Addressing Drinking Water Contamination: A Case Study Comparing Traditional with Model-Based Approaches

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Abstract: Rapid and effective decision-making is crucial during drinking water contamination events to ensure public safety. This paper examines a case study where a water utility, responding to customer complaints, suspected wastewater contamination in its network. We compare the traditional expert judgement approach to a model-based approach using the PathoINVEST tool. The tool performs simulations of contamination events informed by sensor measurements, identifies contamination sources using sampling results, and suggests optimal valve closures for mitigation. Our findings show that the model-based approach significantly enhances response efficiency and accuracy. It identified the contamination source with four samples in 1.3 h, compared to 11 samples in 3.7 h for the traditional approach, and resulted in a lower infection risk (12% versus 20%) at the time of source identification. Regarding valve closure, the model-based approach performed better, resulting in a 3%-point reduction in infection risk compared to the traditional approach. Modeling uncertainty is addressed by considering valve settings uncertainty; despite a 0.7% discrepancy in valve settings compared to the model, the tool accurately pinpointed the contamination vicinity 75% of the time. These findings support the claim that integrating modeling and sensor tools into emergency response protocols for drinking water contamination events can improve early identification and mitigation, potentially safeguarding public health in urban water supply systems. **DOI: 10.1061/JWRMD5.WRENG-6841**.

Author keywords: Drinking water contamination modeling; Source identification; Emergency response; Water utility; Valve manipulation.

Introduction

Ensuring the safety of drinking water is a primary concern of water utilities worldwide. Contamination events in the drinking water distribution network (DWDN) can arise from human error, infrastructure failures, main repairs, or malicious attacks (Winston et al. 2003; Hrudey and Hrudey 2004; Blackburn et al. 2004; Arnone and Walling 2007; Fewtrell et al. 2011; Laine et al. 2011; Cann et al. 2013; Lendowski et al. 2015; Blokker et al. 2018) directly impacting public health and well-being (Kunz 2024). Advancements in monitoring and remediation technologies have enhanced our ability to respond to such events (Erickson et al. 2019), yet there remains a challenge in effectively using real-time modeling tools to aid responsible authorities (Eliades et al. 2023).

Despite already established protocols and tools for emergency response, pathogen-related contamination events in the DWDN continue to affect communities. Communication gaps and the underutilization of available technologies play an important role. Rapid and effective decision-making is crucial during such events; delays or inaccuracies in addressing these situations can lead to more people affected, escalated health risks, economic losses, and prolonged recovery periods (Laursen et al. 1994; Corso et al. 2003; Ailes et al. 2013; Chyzheuskaya et al. 2017; Gude and Muire 2021). Moreover, repeated or mismanaged events erode public trust in the

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Note. This manuscript was submitted on September 11, 2024; approved on October 3, 2025; published online on April 1, 2026. Discussion period open until September 1, 2026; separate discussions must be submitted for individual papers. This paper is part of the ***Journal of Water Resources Planning and Management***, ASCE, ISSN 0733-9496.

safety of drinking water, which is a foundation of urban living and public health (Anadu and Harding 2000).

Currently, when a DWDN is contaminated by wastewater, water utilities activate their crisis management procedures to find the suspected contamination source and minimize as soon as possible the impact of contamination through mitigation measures (USEPA 2003). Traditional decision-making during the crisis management procedure has been predominantly guided by past experience, best practice industry protocols, and expert judgment based on (limited) available information on the contamination event. Regarding their knowledge of the network characteristics, water utilities rely on solvers (e.g., EPANET, WATERGEMS, etc.) to model the hydraulics and water quality dynamics. While experts using those modeling tools are consulted, their input often comes after a critical window of opportunity (sometimes after 24 h have passed). They frequently rely on outdated network characteristics and slower, generic (not dedicated to wastewater contamination events) models, without being able to model the health impact of a contamination.

In this study, a traditional approach represents the status quo of current practices in water utilities (expert judgment, past experience, offline generic modeling), while a model-based approach uses real-time modeling tools for pathogen propagation based on stochastic water demands, health risk assessment, and support in decision-making. Hence, the hypothesis of this study is that the integration of modeling tools (model-based approach) with current practices (traditional approach) can enhance responses and reduce the negative impacts of contamination events.

Recently an analytical tool named the Pathogen contamination INVESTigation decision support system (PathoINVEST) (Paraskevopoulos et al. 2022) was developed as part of the EU-funded Pathogen Contamination Emergency Response Technologies (PathoCERT) project. The objective of the project was to enhance the coordination capabilities of first responders during pathogen contamination emergencies. PathoINVEST is a decision-support tool that helps water utilities during emergencies. It is built as a QGIS plugin and it uses the software EPANET-MATLAB Toolkit (Eliades et al. 2016) and a benchmark hydraulic and quality model incorporating various factors (e.g., pathogen concentrations in contamination sources, pathogen inactivation and chlorine demand kinetics, and stochastic water demands). This tool not only simulates contamination events and their health impact realistically but also suggests potential sampling locations to identify the suspected source of contamination and optimal valve closure strategies for mitigation strategies.

PathoINVEST was applied in three European case studies (Spain, Cyprus, and the Netherlands). Each of the case studies had distinct network characteristics, while the overall goal was to use the tool during the decision-making process of handling a contamination event. Emergency response teams were formed, comprising individuals from relevant sectors (water utilities, civil protection, and health care). The teams incorporated their own network characteristics into PathoINVEST and, in the end, were able to simulate the contaminant transport, find the source of contamination, assess the risk of infection, and finally mitigate the health impact.

This paper addresses the challenge of rapidly finding the contamination source and minimizing the population's health risk through mitigation measures, aiming to improve traditional methods by incorporating modeling tools in the decision-making of emergencies. The objective is to quantify the health protection and operational efficiency benefits of using a model-based approach by systematically comparing it with a traditional approach in responding to a wastewater contamination event in the DWDN when the source is unknown. We focus on understanding how decision-making can be enhanced with the integration of real-time modeling tools and sensors. For the source identification, the comparison metrics include the duration of time needed to find the source, the number of samples required, and the infection risk of the urban population at the time the source was identified. For the mitigation measures, we focus on valve manipulation so that the contamination plume can be isolated or reduced, and the comparison metric is the risk of infection. We also address the problem of uncertainty when using modeling tools. Specifically, we assess how valve settings uncertainty in the DWDN can potentially provide misleading results for decision-making using the model-based approach. We demonstrate a fictional contamination case study, observing how responsible authorities from a water utility in the Netherlands respond to suspected wastewater contamination in their DWDN.

The main contributions of this study are as follows:

1. Demonstration of a realistic contamination case study, revealing the actual steps water utilities take in emergencies.
2. Demonstration of a software tool that simulates real-time contamination events in DWDN and provides decision support for water utilities during an emergency.
3. A comparison between traditional and model-based decision-making for source identification and mitigation measures.
4. Evaluation of valve settings uncertainty in the DWDN and how it influences the accuracy of decisions during emergencies.
5. Quantification of the health protection and operational efficiency benefits of using a model-based approach during emergencies.

Methodology

Study Design and Methodology Structure

This study evaluates the effectiveness of two decision-making approaches (traditional and a model-based) in managing a simulated contamination event in a DWDN. The methodology follows five main steps: (1) simulation of a realistic contamination scenario; (2) contamination detection triggering an emergency response for both approaches; (3) identifying the contamination source; (4) mitigating health impacts through valve manipulation; and (5) comparing both approaches using evaluation metrics.

The model-based approach is enabled by the PathoINVEST decision-support tool, built as a QGIS plugin. PathoINVEST operates on top of the BeWaRE testbed, a simulation framework introduced in Paraskevopoulos et al. (2024) that integrates the following:

- Hydraulic modeling;
- Pathogen fate and transport (e.g., enterovirus, Campylobacter, Cryptosporidium);
- Stochastic residential water demands generated by STREaM (to provide a more realistic understanding of the hydraulics and to isolate the tap water end-use relevant for the calculation of risk of infection); and
- Quantitative microbial risk assessment calculations.

PathoINVEST uses this simulation environment to support contamination tracking, propose strategic sampling locations for source identification, and apply the particle swarm optimization (PSO) algorithm for valve manipulation to contain the spread. Additional details on both PathoINVEST and BeWaRE can be found in Paraskevopoulos et al. (2022, 2024).

The effectiveness of each approach is evaluated using the following evaluation metrics: (1) the number of samples required to identify the contamination source; (2) the time until source identification; and (3) the infection risk at that point. A conceptual overview of this methodology is shown in Fig. 1. It starts with the simulation of a realistic scenario using the BeWaRE testbed, which

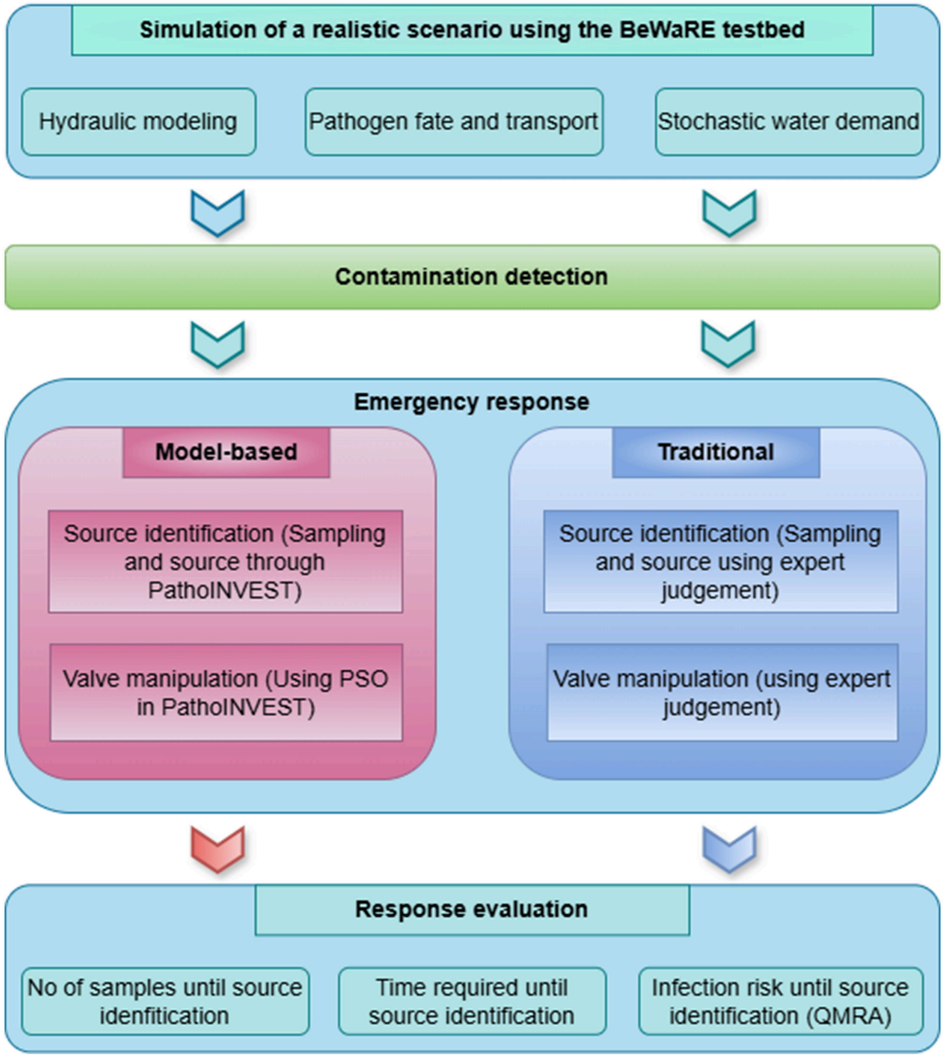


Fig. 1. Conceptual overview of the methodology.

provides the underlying simulation framework (including hydraulic modeling, pathogen transport, and stochastic water demands). Next, we have the contamination detection, which is not addressed further in this work. Contamination detection triggers emergency response in both model-based and traditional approaches. The traditional approach relies on expert judgment for source identification and valve manipulation, while the model-based approach uses simulation-driven sampling and optimization algorithms through PathoINVEST. The outcomes of both approaches are compared using evaluation metrics including the number of samples required, time until source identification, and resulting infection risk.

Emergency Response

In the event of a contamination emergency, the primary goal of a water utility is to rapidly execute a minimal yet effective set of actions to mitigate the incident and restore normal operations. We followed the US EPA Response Protocol Toolbox, which includes a list of recommendations on actions following such an event: (1) detection of contamination; (2) source identification; and (3) consequence management (USEPA 2003; Afshar and Najafi 2014). Contamination can be detected through complaints, manual samplings, or water quality sensor signals (in chlorinated systems). The next step involves identifying the suspected source of contamination. This typically involves determining strategic locations for sampling. Current microbiological testing protocols, such as culture or reverse transcription polymerase chain reaction (RT-PCR), necessitate that samples be transported to a laboratory for analysis. Typically, the time-to-result is approximately 4 h (RT-PCR) to 18–24 h (culture). The positive results from one or multiple samples provide a preliminary indication of the potential origin of the contamination. At the same time, water utilities commonly issue a "boil water" advisory in the potentially affected area as an initial step to mitigate the health impact. While physicochemical parameters such as turbidity, color, taste, or chlorine concentration can serve as early and useful alerts, they are not sufficient for accurately identifying the presence or especially the source of wastewater contamination. They may also fail to detect contamination levels that still pose a health risk, particularly in the case of low-concentration pathogen intrusion. Turbidity can also increase for various reasons that are not related to microbial/wastewater contamination (e.g., due to pipe disturbances, construction, or hydrant flushing). Additionally, in nonchlorinated systems, chemical indicators related to disinfectant residual levels are not available to monitor sudden drops. Therefore, our methodology emphasizes microbiological characteristics that can provide more reliable information on the presence and origin of wastewater contamination. Modeling the contamination (once the contamination source has been identified) provides insights into how the contamination propagates over time. As a result, authorities can issue a boil water advisory to specific areas within the network and strategically close certain valves. This action effectively isolates the contaminated area, preventing further spread (consequence management). Besides valve closure, integral parts of the consequence management step are flushing and chlorination (Poulin et al. 2008), but this paper focuses on the initial response. Following these steps in an emergency event enables a rapid and efficient response to safeguard public health and restore the integrity of the water supply system.

Description of Case Study

DWDN and Pathogen Selection

The case study was simulated using L-Town's DWDN as the water utility's network data were restricted due to sensitive information. L-Town is a modified network from the Battle of the Leakage Detection and Isolation Methods (BattLeDIM) competition (Vrachimis et al. 2022). It is a benchmark network comprising 782 junctions and 905 pipe segments, providing water to an estimated population of 30,000. For this case study, we modeled the waterborne pathogen enterovirus, a common pathogen found in wastewater in high concentrations, for a continuous contamination of 24 h starting at 8 a.m. The water supplied in the network was unchlorinated since this is a common practice in the Netherlands.

Water Demands Generation

The demands of the network were generated using the stochastic residential water end-use model (STREaM) tool (Cominola et al. 2018). This tool simulates household water end-uses, each having distinct consumption patterns and probability distributions for water use volume, use duration, daily frequency, and time of use during the day. Using this tool, each simulated household has a unique demand profile, introducing variability in hydraulic conditions and consequently affecting contaminant transport and infection risk.

Contamination Event

An emergency tabletop exercise was conducted in which a response team dealt with a contamination scenario provided by a supervisor. The supervisor, responsible for running the simulations, was the only one aware of the actual source (and time) of contamination. The supervisor provided feedback (e.g., sampling results, visualization of contamination propagation, health impact) on the proposed activities by the response team (e.g., sampling locations, valve manipulation) while recording the time that would be required for any action. The response team was provided with data on water age and daily average flow directions in the network (Fig. S1). The scenario consisted of multiple customer complaints regarding taste and odor (Fig. 3), which were received at 9:30 a.m. and triggered the emergency response from the team. The response team included an incident commander, a communications manager, advisors specializing in water quality and crisis management, and a modeler. The incident commander implemented a structured decision-making approach, consisting of the following steps: observe, assess, and decide. After reviewing the provided information on water age and flow direction, the response team decided that the contamination likely began around 8 a.m. in the network's eastern part. Additionally, two subgroups were formed to focus on sectioning the network and identifying potential sampling locations. Instead of using the current RT-PCR method (Heijnen et al. 2024), the sampling procedure was undertaken using another PathoCERT tool named PathoTESTICK, a mobile sensor that offers rapid on-site screening of *Escherichia coli*, in less than 5 min (Canciu et al. 2022). For the purposes of this case study, it was assumed that PathoTESTICK can detect wastewater contamination with sufficient sensitivity. Each sampling iteration was estimated to last approximately 20 min, which included the time needed for the field team to reach the location, set up the sampling equipment, await the results, and communicate them back.

Source Identification Using Model-Based Approach

PathoINVEST employs a methodology based on a simplified version of the expanded sampling concept (Eliades and Polycarpou 2012), for the identification of contamination sources in drinking water networks. Their methodology was based on decision trees, expressing conditional statements such as *if–then–else* rules, to return a sequence of nodes for manual sampling.

Valve Manipulation Using Model-Based Approach

The PathoINVEST methodology on valve manipulation expands the work of Moghaddam et al. (2022) focusing particularly on the application of PSO for the strategic closure of pipes within a DWDN to mitigate a contamination event. Diverging from their original model, which includes both pipe closures and hydrant activations, we refined our approach to solely concentrate on pipe closures with a primary objective of minimizing the infection risk, rather than minimizing the number of contaminated nodes. In this application, the PSO algorithm was fine-tuned to identify optimal pipe closure strategies that effectively reduce the infection risk once the contamination source is known. By simulating the movements of particles within a swarm, each particle represents a potential solution. Through iterative refinements and adjustments to particle positions and velocities, our modified PSO model searches the most effective configuration, emphasizing the minimization of infection risk while also incorporating a penalty function to ensure system pressures are maintained above critical thresholds. Another modification compared to the original work of Moghaddam et al. (2022) is that we restricted the PSO algorithm to recommend closing only three pipes in response to real-time contamination events. This limitation aims to increase realism and feasibility for water utilities, recognizing the practical challenges of implementing extensive infrastructure modifications during an emergency. Moreover, by narrowing the potential actions to three pipe closures, we significantly reduce the solution space, which, in turn, decreases computational demands and time. This adjustment not only aligns with the operational capabilities of water utilities but also reduces the significant computational resources typically required by evolutionary algorithms, including the need for advanced processing power and memory capacity to efficiently manage iterative optimizations.

Valve Settings Uncertainty

In a previous study (Paraskevopoulos et al. 2024), the authors assessed the effect of hydraulic uncertainty on the infection risk by applying $\pm 10\%$ water demand variation at each node and examining its influence on the total infection risk. The results showed that this level of uncertainty had minimal impact (1%–3% variability). The current study explores valve settings uncertainty, which can have a substantial influence on model-based hydraulic predictions since it may lead to flow reversals within pipes of the DWDN. This type of uncertainty reflects a real-world operational challenge since many water utilities do not have an accurate overview of their actual network configuration, particularly regarding which valves are open or closed.

In hydraulic modeling, the fidelity of the network representation is very important. When the aim is to model contaminations, predict

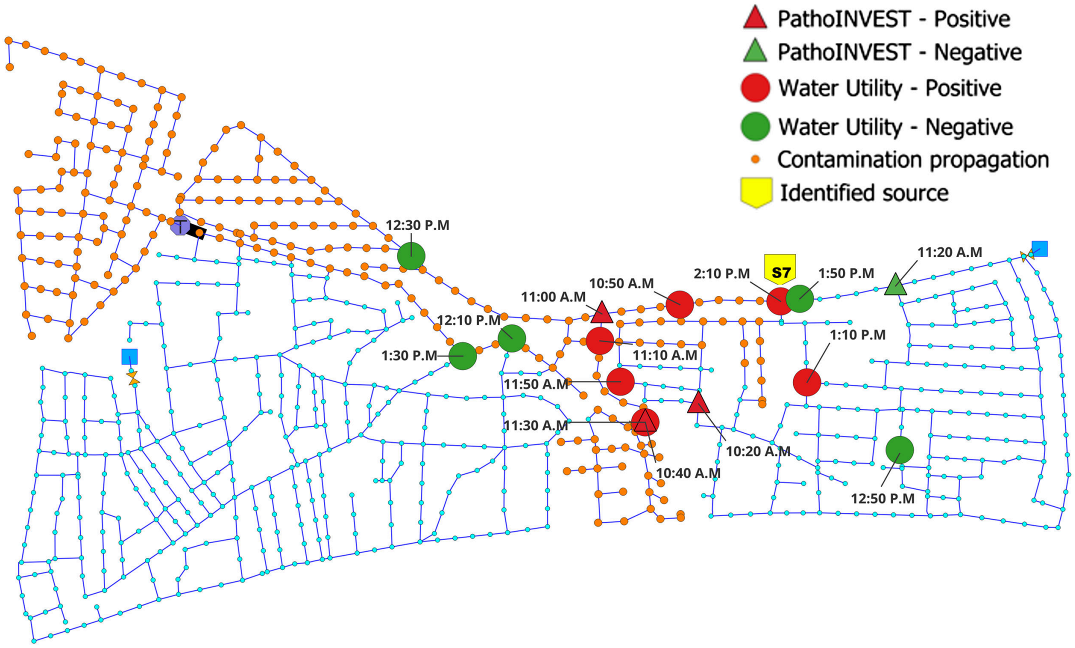


Fig. 2. Identified source, contamination propagation, and sampling results for both traditional and model-based approaches.

realistic outcomes, find the contamination source, and suggest adequate mitigation actions, there must be an accurate representation of the most current network configurations, including valve settings. Inaccurate or outdated models can produce misleading results, making them unreliable for decision-making processes. This unreliability is particularly pronounced in scenarios where valve settings vary significantly between the actual network and the model (e.g., a valve is open in reality but closed in the model). These discrepancies can drastically change the simulated hydraulics and flow directions, thus providing inaccurate results. Previous studies highlight that there can be discrepancies of up to 0.7% between the model and actual valve settings (Mesman et al. 2016).

To explore the potential effect of this inherent uncertainty in valve settings, we developed an approach involving the generation of multiple hydraulic profiles. Specifically, we created 1,000 distinct hydraulic profiles for L-Town, each incorporating a different 0.7% variation in closed valve settings (six out of 905 valves). These profiles were then used to simulate a contamination scenario with a known contamination source. This approach generated 1,000 unique uncertainty scenarios ensuring that both hydraulic and pressure requirements of the system were met. For each scenario, we calculated the risk of infection, allowing us to quantitatively assess the impact of valve uncertainty on the overall risk of infection and compare them with the base scenario (the scenario that was used in the pilot case study without any mitigation action). Furthermore, we evaluated the impact of valve uncertainty, as represented by the 1,000 uncertainty scenarios, on the efficacy of the model-based approach in identifying the contamination source.

Results and Discussion

The case study simulated the emergency response from the water utility using two different approaches: a traditional based on expert judgment, and a model-based using PathoINVEST. Subsequently, we present and compare the results of these two approaches in terms of source identification and mitigation measures.

Fig. 2 shows the contamination source (S_7) and the potential contamination propagation to its full extent by midnight (14.5 h after the complaints were received) without any action by the water utility. The figure also displays the sampling times and results for both approaches (traditional and model-based).

Source Identification

Traditional Approach

After discussing with the response team and based on the insights of Fig. S1 (average flow direction, water age), the incident commander initiated two sampling rounds and designated 11 strategic sampling locations for the field team across the network (Fig. 3). The incident commander had to wait for the results of the first designated sample before deciding on the next sampling location, and the first sample was taken at 10:30 a.m., approximately 1 h after the complaints. The objective was to leverage the information obtained from the samples (indicating either the presence or absence of contamination) in each round, thereby leading to the exclusion of segments of the network and, finally, the identification of the contamination source.

Model-Based Approach

The model-based approach involved analyzing potential contamination sources and the strategic selection of sampling locations, each marked with a binary signature dependent on the outcome—positive (1) or negative (0). A positive binary signature at a sampling location means that a given contamination source's trajectory has intersected that point, indicating that any sample retrieved from a field team at this site would be positive. Therefore, the first step for the model-based approach was to identify potential contamination sources. This was achieved by finding any upstream node from the location of the complaints (Fig. 4). The desired outcome was obtained using an additional feature of the tool, a function $f(\mathcal{G}, s, d)$ able to identify potential upstream contamination nodes in a network. This function finds all nodes within a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V}$ and $\mathcal{E}$ represent the nodes and edges, respectively. Specifically, it locates nodes within an infinite distance d from a specified node s (the complaint node), effectively capturing any node in the network that could contribute to upstream contamination of s.

J. Water Resour. Plann. Manage., 2026, 152(6): 05026010

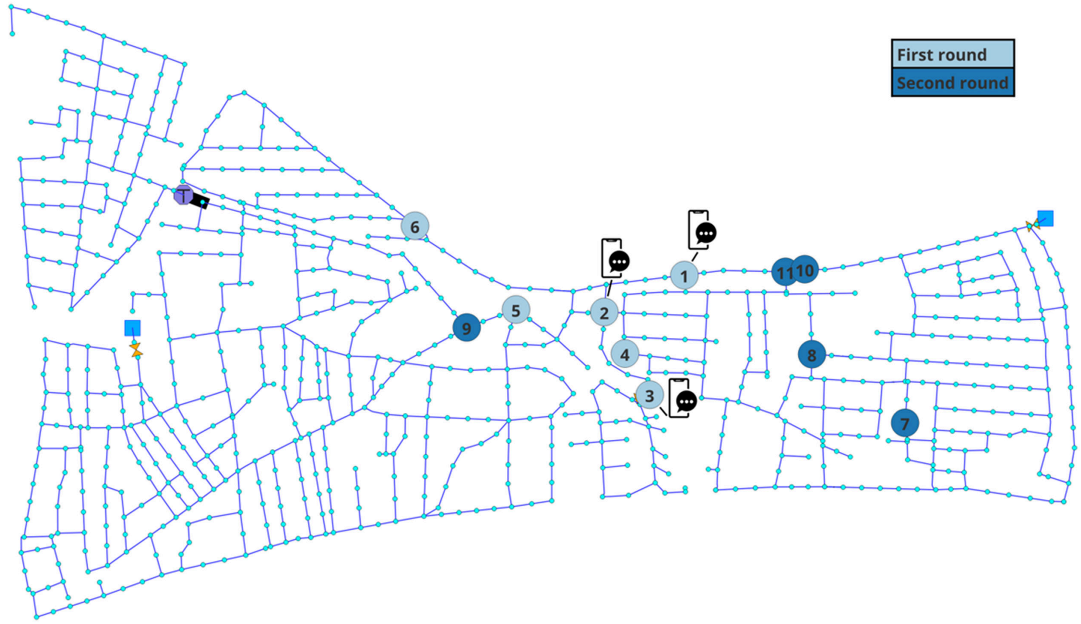


Fig. 3. Proposed sampling locations in two rounds (light and dark blue) along with the customer complaints (smartphone).

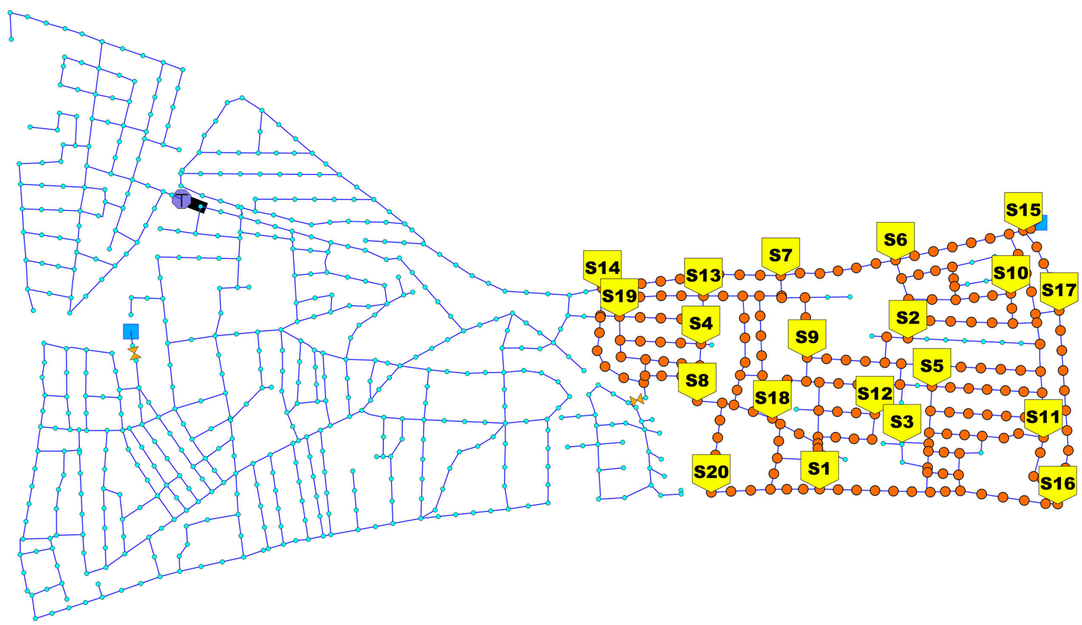


Fig. 4. Upstream potential contamination sources (orange circles) using complaints as a starting point and the 20 most probable contamination sources.

After identifying and highlighting all the potential sources of upstream contamination, 20 strategic locations were selected as the most probable contamination sources by the response team (Fig. 4). The next step was to select strategic locations for sampling. All the potential upstream contamination sources from Fig. 4 were also considered sampling locations (243 nodes in total). Again, the time-to-result of the PathoTESTICK tool was used.

To find the suspected contamination source, the hydraulics and quality dynamics of the DWDN were simulated for 20 scenarios, representing all 20 contamination sources. This enabled the generation of binary signatures for all sampling locations corresponding to the simulated contamination trajectories (Fig. 5). The simulation of the 20 contamination scenarios took approximately 5 min. Consequently, after accounting for a 25-min discussion with the team regarding the 20 strategic locations, the binary signatures and hydraulics were successfully computed by 10 a.m. The temporal dynamics of contamination play a critical role in this process. For instance, a node, say N_{220}, may not be associated with a contamination source at 10 a.m. but may become contaminated by 11 a.m. due to the progression of contamination.

After the generation of binary signatures in all sampling locations for each of the 20 contamination scenarios, the tool indicated the first sampling location. To prioritize the optimal sampling location, the tool utilizes the theory of entropy, which measures the uncertainty or unpredictability in a system. In our context, each sampling location can either be contaminated (1) or not contaminated (0). We calculate the probabilities $p1$ and $p0$ based on the frequency of positive and negative outcomes from the 20 contamination simulations. The entropy H at each node, v, is computed using the formula

J. Water Resour. Plann. Manage., 2026, 152(6): 05026010

Scenario	n_{220}	n_{221}	n_{222}	n_{223}	n_{224}	n_{225}	n_{228}	n_{229}	n_{230}	n_{232}	n_{235}	n_{238}	n_{239}	n_{240}	n_{241}	n_{244}	n_{245}	n_{248}	n_{249}	n_{250}
S1	1	1	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
S2	1	1	1	1	0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1
S3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S4	0	0	0	0	0	1	0	0	0	0	1	1	1	0	1	1	0	0	0	0
S5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
S6	0	1	1	1	1	1	0	1	0	0	1	1	1	0	1	1	0	0	0	0
S7	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
S8	0	1	1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	0	0	0
S9	0	0	0	0	0	0	0	0	0	0	1	1	1	0	1	1	0	0	0	0
S10	0	1	1	1	1	1	0	0	0	0	1	1	1	0	1	1	0	0	0	0
S11	0	1	1	1	1	0	1	1	0	1	1	1	0	0	0	0	0	0	0	0
S12	0	1	1	1	1	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0
S13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0
S15	0	1	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
S16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S17	1	1	1	1	0	0	1	0	1	1	0	0	0	1	0	0	1	1	1	1
S18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S19	0	1	1	1	1	1	0	1	0	0	1	1	1	0	1	1	0	0	0	0
S20	0	1	1	1	1	1	0	0	0	0	1	1	1	1	1	1	0	0	0	0

Fig. 5. Simulated binary signatures of a snippet of the sampling locations for each of the 20 contamination sources at 10 a.m. Node n_241 is the selected sampling location based on the entropy results. The rows marked with shading indicate the scenarios that are not consistent with the sampling result. The sampling result was positive (1); therefore, the shaded scenarios can be discarded.

	n_{241}	n_{235}	n_{223}	n_{229}	n_{244}	n_{238}	n_{239}	n_{222}	n_{224}	n_{221}	n_{225}	n_{228}	n_{232}	$n_{\{240}$	n_{220}	n_{230}	n_{245}	n_{248}	n_{249}	n_{250}
$P(1)$	0.5	0.55	0.55	0.55	0.55	0.55	0.55	0.6	0.4	0.6	0.35	0.25	0.25	0.25	0.2	0.18	0.15	0.15	0.15	0.15
$P(0)$	0.5	0.45	0.45	0.45	0.45	0.45	0.45	0.4	0.6	0.4	0.65	0.75	0.75	0.75	0.8	0.85	0.85	0.85	0.85	0.85
H	1	0.99	0.99	0.99	0.99	0.99	0.99	0.97	0.97	0.97	0.93	0.81	0.81	0.81	0.72	0.6	0.6	0.6	0.6	0.6

Fig. 6. Results of entropy for the selected snippet of sampling locations.

$$H(v) = -p(0)\log_2(p(0)) - p(1)\log_2(p(1))$$

where $p(0)\log_2(p(0))$ and $p(1)\log_2(p(1))$ = information content or uncertainty when the location is not contaminated and when the location is contaminated, respectively.

High entropy indicates a high level of uncertainty about the contamination status at a location, meaning it is equally likely to be contaminated or not. Sampling at locations with high entropy maximizes the informational yield, reducing uncertainty most effectively. By focusing on high-entropy sampling locations, this methodology aims to maximize the informational yield from each sample and, thus, efficiently narrow down the possible contamination sources.

After entropy analysis, node n_{241} exhibited the highest entropy, signaling it as the prime candidate for sampling (Fig. 6). In cases where multiple locations exhibited equivalent maximum entropy, the selection of the next sampling site was left to the discretion of the user.

The field team was instructed to take the first sample in the designated location (node n_{241}) at 10 a.m. The result was positive, and that allowed for the exclusion of simulated contamination scenarios that do not align with this outcome (Fig. 5). This iterative process continued until the set of potential contamination sources was sufficiently narrowed, facilitating the identification of the actual source of contamination. The remaining procedure (identification of the sampling node with the highest entropy and exclusion of simulated contamination scenarios) can be found in Figs. S2–S4).

Valve Manipulation

Based on the network topology and discussions with the team, the incident commander proceeded to the closure of valves at strategic locations. The first mitigation action (for both traditional and model-based approaches) was the closure of valves V_1 and V_2, located near the complaint site [Fig. 7(b)], at 10:40 and 10:45 a.m., respectively (Action 1). This action was aimed at preventing further contamination spread to the network's western part even though the contamination source was not found yet. This was considered an appropriate action because it would keep the water supply intact for all customers while separating the network into two parts. Each part would be supplied by its own water source, preventing contamination from moving between these two sections of the network. As soon as the contamination source was identified, the second mitigation action from the water utility (again for both traditional and model-based approaches) was to immediately close the pipes surrounding the source to prevent further spreading (Action 2).

Traditional Approach

Although the traditional Action 2 stopped the contamination source at 2 p.m. [Fig. 7(a)], pathogens were still present and spreading in the eastern part of the network. Therefore, the water utility decided to implement Action 3, which involved closing an additional three valves. Subsequently, valves V_3, V_4, and V_5 were closed at 2:20, 2:25, and 2:30 p.m., respectively, to contain the spread in the network's eastern part. At this point, it was time to run a model simulation to evaluate the performance of

J. Water Resour. Plann. Manage., 2026, 152(6): 05026010

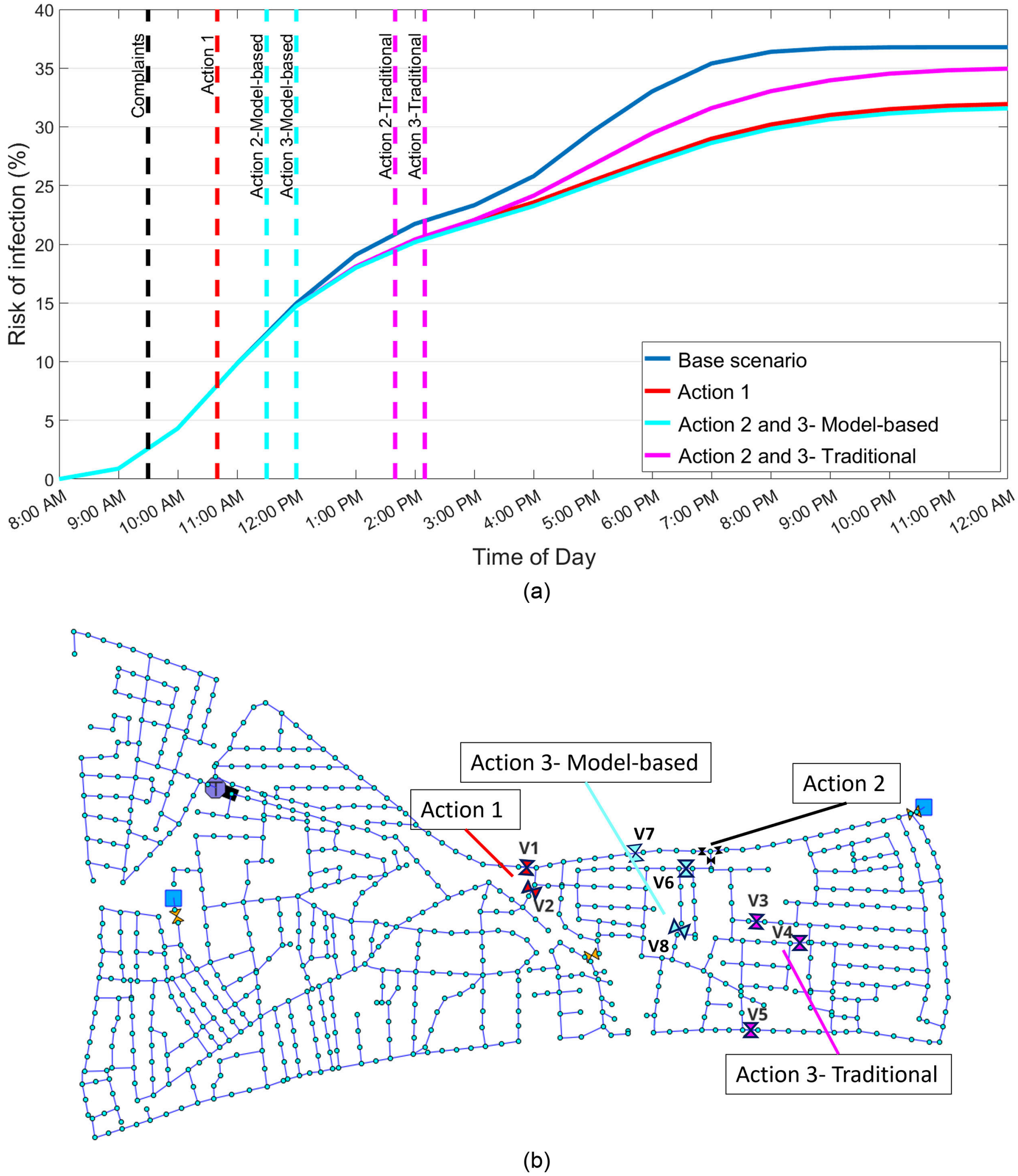


Fig. 7. (a) Risk of infection comparison between the base scenario and the mitigation Actions 1–3; and (b) closure of valves (actions) by the water utility and PathoINVEST.

the traditional approach. The identified contamination source was incorporated to calculate the infection risk (defined as the percentage of people being infected) and assess whether the health impact was mitigated. This simulation specifically factored in which valves to close (spatial resolution) and the timing of their closure (temporal resolution).

Model-Based Approach

For the model-based approach, Actions 1 and 2 are identical to the traditional approach. However, the model-based Action 2 occurred earlier at 11:20 a.m. since the source was identified earlier. The additional closure of three valves (model-based Action 3) was suggested by the PathoINVEST tool. Utilizing the modified PSO algorithm, the model-based approach identified the optimal three valves, V_6, V_7, and V_8, for closure, as shown in Fig. 7(b). These pipes were closed around noon, considering the travel time for the field team and the time needed for valve closure.

Comparison

Source Identification

Table 1 compares the traditional and the model-based approach, detailing the number of samples and the time needed to find the contamination source. In addition, it assesses the estimated infection risk starting from the onset of contamination (8 a.m.) until the moment the contamination source was finally identified. As a point of reference, we also calculated the infection risk using the RT-PCR method (4 h) instead of the PathoTESTICK, which yields results in 20 min. Although considerably faster than the culture-based approach, the RT-PCR approach would still mean that the field team would face a 4-h wait for each round of results. Since two sampling rounds were performed, this would result in a total waiting time of at least 8 h.

The model-based approach is more efficient and rapid in locating the source, as it takes only four samples and 1.3 h,

Table 1. Comparison between traditional and model-based approaches to find the source of contamination

Approach	No. of samples	Time to find the source (h)	Infection risk with Action 1 (%)	Infection risk w/o Action 1 (%)
Traditional (RT-PRC)	11	8	27	33
Traditional (PathoTESTICK)	11	3.7	20	22
Model-based (PathoTESTICK)	4	1.3	12	12

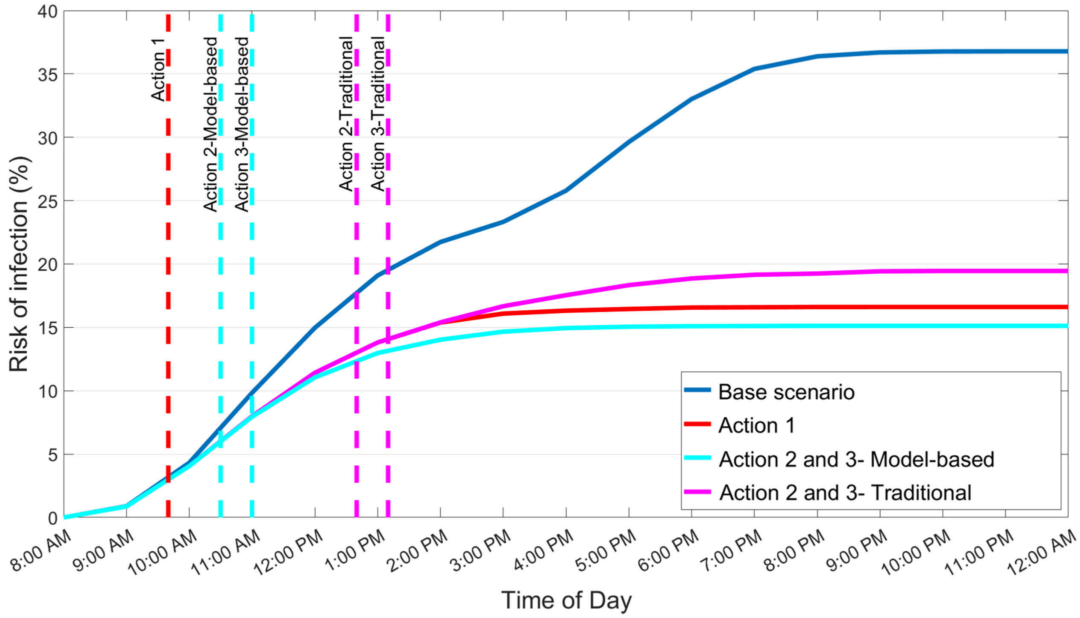


Fig. 8. Risk of infection comparison between the base scenario and mitigation Actions 1–3 in the alternative simulation where all actions are advanced by 1 h.

compared to 11 samples and 3.7 and 8 h for the traditional approach, using the PathoTESTICK and RT-PCR, respectively. Calculating the risk of infection until the time the contamination source was identified (and any potential mitigation measures could have started) for all three approaches, we see that the model-based approach is again better here as the risk of infection is 12% compared to 20% and 27% for the traditional approach with the PathoTESTICK and RT-PCR, respectively. Finally, a key observation is the (moderate) reduction of the health impact of the contamination by the water utility's rapid action on closing the first two valves (Action 1) compared to the base scenario [Table 1 and Fig. 7(a)].

Valve Manipulation

Regarding the traditional approach, the closure of two valves identified as V_1 and V_2 (Action 1), at 10:40 and 10:45 a.m., respectively, effectively reduced the infection risk, as shown in Fig. 7(a). However, since the contamination was initiated at 8 a.m. a certain extent of contaminant spread had occurred before Action 1 was implemented. As a result, the valve closures, while appropriate, were late, leading to considerable contamination in L-Town's western region. Additionally, the traditional Action 3 inadvertently redirected the contamination plume, reaching previously unaffected zones. This misdirection increased the potential risk of infection, as can be seen in Fig. 7(a).

Regarding the model-based approach, as shown in Fig. 7(a), the model-based Action 3 reduced the infection risk when compared to the base scenario as well as the traditional Action 3. However, the infection risk remains relatively high. Due to the timing of this action, those at risk had likely already been exposed.

Importance of Rapid Response

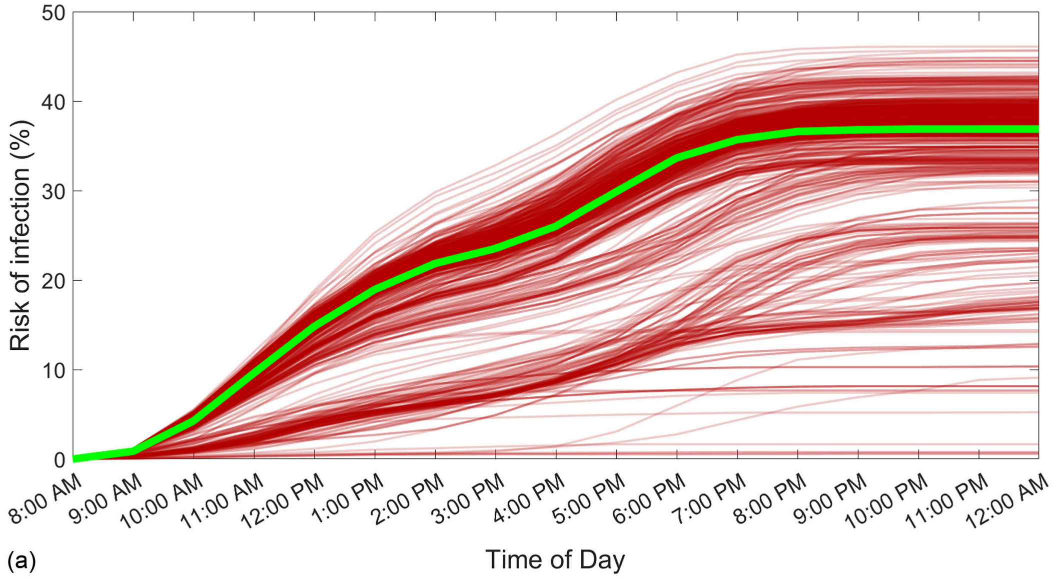
Fig. 7(a) shows that the infection risk, although reduced, remained high regardless of mitigation actions from the water utility. This indicates that to significantly minimize the infection risk, interventions should have been earlier. A reevaluation of the event timeline, featuring an alternative simulation of the same contamination scenario where actions were initiated 1 h earlier, sheds light on the importance of rapid response. In this revised scenario, valves V_1 and V_2 were closed at 9:40 a.m., immediately following the customer complaints, as a *no-regret* preventative mitigation action. Using PathoINVEST to select the sampling locations also moved subsequent mitigation Actions 2 and 3 to 1 h earlier. This quicker response led to a significant decrease in the infection risk (a 17%-point reduction in total infection risk), indicating that immediate valve closure after contamination detection (or even suspicion) can significantly contain the contamination (Fig. 8). This highlights the importance of strategic sensor placement, rapid response actions (automated valve closures), and sensors that offer screening of fecal contamination during such emergencies.

Valve Settings Uncertainty

Infection Risk Uncertainty

To evaluate the potential impact of valve settings uncertainty, Fig. 9(a) demonstrates the infection risk across 1,000 uncertainty - scenarios with the solid line representing the base scenario.

J. Water Resour. Plann. Manage., 2026, 152(6): 05026010



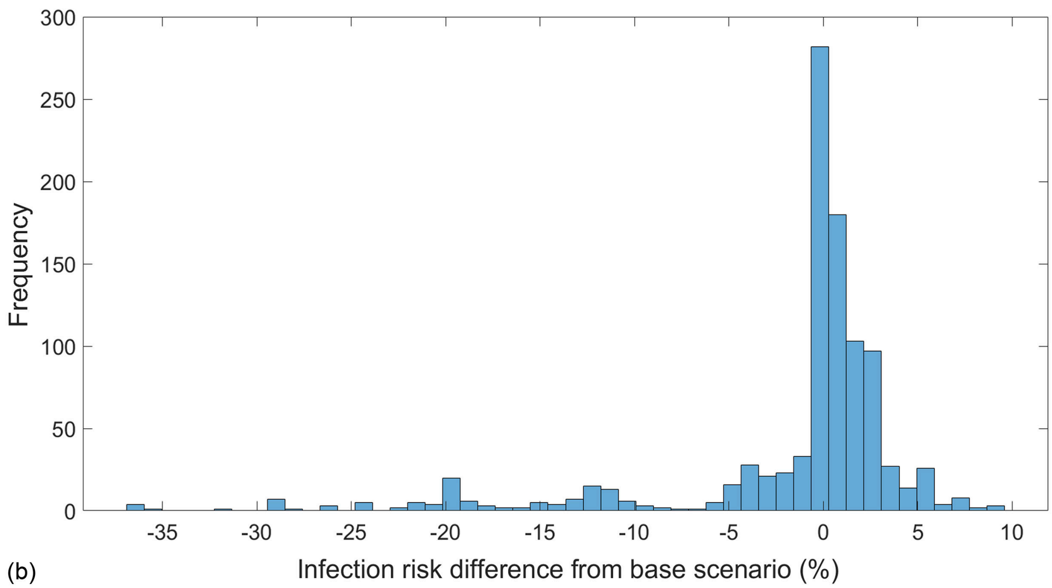


Fig. 9. (a) Risk of infection for the 1,000 uncertainty scenarios and the base scenario (shown with a solid line); and (b) histogram showing the difference between the 1,000 uncertainty scenarios in infection risk compared to the base scenario.

The 0.7% uncertainty in valve settings yields variability in the projected infection risk. Fig. 9(b) shows the infection risk difference of the 1,000 uncertainty scenarios from the base scenario. The histogram indicates that about 80% of the uncertainty scenarios are within the range of −5% to +5% from the base scenario infection risk. Also, the majority of the 1,000 uncertainty scenarios cluster around the base scenario. This suggests that modeling with a 0.7% uncertainty in valve settings generally does not result in significantly different or underestimated infection risk outcomes.

The scenarios with significantly lower infection risk (below 10%) are observed when one or more pipes downstream of the eastern reservoir are actually closed, or in cases where pipes located immediately downstream of the contamination source are closed. These scenarios effectively limit the spread of contamination, thereby significantly reducing the infection risk.

Source Identification Uncertainty

Valve settings uncertainty may also impact the reliability of the PathoINVEST contamination source identification feature. Fig. 10 showcases how a 0.7% uncertainty in valve settings influenced the performance of the model-based approach in identifying the contamination source. This analysis was conducted for each of the 1,000 uncertainty scenarios, following the expanded sampling methodology subsection for the 20 potential contamination sources. The results indicate that, despite the valve settings uncertainty, the model successfully identified the exact source of contamination, S_7, in 57% of the uncertainty scenarios. The next most frequently identified source was S_6 with 18%, which is adjacent to the exact source, S_7. This implies that even if PathoINVEST incorrectly pinpoints S_6 as the contamination source, it would still guide the investigation toward the correct vicinity for further inspections. Considering this, the effectiveness of the PathoINVEST source identification feature in correctly identifying the source of contamination stands at 75%.

Valve Manipulation under Valve Settings Uncertainty

The influence of valve settings uncertainty on valve manipulation was evaluated only for Action 1. Fig. 11 shows the mean (derived

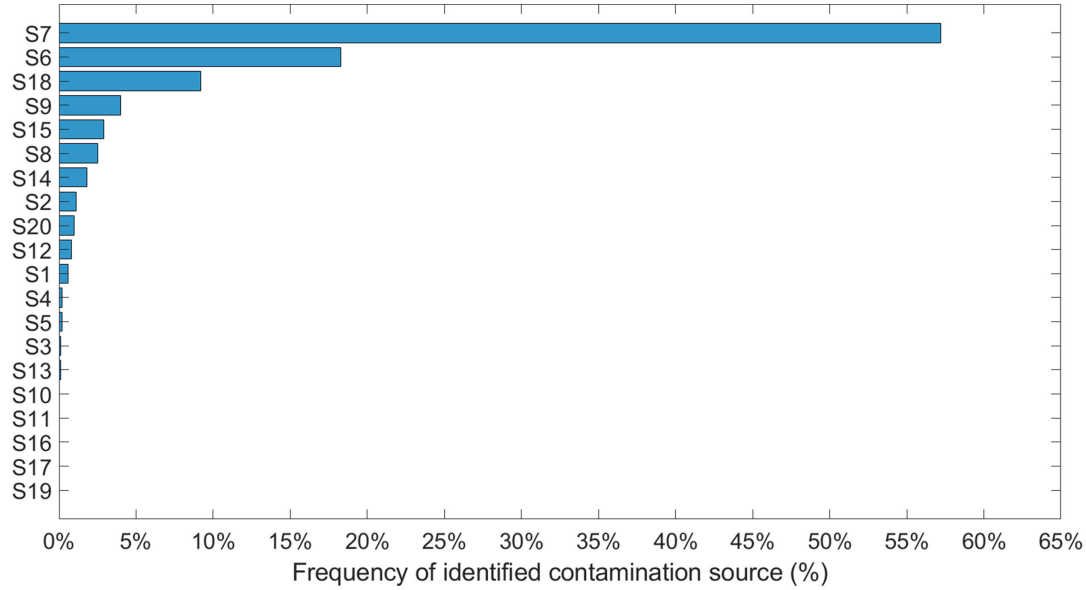


Fig. 10. Frequency of the 1,000 uncertainty scenarios in identifying the contamination source using PathoINVEST.

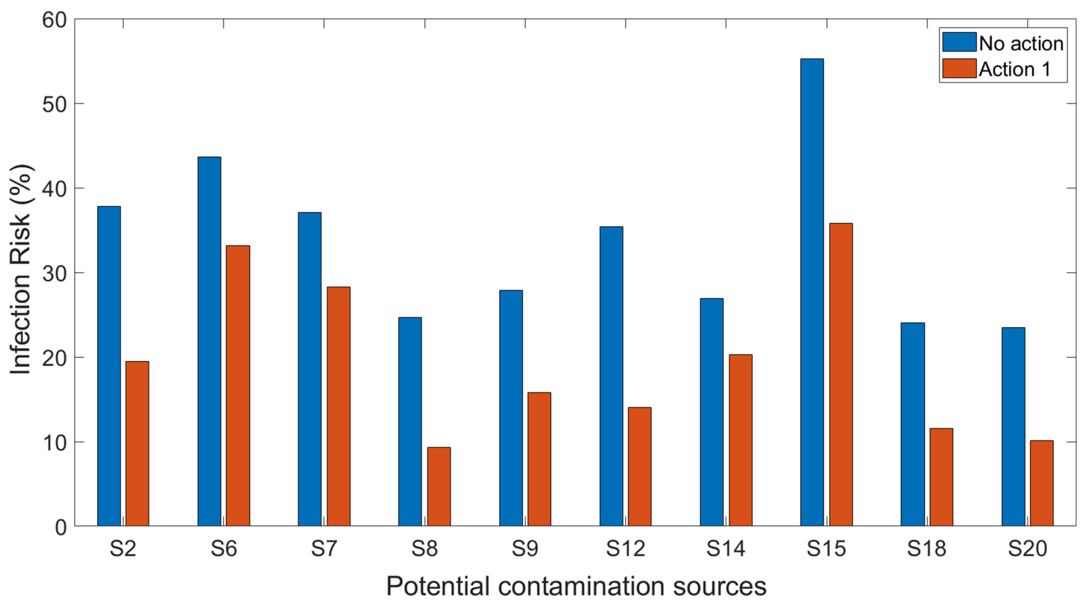


Fig. 11. Comparison of mean infection risk (derived from 1,000 uncertainty scenarios) between the base scenario (no action) and Action 1 for the most frequently identified contamination sources by PathoINVEST.

from the 1,000 uncertainty scenarios) total infection risk associated with 10 of the potential 20 contamination sources, comparing the base scenario (*no action*) with the original closure of two pipes (V_1 and V_2) by the water utility (Action 1). This comparison demonstrates that, regardless of the contamination source and its accurate identification by the PathoINVEST source identification feature (due to any potential valve settings uncertainty), the strategic closure of two pipes (Action 1) consistently reduced the relative risk of infection, ranging from 23.8% (S_7) to 62.4% (S_8) reduction. This outcome highlights the effectiveness of strategic valve closure during a contamination event.

Approach Assessment

Assessing traditional and model-based approaches to managing such emergencies allows identifying their respective strengths and weaknesses.

Traditional Approach

The decisions made in the traditional approach rely heavily on the experience and intuition of the response team, whereas the need for a good understanding of the network characteristics is imperative. This approach, while it does not possess the sophistication of advanced technologies, offers reliability and independence from modeling tools, which is important in situations where such technologies may be unavailable or slow. We saw that the response team's quick decision to close the two valves at the beginning of the event (Action 1) led to a reduction in infection risk. However, this approach tends to be more time intensive. This is demonstrated by the 11 samples required to identify the contamination source, compared to just four from the model-based approach, resulting in an additional 2 h and 20 min. During this time, there was an additional 8%-point infection risk. It can also sometimes lead to mistakes, such as the wrong closure of the remaining three valves

J. Water Resour. Plann. Manage., 2026, 152(6): 05026010

(traditional Action 3), which resulted in a 3%-point higher infection risk compared to both Action 1 and model-based Action 3. The lack of predictive capabilities inherent in this approach often results in slower decision-making processes, extensive response times, and mitigation measures of diminished efficacy. This issue becomes even more pronounced when considering current detection and sampling methods (such as RT-PCR), which require considerably more time to deliver results, further slowing down the decision-making process during emergencies.

Model-Based Approach

Having an on-site mobile device capable of detecting pathogens in water with 20 min time-to-result is extremely valuable and important during emergencies. The model-based approach demonstrates significant improvements in response speed since it takes 2 h and 20 min less to find the source in the presented case study. Being able to simulate multiple real-time contamination events, propose sampling locations for source identification, and suggest valve closures to mitigate the event offers valuable insights to a water utility, resulting in more effective decision-making. Nonetheless, the model-based approach also has limitations. The accuracy of a model is heavily dependent on the quality and current state of network data. An inaccurate or outdated network can compromise the model's outputs, leading to potentially flawed decision-making by the response team. Additionally, these tools require constant updates and maintenance, which requires a commitment of resources. The deterministic nature of models also presents a limitation, as they might not fully capture the complexity and variability of real-world scenarios. While the application of PSO for valve manipulation demonstrates an efficient outcome, it may not represent the optimal approach. Alternative metaheuristic algorithms (e.g., multiobjective evolutionary algorithms) could potentially offer improved results for valve closure (Nouiri 2017; Quintiliani et al. 2019). The constraint within our PSO application, specifically to close only three valves, introduces another layer of limitation. However, the primary aim of this paper was to investigate the added value of using modeling tools and rapid sensors during emergencies. Further improvements in the sensor and the presented methodology (source identification, valve manipulation) can enhance the benefits of using mobile devices for on-site contamination screening and models in the decision-making of crisis scenarios. Additionally, the optimization procedure used to select which valves to close does not incorporate any knowledge regarding uncertainties in water demand or valve settings, even though bounds on these uncertainties may exist. Robust optimization approaches, e.g., as proposed by Marquez Calvo et al. (2018) for valve management under demand uncertainty, could provide a valuable extension to this methodology and increase the robustness of the mitigation strategy. While this study focused specifically on valve settings uncertainty, and previous work by the authors addressed water demand variability independently, a combination of both sources of uncertainty is recommended as a future step. This approach could offer a more comprehensive evaluation of model robustness and provide real-world complexity in the model-based approach. Moreover, while the current source identification method in PathoINVEST relies on topological proximity and hydraulic flow direction, the integration of data such as pressure or flow anomalies could enhance the process. For example, a sudden pressure drop at a specific location could indicate a potential contamination location and be included in the candidate nodes considered in the strategic sampling process. This could further improve the accuracy and efficiency of the model-based approach, especially in systems where such SCADA data are routinely available. Pressure and flow data could also be used to calibrate the hydraulic model more frequently or support the development of a digital twin of the system to make sure that the model used by PathoINVEST reflects the current network characteristics. After mitigation actions such as valve manipulation, real-time hydraulic sensor feedback could also be used to recalibrate the model and improve subsequent decision-making. Finally, we note that the effectiveness of the source identification process in the model-based approach also depends on the duration of the contamination event. In cases where a contamination lasts only a few minutes (e.g., 15 min), the contamination plume may no longer be present in the DWDN by the time the emergency response is initiated and the sampling team is on the field. This limits the usefulness of field sampling, as there is a higher chance of missing the plume entirely. Incorporating additional water quality parameters such as turbidity for preliminary screening could further improve response times overall. However, these indicators should be carefully integrated and perhaps in combination with microbiological confirmation since they are not specific or reliable indicators of wastewater contamination. While this study focuses on sudden contamination events, future work could explore how gradual mechanisms such as biofilm sloughing and the different simulation approach they require (e.g., modeling microbial growth, detachment kinetics) affect contamination detection, source identification, and, overall, model-based decision-making.

Conclusions

This study compared traditional and model-based approaches in managing DWDN contamination events, revealing several key insights:

- The water utility's rapid response action to close the first two valves (traditional approach), despite not knowing the contamination source, effectively prevented the spread of contamination and reduced the health impact.
- The model-based approach was shown to be more efficient than the traditional approach in identifying the source of contamination (1.3 versus 3.7 h), requiring fewer samples (four versus 11) and resulting in lower infection risk by the time the source was identified (12% versus 20%) in this case study.
- The model-based approach was more effective in finding the best valves to close in the network since it resulted in a 3%-point infection risk reduction.
- Having up-to-date valve settings in the DWDN schematization is important to provide reliable results on source identification. Discrepancies between the actual network and the model can lead to inaccurate infection risk estimates when using modeling tools to support decision-making.
- Rapid actions and decision-making are crucial upon detecting contamination in the DWDN, as a 1-h faster response from the water utility can lead to a 17%-point reduction in total infection risk. One example of such rapid actions is the use of mobile rapid testing devices for on-site contamination screening, as they deliver immediate results and enable quicker responses.

This study underscored the potential advantages of integrating modeling and sensor tools for managing DWDN contamination events. It demonstrated the improvements in the efficiency and speed of model-based approaches, dependent on the network model's accuracy and effective management of uncertainties, such as valve settings. Furthermore, the study highlighted the essential value of traditional knowledge and human intuition in emergency responses, illustrating how quick, expert decisions remain critical. The deployment of mobile devices for rapid on-site contamination screening represents a significant advancement, facilitating immediate response actions. By combining model-based strategies with traditional expert insights, our approach provides a robust framework for improving water contamination management and decision-making processes, thus ensuring public health during emergencies. The development of real-time modeling tools such as PathoINVEST further exemplifies this approach, showing great potential for promoting operational improvements in drinking water crisis management. Our case study showed that when a contamination event unfolds, the window of opportunity for meaningful interventions is small (within a few hours), while the risk of infection can be quite high since many people can be exposed to pathogens.

Data Availability Statement

Some or all data, models, or code generated or used during the study are available in a repository or online in accordance with funder data retention policies (https://github.com/KIOS-Research/PathoINVEST-WDSA-CCWI-2022).

Acknowledgments

This research was funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 883484 (PathoCERT) and the European Research Council (ERC) under the ERC Synergy grant agreement No. 951424 (Water Futures) and was supported by the European Union's Horizon 2020 Teaming programme under grant agreement No. 739551 (KIOS CoE) and the Government of the Republic of Cyprus through the Deputy Ministry of Research, Innovation and Digital Policy.

Author Contributions

Sotirios Paraskevopoulos: Conceptualization; Data curation; Formal analysis; Investigation; Methodology; Visualization; Writing – original draft; Writing – review and editing. Stelios G. Vrachimis: Conceptualization; Data curation; Investigation; Methodology; Validation; Writing – review and editing. Marios S. Kyriakou: Data curation; Resources; Software; Visualization. Demetrios G. Eliades: Formal analysis; Funding acquisition; Methodology; Project administration; Resources; Validation; Writing – review and editing. Patrick Smeets: Conceptualization; Formal analysis; Investigation; Methodology; Supervision; Validation; Writing – review and editing. Mirjam Blokker: Formal analysis; Investigation; Methodology; Supervision; Validation; Writing – review and editing. Marios Polycarpou: Formal analysis; Funding acquisition; Validation; Writing – review and editing. Gertjan Medema: Conceptualization; Formal analysis; Investigation; Methodology; Supervision; Validation; Writing – review and editing.

Supplemental Materials

Figs. S1–S4 are available online in the ASCE Library (www.ascelibrary.org).

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