# QUICS: Quantifying Uncertainty in Integrated Catchment Studies

## *D4.6 Concept and methodologies to guide surrogate modelling for real-time control (RTC) of urban drainage systems under uncertainty*

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## Executive Summary

In this project deliverable, in part 1, an extensive literature review has been done in order to categorise and introduce some of the most relevant surrogate modelling approaches in water and waste-water modelling domain. Advantages and disadvantages of each category is discussed briefly and finally some recommendations are proposed.

Second part is focused on summary of a publication introducing an analytical surrogate modelling technique to develop simple and fast surrogate models for real-time control (RTC) purpose of combined urban drainage networks based on model predictive control (MPC) approach.

# CONTENTS

# Part 1: Proposal for surrogate modelling approaches

## 1 Introduction

Computationally expensive models hinder various tasks such as: integrated modelling, calibration, sensitivity analysis, uncertainty propagation analysis, inverse modelling, decision support and Real Time Control. A possible way to tackle this problem is to develop surrogate models. Surrogate modelling is an approach in order to develop a simpler, and hence faster, model which emulates the specified output of a more complex model in function of its inputs and parameters (Asher *et al.*, 2015).

In the literature, the surrogate models are also known as meta-models (e.g. R. V. Blanning 1975), reduced models (e.g. Willcox and Peraire 2002), emulators (e.g. O'Hagan 2006), proxy models (e.g. Bieker et al. 2007), low fidelity models (e.g. Robinson et al. 2008), response surfaces (e.g. Regis and Shoemaker 2005) and so forth.

The main motivation for developing a surrogate model is to achieve computational efficiency and reduce the number of model inputs due to data unavailability and model parameters which are often hard to calibrate if not measurable (Razavi, Tolson and Burn, 2012c). In the literature, there are several categorizations for surrogate modelling. The most general way for this classification is to consider them as either data-driven or model-driven approaches (Siade and Putti 2010). In data-driven techniques a statistical model is built by fitting the input and output data through a machine learning process; while, in model-driven approaches the focus is on how to reduce the number of parameters and sub-models through e.g. mathematical reduction.

A comprehensive taxonomy of surrogate modelling approaches is addressed in (Asher *et al.*, 2015). Three main categories of surrogate models can be identified:

1. Data-driven approach, in which the complex model is approximated through an empirical (statistical) model which captures the input-output mapping of the original model.
2. Projection-based approach, in which the dimensionality of the parameter space is reduced by projecting the governing equations onto a basis of orthonormal vectors.
3. Hierarchical or multi-fidelity approach, where the surrogate is developed by R For example, by ignoring some of the processes which are less relevant or by reducing the numerical resolution.

Based on this categorization, relevant literature is presented in the following sub-sections. At the end of each sub-section, the advantages and disadvantages of each method are addressed.

## 2 Data-driven Approaches

Data-driven approaches are also known as response surface, statistical and black box methods (Asher *et al.*, 2015). This category covers rather a broad range of methods. It is not the purpose to go into the details of all methods but rather provide a concise overview.

Hence, the main focus is to introduce the most relevant and promising examples that have applied surrogate modelling techniques in the field of water and wastewater engineering.

## 2.1 Artificial Neural networks (ANN)

By definition, ANN is "a computing system made up of a number of simple, highly interconnected processing elements, which process information by their dynamic state response to external inputs" (Hecht-Nielsen, 1987). ANN is able to solve complex problems by mimicking the human brain problem-solving mechanism. The main challenging and important task in developing an ANN-based surrogate model is to determine the optimal structure of the network (Razavi, Tolson and Burn, 2012c). There are several recommended methods in this regard based on different given problems, see e.g. (Reed, 1993), (Vila, Wagner and Neveu, 2000), (Xiang, Ding and Lee, 2005), (Teoh, Tan and Xiang, 2006), (Xu, Wong and Leung, 2006) and (Kingston, Maier and Lambert, 2008).

Applications of ANN and Genetic Algorithms (GA) is also considered in the field of groundwater modelling, which normally is accompanied with extremely time-consuming simulations. For example, (Yan and Minsker, 2006) introduced an Adaptive Neural Network Genetic Algorithm (ANGA) to replace computationally expensive models such as MODFLOW and RT3D. The results for the case study showed about 90% reduction in the required simulations to achieve the optimal solutions. Some of the other examples in this field are e.g. (Kourakos and Mantoglou, 2009), (Yan and Minsker, 2011) and (Razavi, Tolson and Burn, 2012a).

Khu and Werner (2003) took advantage of neural network to automatize calibration of the SWMM rainfall-runoff model, based on uncertainty quantifications. A new method was proposed to reduce the number of Monte Carlo model simulations in the Generalized Likelihood Uncertainty Estimation (GLUE) technique. The proposed ANN based method reduced substantially the number of model simulations and yielded 80% computational saving.

Another example of applying ANN for uncertainty analysis purpose is the research of Shrestha et al. (2009) They used ANN for emulating a time-consuming Monte Carlo simulation for parametric uncertainty assessment of a lumped conceptual hydrological model, HBV.

Broad et al. (2005 and 2010) used ANN in combination with a genetic algorithm (GA) for design optimization of the water distribution systems. A similar approach is taken into account in another study in order to optimize the monitoring locations in the water distribution systems (Behzadian *et al.*, 2009).

Zou et al. (2007) developed an adaptive ANN-GA approach for inverse water quality modelling and automatic calibration of the WASP model which resulted in a considerable reduction in CPU time (97%). They applied the same approach for parameter identification and uncertainty analysis (Zou, Lung and Wu, 2009).

An example of application of ANN for RTC is (Zhang & Stanley 2000). In this research, a feed-forward scheme is introduced for RTC of water treatment process considering coagulation, flocculation and sedimentation. Several inputs describing the raw water quality are considered to define the control actions regarding alum and PAC dose. The network performed well for the trained data (2000 sets of process control data). However, a generalization can be made after application for a real on-line process control operation. ANN is also applied in practice for real-time operational management of sewage systems (HR Wallingford, 2012).

## 2.2 Deep Learning (DL)

These techniques are the newest generation of ANNs. Their difference with the conventional ANNs is on the 'credit assignment paths' which are the chains of possible learnable, causal links between actions and effects (Schmidhuber, 2015a). Their purpose is "to model high level abstractions in data by using a deep graph with multiple processing layers, composed of multiple linear and non-linear transformations" (Deng and Yu, 2013). A comprehensive review of DL techniques is given in (Schmidhuber, 2015b). Although application of DL techniques is growing very fast in many fields, rare studies have been carried out in the domain of water engineering so far. An example is application of Deep Belief Network (DBN) for simulation of a water distribution network. The DBN outperforms the conventional ANNs for the given case study, without the necessity of performing initial sensitivity analysis for construction of the network (Wu, El-Maghraby and Pathak, 2015).

## 2.3 Radial Basis Functions (RBF)

RBF surrogate models typically consist of two main elements: A polynomial; and a weighted sum of n correlation functions (or radial basis functions) where n is the number of design sites. An RBF model is formed after defining the coefficients of the polynomial as well as the weights of the basis functions (Razavi, Tolson and Burn, 2012c).

This method is vastly used for automatic calibration of different models such as: MIKE11/NAM e.g. (Khu et al. 2004); groundwater models e.g. (Mugunthan et al. 2005 and 2006) and (Razavi, Tolson and Burn, 2012b); SWAT watershed models e.g. (Regis and Shoemaker, 2007) and (Razavi, Tolson and Burn, 2012b); and other environmental models, for example a model for pollution of the soil and groundwater (Regis *et al.*, 2008). Computational saving in these cases ranges from 50-90% of the full evaluations for calibration purpose. In a more relevant and interesting study, Han et al. (2012) applied this method to develop a self-organizing neural network to be applied in model predictive control (MPC) of dissolved oxygen (DO) concentration in a WWTP using the BSM1 model. In this technique the neural network's structure can be adapted according to the changes in the system dynamics to maintain the prediction accuracy. It is proven that this technique has improved the control performance in comparison with the traditional MPC approach. See also e.g. (Bagheri *et al.*, 2015) and (Heddam, 2016).

## 2.4 Kriging

Kriging is very similar to RBF with the same main elements. The polynomial, which is considered as a global function over the input space, and the correlation model (basis functions) which is in fact a deviation model. The main difference between these two methods is that, thanks to its stochastic structure, Kriging is able to produce an approximation of the prediction uncertainty. This method is widely used for optimisation purpose. For example, multi-objective design optimisation for water distribution systems (Dipierro *et al.*, 2009); well field design optimisation (Hemker *et al.*, 2008); pump-and-treat (PAT) optimisation (Baú and Mayer, 2006); and a simulation-optimisation approach in groundwater modelling (Zhao, Lu and Xiao, 2016).

## 2.5 Gaussian Processes Emulator (GPE)

This method can be considered as an extension of the kriging method, but in a Bayesian setting (Stone, 2011a). Generally speaking, an emulator is a probability distribution of a simulator which estimates the simulator's output and also quantifies the uncertainty in this estimation (MUCM Community 2011). More specifically, a GP emulator is built based on defining a prior for the simulator as a Gaussian stochastic process, decomposed into a mean function, such as a regression function, and a stochastic process with zero mean and a covariance function. Afterwards this process is conditioned on some selected design data to produce a posterior which is called the emulator (Machac *et al.*, 2016).

Stone (2011) took advantage of GP emulators in the field of groundwater modelling and risk assessment for radioactive waste disposal. The computer models in this field are extremely computationally expensive (e.g. WIPP) and this fact makes the uncertainty propagation analysis challenging. Traditional methods such as Monte Carlo (MC) simulations can be enormously time-consuming. Based on the final results, the developed emulators in this research were able to estimate the uncertainty bounds similar to MC methods, but in a considerably shorter time. A dynamic emulation approach, which preserves the dynamic behaviour of the original complex model, is presented by (Castelletti et al. 2011 and 2012). This approach was applied successfully to emulate a 1D-hydrodynamic-ecological model for optimal operation of a dam as a case study. More recently, this approach was applied in order to emulate the computationally expensive Delft3D-FLOW model. The resulting emulator, which was four orders of magnitude faster than the original complex model, was applied for Real-time Model Predictive Control (RT-MPC) of a reservoir in Singapore considering water quantity and quality control (Galelli, Castelletti and Geodbleod, 2015).

More recently, Machac et al. 2016 developed an emulator for the SWMM model which is used in urban drainage modelling domain. They introduced a mechanism-based emulator in which in addition to the information gained from the design data, the knowledge about the mechanisms of the simulator is used as well. This was done in order to investigate if the accuracy of the emulator increases in this way. The main motivation for this research was to facilitate the calibration of the SWMM model. Based on the results, the calibration time decreased from weeks to hours by introducing this mechanism-based emulator. An earlier version of this research with application to shallow water equations can be seen in (Machac, Reichert and Albert, 2016).

Other popular data-driven approaches examples are: Polynomials, e.g. (Schultz et al. 2004 and 2006), (Creaco *et al.*, 2016); Linear regression, e.g. (Johnson and Rogers, 2000) (Schultz et al. 2004 and 2006) (Herrig *et al.*, 2015).

## 2.6 Advantages and disadvantages of the data-driven methods

The main advantage of the ANN methods is their non-intrusive nature. Besides, they result in fast runtimes once the model has been calibrated. This method provides valuable techniques for applications in integrated modelling or decision support modelling which require a limitation in number of parameters or ranges which they vary.

Apart from the popularity, ANN methods have some disadvantages as well. The main disadvantages are: subjective (data depended) structure, time-consuming calibration, risk of over-fitting, risk of getting trapped in local minima, and considering a relatively small number of parameters (Asher *et al.*, 2015).

# 3 Projection-based Approaches

These approaches are also known as model order reduction (MOR). Consideration and application of MOR in the field of water engineering and management is relatively new. Some of the recent works appear in the fields of fluid control (e.g. Ravindran 2000), groundwater modelling (e.g. (Siade and Putti 2010), (Boyce et al. 2015), (Vermeulen et al. 2005), (Winton et al. 2011)); and tsunami modelling (e.g. Ha and Tkalich 2008). One of the earlier works can be found for climate modelling in (Young 1970).

MOR is a mathematical technique to reduce the order of a dynamical system described by a set of ordinary or differential-algebraic equations (ODEs or DAEs) to facilitate or enable its simulation; the design of a controller; or optimization and design of the physical system modelled. In other words, a large-scale set of describing ODEs/DAEs can be replaced by a much smaller set without sacrificing significantly the accuracy of the input-to-output behaviour of the original model (Benner, 2014). Introduction to MOR concepts and application can be seen in (Schilders 2008) and (Schilders and Rommes 2008). Two of the main techniques that are most promising in the field of systems and control engineering are described here:

## 3.1 Balanced Truncation (BT)

BT is the most common MOR technique in the field of control and systems engineering. The reason for its popularity is because it preserves the ‘stability’ of the original high-order model and provides an ‘error band’ which gives a direct measure for the quality of the reduced model. In this technique, the input (actuator)-output (sensor) behaviour of the systems plays the main role and the model does not need to describe the detailed behaviour of the system (Besselink *et al.*, 2013).

The main steps of BT:

1. *Balanced realization*: in this step the states of the model are ordered according to their contribution to the input-output behaviour. For balanced realization two factors are quantified including: *controllability* and *observability* functions. Combination of controllability and observability Gramians defines the importance of different states of the model. Namely, the realization is balanced i.e the states that are easy to control are easily observed as well.
2. Discarding the states with the smallest influence to achieve the reduced model.
3. Check the error bound to quantify the quality of MOR. The error bound is expressed in terms of discarded Hankel singular values. States with the largest Hankel singular values are the most important ones according to input-output behaviour.

Few researchers in the field of urban drainage modelling have applied BT method and the main focus has been on model reduction for WWTPs. Mulas (2006) implemented the BT technique for model reduction of Activated Sludge Processes control. More recently, Sahlan and Darus (2013) investigated and compared three Frequency Weighted Model Reduction Techniques (FWMRT) for an Activated Sludge Process model and its PI-controller application (Sahlan *et al.*, 2013).

## 3.2 Proper Orthogonal Decomposition (POD)

MOR in this method is based on calculating the basis function. It can be applied for linear as well as non-linear models, see e.g. (Hinze and Volkwein 2005) and (Chen and Li 2010). POD is a very efficient technique based on projection of the original model onto a subspace generated by so called 'snapshots' from the full model. These snapshots should be significantly different from each other and they should cover the overall range of variability of the full model. After taking these snapshots a 'covariance matrix' is formed. In POD method, selection of the optimal snapshot set is the main challenge. This optimal snapshot set is found by maximizing the minimum eigenvalue of the snapshot covariance matrix (Siade and Putti 2010).

Accuracy of this MOR technique is dependent on which snapshots are taken into account. It should be noted that a large number of snapshots does not necessarily guarantee a better MOR with higher accuracy. So the objective is to find the best sampling strategy for a given snapshot size such that the accuracy of the reduced model is maximised (Siade, Putti and Yeh, 2010).

The number of snapshots is optimal when adding a new snapshot will not add a significant information to the reduced model, because it may be approximately a linear combination of other snapshots that have already been considered. More detailed description of the POD method can be found in (Willcox and Peraire, 2002) and (Pinnau, 2008).

Liang et al. (2002) have a detailed comparison between three popular POD methods including: Karhunen-Loeve Decomposition (KLD), Singular Value Decomposition (SVD) and Principal Component Analysis (PCA) and they prove the equivalence of these methods (Liang et al. 2002).

In the field of water management and engineering, the snapshot method has been applied in a few studies by focusing on water quantity modelling, see e.g. (Ravindran 2000), (Ha et al. 2007), (Ha and Tkalich 2008), (Ştefănescu and Navon, 2013), (Bistrian and Navon, 2008) and (Luo, Gao and Xie, 2015). To give a more detailed example, Min Xu (2013) applied this method for model reduction of a combined water quantity and quality model in open channels. The initial model was based on Saint-Venant equations and transport equation for water quantity and quality respectively. The reduced model in this study was implemented in MPC and the influence on the control performance was analysed. The conclusion was that, for the employed case study, MPC using the reduced model is a good trade-off between control effectiveness and computation time. Hence, the proposed MPC procedure in this study is considered as a successful method for MPC implementation, (Xu et al. 2013b).

### 3.3 Advantages and disadvantages of projection-based approaches

Generally speaking, the main advantages of these approaches are: their computational efficiency once constructed; as well as producing an error bound after MOR in most of these techniques (Willcox and Megretski, 2005).

The main disadvantage of these methods is that they are highly intrusive; meaning that one should initially define a clear mathematics description of the given model which is subject to MOR. Besides, it is difficult to implement these techniques for inverse modelling and uncertainty analysis; solving the reduced model normally involves editing the model code; and the basis vectors depend on the snapshots used to compute them (Asher *et al.*, 2015). These approaches are rather difficult to be implemented for practitioners and difficult if commercial modelling software does not provide access to the source code and its implemented underlying equations.

## 4 Hierarchical or Multi-fidelity Approaches

These approaches are normally the surrogate modelling techniques which are implemented by neglecting less-important processes, decreasing the numerical resolution, or increasing some tolerances in the model. Probably, the simplest and most common approach in this regard is to reduce the numerical discretisation of the original complex model. Decreasing the overall numerical resolution of the complex model (such as upscaling) might not be a proper way when we need some specific output(s) of the model in finer resolution. Hence, one would consider developing multiple resolutions in different levels, to achieve the same accuracy but with a faster runtime (i.e. the global problem with coarse resolution and local problem with finer resolution) (Asher *et al.*, 2015).

There has been few studies in this regard in the field of urban drainage systems modelling. Two of the relevant works are explained in the following paragraphs.

Meirlaen and Vanrolleghem (2002), introduced a model simplification method through boundary relocation in order to facilitate RTC of integrated urban drainage systems. The main steps of their technique, which is called dependency-structure base model reduction, is as follows:

1. Relocation of the upstream system boundaries to upstream of the first control point.
2. Relocation of the downstream boundaries to the downstream of the last measurement point.
3. More simplification based on sensitivity analysis of control actions and sub-model elimination.

The idea in this study was to control the sewer system (SS) and wastewater treatment plant (WWTP) based on the information related to the receiving water body (river).

Leitão et al. (2010) were interested in an investigation on the model network simplification of urban drainage systems for flood forecasting, based on simulation time and model accuracy. In this study, initially two types of models are selected including a 1D/1D and a 1D/2D model. Further, the 1D/1D model network is simplified based on 1) pruning; 2) merging; and 3) combination of both. Then, these three simplified networks are compared with the original 1D/1D model as well as the 1D/2D model. Comparison criteria are including: Mean absolute error (MAE), modified index of agreement, and Bias goodness of fit. Results of this study are promising regarding reduced time and accuracy.

## 4.1 Advantages and disadvantages of hierarchical or multi-fidelity approach

The main advantage is that *sometimes* these methods (if developed correctly) are able to maintain the detail and accuracy of the original complex model; for instance, by defining multiple resolutions as mentioned earlier. The main disadvantage is that, these methods are also highly intrusive and difficult to implement for practitioners. Besides, normally they are case-specific and it is difficult to generalize and automatize them for other given models of interest.

# 5 Comparison and Recommendations

None of the introduced categories for model simplification are universally superior for all applications. The method selection depends on the field of interest and ultimate purpose of the model simplification. Besides, one would consider a combination of two or more methods as well (Asher *et al.*, 2015). There are various criteria to evaluate different methods and select based on the needs of the project. The method should firstly, reduce the runtime significantly and increase the computational efficiency, and secondly, give a quantification of the uncertainty induced by surrogating in a probabilistic framework, and thirdly, be easily applicable in practice in conjunction with commercial and non-commercial, closed and open source software.

Asher et al. (2015), suggest in their comprehensive review of surrogate modelling approaches, that for decision support systems, where a very short runtime is required, data-driven approaches are the obvious choice. This is mainly because in decision support systems typically a small number of parameters are involved to keep the decision algorithms feasible and reach a solutions. Therefore, several drawbacks of the data-driven approaches which was addressed earlier are irrelevant.

# Part 2: Summary of journal paper on surrogate modelling using an analytical method

## 1 Problem statement

A common approach, in practice, to deal with computational burden of complex/detailed models for RTC purpose is to develop an alternative simple model based on the basic understandings about the physics of the system under study. This model should be able to model/approximate the main behaviour of the system which is subject to RTC. Since, this is an alternative approach to achieve fast surrogate models, it was interesting for my research to start with a brief study in this regard. Therefore, I followed a collaborative study on the concepts of an ongoing project at LIST. In this study, two types of controllers are proposed and compared to attain a better understanding of the potential of RTC approach based on wastewater quantity and quality for combined sewer networks. The first controller is solely based on a wastewater quantity control approach, whilst, the second one is also considering wastewater quality modelling, as well as its uncertainty propagation.

## 2 Research Question

How can we develop a simple analytical and fast surrogate model for the purpose of wastewater quantity and quality control in a combined sewer network? What are the possibilities to include uncertainty propagation in RTC based on this simple model?

## 3 Approach/Method

In this research, a simple but fast tank model was developed for combined sewer networks to be applied within an MPC approach. The model was based on volume balance and mass balance laws in the tanks and time delay concept in the pipes (See Figure 1). This model was applied to a small case study in Luxembourg to illustrate and discuss the results. The uncertainty propagation in the second controller was based on Taylor series of first order approximation. This quantified uncertainty, was incorporated inside the objective function of the optimisation problem in the MPC, which was subject to minimisation. Hence, for instance, if two tanks in the network are subject to CSO in the same time step, the one with less uncertainty is privileged to occur by the controller. The overall schema of the methodology in this sub-project is illustrated in Figure 2.

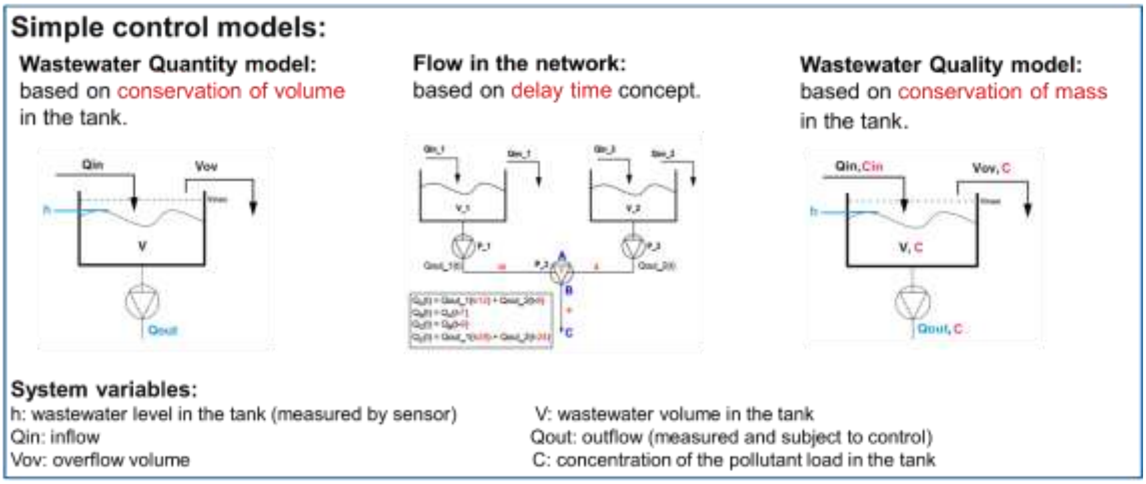


Figure 1. Simple control models and their system variables

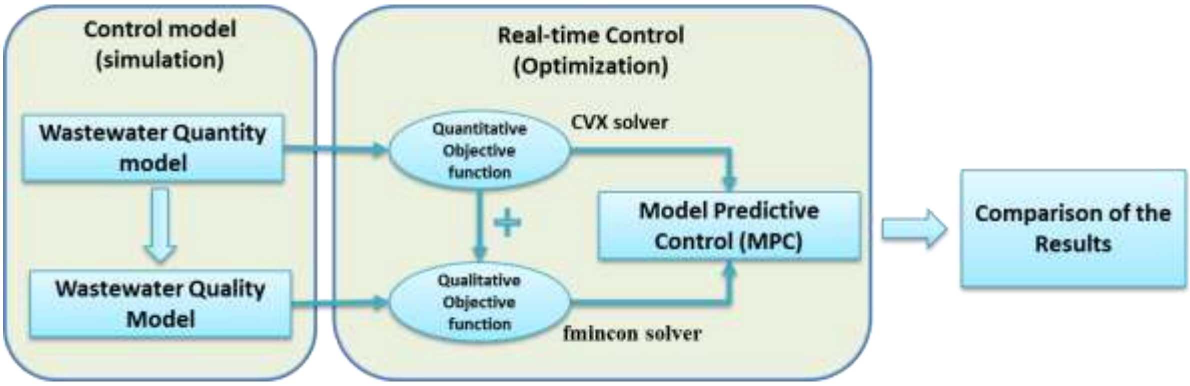


Figure 2. Overall schema of the methodology

## 4 Results

The main idea of this study was to develop a simple surrogate model for wastewater quantity and quality control and understand if the quality-based controller can improve the efficiency of the former quantity-based MPC controller. An uncertainty propagation method was introduced for the unmeasured variable of a global pollution load in the network and included in the objective function of the quality-based controller. In conclusion, the results showed a positive contribution of the new quality-based controller in decreasing the overflowed pollution mass as well as CSO volume during the selected rain scenarios.

## 5 Expected Impact for scientific and practitioners community

In fact, the results were promising and the introduced MPC approach could be considered as a ‘soft’ solution for combined sewer network management. Because, the new controller reduced the pollution load and overflow volume without the need to add new physical elements (e.g. sensors) to the system which are normally expensive to purchase and maintain.

## 6 Journal paper

Details of this approach can be found in: "Pollution-Based Model Predictive Control of Combined Sewer Networks, Considering Uncertainty Propagation", International Journal of Sustainable Development and Planning, Volume 12 (2017), Issue 1, (https://www.witpress.com/elibrary/sdp-volumes/12/1/1446).

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