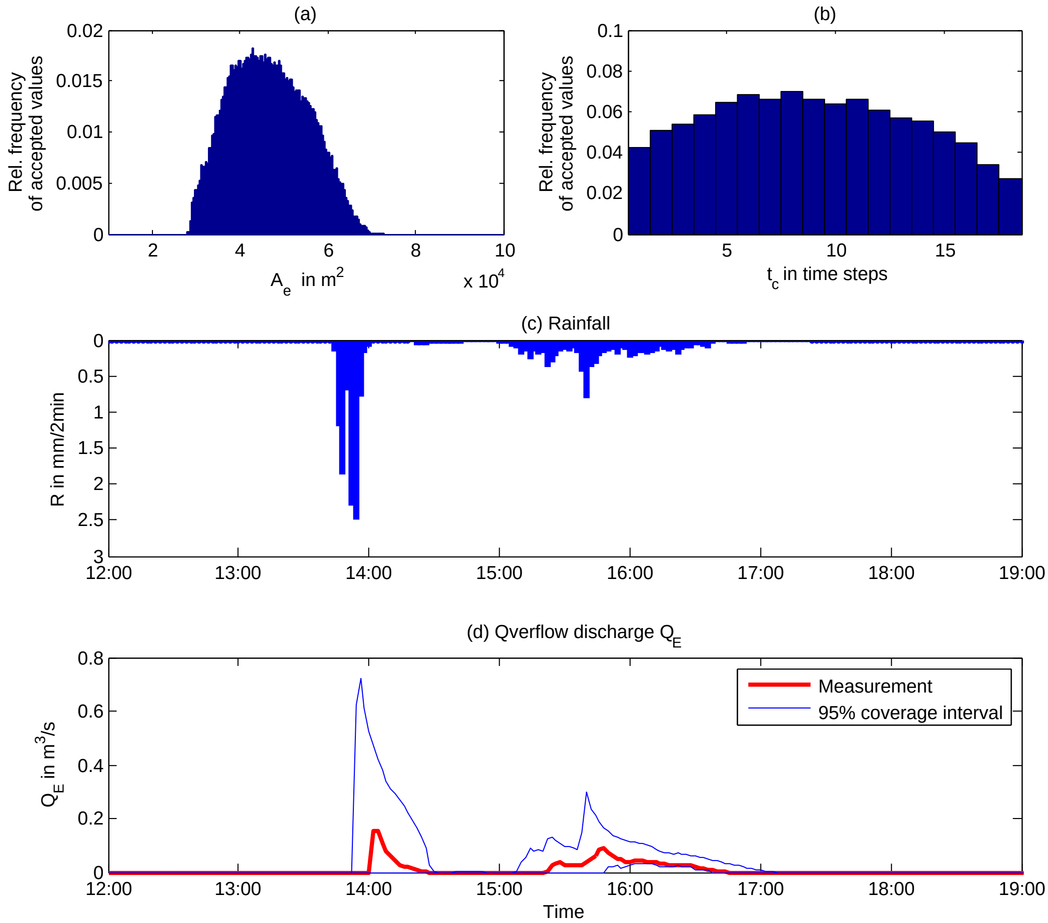

Figure 6.2: Results of an event-based calibration of the parameters of the time-area method using binary data on overflow occurrence: Posterior parameter distributions of the rainfall-runoff model parameters (a, b), measured rainfall (c), and overflow discharge simulated based on posterior distributions (d).

time step. The parameter distribution is updated based on the model's performance in the same period. The distribution is thus not changed in the course of a single simulation, but as soon as new information is available, i. e. in the course of an event. As each simulation starts at the beginning of an event, consistent model states and mass conservation are ensured. This corresponds to a repeated calibration. As a result, the updated online model provides an estimate of overflow discharge and the corresponding uncertainty range.

An important issue is the sample size used for the Monte Carlo simulations. The sample size is limited by the available computation time but should nevertheless be sufficiently large to explore the parameter space. **Paper 5** thus provides a detailed discussion of the stability of the results. Furthermore, the consequences of uncertainties in the water level data are investigated and two different objective functions are compared.

6.2.1 Summary of results and discussion

A good example for the performance of the updating algorithm presented in **Paper 5** is shown in Fig. 6.3. It shows the rainfall data, the development of the parameter distribution in the course of the event and estimated overflow volume. Fig. 6.4 depicts updated parameter distributions at different time steps. The results were obtained in a simulation based on 3000 Monte Carlo samples.

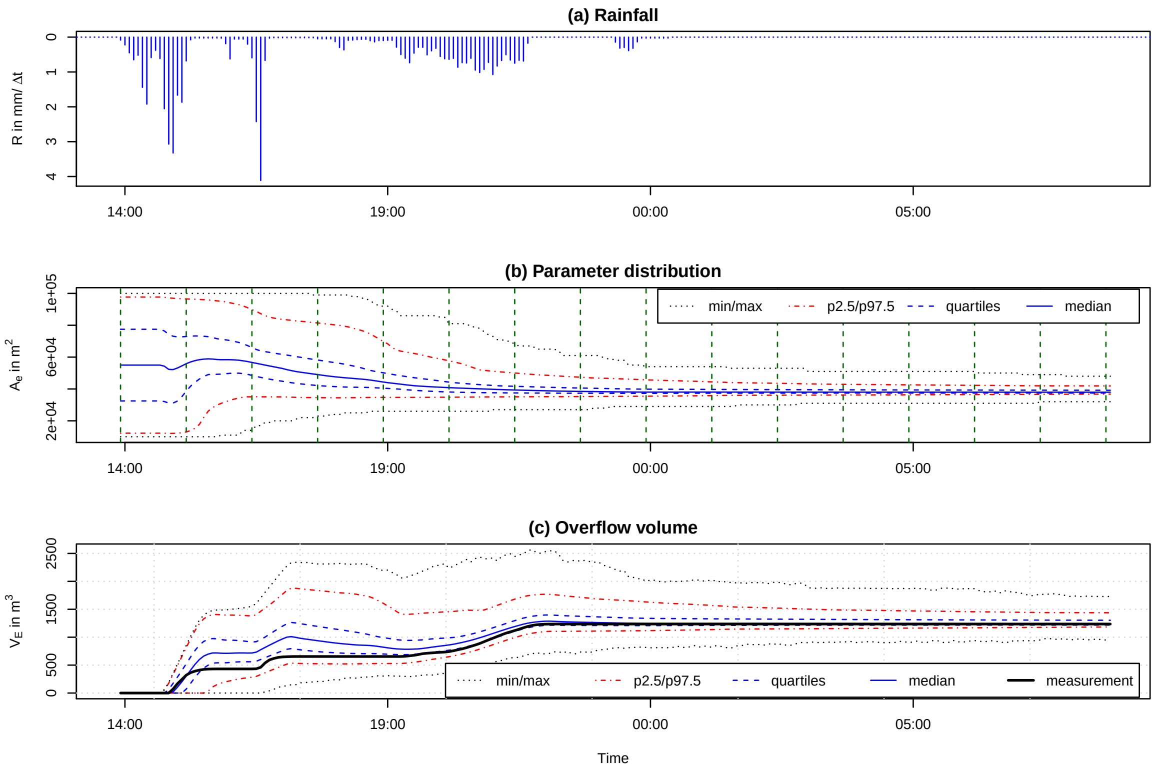

Figure 6.3: Results of an updating simulation for an overflow event: measured rainfall (a), percentiles of the distribution of parameter A_e (b), and estimated overflow volume (c). The dashed vertical lines in plot (b) indicate the time steps of the distributions in Fig. 6.4.

The updating methodology can provide estimates of combined sewer overflow discharge and corresponding uncertainty in real time. As intended, the algorithm improves the estimation in the course of an event, and the distribution of the parameter A_e could be clearly identified. In the presence of uncertainties in the binary measurement data, the prediction intervals can be rather large. The binary data used for updating should thus be reliable and provide unique information.

In the case of binary information on model states, the flexibility of the GLUE methodology with regard to distributions and the likelihood function is an advantage. However, the computational effort of Monte Carlo simulations is an important issue in an online application. A sufficient number of samples is required to ensure stable and reproducible results. In the presented case study, a sample size in the range of 3000 to 5000 provided results which can be considered as stable from a practical point of view. As in the case of model calibration with GLUE, the choice of the acceptance limit and the likelihood function are important issues, which require sound preliminary tests of the model based on real data. The technical implementation of the method must also consider the possible degeneration of parameter distributions or the failure of updating.

A more detailed model structure could probably improve the estimation of overflow discharge. Furthermore, the update of other and/or more parameters should be considered. The application of other sampling strategies might bring further improvement. A further assessment of the methodology, including e. g. a comparison to forward uncertainty propagation based on fixed parameter distributions, should include evaluation of the long-term performance.

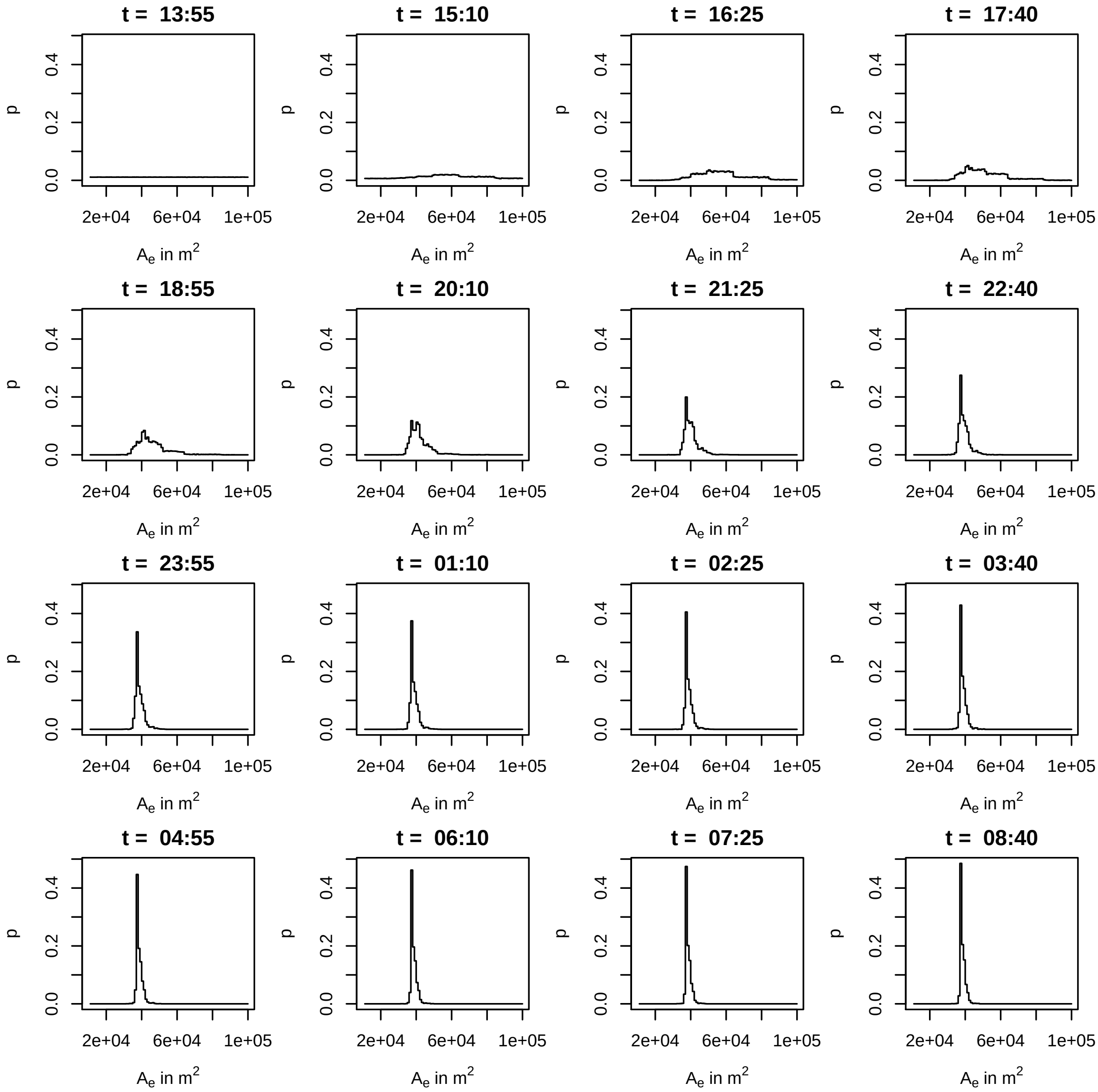

Figure 6.4: Updated distributions of the parameter A_e at different time steps during the event shown in Fig. 6.3.

7 What about water quality?

With regard to one of the main objectives of urban drainage - the protection of water resources - software sensors for water quality in sewer systems and receiving waters would be very attractive, either to quantify emissions or assess the immissions in receiving waters. The aim of the following chapter is not to provide a comprehensive review about water quality issues in urban drainage modelling, but a brief critical discussion of experiences regarding water quality from research projects related to this dissertation.

Following the previous chapters, the preconditions for software sensors - similar to those for environmental modelling in general - can be summarized as follows:

- A reliable mathematical description of the underlying processes. This requires sufficient knowledge of the system boundaries and the relevant processes.
- Reliable measurement data on driving forces, system output, and possibly further system states. In case of model applications in real time, online measurements are required.

With regard to the estimation of pollutant loads and concentrations, useful water quality models and reliable measurement technologies are thus required. Using models and measurement of hydrologic processes in urban catchments as a reference, there is a considerable gap between quality and quantity (hydrologic) issues. Ashley et al. (1999) identified a list of principal problems in the development of models for sewer processes, including among others

- *"The difficulty of actually measuring the processes in the field.*
- *The limited amount of observations economically and logistically possible even when measurement methods are effective.*
- *The extreme temporal and spatial variability of all aspects of the phenomena related to sewer processes."*

The selection from the list also holds for processes on catchment surfaces, and partly for receiving waters. Furthermore, the processes involve not only transport of substances, but also their reaction and thus conversion (Ashley et al., 1999). It might thus be necessary to consider not only a single pollutant, but a relevant set of interacting substances. Measurements might only indicate the cumulated effect of several interdependent processes.

A lot of effort has been and is still spent on water quality monitoring (e.g. Gruber et al., 2005; Francey et al., 2010; Métadier and Bertrand-Krajewski, 2012). However, the results did not only provide more insight, but highlighted also the large variability. Monitoring as currently performed might thus not be the single key to the development of better models (Bertrand-Krajewski, 2013).

Nevertheless, many concepts to model quality of storm- and wastewater in sewer systems as well as the effects in receiving waters have been introduced, ranging from simple lumped models to rather detailed approaches (see also Sec. 2.2.3.4). Issues of model structure in relation to knowledge of the processes are e. g. discussed in Ashley et al. (1999); Bertrand-Krajewski (2007). No clear conclusions on the performance of stormwater quality models can be drawn from the literature. To summarize a few examples with regard to “classical” quality parameters (TSS, COD), Dotto et al. (2010a, 2011) reports poor performance of rather lumped model, and Métadier (2011) confirms the requirement of a large local data base for regression models and difficulties to simulate measured pollutographs with accumulation-erosion-transfer models. Freni et al. (2010), Mannina and Viviani (2010), Willems (2010) and Gamerith (2011) present examples of more successful applications. The level of complexity of the investigated models is of course different, but does not fully correlate to their performance. Furthermore, the size of the data sets used for model calibration and assessment vary considerably.

In 2009 and 2010, a measurement campaign was performed in the case study catchment Zirl, Austria (see Sec. 4.1). At four CSO structures, grab samples were collected during dry and wet weather using automatic samplers. The aim of the monitoring campaign was to estimate pollutant loads in CSO emissions. Details on the sampling locations and comprehensive results can be found in Fach et al. (2010) and Engelhard et al. (2011). The results showed a large variability with respect to different events and sampling sites. An example is shown in Fig. 7.1. Furthermore, practical, logistic and economic limits of the measurement campaign were reached fast, as the equipment requires a lot of maintenance and thus manpower.

A few results from the application of the water quality data for modelling are presented in Leonhardt et al. (2011b,a). An attempt was made to include the estimation of emitted pollutant loads in the overflow discharge in the software sensor presented in **Paper 1**. Fig. 7.2 shows an example of results. The quality model is based on the

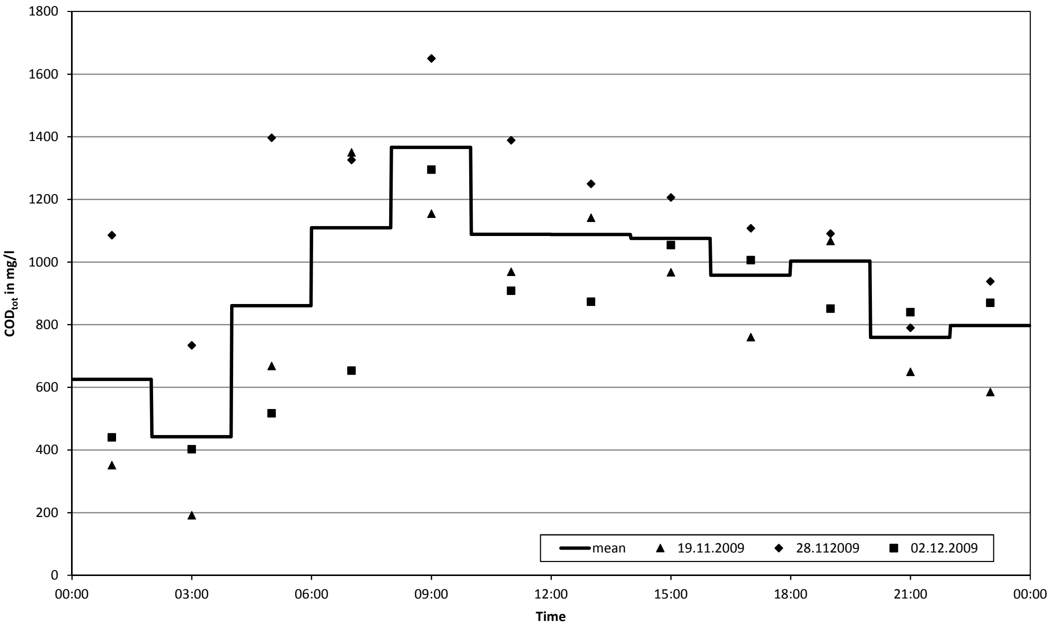

Figure 7.1: COD in hourly dry weather samples from three differnt days in a sub-catchment with considerable industrial activity (adapted from Engelhard et al., 2011).

results from dry weather monitoring and a build-up - washoff model (Sec. 2.2.3.4) calibrated based on wet weather samples. However, a reliable estimation would require significantly more data, in terms of longer measurement periods including more events and more monitoring sites.

Another large research project on integrated assessment of receiving water quality, with a focus on monitoring and modelling, was performed in the Schwechat catchment in the province of Lower Austria (IMW, 2013). Despite the use of state of the art monitoring equipment, comprising four monitoring sites equipped with online sensors, the practical limits were clearly demonstrated. The sensors can provide data in high temporal resolution, but they require a large amount of maintenance, including a sound calibration over the entire possible concentration range, based on laboratory analysis of samples. As discussed in Gamerith et al. (2013a), post-processing is also highly recommended before using the data for modelling. With regard to modelling it was demonstrated that the basic processes can be represented using a river water quality model including transport and conversion processes. However, in particular during rainfall events the identification of processes remains difficult. The reliability of model predictions is thus limited. A more detailed description and discussion can be found in Leonhardt et al. (2013) and the final report (IMW, 2013).

Although water quality data, in particular long term high resolution data sets, are

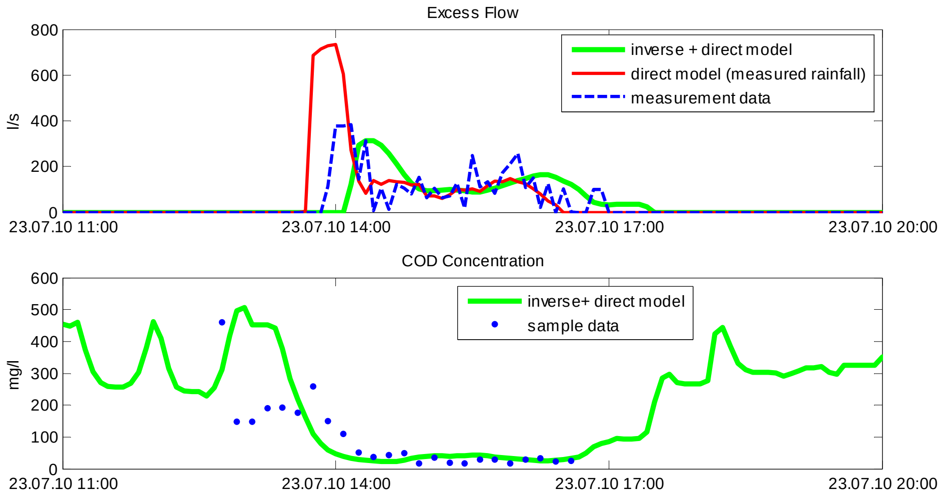

Figure 7.2: Estimates of the software sensor compared to measurements; top: CSO discharge; bottom: COD concentration in the inflow to the CSO from sub-catchment A (see Fig. 4.1); adapted from Leonhardt et al., 2011a.

a prerequisite for water quality modelling, the currently available technologies are still facing tight practical limits. Furthermore, an immediate use of online water quality data could lead to wrong results. Together with the currently known modelling approaches, the methods to address water quality issues cannot be regarded to be fully suitable for the general application of software sensors. Their application might however be considered in very specific cases. The use of stochastic models (forward uncertainty propagation) to estimate a possible range of pollutant loads or concentrations could be another alternative.

8 Conclusions and outlook

8.1 General conclusions

In this dissertation, the application of mathematical models as software sensors for the estimation of different quantities in urban catchments and sewers systems has been investigated based on different case studies. The models are conceptual, but physically based, and are applied either offline or online. To serve as software sensors, the models are used as *reverse models,* or as forward model which is updated during online operation.

Reverse modelling was applied for the estimation of *net areal rainfall*, *inflow to storage and CSO structures*, and in the frame of a deterministic online model for the *estimation of CSO discharge.*

Updating was applied to a rainfall-runoff model for *online estimation of CSO discharge* and associated uncertainty.

All methods enable or even require the consideration of different sources of uncertainties. Furthermore, they are based on standard measurement data, which is already available in many sewer systems.

Altogether the presented methods and their applications show that software sensors can derive reliable and valuable information from existing data. They can thus increase the benefit of measurements performed with real sensors. The derived information can support the operation of urban drainage systems, as well as the assessment of other measurement methods and data sets. The methods cannot replace measurements in urban drainage systems, but will, as modelling in general, always benefit from the improvement of monitoring systems and measurement devices. As all mathematical models, the methodologies must be applied carefully. Even though the input data should have passed some validation, the estimated results require critical review.

Further work should explore the application to different case studies and the adaptation of the presented methods to other sub-systems and structures. Today, the application of models is usually considered after the installation of sensors. The modeller adapts methods for identification, calibration or updating to the available data and devices. In future, online modelling could greatly benefit from its consideration in the planning of monitoring networks. Furthermore, software sensors could support the development of new monitoring concepts. In the long term, an application to water quality issues might not only be desirable, but also possible and thus provide a huge potential for software sensors.

8.2 Reverse modelling

Reverse modelling has been applied to different sub-systems in urban catchments. Based on the results and experiences, a comprehensive introduction and systematic overview of methodologies for reverse modelling in urban hydrology has been developed. In addition, a review of the relevant literature on applications in urban drainage and related fields in hydrology is provided.

Regardless of the specific application of reverse models, their property to amplify high frequency variations in input data to often unrealistic oscillations has been identified as a common challenge. This is of particular importance in highly dynamic urban drainage systems. The property is related to their mathematical structure and concerns many hydrological models. Furthermore, two basic strategies for reverse modelling have been identified: the reformulation of the forward model (strategy 1), and the estimation of forward model input based on measurements of output (strategy 2). Regardless of the applied strategy the above mentioned issue of the amplification of variations has to be considered.

Based on the application results, possibilities and limitations of reverse modelling in urban drainage have been identified. Conclusions and outlooks for the specific applications are summarized in the following sections.

8.2.1 Reverse rainfall-runoff modelling

Estimates of effective areal rainfall obtained with the second strategy can be considered as realistic and plausible results. This judgement is based on comparison with rain gauge data. The consideration of uncertainties is considered as an essential part of the methodology. Uncertainties of estimated rainfall are large, but they reflect the low-pass filter property of the forward model. As already mentioned by other authors (Sun and Bertrand-Krajewski, 2013), and although contradictory to other results, this issue should be considered in discussions on the required accuracy of a single rainfall measurement (i. e. the rainfall depth in an interval of a few minutes). As the method requires knowledge of model parameters, i. e. a calibrated model, a certain amount of rainfall data is required prior to application. However, it is also a suitable method to assess rainfall measurements and fill data gaps.

The performance of reformulated rainfall-runoff models (first strategy) cannot be considered as satisfactory, as rainfall intensities cannot be estimated accurately. This is mainly caused by the loss of information in case of filtering of input data. The suitability of the results remains thus rather limited.

As the second strategy can only be applied offline, a suitable method for online application is still missing. New techniques for filtering of input data could be a potential key to the development of methods for online application. Suitable filtering techniques might be found in image processing, where deconvolution is applied for image denoising and deblurring (e.g. Chan and Shen, 2005). However, a real online application is always limited to small catchments where the answer to rainfall, i. e. the increase in runoff, can be measured without time delay.

Although the “true” areal rainfall will remain unknown, and the estimated net areal rainfall is a quantity related to modelling concepts, an assessment of the results based on indirect rainfall measurements (e. g. radar) should be aspired.

8.2.2 Reverse routing

The reverse estimation of flow enables the use of other methods, as hydrographs - in contrast to hyetographs - show a certain degree of smoothness (autocorrelation). Methods based on the estimation of forward model input (the second strategy) can thus make use of regularization.

A Bayesian approach, using the assumption on the structure of a covariance model for the estimated inflow as prior knowledge, has proven to be suitable to estimate inflow to a CSO storage tank. In the case of simple forward models, it can also be used online. The method might also be applied to other sub-systems of urban drainage infrastructure. Future work should thus focus on methods for the approximation of the sensitivity matrix of the forward model, in order to apply more complex model structures.

In the case of level-pool routing, a reformulated model (first strategy) can be suitable in specific cases, depending on the quality and resolution of the data. The method would also benefit from improved filtering techniques mentioned above. However, the problems are not only caused by measurement noise (which can be removed by filtering), but also by model simplifications and local phenomena.

8.3 Model updating

Model updating aims to improve the prediction of an online model based on measurements from the represented system. The presented methodology uses data in binary form, which can be obtained at low cost, but contains limited information. Suitable measurement devices, as e. g. water level sensors or on/off switches, are already installed in many sewer systems. The method could thus support a more widespread use of updated online models. In contrast to other examples, distributions of model parameters are updated to improve the estimation of past and current model states. As the method is based on Monte Carlo simulations it is flexible with regard to distributions and likelihood functions, but also limited by the available computational resources.

The results show that realistic estimates of the overflow volume and associated uncertainty can be provided, but also suggest further evaluations. Future work should focus on computationally fast implementations, the use of different data for updating, and the choice of model parameters to be updated. Furthermore, there is probably more potential for the use of “cheap data” and surrogate data in urban drainage modelling in general. This would certainly support model applications in practice and improve their quality.

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Papers

Paper 1

A software-based sensor for combined sewer overflows

Leonhardt, G., Fach, S., Engelhard, C., Kinzel, H., Rauch, W.

Water Science and Technology (2012) 66(7): p. 1475-1482

Paper 2

Comparison of two model based approaches for areal rainfall estimation in urban hydrology

Leonhardt, G., Sun, S., Rauch, W., Bertrand-Krajewski, J.-L.

Journal of Hydrology (2014) 511: p. 880-890

Paper 3

Estimating Areal Rainfall and Accompanied Uncertainty by Combining Two Model-Based Approaches

Sun, S., **Leonhardt, G.**, Bertrand-Krajewski, J.-L., Rauch, W.

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Paper 4

Estimating inflow to a CSO structure with storage tank in real time - evaluation of different approaches

Leonhardt, G., D'Oria, M., Kleidorfer, M., Rauch, W.

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Paper 5

Using "cheap data" for model updating in online simulation

Leonhardt, G., Kleidorfer, M., Rauch, W.

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