Sachbericht zum Verwendungsnachweis

Verbundprojekt

Online-Monitoring und digitale Steuerung in Trinkwasserversorgungssystemen

MoDiCon

in der Fördermaßnahme

CfP 2019 Digital transformation of the water sector

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GEFÖRDERT VOM

Bundesministerium für Bildung und Forschung

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I. Teil I Kurzfassung

Das MoDiCon-Projekt zielte darauf ab, ein digitales Online-Überwachungssystem für Wasserversorgungssysteme (WVSs) zu entwickeln, das in Echtzeit-Veränderungen der Wasserqualität erkennt und darauf automatisch reagiert. Fest installierte Wasserqualitätssensoren für z.B. pH, Trübung und freies Chlor haben sich in den meisten Ländern als effektive Methode zur Überwachung der Wasserqualität erwiesen. Jedoch gibt es kaum Anwendungen zur Echtzeit-Überwachung von organischen Parametern und der Erkennung mikrobiologischer Kontamination im WVS, welche für gesundheitsrelevante Auswirkungen verantwortlich sind. Entsprechende, auftretende Veränderungen sind jedoch zukünftig zu erwarten. Der Klimawandel und seine Folgen werden langfristig zu neuen Herausforderungen hinsichtlich der Qualität des Trinkwassers führen. In diesem Zusammenhang können auch Naturkatastrophen wie starke Regenfälle oder Überschwemmungen zu Kontaminationen im Trinkwassernetz führen. Auch veraltete Rohrleitungssysteme - teilweise 60 Jahre und älter - erhöhen das Risiko von Leitungsschäden und damit eventuellen Verunreinigungen im VWS. Schließlich können auch menschliche Fehler, Cyberattacken oder reale physische Angriffe die Wasserqualität im Netz gefährden. Neben der Etablierung eines Echtzeit-Monitorings, galt es im MoDiCon-Projekt Daten mit Echtzeit-Simulationen und -Steuerung der Hydraulik des WVSs zu verknüpfen. Ein digitales WVS bietet die zentrale Voraussetzung, einen automatischen und unmittelbaren Kontrollmechanismus bereitzustellen, um angemessen auf ungewöhnliche Veränderungen in der Wasserqualität zu reagieren und somit die Hausanschlüsse sicher zu schützen.

Methoden und Ergebnisse: Im Rahmen des MoDiCon-Projekts hat das Konsortium einen integrierten Rahmen entwickelt, der gleichzeitig das Monitoring von Wasserqualitätsparametern, deren Simulation im WVS sowie die automatische Reaktion und Steuerung ermöglicht. Die Umsetzung erforderte neben Labor- und Pilotversuche zur Echtzeit-Analyse mikrobieller und organischer Wasserqualität (TUHH), die Entwicklung von Modellen zur Vorhersage der Wasserqualität an jedem Punkt im VWS (Technion) sowie die Entwicklung von automatisierten Kontrollstrategien (TU Ilmenau).

Ein innovatives Sensorsystem zur gekoppelten Echtzeit-Überwachung mikrobieller und organischer Parameter wurde durch die Kombination von Durchflusszytometrie und Fluoreszenzspektroskopie entwickelt. Es ermöglicht die Generierung individueller Wasser-Fingerabdrücke und erkennt daher schnell Veränderungen der Wasserqualität (<15 min). Hierfür wurde das Sensorsystem in einem Laborversuchsumfeld angepasst und kalibriert, bevor es in eine reale Pilotanlage integriert wurde. Die Pilotanlage ermöglichte die erfolgreiche Validierung des Fingerprint-Ansatzes unter den realen Strömungsbedingungen eines Trinkwassernetzwerks. Die assoziierten Partner Hamburg Wasser und bbe moldenke unterstützten diese Umsetzung mit Hardware und technischem Know-how. In diesem Zusammenhang umfasst das automatisierte Monitoring Probenahme, Messung, Datenanalyse und Visualisierung. Die Entwicklung eines automatisierten PARAFAC (Parallelfaktoranalyse)-Modells bietet insbesondere eine detaillierte Charakterisierung organischer Substanzen. Der Automatisierungscode der Überwachungsmethode ist ein wichtiges Projektergebnis. Dieser wird nach Projektende als Open-Access-Code zur Verfügung gestellt. Der Visualisierungsteil gibt einen Ausblick auf die mögliche Darstellung der automatisierten digitalen Wasserqualitätsüberwachung.

Zuverlässige Vorhersagen der Trinkwasserqualität im Netz erfordern mathematische Modelle eine genaue Interpretation der Hydrodynamik und der mit den vielfältigen Austauschprozessen innerhalb der Rohrleitungen verbundenen Unsicherheiten. Gerade das Wissen über Austauschprozesse ist limitiert.

Hierfür existieren komplexe Modelle lediglich als theoretische Rahmenwerke, es fehlt die Möglichkeit zur allgemeinen Anwendung. Daher wurden physikalische Modelle (innerhalb eines neuen Softwarepakets – EPANET-C) entwickelt, um die Wasserqualitätsdynamik in einem realen VWS genau zu beschreiben. Über integrierte und anpassbare Verzeichnisse für konzeptionelle und mathematische Modelle erleichtert EPANET-C die Modellierung bzw. Simulation der Wasserqualität im VWS, auch ohne spezifische Programmierkenntnisse. Für die untersuchten Testbedingungen zeigte sich, dass einfache Einphasenmodelle mikrobiologische Qualitätsvorhersagen ähnlich genau zu denen relativ komplexer Zweiphasenmodelle treffen. Die Untersuchung verdeutlichte, dass die Unsicherheit (hauptsächlich aufgrund von Datenknappheit) in Bezug auf Mechanismen des heterotrophen Bakterienwachstums in der Bulk-Phase und der Ablösung des Biofilms an der Wandphase entscheidend ist, um die Zuverlässigkeit der Wasserqualitätsmodelle zu kontrollieren. Aufgrund seiner Flexibilität kann EPANET-C zu einem De-facto-Standardwerkzeug in der Modellierung der Wasserqualität im VWS sowohl für industrielle als auch akademische Anwendungen werden.

Detektierte als auch simulierte Hinweise auf Änderungen der Wasserqualität erfordern Untersuchungen zu einem optimierten Steuerungsstrategierahmen, um Kontaminationen schnell zu isolieren bzw. zu entfernen. Im ersten Schritt wurde eine modellbasierte, optimale Steuerungsstrategie entwickelt, um das Problem einer Kontamination, unter besonderer Berücksichtigung verschiedener hydraulischer und wasserspezifischer Parameter zu lösen. Für dieses Modell wurden die Gesetze der Massen- und Energieerhaltung verwendet. Zunächst wurde ein eindimensionales, advektives Transportmodell zu einer differentiellen Gleichung vereinfacht, um die Chlorzehrung in einem Rohrleitungssystem zu beschreiben. Anschließend konnte ein nichtlineares Programmierungs (NLP)-Optimierungsproblem formuliert und gelöst werden, um eine vorgegebene Chlorkonzentration an jedem Punkt des Netzes zu erreichen. Darauf basierend wurde ein gemischt-ganzzahliges, nichtlineares Programmierungs (MINLP)-Modell entwickelt, um die optimale Position von Isolationsventilen und Steuerungsstrategien nach einer Kontamination im VWS festzulegen. Der anschließende Spülprozess wurde mithilfe des etablierten EPANET-Modells der Hamburg Wasser Pilotanlage implementiert. Ein digitales System zur Online-Überwachung und Steuerung der Wasserqualität wurde ausgelegt, in Betrieb genommen und extensiv getestet. Die Validierung des Systems erfolgte durch gezielte Kontaminationsszenarien an verschiedenen Positionen im Pilot-VWS. Die hydraulischen Komponenten konnten innerhalb einer optimalen Steuerungsstrategie erfolgreich gesteuert und dadurch die Kontamination isoliert sowie aus dem System entfernt werden.

Zusammenfassung: Die Partner des MoDiCon-Projekts haben einen neuartigen Ansatz für ein vollautomatisiertes Überwachungs- und Vorhersagesystem für die Trinkwasserqualität in Versorgungssystemen entwickelt. Die entwickelte Schnittstelle zwischen der physischen Überwachung und den Simulations- und Optimierungstools ermöglicht es Wasserversorger potentiell, die Sicherheit ihrer Wasserverteilungssysteme zu gewährleisten. Allerdings bedarf die endgültige Anwendung einer Testphase in einem realen WVS. Herausforderungen für eine reale Umsetzung des MoDiCon-Ansatzes sind Umbaumaßnahmen in den Bereichen Sensorik, Aktoren (Ventile, Schieber, Pumpen, etc.) sowie weiterer Steuerungselemente (Hydranten, Behälter, etc.). Weiterhin könnte die Umsetzung eine bisher noch nicht durchgeführte Berücksichtigung verschiedener Druckzonen im Netz sowie den Umgang im Fall von Notfallentnahmen (z.B. Feuerhydranten) erfordern. Diese Punkte gilt es in zukünftigen Forschungsvorhaben zu adressieren.

Teil II Eingehende Darstellung

In the last two decades over 70 cases of contaminated drinking water with harmful impacts on consumers' health were reported (Efstratiou et al., 2017; Moreira & Bondelind, 2017). All cases could be related to bacteria spreading into the WDS, with various origins of the contamination entering the system. The rapid detection as well as the reaction to the contaminant failed or were not able due to missing online monitoring systems, respectively. Scenarios like this are expected to increase in the future because of several reasons. Climate change and its secondary effects might deteriorate the drinking water quality (i), natural disasters like heavy rainfall or floods can overflow and contaminate water reservoirs and tanks (ii). Furthermore, aging infrastructure can lead to pipe damage and associated occurrence of contamination (iii). Last, human errors or cyber- and physical attacks may infiltrate the system and have to be avoided (iv). That is where the MoDiCon idea starts about what future digitalized water supply and water supply security could be like. Aiming for the assurance of drinking water quality all over the WDS via automized methods requires different actions:

Autonomous water quality monitoring systems at several locations in the WDS

Minimizing the consumers' risks in case of contamination requires the determination of the optimum location for monitoring systems. These monitoring systems must be able to rapidly detect even little changes in the water matrix considering organic and microbial content. In case of a water quality change, the monitoring systems must communicate with controlling mechanisms.

Predictions for water quality all over the WDS

Since actual measuring of the water quality is not feasible at any time and at any location in the network, advanced water quality simulating tools are required to predict the water quality for every part of the WDS. Further data-driven algorithms must be developed and trained to recognize water quality anomalies even before they appear in the monitoring systems

Reaction and control in case of a contamination

To react appropriately in case of a contamination, optimum control strategies in terms of closing valves, and flushing the system must be developed. This requires the optimal location of automatic control instruments like vales in the WDS.

Aiming a solution for this pictured "Future WDS" needs expertise in different fields which can ideally be served by the three research groups TUHH, Technion, and TUIL. Within the MoDiCon project, the research groups developed some individual approaches and objectives to achieve the above points. The research results of each group are highlighted in the following subsections.

TUHH, Jonas Schuster and Mathias Ernst

In the following, the contribution of the TUHH research group to the overall MoDiCon project is presented. For this purpose, it is subdivided into the three main work packages that were essential for the successful implementation of the project.

WP1: Further development of a Flow Cytometry and Fluorescence Spectroscopy (EEM) data analysis (EEM based on PARAFAC), and generating real water quality database

WP2: Developing a laboratory environment for continuous and autonomous real-time (<15min) measurement

WP3: Application of developed methods in a pilot plant setup

WP1: Further development of Flow Cytometry and Fluorescence Spectroscopy (PARAFAC) data analysis, and generating real water quality database

Both methods, flow cytometry, and fluorescence spectroscopy, are not part of either German or Israeli standard operation procedures in drinking water quality analysis, although they find application in several other research fields (medicine, biochemistry, etc.). The transmission of continuous monitoring methods into a real environment for a water supplier such as Hamburg Wasser requires standard handling procedures as well as an added value to state-of-the-art methods. Therefore, the initial step was to characterize measuring range, sensitivity limits, etc.

Flow Cytometry

By the start of the MoDiCon project, TUHH acquired and installed a new flow cytometer (Cube 6 – Sysmex) with an additive automation unit (OC300 – onCyt). Flow cytometric parameters that play a role in the MoDiCon project are Total cell count (TCC), high nucleic acid cells (HNA), low nucleic acid cells (LNA), viable cells, and dead cells. These parameters were analyzed by following steps: Adding up to two fluorescent dyes (SYBR Green I and Propidium Iodide) to the water samples, incubating the samples (13 min), and analyzing them with the flow cytometer. Within the first experiments, the detection range of cells was successfully defined considering cells with different sizes, viable/dead, as well as different cell concentrations. Test series were performed with solutions containing isolated bacteria (Escherichia coli, 1 – 6 µm, and Brevundimonas diminuta, 0.3 – 2 µm), drinking- and groundwater samples from different Hamburg Wasser utilities. A detailed Python-based data analysis tool was developed using the open-source software FlowKit (White et al., 2021).

Fluorescence Spectroscopy

Natural water samples generally contain fluorophores as part of the natural organic matter, which all types of natural waters obtain. Fluorescence spectroscopy can detect and quantify these fluorophores. It is known as a robust method for rapid organic characterization, although the quantification of qualification of fluorophores and its influence on the microbiological environment in the water is still under research. An innovative approach to standardize the data evaluation is the parallel factor analysis (PARAFAC), whose research impact increased recently regarding natural water characterization (Murphy et al., 2013). PARAFAC is a mathematical decomposition tool that enables the subdivision of total fluorescent organic matter signals. The goal of the MoDiCon project was to further develop the PARAFAC method into a standardized automatic procedure that can be established for continuous monitoring of fluorescent organic matter in drinking water. The PARAFAC model which was developed during the project can distinguish the total fluorescent signal in between five and seven different organic components, standing for several types of fluorophores. Figure 1 shows the excitation and emission matrix (EEM) of all (here: six) decomposed organic components. Each water sample can thus be analyzed by PARAFAC for the intensity of these six components providing an individual organic fingerprint. The unique character of the developed six-component PARAFAC model was successfully applied to all investigated natural water samples (drinking water, wastewater, rainwater).

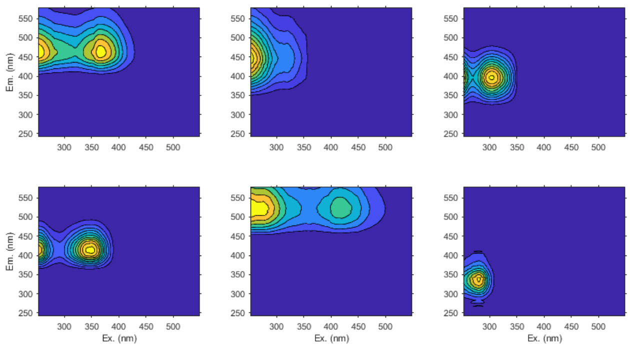

Figure 1: Developed six-component (C1 – C6 from top left to bottom right) PARAFAC model, validated for all kinds of investigated water samples. The peak excitation and emission wavelengths for each component are C1 λex = 250/370 nm and λem = 465 nm, C2 λex = 250/325 nm and λem = 450 nm, C3 λex = 250/305 nm and λem = 400 nm, C4 λex = 250/350 nm and λem = 420 nm, C5 λex = 250/275/420 nm and λem = 525 nm, C6 λex = 280 nm and λem = 335 nm.

^^Table 1: Overview of microbial and organic parameters from a few different natural water bodies. PARAFAC components based on the model (introduced in Figure 1).

Water body	Flow Cytometry			Organics	PARAFAC components					
	TCC	HNA	LNA	TOC	C1	C2	C3	C4	C5	C6
	in cells/mL			in mg/L	Fluorescence score in R.U.					
Drinking water 1	1.4×10^5	0.9×10^5	0.5×10^5	4.6	0.61	0.78	0.89	0.66	0.21	0.21
Drinking water 2	8.2×10^5	1.7×10^5	6.5×10^5	3.1	0.47	0.58	0.54	0.41	0.19	0.21
Wastewater	1.7×10^7	0.5×10^7	1.2×10^7	16.3	5.03	0.00	4.84	3.67	2.08	2.19
Rainwater	1.0×10^7	9.5×10^6	0.5×10^6	2.5	0.44	0.42	0.42	0.31	0.18	0.34

By combining both techniques, the TUHH group generated individual microbial and organic fingerprints for different waters. An insight into these data is given in Table 1 for some chosen water samples.

However, even little changes in the water matrices can influence the harmlessness of the drinking water quality. The detection of these little changes via continuous monitoring was part of the second and third work packages.

Another part of the first work package was the generating of bacteria growth rates which were needed for water quality simulation tools (Technion). The growth behavior of different drinking water bodies microorganisms was analyzed via online flow cytometry and maximum growth rates were calculated. These results are shown in the WP1 of the Technion group.

WP2: Developing a laboratory environment for continuous and autonomous real-time (<15min) measurement

Regarding a standardized application of monitoring microbial and organic fingerprints WDS via flow cytometry and fluorescence spectroscopy, an automated process was needed. This process includes 1. sampling, 2. pre-treatment, 3. measuring, 4. data analysis, and 5. visualization. Whereas the installed flow cytometric devices include steps 1. – 3., the entire process was developed for fluorescence spectroscopy (Figure 2). Time-limiting steps are the pre-treatment step of flow cytometry (13 minutes of dye incubation), as well as the fluorescence measurement and PARAFAC modeling, each takes approximately 7 minutes. Thus, the total duration of the automatic procedure for one sample, from sampling to visualization, was minimized to approximately 15 minutes which can be described as real-time regarding conventional microbiological drinking water investigations that require days of responses. However, this fact must be considered as limiting for the MoDiCon approach of autonomous reaction in case of a WDS contamination (TUIL).

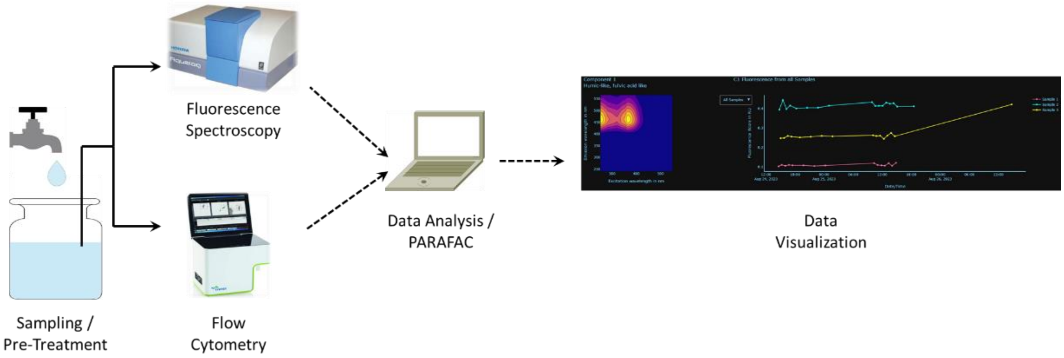

Figure 2: Schematic overview of automatic water quality monitoring on a lab scale. Data visualization shows an example of monitoring one PARAFAC component.

Besides the physical development of an automation unit for fluorescence spectroscopy, a very challenging part was the automation of PARAFAC data analysis in combination with data postprocessing. PARAFAC modeling was performed in MATLAB (version R2021b) using drEEM (version 0.6.5) toolbox, implementing little adjustments. For visualizing the PARAFAC data, the TUHH group developed a Python-based dashboard solution that also shows flow cytometric results. Furthermore, it is flexible for adding more real-time data from other devices (e.g., conductivity, turbidity, UV absorption, etc.). The real-time setup was successfully tested and experimental data was published in Schuster et al. (2022). Figure 3 shows some correlations that were investigated between organic matter and bacterial growth behavior.

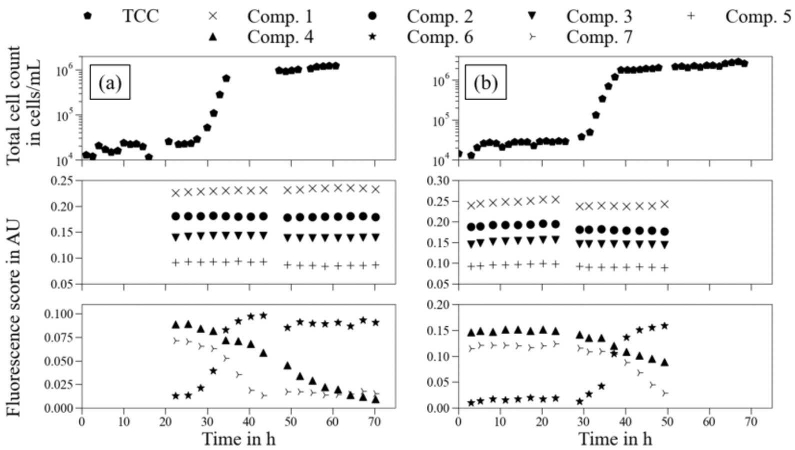

Figure 3: Experimental results from drinking water real-time monitoring via fluorescence spectroscopy (PARAFAC components 1- 7) and flow cytometry (Total cell count – TCC). The drinking water was spiked with organic nutrients to observe cell behavior in the presence of nutrients. Figure from Schuster et al., 2022.

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The overall objective of this part was the development of a reliable and comparable method that can be adopted into WDS quality monitoring. For the introduced method, it is important to understand that it does not work with absolute limit values. Instead, it is necessary to generate water individual baseline values for all fluorescence components and flow cytometric parameters, respectively. Considering continuous monitoring, this approach detects even little discrepancies from the baseline values. Due to the type of changing fluorescence component / flow cytometric parameter and its intensity, it may be possible to identify the origin of the contamination and its criticality (e.g., sewage contamination and its amount). Due to the automated process, any critical changes can be reported immediately to the optimized control system (TUIL). Another offline application of this method is the building of a database for several wells or water work exits. The rapidity of the methods allows total monitoring over a long period, even for larger water suppliers such as Hamburg Wasser. Since defining water-specific limit values is one of the future key challenges of applying these methods to a real WDS, the next work package describes an initial approach for the implementation.

WP3: Application of developed methods into a pilot plant setup

In collaboration with Hamburg Wasser, the developed system was tested in a pilot plant flowing system. This pilot plant can simulate flow circumstances similar to the one in a real WDS. The pipe system, filled with approximately 4 m3 of local drinking water (TCC = $1 - 2 \times 10^5$ *cells/mL, TOC = 2.4 – 4.8 mg/L), flows in a circular closed loop with approximately 150 m length. With the adjusted volumetric flow rate of around 60 L/min, one round of the flowing water in the pilot plant took approximately 75 min. Under these stable conditions, small amounts (1 v%) of different natural waters ("contaminants") were injected into the system. Table 1 contains an overview of the cell count (TCC) and total organic carbon (TOC) of the injected waters.*

The objectives of the injection experiments were both, defining sensitivity limits of the methods in a flowing system and finding a way to characterize the injected water regarding its origin and potential hazardous components or general cases of contamination. To perform these experiments, the pilot plant had to be adapted (sampling points, new pipes for closed loop, injection point, etc.). Figure 4 shows a flow chart sketch of the final pilot plant version.

(a) (b)

Figure 4: Picture (a) from the indoor part and total flow chart sketch (b) of the Hamburg Wasser pilot plant.

The water quality of the system water was continuously monitored at the first sampling point (S1), located approximately 10 m (approximately 7 min under corresponding flow conditions) behind the injection point. The developed approach of simultaneous flow cytometric and fluorescence spectroscopic PARAFAC analysis (WP 2) was applied to these experiments as well. The monitoring of both was proven powerful in detecting little changes in drinking water. In combination, neither a microbiological change nor a change in organic matter content can be missed. Some exemplary results of the rainwater and wastewater injection experiments are shown in Figure 5. Both experiments simulated kind of contamination scenarios in a pipe system.

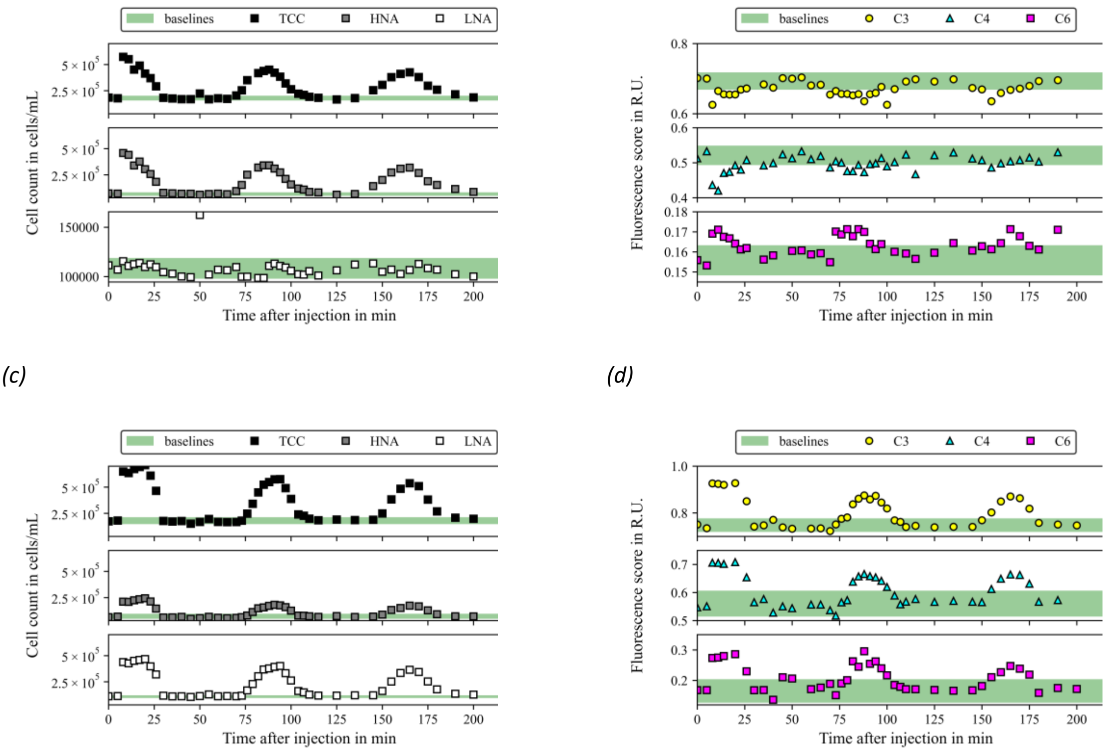

Figure 5: Particular monitoring results of the injection experiments. Cell count (TCC, HNA, and LNA) over time (a, and c), as well as the fluorescence score of three selected PARAFAC components (b, and d). The injected waters had their origin in collected rainwater (a, and b), and treated wastewater (c, and d).

All results show a significant deviation from the pilot plant baselines after approximately 7, 75, and 150 minutes. This correlates with the time duration needed for the water to pass the sampling point (S1) and for the flow circulation two times afterward. Thus, it was possible to detect a little change in the water matrix which was enforced by injecting another type of water into the system. The microbial cell count of both injected waters was higher (> 1.0×10^7 cells/mL) than in the pilot plant water (approximately 2×10^5 cells/mL). However, they differ in the distribution of HNA and LNA cells (see Table 1). Rainwater was dominated by HNA cells, whereas wastewater was by LNA cells. This differentiation is shown by the monitoring results in (a) and (c). It explains how flow cytometric fingerprinting can not only detect contamination but also characterize it. The same was proven for fluorescence spectroscopic PARAFAC analysis. The lower amount of organic matter in rainwater - compared to the pilot plant- results in a reduction of the fluorescence score for C3 and C4 (b). In contrast to this, C6 showed a different behavior for all experiments. This component stands for protein-like organic compounds, and could slightly be correlated to TCC for all experiments. However, it does not show as high sensitivity as the determination of TCC by the flow cytometry. For a higher amount of organic matter in wastewater, all three components show an increase in the fluorescence score in the expected region (d).

The successful performance of this work package is fundamental when it comes to future application in a real WDS. Flow cytometry and Fluorescence spectroscopy including PARAFAC modeling can generate a unique microbial and organic fingerprint of a flowing system. Achieving baseline limit values for parameters, such as TCC, HNA, LNA, and PARAFAC components is significant for detecting critical deviations. In case of an unexpected event/increase/decrease of some parameters, the information must be transferred to the controlled system and the respective reaction will be launched (TUIL). TCC in particular can be used for continuous simulation for predicting the microbial load all over the WDS (Technion).

Technion

Gopinathan R. Abhijith, Leonid Kadinski, and Avi Ostfeld

The efforts of the Technion working group in the project consisted of four working packages. They are explained in detail below:

WP1: Interface between simulations and experiments:

The chosen model by Zhang et al. (2004) was adjusted for MoDiCon by excluding the chlorine compounds from the water quality simulation. The simulations were conducted using EPANET 2.0, including a MATLAB Toolkit for EPANET toolkit (Eliades et al. 2016) via MATLAB 2020a. The simulated main compounds included the mass concentration or total cell count (TCC) of bacteria in the drinking water as well as the substrate concentration utilized for bacterial growth. The model of Zhang (2004) uses a simple Monod kinetics approach where the growth rate of bacteria can be determined, as seen in (1), and the concentration of the substrate is expressed in (2).

$$\frac{\mathrm{dX}}{\mathrm{dt}} = \mu \cdot X \tag{1}$$

$$\frac{\mathrm{dS}}{\mathrm{dt}} = \frac{\mu \cdot X}{Y} \tag{2}$$

Where X is the total count of bacterial cells and S is the concentration of the substrate. In the specific case of the model in Zhang et al. (2004), S represents the biodegradable fraction of dissolved organic carbon (BDOC, dissolved organic carbon: DOC), Y is the growth yield coefficient of bacteria, and μ is the specific growth coefficient. While the model used biodegradable organic carbon (BDOC) as the substrate to model bacterial growth, the challenge for this WP was to simulate parameters that can be validated in online measurements with flow cytometry and fluorescence spectroscopy. The first measurements by the laboratory in the TUHH indicated bacterial growth behavior and the respective DOC. As only a fraction of DOC can be utilized by bacteria as an energy source for growth (Prest et al. 2016), the sole measurement of DOC cannot be used to validate the conducted simulations. Assimilable Organic Carbon (AOC) is a parameter that describes the fraction of easily accessible carbon for present bacteria in drinking water. It is a maximum of up to 5% of DOC. For drinking water analysis, the AOC parameter is more convenient than BDOC. Hammes and Egli (2005) introduced a methodology to determine AOC using flow cytometry where bacteria concentration is observed over several days. To initialize the water quality simulations, the dependency of the specific growth coefficient to the substrate is required, which the bacteria use for growth for correctly modeling regrowth in the WDS model. This specific bacterial growth coefficient μ can be calculated as follows:

$$\mu = \frac{\mu_{max}}{S + K_s} \tag{3}$$

Where μ_{max} is the maximum bacterial growth rate respective to utilized substrate and K_s, the half-saturation constant, is the substrate at μ_{max}/2.

To retrieve the specific growth rate that corresponds to the laboratory experiments of the TUHH, the maximum growth rate of various bacterial growth rate experiment series was plotted over the respective initial substrate concentration as seen in Figure 6. The substrate for these experiments was determined to be AOC. Each data point stands for one growth experiment. To calculate the specific growth rate μ with equation (3), a non-linear parameter estimation was conducted with the conducted. From these data μ_{max} was determined, as well as K_s.

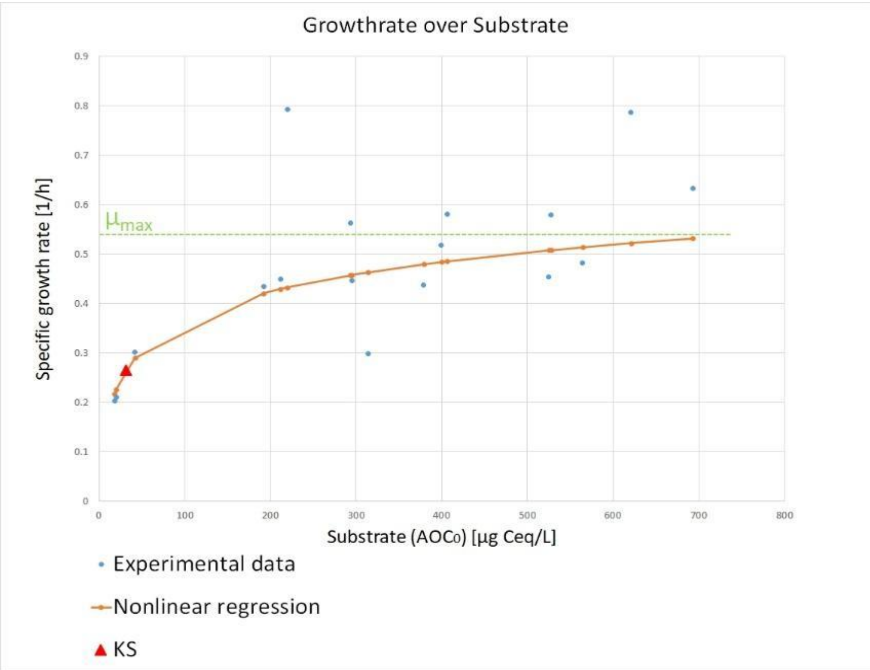

Figure 6: Maximum bacterial growth rate plotted over respective initial substrate concentration (AOC) from 17 experiment series. The non-linear regression was used to determine the parameters for the specific bacterial growth rate.

The calculated values were used for the first simple water quality simulation, which is described below. Monod kinetics was used to model the bacterial growth in the water network inside the simulation tool EPANET-MSX. The various equation coefficients were taken from the laboratory experiment evaluation of the TUHH. The WDS model chosen is the EPANET Net3 network. This study places fixed water quality sensors at nodes 159, 113, 184, 173, and 211, as seen in Figure 7. The presented scenario considers a substrate/organics injection at three network sources (see Figure 7). A minimal specific global level of bacteria in the system must be defined; otherwise, the equilibrium equations cannot be solved. The simulation time was 24 hours, and the duration of the substrate injection in scenarios 1 and 2 was 6 hours from the beginning of the simulation. The substrate concentration, which was injected, was 300 µg/L per minute.

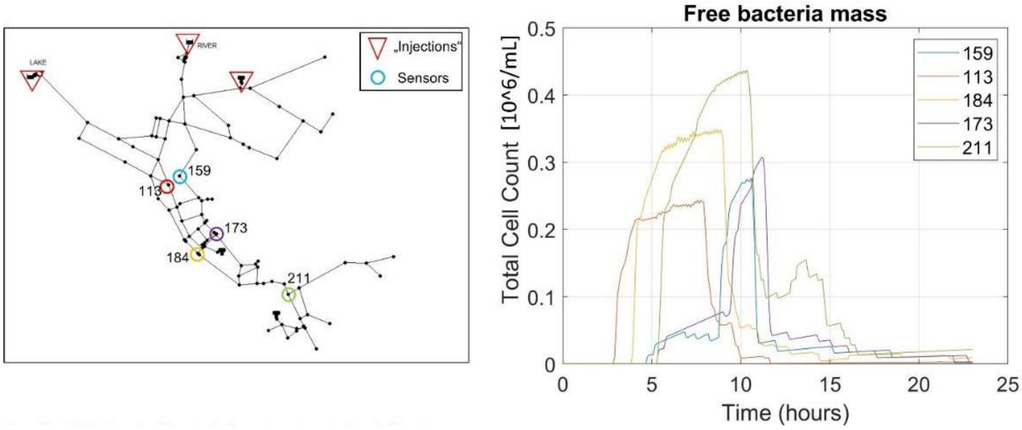

Figure 7: Example scenario simulated applying the bacterial regrowth model.

After establishing the interface between the laboratory experiments and the water quality simulations, the overarching goal was to validate the model through a sensitivity analysis using flow experiments. After the validation, the model was fused with deepened simulations (see WP-2) and expanded continuously.

WP2: Deepened, complex water quality simulations with chemical and biological compounds.

The tasks completed for WP-2 involved a comprehensive review of relevant literature pertaining to chemical and biological water quality parameters in WDS, building an environment (EPANET-C) for performing flow and transport simulations of relevant water quality parameters, and conducting deepened simulations in drinking WDS. EPANET-C is designed to be an advanced open-source extension of EPANET–EPANET-MSX modeling. It uses function directories to integrate the necessary resources for implementing multi-species reactive-transport (MSRT) models via the well-established EPANET–EPANET-MSX framework.

EPANET-C incorporates fifteen multi-species reactive-transport (MSRT) modules, each integrating the transport (via advection) and exchanges (physical, chemical, physicochemical, and biochemical reactions) of different combinations of the eleven reacting constituents i.e., nine abiotic constituents – chlorine, total organic carbon (TOC), biodegradable dissolved organic carbon (BDOC), trihalomethanes (THMs), 2,4,6-trichlorophenol (2,4,6-TCP), 2,4,6-trichloroanisole (2,4,6-TCA), perfluorooctaneamido betaine (PFOAB), perfluorooctaneamido ammonium salt (PFOAAmS), and perfluorooctanoic acid (PFOA) – and two biotic constituents – planktonic and biofilm microorganisms. The scientific information reported in our works was comprehended to establish the theoretical backgrounds of these modules. The conceptual model graphic of the comprehensive EPANET-C module (named 1234) is illustrated in Figure 8.

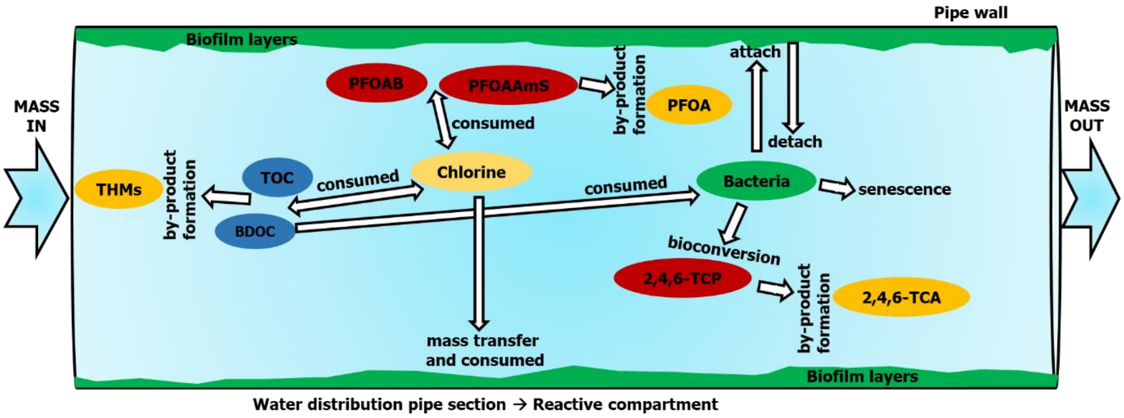

Figure 8: Conceptual framework of EPANET-C MSRT Module 1234.

EPANET-C is developed to be used as a shared object library. Thus, the programming interface of MATLAB was utilized for its calling and for water quality model implementation. However, to make the programming necessities in MATLAB more effortless or altogether bypass the same, the EPANET-C function directories were devised and operated. These in-built function directories of EPANET-C comprise every information concerning the MSRT modeling. This includes the type and number of reacting constituents, conceptual information about the multi-species reactions, values of reaction rate coefficients, and the governing equations for all the contamination events simulated by applying EPANET-C.

Presently, EPANET-C is developed to function as an advanced extension of EPANET – EPANET-MSX modeling. A MATLAB (not older than the 2017b version) interface was created to attain this. The EPANET-C–MATLAB interface facilitates the loading and opening of the EPANET-C function libraries, provides input information, and implements hydraulic and water quality modeling. The hydraulic modeling and water quality modeling, precisely MSRT modeling, are executed using the EPANET and EPANET-MSX dynamic link libraries (DLL) for Windows. The EPANET-MATLAB toolkit was employed in this direction to utilize the EPANET and EPANET-MSX DLL. In total, the EPANET-C–MATLAB interface integrates the internal functions to make direct calls to the EPANET-MATLAB toolkit and performs MSRT modeling of WDS.

WP3: Data-driven event detection algorithms

A brief overview of the second work package, which deals with training machine learning algorithms with real-life water quality data to determine possible water quality anomalies, is given below. Recent studies have used machine learning methodologies to detect water quality anomalies and their sources by training these algorithms with specific water quality parameters as input features to predict possible water events. Artificial and convolutional neural networks (ANN/CNN) and support vector machines (SVM) have been used to detect whether a contamination event has occurred in a water network (Asheri et al., 2019; Ashwini et al., 2019). MoDiCon´s associate partner, Hamburg Wasser, the water utility of Hamburg, provided the project with a significant amount of water quality data for five years. The data from 22 sampling points in 19 waterworks was pre-processed and analyzed with various data evaluation packages in Python. The overarching goal was to train an ANN and a random forest algorithm with parameters that can be measured online to determine whether there is an anomaly in the water network. Figure 9 shows a conceptual layout of an ANN where the respective data for the input and output layer of the neural network is shown. The overarching goal was to create a support tool for water utilities to explore water quality online and in real-time and understand whether additional laboratory check-ups of the water quality need to be conducted.

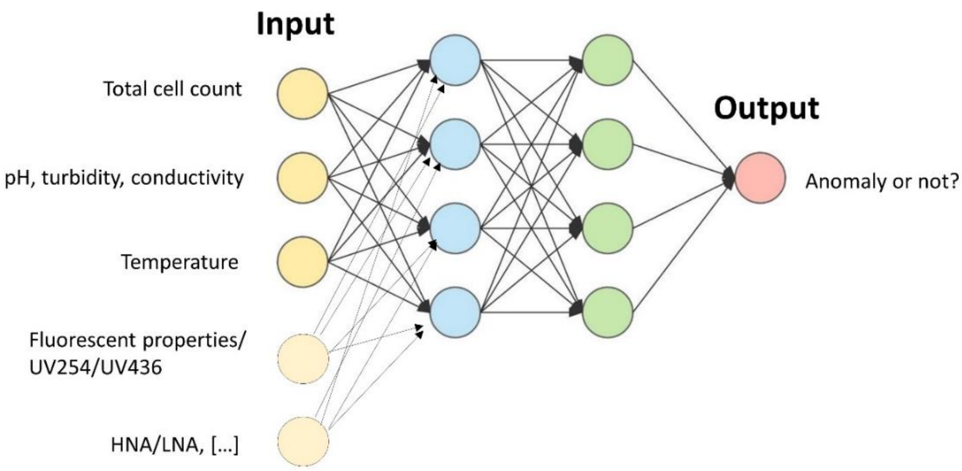

Figure 9: Conceptual layout of ANN where input features are water quality parameters that can be measured online and the output is a prediction of a possible anomaly in the water network system.

WP4: Modeling framework for sensor placement and source detection.

After the first pre-processing and evaluation of the water quality data, the correlation of various parameters was conducted to understand for which parameter it is reasonable to train the ANN. Although a significant amount of data was provided, there was still a lack of various organic water quality parameters in the dataset. The sparse dataset was imputed with the k-Nearest Neighbor Imputation method. After preparing the data, an ANN and random forest algorithm were trained to predict water quality anomalies. The accuracy of the random forest algorithm for predicting a water event came out to 97% which is considerably very high. However, it must be acknowledged that it came from primarily true negatives, not true positive water event predictions.

Utilizing a data-driven model as a support tool for water utilities is a promising technology. It should be explored further with support from Hamburg Wasser, who can evaluate the use they could have from it as a water utility. However, due to insufficient data, WP-3 was not explored further for contamination detection in WDS in this project.

Computer-based physical modeling tools that simulate water quality variations in WDS are functional solutions for monitoring WDS integrity and adequately fit the framework for sensor placement locations identification and detecting contamination events. WP-4 developed EPyT-C (in which C stands for any contaminant), a Python-based package allowing the simulation of the transport and fate of multiple water quality parameters in WDS. EPyT-C constitute in-built modules that conceptualize the scientific understanding of the physical, physicochemical, and biochemical interactions concerning water quality parameters within the distribution network realm, mathematize them as one-dimensional advective-reactive equations, and numerically solve them to emulate the spatiotemporal distribution of the quality of water delivered via WDS.

EPyT is an open-source software, initially developed by the KIOS Research and Innovation Center of Excellence, University of Cyprus, operating within the Python environment to provide a programming interface for the latest version of EPANET 2.2 (Rossman et al., 2020). It calls EPANET a shared object and employs an Object-Oriented approach for interfacing EPANET with Python. Though EPyT can be employed for performing single-species water quality analysis, which comes within the scope of EPANET 2.2, it lacks MSRT modeling capability in its current form. In other words, EPyT can only analyze one water quality parameter at a time. Consequently, the water quality modeling compartment of EPyT needs to be improved to solve several real-world problems concerning water quality variations during delivery via WDS. A fully independent water quality modeling extension, EPyT-C, is developed in this direction. The source code of EPyT-C calls EPyT and employs the hydraulic solver of EPANET 2.2 for performing hydraulic simulation, which the in-built water quality solver then utilizes for performing MSRT modeling.

In its current form, EPyT-C comprises two in-built modules - the 'Chlorine decay and Trihalomethanes formation' module and the 'Bacterial regrowth' module. The former EPyT-C module encompasses all the required details on the physical and physicochemical interactions of the following three water quality parameters: free available chlorine (FAC), total organic carbon (TOC), and trihalomethanes. The latter contains details on the physical, physicochemical, and biochemical interactions of the five water quality parameters: FAC, recalcitrant dissolved organic carbon, biodegradable dissolved organic carbon, free-living bacteria (suspended heterotrophic bacteria), and free dead bacteria. Based on the module selected for WDS analysis, EPyT-C evolves partial differential equations and ordinary differential equations governing the propagation and formation/ degradation of the corresponding water quality parameters within the distribution network realm. Once the governing equations (advective-reactive equations) are framed, the numerical method that involves the explicit method of characteristics and the fourth-order Runge-Kutta method is applied to derive numerical solutions – spatiotemporal distribution of complex water quality parameters in WDS.

EPyT-C offers the following flexibilities, making it a handy tool for research and industry: 1. Allows time-series variations in the input values for the water quality parameters at the sources (reservoirs and booster nodes). 2. Customize the random fluctuations in the input values for the water quality parameters at the sources. 3. Customize the perturbations in the reaction rate coefficient values. 4. Customize the outputs and export the data as Excel files or other formats (Figure 10). 5. Customize the numerical accuracy by altering the model parameters (time step, velocity tolerance, etc.). 6. Control the computational efficiency by adjusting the accuracy of the numerical solutions.

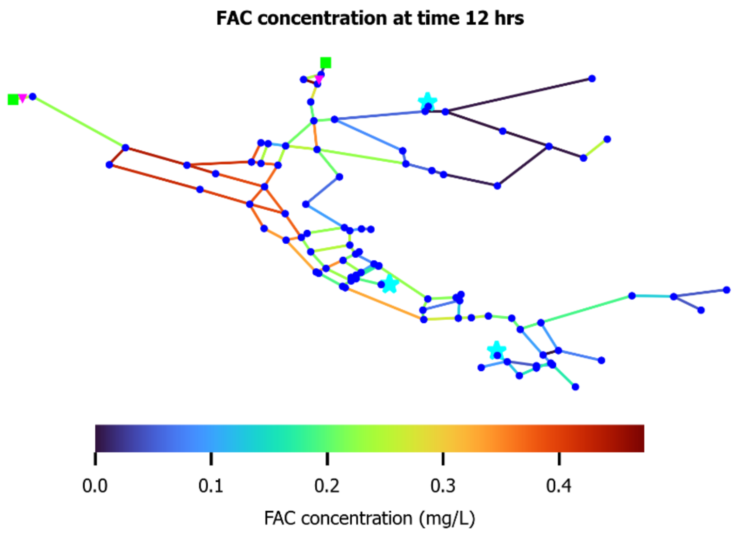

Figure 10: Spatial distribution of FAC at time = 12 hours within the benchmark test network (EPANET Network 3) corresponding to FAC concentration 0.5 mg/L at the river and lake water source outlets. The TOC concentration values at the river and lake sources outlets were maintained at 3 mg/L and 1 mg/L, respectively. The simulations were performed using the 'Chlorine decay and Trihalomethanes formation' module of EPyT-C. The squares denote reservoirs, stars indicate tanks, and circles indicate junctions. The lines specify links connecting reservoirs, tanks, and nodes.

In conclusion, EPyT-C is a practical tool that can assist the scientific community and water utility managers in examining WDS performance under different operating scenarios. EPyT-C scripts are under continuous development and can be further extended and improved by users and developers for specific applications. Forthcoming works involve advancing EPyT-C modeling capability to simulate dispersive transport.

TUIL

Hao Cao, and Pu Li

WP1: Modeling of the water quality

In the first working package, a water quality model has been developed for the optimization model in the following. For the water quality of WDS, a one-dimensional advection equation with reaction is very common to be used:

$$\frac{\partial C_i(x,t)}{\partial t} u_i \frac{\partial C_i(x,t)}{\partial x} + rC_i(x,t) = 0 \qquad (4)$$

where $C_i(x,t)$ = chlorine concentration inside the pipe i at point x and time t ; u_i = flow velocity in the pipe i with changing sign as the flow changes its direction, r = reaction coefficient which is pipe-dependent for a component such as chlorine for example, which is named as bulk and wall reaction (Rossman et al. 1994). Since

$$\frac{\partial C_i}{\partial t} = \frac{\partial C_i}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial C_i}{\partial t}$$

$$= u\frac{\partial C_i}{\partial x} + \frac{\partial C_i}{\partial t} = rC_i \qquad (5)$$

$$C_i(x(t),t) = C_{i0}e^{rt}$$

Function (5) reveals that the chlorine concentration change in a WDS is a decay process, i.e. the concentration at a position within a pipe can be calculated by the time it takes for the water to travel from *the starting of the pipe to this position. With the help of this function, the component (chlorine) concentration at every node depends on the initial value, reaction coefficient r and time t.*

In the work that followed, Function (5) is used as a simplified water quality model in optimization models.

WP2: Nonlinear optimization model

In this working package, a nonlinear optimization problem was formulated based on hydraulic and water quality, numerically implemented, and solved to achieve the specified chlorine concentration within a reasonable range in a WDS.

Hydraulic characteristics include several parameters of the WDS, such as pressure, head loss and flow. One of the most important parameters for water quality control is the flow velocity in the pipes. EPANET can be used for calculating the velocity, but it is challenging to use its results for solving optimization problems. Two new methods were proposed to obtain a suitable form that can be applied to the water quality model and optimization. The Hardy cross method (Brkić et al. 2019) is a classic iterative method for determining the flow in pipe networks. We proposed the maximization of energy conservation as a novel method to compute the flow in a pipe network. In addition, the flow control valve (FCV) is one of the most critical actuators of the WDS with the control system. Therefore, we proposed to manipulate and redistribute the flow velocity in the pipelines with the FCV.

For this purpose, a nonlinear optimization problem was formulated based on the hydraulics and water quality model, numerically implemented, and solved to achieve the specified chlorine concentration within a reasonable range in a WDS. The mass and energy conservation laws were employed to describe the hydraulic properties of WDSs. The one-dimensional advection transport model was simplified to describe the decay of chlorine in the pipelines. The chlorine concentration limits at the nodes were formulated as inequality constraints which will be satisfied by manipulating the flows and their directions in the pipelines. The optimization problem is expressed as follows:

$$\begin{aligned} &\min_{q_1 \cdots q_{np}} \frac{1}{2}\sum_{c=1}^{n_c}\Big(\sum_{j=1}^{n_p} L_{cj} k_j \left|q_j\right|^{1.852}\Big)^2 \\ &subject\ to: NQ = D \\ &Lower\ limit < Ci < Upper\ limit \\ &0 \le \left|q_j\right| \le q_{max}, \forall j = 1, \ldots, n_p \end{aligned} \tag{6}$$

where $|q|_j$ is the flow rate in pipe j. The absolute value here is to consider changes in the flow direction. The equality constraint and the inequality constraint are used to describe the constraint of flow rate in each pipe and chlorine concentration at certain nodes. A model-based optimal control strategy was developed based on this optimization model. The interior point solver (IPOPT) for large-scale nonlinear optimization (Waechter et al. 2006) was used to solve the nonlinear optimization problem. Figure 11 shows a selected benchmark network model 1 with two loops, A-B-F-E and A-C-D-B as a case study.

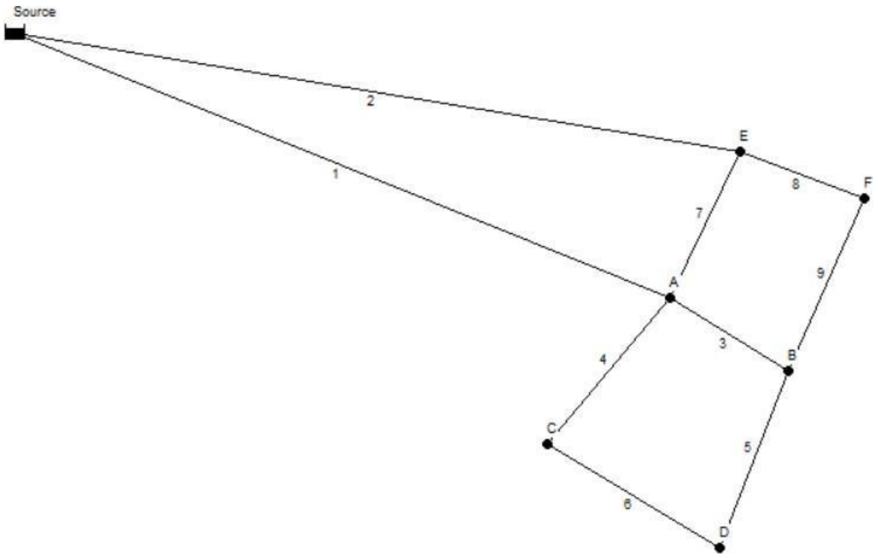

Figure 11: WDS with two loops.

The whole system has one reservoir, 6 nodes, and 9 pipes. Assuming a chlorine concentration of 1.2 mg/L in the reservoir and node concentrations should be between 0.1 - 0.3 mg/L. In the operation, the concentrations at some nodes are outside this range and we aim to compute a new operation strategy so that they go back to the specified range. The elevation of the reservoir and all other nodes are 80 m and 5 m, respectively. All pipes have the same diameter and roughness of 500 mm and 100. The length of pipes 1 and 2 is 13,608 m and all other pipes are 2,268 m.

Table 2: Results of model 1.

Node ID	**Demand**)$(\mathbf{m^3/h}$	**Chlorine concentration (mg/L)**		**Pipe ID**	**Flow rate** $(\mathbf{m^3/h})$	
		Original system	After FCV Placement		Original system	After FCV Placement
Reservoir		1.2	1.2	1	100.2	114.5
A	0	0.35	0.45	2	99.82	86.10
B	30	0.21	0.24	3	54.23	54.55
C	30	0.26	0.30	4	63.53	44.81
D	80	0.14	0.16	5	46.46	65.38
E	30	0.39	0.30	6	33.53	14.71
F	30	0.27	0.23	7	17.59	-15.02
				8	52.22	71.03
				9	22.23	40.93

Table 2 shows the results of solving the optimization problem. In the original operation, at node E, the concentration is higher than 0.3 mg/L. Using the optimized operation with the FCVs placement, each node now has an acceptable chlorine concentration. In comparison to the original operation, there is a significant change in the flow rate in each pipe, even with a change in flow direction in pipe 7. This means that chlorine concentration has been effectively controlled by the FCVs placement.

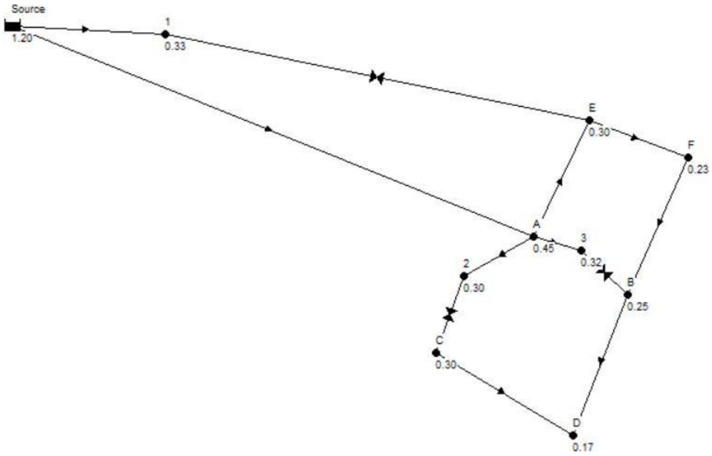

Figure 12: WDS with two loops with FCV placement.

Figure 12 shows the FCV arrangement and the simulation result from EPANET, with three FCVs installed in the WDS, and the chlorine concentration of each node. Compared to the calculation results in Table 3, the error of concentration of chlorine at each node from the simulation is very small. The results of this section give us a way to use FCV in water quality control and thus water quality management by controlling the flow rate as well as the direction in the pipes.

WP3: MINLP Optimization model

A MINLP approach was developed in this working package to optimize the placement of isolation valves. We aim to keep the chlorine concentration in the specified range in the network. The simplified one-dimensional advective transport model describes the decay of chlorine in the pipes, and the mass and energy conservation laws are enforced as nonlinear constraints. In addition, binary variables are used to describe the placement of valves as possible isolation valves that can either be opened or closed. The MINLP problem is defined as follows:

$$\min Amount(i) \tag{7a}$$

$$\text{subject to: } Nq - D = 0, \tag{7b}$$

$$q(-N^T P - N^T e - h_f(q)) \geq 0, \tag{7c}$$

$$-N^T P - N^T e - h_f(q) - Mz \leq 0, \tag{7d}$$

$$z_j + z_{n_p+j} \leq 0, \qquad \forall j = 1,\dots,n_p, \tag{7e}$$

$$\sum_{j=1}^{2n_p} z_j = n_v, \tag{7f}$$

$$\sum_{j=1}^{2n_p} q_j z_j = 0, \qquad \forall j = 1,\dots,n_p, \tag{7g}$$

$$P_{\min} \leq P_i \leq P_{\max}, \qquad \forall i = 1,\dots,n_n, \tag{7h}$$

$$0 \leq q_j \leq q_{\max}, \qquad \forall j = 1,\dots,n_p, \tag{7i}$$

$$Concentration_{\min} \leq Concentration_i \leq Concentration_{\max}, \quad \forall i = 1,\dots,n_n, \tag{7j}$$

$$z \in \{0,1\}^{2n_p}, \tag{7k}$$

where the objective function (7a) is to minimize the chlorine amount to be injected into the WDS at position i. n_n and n_p are number of nodes and pipes in the WDS. To ensure the hydraulic feasibility of the solution, (7b) expresses the mess conservation law of each node, (7c) and (7d) consider the energy conservation law of each pipe with and without isolation valve, respectively. The flow direction can be changed due to the valve arrangement, therefore the node-pipe incidence matrix is N ∊ R2np×nn. $h_f(q)$ is the head loss of each pipe, for which the Hazen–Williams equation is used in this study. q_j and P_i are flow and pressure on every pipe or node. z_j is a {0, 1} vector, that expresses there is no isolation valve or there is one. Each segment is a constant to express the head loss on isolation valves, since the valves are closed after placement, M in (7d) is a large enough value in this study. The inequality (7e) is a constraint to guarantee that only one valve is allowed to be placed on each pipe, and the quality constraint (7f) considers the total number of valves to be placed in the network n_v. The equality (7g) describes the pipe with an isolation valve having no more flow. The minimum and maximum pressure and flow in each node and pipe are defined by (7h) and (7i), respectively. (7j) is the constraint of chlorine concentration at a certain node. (7k) is the binary constraint to specify whether or not a valve is fitted on a pipe. In this study, Bonmin has been used to solve the MINLP model (Bonami et al. 2011.)

The MINLP model is implemented and validated by using a benchmark WDS shown in Figure . The lower bound of residual chlorine concentration and pressure was set to 0.45mg/L, and 20m, respectively. The optimization result is shown in Table 3 and Table 4. In the first step, no valve is considered in the WDS as the initial scenario, i.e., in the MINLP model$n_v = 0$. It can be seen from Table that the minimum chlorine concentration is maintained, but the sum of residual chlorine in the WDS is quite high. Generally speaking, the more valves installed in the WDS, the less the total amount of chlorine that needs to be injected into the water source to maintain the minimum concentration of WDS residual chlorine, and the lower the maximum concentration, as well as the total sum of residual chlorine in the system. However, the difference between the results of using 1 to 3 valves and 4, to 5 valves is not significant, as shown in Table 3. The reason may be due to the fact that the MINLP model is not convex and thus the solver cannot guarantee a global solution.

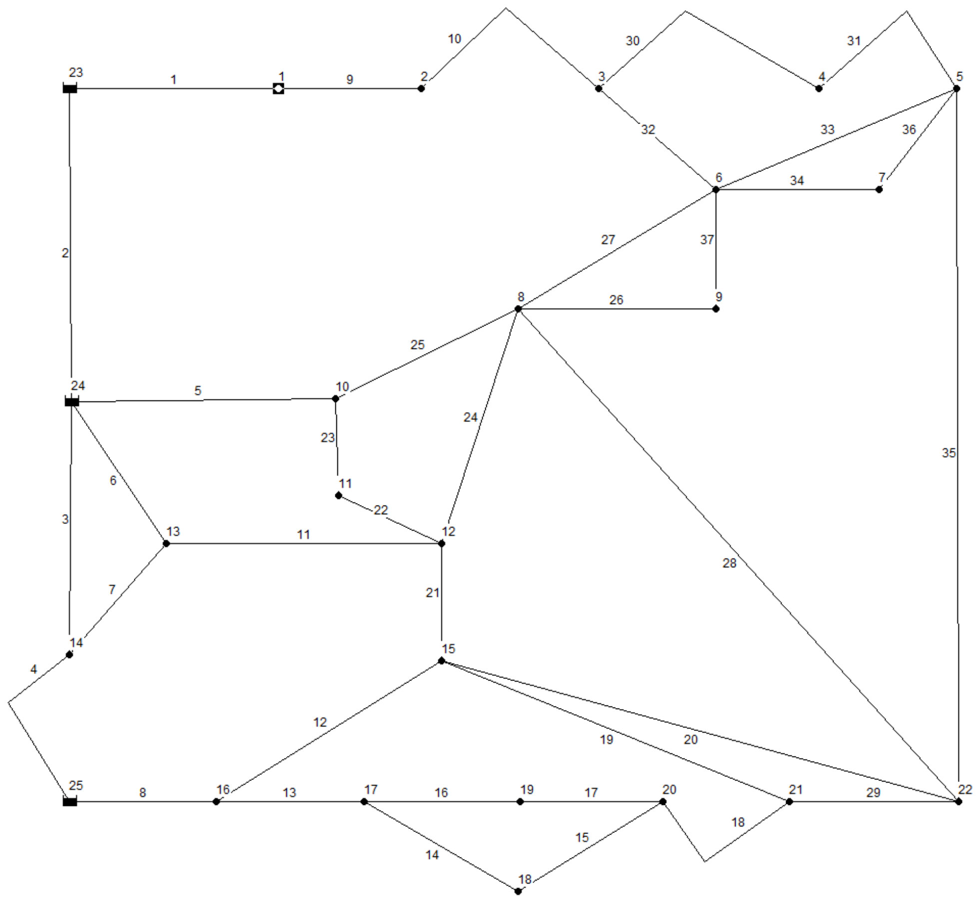

Figure 13: A benchmark water network.

Table 3: Number of valves to be used and the corresponding chlorine concentration.

Concentration (mg/L)	0 valve (Initial)	1 valve	2 valves	3 valves	4 valves	5 valves
Reservoirs (23,24,25)	1.35	0.96	0.96	0.96	0.7	0.7
Minimum in WDS	0.45	0.45	0.45	0.45	0.45	0.45
Maximum in WDS	1.30	0.93	0.93	0.93	0.68	0.68
Sum of residual Chlorine	22.42	16.19	16.19	16.5	12.56	12.63

Table 4: Number of valves and their position.

Number of valve(s)	Position of the valve (Pipe ID)
1	31
2	31,35
3	12,31,35
4	10,20,31,35
5	10,19,20,31,35

Table 4 shows the resulting optimal positions of the valves. It can be seen that there are several pipes, such as 31, and 35, have always been chosen, which means that such pipelines have a higher potential to affect the residual chlorine.

The results of this section lead to a method to place isolation valves in water quality control so that the concentration of disinfectant in the water can be controlled by closing or opening specific pipes, thus affecting the quality of the water. This method can also be used to design control strategies after contamination in the WDS to separate the contaminants and reduce their impact.

WP4: Testbed design and construction

A testbed to verify the computed control strategy was designed and constructed. Figure 14 shows the structure of the testbed.

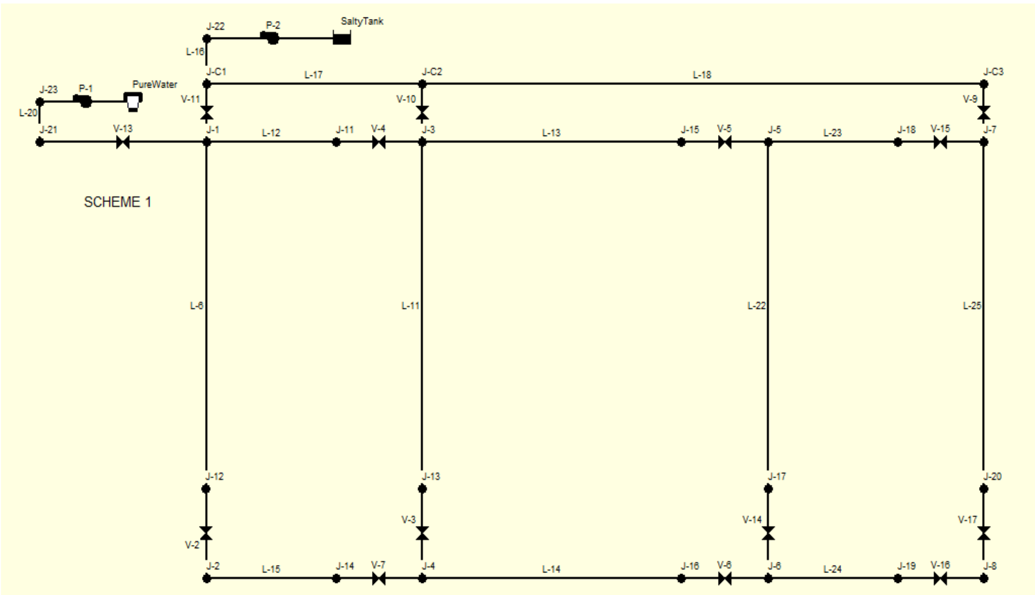

Figure 14: Structure of the testbed.

The entire network includes water tanks, pumps, valves, pressure sensors, water quality sensors, and flow sensors. For the first study, we plan to study the case of bringing salty water into the system as a contaminant and detected by the conductivity sensors in the system. Then the valves and pumps are manipulated by the control strategy to reduce the contamination in the possibly shortest time.

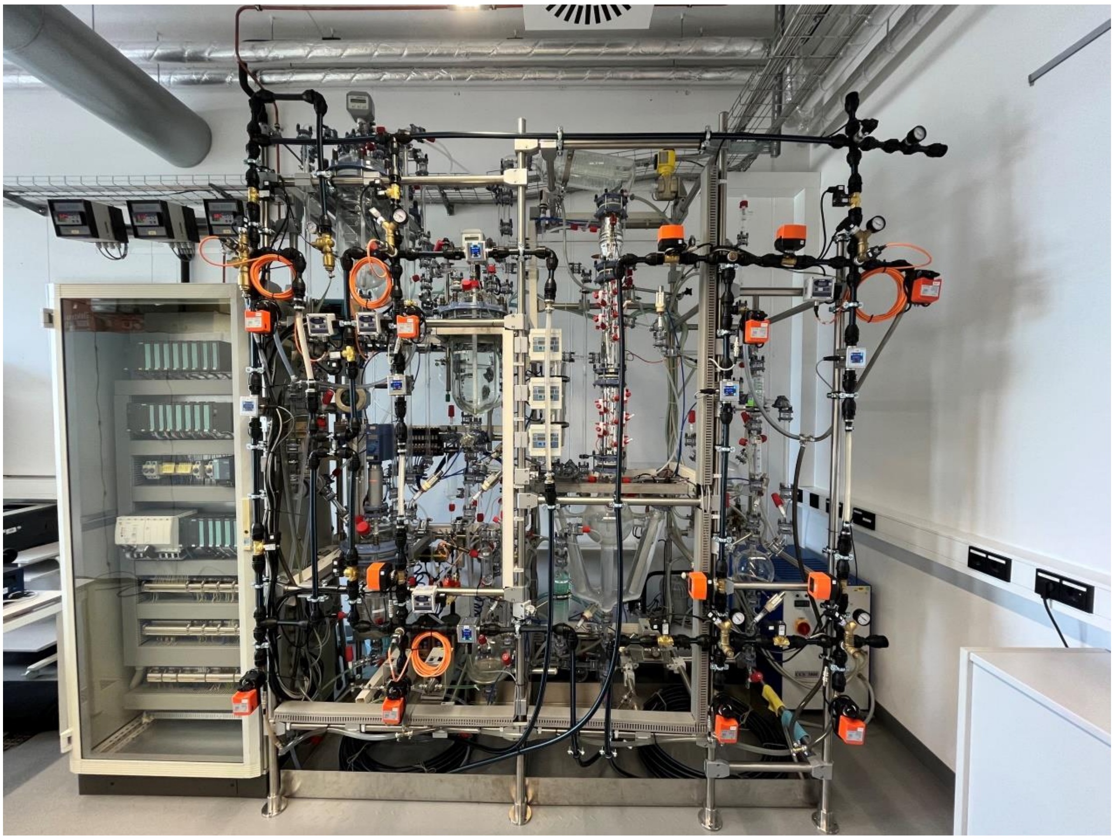

Figure 15: TU Ilmenau testbed.

Figure 15 shows the constructed testbed. Figure 16 is the monitoring software interface of the testbed established.

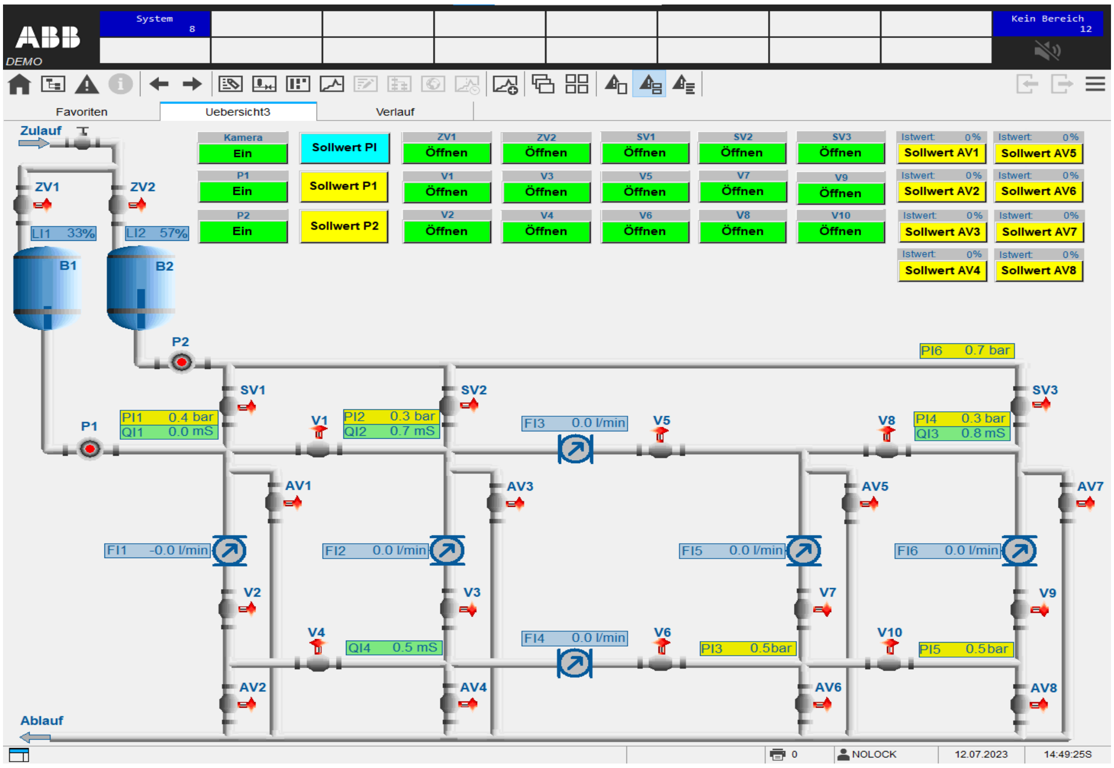

Figure 16: Monitoring interface of the testbed.

WP5: Experiment on testbed

After the testbed construction was completed, experiments were conducted to test the pipe flushing in case of contamination. In addition, we designed a control system to realize the manipulation of this testbed.

Many different scenarios of contamination were tested. Fig. 17 shows the experimental results of one scenario of contamination. It includes 8 time-dependent trajectories, which are the water quality, water pressure, and control signal of the valves and pumps, respectively. At the bottom of the last graphic, the time points of T1 to T5 are marked. In this scenario, we assume that the contamination happened from T1 to T2, then an alarm was given at that moment. From T3 to T5 different actions of the valves separated (isolated) the contamination and then flushed the pipes. It is seen from the first graphic that, from T5, the water quality was within the specified range, i.e., the WDS was recovered to normal operation.

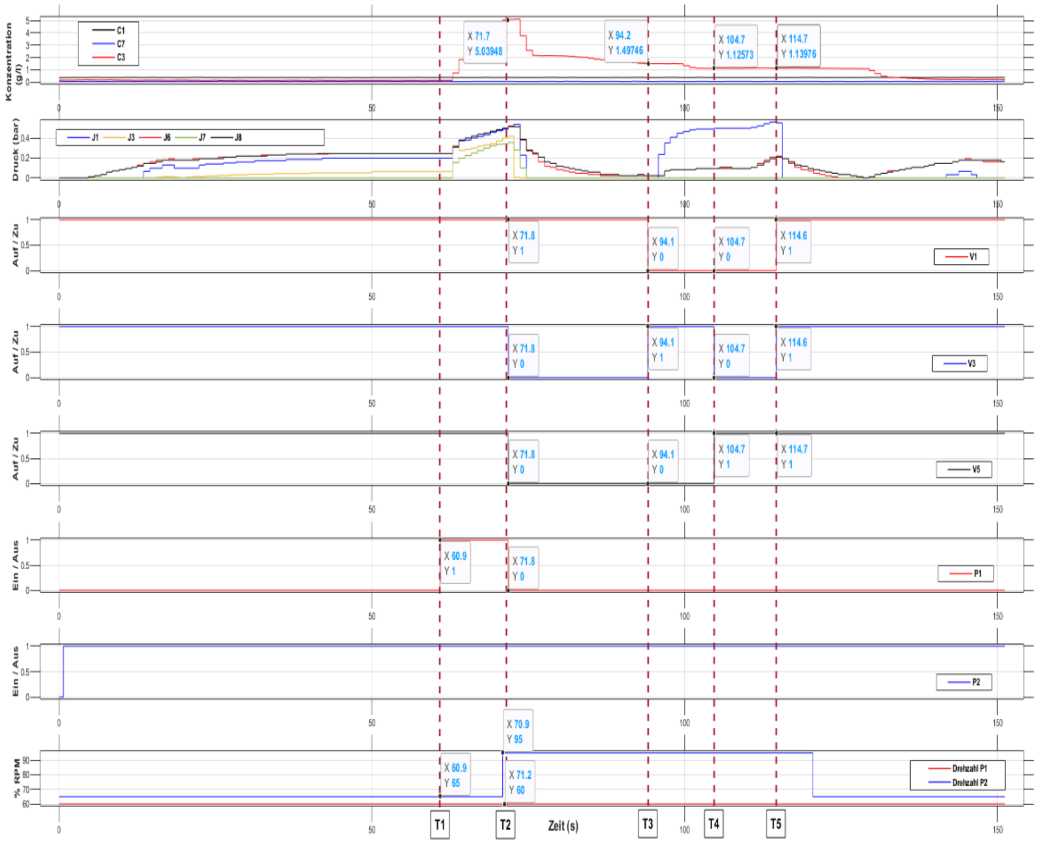

Figure 17: Signals of pollution and flushing process of the testbed.

Joint conclusions

The MoDiCon project aimed the development of a future digitalized WDS and its main challenges of dealing with crucial water quality change. With respect to the rapid characterization of the water quality, the combination of flow cytometry and fluorescence spectroscopy (including PARAFAC) was proven as a successful method that can be implemented in future standardized applications. The further development showed the opportunities for detailed organic and microbial fingerprinting. Even little changes in water matrices are possible to detect, thus, contaminated water can be further characterized. The computer-based tools capable of simulating the quality fluctuations that can act like digital twins are critical for developing digitized WDS. The real-world data paucity is a limiting factor in developing data-driven modeling tools in this regard. Conversely, the development and performance of physics-based models were found to be significantly impacted by numerous factors such as water temperature, type of *microbial species present, growth-limiting nutrients availability, the presence of residual disinfectant and other inhibitory substances; microbial attachment/ detachment to/from the pipe walls; biofilm formation; particle deposition; and sediment re-suspension. Within these limitations, the physics-based models developed could adequately forecast microbiological water quality in WDS, specifically total cell count (TCC). Due to the many processes considered and the interrelation between the model parameters signifying the mechanisms governing water quality, the reliability of predictions of the physics-based models was found to be highly sensitive to epistemic uncertainty. Forthcoming works involve advancing modeling capability to simulate and predict different water quality parameters within the WDS. These computer-based simulation tools, combined with installed flow cytometry and fluorescence spectroscopy, enable the monitoring and prediction of water quality all over the network. Actual measuring, as well as simulating of water quality, were interfaced with reaction and controlling methods. Therefore, individual characteristic baseline limits were established for flow cytometric and fluorescence spectrometric (PARAFAC) parameters. Considering autonomous controlling, two new optimization methods were proposed. For both, successful simulations were performed and showed the potential of those implanting in a real WDS. Furthermore, a newly designed test bed was used to simulate different automated contamination and reaction processes in a small-scale network.*

In terms of applying the MoDiCon outcomes to the real world, it has to be mentioned, that the developed systems need to be further tested under real circumstances such as in a real WDS. Although the individual methods are sufficiently developed and evaluated in a common laboratory and pilot plant framework, especially the communication between measured values, simulation, and reaction must be validated for a real WDS. Furthermore, bringing the developed methods into practice faces several application challenges. In particular, the conversion of automated monitoring stations, valves, and control equipment required a great deal of work as well as expenses. In addition, employees of water utilities must also have the appropriate qualifications to be able to work with such automated systems. However, other research groups and water suppliers can use published methodologies based on the MoDiCon outcome to improve water quality surveillance.

Publications, patents, inventions:

Journal publications:

Abhijith, G. R., and Ostfeld, A. 2023. Assessing uncertainties in mechanistic modeling of quality fluctuations in drinking water distribution systems. ASCE Journal of Environmental Engineering (Accepted for publication).

Ostfeld, A., and Abhijith, G. R. 2023. Digital Twin for Water Distribution Systems Management—Towards a Paradigm Shift. ASCE Journal of Pipeline Systems Engineering and Practice Forum, 14(3), 02523001. https://doi.org/10.1061/JPSEA2.PSENG-1486 Date of publication: May 13, 2023.

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