CONTROL THEORY FOR WATER QUALITY REGULATION IN DRINKING WATER DISTRIBUTION NETWORKS

by

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To my dad, mom, sister, and wife

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We encountered on the sea on a dark night,
When we sailed for our own light.
It would be nice if you remember,
But I hope you'd rather forget
The spark we mutually sent when we met.

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A drinking water distribution network (WDN) is designed to adequately carry quantities and qualities of potable water from treatment plants or reservoirs to consumers. To ensure safe drinking water, the most used disinfectant in WDNs is chlorine, and a minimum chlorine residual is typically maintained according to the regulations enforced by the U.S. Environmental Protection Agency (EPA). However, maintaining minimum chlorine concentrations or performing real-time water quality control (WQC) and regulation are challenging tasks due to the lack of *(i)* a proper control-oriented model considering complicated components in WDNs (e.g., junctions, tanks, pipes, and valves) for water quality modeling (WQM), and *(ii)* a corresponding scalable control algorithm that performs real-time water quality regulation.

The objective of this dissertation is to propose a control-oriented state-space representation of the water quality model that is friendly to the state-of-the-art algorithms to model, control, and estimate water quality state in WDNs. Based on the proposed state-space model, this dissertation solves two essential research challenges — optimal water quality control and sensor placement problems. Furthermore, this dissertation explores other potential ways to create more compact water quality models by reducing the system order of proposed control-oriented water quality model and identifying system models only by data-driven methods.

In particular, water quality models depict the decay and transport of disinfectants (e.g., chlorine) in WDNs. However, traditional water quality models fail to describe the explicit relationship between inputs (chlorine dosage at booster stations) and states/outputs (chlorine concentrations in the entire network) from the perspective of control theory such that the advanced control algorithms are prohibited from being applied in WDNs. This dissertation proposes a control-oriented

state-space form of water quality model that not only can describe the spatiotemporal evolution of disinfectants accurately but also is friendly for existing control algorithms. With such proposed WQM, a highly scalable model predictive control algorithm that showcases fast response time and resilience against some sources of uncertainty is developed. The goal of maintaining the minimum chlorine residual in entire WDNs, that is, the requirements of water quality control (WQC) are met.

Furthermore, real-time water quality sensors in WDNs have the potential to enable contamination event detection, closed-loop feedback control of water quality dynamics/models, and network-wide observability of water quality indicators. However, this objective is overlooked in recent research studies. Hence, this dissertation also provides a computational water quality sensor placement (WQSP) method considering improve the network-wide observability of the water quality dynamics with the assistant of the proposed WQM. This metric finds the optimal WQSP that minimizes the state estimation error via the Kalman filter for noisy water quality dynamic — a metric that quantifies WDN observability.

With the proposed WQM and solving the corresponding WQC and WQSP problems, this dissertation revisits the WQM problem and explores several methods (such as reducing system orders and identifying system dynamics using data-driven techniques) to obtain a more compact water quality model that potentially reduces computational load.

Specifically, model order reduction (MOR) methods for water quality dynamics are investigated. The presented investigation focuses on *(i)* reducing state-dimension by orders of magnitude while retaining the input-output relationship and stability of the MOR methods and *(ii)* combining the reduced-order model with model predictive control. System identification (SysID) algorithms, seeking to approximate models using only input-output data without relying on WDN parameters/typologies, are explored while overcoming several challenges. Such challenges are the complex water quality and reaction dynamics and the mismatch between the requirements of SysID algorithms and the properties of water quality dynamics. Through case studies, we demonstrate the applicability of SysID algorithms and show the corresponding performance in terms of accuracy and computational time by comparing it with the proposed WQM. Moreover, the possible factors impacting water quality model identification are explored.

In short, this dissertation is the first thorough system, network, and control-theoretic attempt at modeling water quality dynamics, controlling them, and scaling their implementation via model-free methods. Future work will focus on more complex and nonlinear multi-species models as well as feedback control problems that regulate such complex models.

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CHAPTER 1: INTRODUCTION

A drinking water distribution network (WDN) is composed of complex components that adequately carry quantities and qualities of potable water from treatment plants or reservoirs to consumers to satisfy the demands and requirements from residential, industrial, commercial, and fire fighting. Water quality is typically ensured by chemical disinfection such as injecting chlorine-based disinfectants. Moreover, residual chlorine concentrations are routinely monitored by water quality sensors to verify that a sufficient residual is maintained throughout WDNs. Maintenance of a detectable residual is also typically mandated by state and federal regulations in many countries. For example, water utilities in the US are required to preserve detectable chlorine residual throughout the WDNs under the Surface Water Treatment Rule (SWTR) [47], the Safe Drinking Water Act of 1974 and its amendments in 1986 also require that a measurable disinfectant residual (i.e., 0.2 mg/L of chlorine residual) must be present at points of water consumption such as the end of users [2]. In addition, many states have established even more stringent numerical thresholds on the minimum residual concentration [109].

1.1 Motivations and challenges

WDNs should be capable of meeting the demands at all times and with satisfactory water quality. However, in our modern era, it is challenging to achieve the aforementioned goals due to the lack of *(i)* a proper control-oriented water quality modeling (WQM) considering complicated components (junctions, reservoirs, tanks, pipes, pumps, and valves), *(ii)* a corresponding scalable control algorithm that performs real-time water quality control (WQC), and *(iii)* an effective, optimal water quality sensor placement (WQSP) strategy to place sensors that can monitor chlorine concentration to improve the observability of the WDNs instead of installing the more expensive water quality sensors at random locations.

The main objective of this dissertation is addressing the modeling problem of water quality dynamics from the perspective of control theory and solving the corresponding optimal control and sensor placement problems in WDNs. We discuss the detailed challenges of each problem next.

- The **WQM problem** depicting the decay and transport of chlorine-based disinfectants in WDNs is hard to tackle because the network components are complex. A WDN mainly consists of pipelines, storage facilities (i.e., tanks and reservoirs), pumps, and other accessories (e.g., various types of control valves). The mathematical models of these components introduce more intractable problems. For example, the water quality models in pipes are described PDEs. Additionally, the topology of these components is also very diverse and complex, and there exist four typical typologies: grid, ring, tree or radial, and dead-end. Furthermore, the hydraulics in WDNs are dynamic and the dynamic comes from multiple aspects such as the time-varying demands and uncertainty caused by leaks.

- The **WQC problem** — maintaining the minimum chlorine residual in WDNs while satisfying specific constraints—is also a challenging task since it needs advancing control algorithms to determine the appropriate chlorine dosage to ensure a sufficient residual, particularly at the far ends of WDNs where the water age is the highest. Applying large doses of chlorine-based disinfectants at the treatment plant has been associated with multiple issues, including the excessive formation of disinfection byproducts as well as aesthetic issues with water taste and odor [40]. Alternatively, the disinfectant can be injected in smaller doses at multiple locations in the network, a practice commonly known as booster disinfection, to maintain a uniform disinfectant concentration throughout the WDNs [128].

- The **WQSP problem** that maximizes the observability or state estimation metrics of the monitored WDNs given a limited number of sensors is NP-hard in general when searching over all possible sensor combinations. Herein, observability is defined as the ability to estimate water quality model states from available measurements via a state estimation routine. This provides situational awareness for the operator given data from a few water quality sensors. Although the WQSP problem considering different purposes such as detecting contamination events has been studied in water quality literature [48, 59], the sensor placement to improve the observability has not been explored yet.

Revisiting water quality modeling for more compact models

Even if we could successfully develop the water quality model and propose effective algorithms that can potentially solve the corresponding WQC and WQSP problems for WDNs. The efficiency or scalability of such models and algorithms is still an issue. This is because the dimension (or system order) of the water quality model can reach 10^4 or 10^6 even for small-to-midsize due to ensuring high fidelity after discretizing the PDEs describing the spatiotemporal evolution of disinfectant concentration in pipes. It implies that high-accuracy models, though effective for predicting system dynamics, are not amenable to controller or estimator design for large-scale networks — especially in the presence of state or input constraints.

To that end, **model order reduction** (MOR) is necessary to derive a compact model for fast simulation and efficient synthesis of controllers and state estimators. The motivation of MOR is to reduce the *full-order model* to a *reduced-order model* that has a much smaller number of states or order without significantly decreasing model accuracy while maintaining input-output relationships and retaining certain properties of the system such as controllability and observability [13, 110, 146].

Traditional water quality modeling including the proposed WQM method in this dissertation is analysis-based [44, 60]. However, the analysis-based methods either rely on cumbersome, extensive water/chemistry-based modeling or are based on obtaining hydraulic and many other parameters—or require both. This is because the water quality analysis depends on the results of hydraulic analysis such as the flow rates in all links. Since we already have the booster stations installed to regulate the water quality and have the water quality sensors installed to monitor the WDNs, an intuitive idea is to take advantage of these actuators and sensors by collecting experimental data to identify the water quality models. In this way, a compact model could be obtained because only a few actuators and sensors would be deployed in WDNs. Moreover, the process of obtaining the full-order of the water quality model first and reducing the system model using

MOR algorithms to generate a compact model can be avoided. **System identification** (SysID) algorithms for generic dynamic system models seek to approximate such models using only input-output data without relying on network parameters. This dissertation also investigates SysID algorithms for water quality model approximation to obtain a compact water quality model. This research problem is complicated and mainly caused by the mismatch between the requirements of SysID algorithms and the properties of water quality dynamics.

1.2 Literature review

In this section, we only provide a brief review of the literature related to the topics aforementioned in the Introduction section since a separate, thorough literature review on each topic is provided accordingly in the ensuing chapters of this dissertation.

1.2.1 Literature review of WQM

Over the past two decades, many studies have investigated the WQM problem in WDNs. Water quality modeling depicts the decay and transport of chlorine-based disinfectants in WDNs. This can be expressed via the advection-reaction dynamics for which three different families of numerical schemes can be used to obtain the numerical solution: Eulerian-based schemes [106], Lagrangian-based schemes [19, 78], and hybrid Eulerian-Lagrangian schemes [11]. For example, EPANET [107] is a widely used modeling software using a Lagrangian-based approach. For example, the studies [117, 150] derive an input/output (I/O) water quality model giving an explicit relationship between inputs and outputs based on Lagrangian scheme.

All these studies have their limitations. Most of these studies fail to describe the input and output relationship and are not designed for control-related purposes. For example, the I/O model does not explicitly model the states, which results in a model that only captures the output performance rather than all state variables in the network, and has to be updated once the locations of inputs (boosters) and outputs (sensors) change. In this dissertation, we overcome these issues by showcasing that the formulation of the state-space representation/form of water quality model