Evaluation of chlorine booster station placement for water security

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ABSTRACT

Drinking water utilities use booster stations to maintain chlorine residuals throughout water distribution systems. Booster stations could also be used as part of an emergency response plan to minimize health risks in the event of an unintentional or malicious contamination incident. The benefit of booster stations for emergency response depends on several factors, including the reaction between chlorine and an unknown contaminant species, the fate and transport of the contaminant in the water distribution system, and the time delay between detection and initiation of boosted levels of chlorine. This article takes these aspects into account and proposes a mixed-integer linear program formulation for optimizing the placement of booster stations for emergency response. A case study is used to explore the ability of optimally placed booster stations to reduce the impact of contamination in water distribution systems.

KEYWORDS

Chlorine booster stations; optimization; water distribution systems; security

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1. Introduction

Chlorine degradation and other reaction dynamics can cause significant variation in chlorine concentration throughout a water distribution system. Chlorine booster stations are commonly used to maintain drinking water standards. Booster stations are designed to inject chlorine at strategic locations, helping to maintain residual chlorine levels that can prevent pathogen re-growth. Chlorine booster stations are typically installed at pump stations or other facilities but could also be added throughout the water distribution system. While boosting chlorine levels can improve water quality, harmful disinfection by-products can form when chlorine reacts with different chemicals. Several optimization methods have been suggested to place booster stations and to schedule booster operations for water quality objectives (Boccelli et al. 1998; Kang and Lansey 2010; Lansey et al. 2007; Maheshwari et al. 2018; Munavalli and Kumar 2003; Ostfeld and Salomons 2006; Ozdemir and Ucaner 2005; Prasad, Walters, and Savic 2004; Propato and Uber 2004a,b; Tryby et al. 2002; Uber, Polycarpou, and Subramaniam 1998). The water quality objectives used in these approaches include: minimizing the total injected chlorine while maintaining a limit on the chlorine residual throughout the water distribution system, minimizing the squared deviation from a target chlorine concentration, maintain bounds on chlorine residual and disinfection by-products, minimizing the number of booster stations that provide maximum coverage, and minimizing the capital and operational costs associated with booster stations.

Given that water distribution systems are critical infrastructure, vulnerable to intentional attacks as well as accidental contamination (Murray et al. 2009), water security objectives could also be used to identify booster station locations. In the event of a contamination incident, an effective emergency response plan could include injecting chlorine at fixed booster locations to inactivate or destroy a potentially harmful contaminant. Unlike booster station placement for water quality objectives, optimal booster station placement for water security should take into account a wide range of possible contamination injection scenarios. Additionally, booster station placement for water security should also account for two time delays: 1) the time between the

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start of the contaminant injection into the water distribution system and the detection of the contamination, and 2) the time between the contamination detection and the injection of chlorine from booster stations.

One of the biggest challenges associated with the booster placement problem for water security is modeling the reaction between chlorine and an unknown contaminant species. Booster stations are only effective for response to water contamination incidents if the contaminants ability to cause harm can be reduced by chlorine. Many biological contaminants are inactivated in the presence of sufficient chlorine; meaning that they are killed or damaged to the extent they cannot cause human disease or death. Some chemical contaminants are oxidized in the presence of chlorine, reducing the toxicity of the contaminant. However, harmful disinfection by-products might be formed in this reaction. For example, chlorine can react with some organophosphate pesticides to form oxons, which might be more toxic than the original compound. Understanding these complex reactions is critical in order to estimate the benefits of booster stations in the context of water security. However, with limited knowledge at the planning stage, reasonable assumptions would have to be made to approximate the reaction between chlorine and an unknown contaminant. Additionally, during a real-world contamination incident, the contaminant species is typically unknown at the time of detection. Current monitoring technologies rely on standard water quality parameters (i.e., pH, turbidity, residual chlorine), which do not indicate the type of contaminant in the system. For this reason, the exact reaction between the contaminant and chlorine cannot generally be modeled at the time of response.

A limited amount of research has explored the application of booster stations with water security objectives. Ostfeld and Salomons (2006) used a genetic algorithm to minimize the difference between chlorine concentration and a residual chlorine upper bound. Islam et al. (2017) couple multi-species simulations with a genetic algorithm to optimize booster locations and dosage to minimize exposure to Escherichia coli (E. coli). While these studies show that booster stations for water security applications are feasible, the methods are computationally intensive, specific to one type of contaminant, and there is no guarantee that the genetic algorithm will achieve an optimal solution. Seth et al. (2017) used a mixed-integer linear program (MILP) to identify

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booster station locations that minimized the mass consumed by the population or the population that dosed more than a specified mass threshold of the contaminant. The MILP was able to find optimal locations for boosters in large water distribution network models by considering a large ensemble of contaminant scenarios, but the optimization method greatly simplified reaction kinetics by assuming that any type of contamination is completely neutralized when it comes in contact with chlorine. Parks and VanBriesen (2009) and Propato and Uber (2004c) analyzed the effectiveness of booster stations to reduce the impact of contamination in the system. These two articles evaluated the performance of booster stations in water security applications, but optimization methods were not used to select the locations for the booster stations.

The objective of this article is to introduce a new booster station optimization method that uses a limiting reagent reaction model and compare the results to the method from Seth et al. (2017). Both methods assume approximate reactions to simplify the optimization problem. Both methods also propose optimization formulations that include stochasticity in the location and time of the contamination incident. Unlike the method in Seth et al. (2017), which assumes that chlorine is always in stoichiometric excess as it neutralizes contaminant, the formulation proposed in this article can be used to model different stoichiometric ratios between the contaminant and chlorine. Different levels of contaminant-chlorine reactivities are approximated using the proposed formulation and their impact is studied on both the booster placement layout and the effectiveness of the booster stations in reducing impact on the population. Additionally, this article investigates how the location of online sensors can influence detection time and therefore the performance of disinfectant booster stations. A case study is used to explore the impact of optimally placed booster stations to reduce contamination in water distribution systems. Booster placements were further evaluated given a range of stoichiometric ratios to determine how the methods could be used to develop response action plans.

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2. Methods

The optimization method introduced in this article, referred to as the 'Limiting Reagent' method, builds upon and adds more realism to the method described in Seth et al. (2017), referred to as the 'Neutralization method.' Both methods are formulated to minimize the expected population dosed given a ensemble of contamination scenarios. Population dosed is defined as the number of people who ingest contaminated tap water above a specified mass threshold.

The Neutralization and Limiting Reagent methods approximate the unknown reaction between a contaminant and chlorine. For both methods, the contaminant and chlorine concentrations are calculated using water distribution hydraulic and water quality models. For the results shown in this article, the hydraulics are computed using EPANET 2.0 (Rossman 2000) and Merlion (Mann, Hackebeil, and Laird 2014; Wong et al. 2010) is used for the water quality analysis. EPANET could be used for the hydraulic and water quality simulations for the Neutralization method. However, the linear water quality equations from Merlion are necessary for the Limiting Reagent method. In the interest of using the same simulation engine for both methods, Merlion was used in both the Neutralization and Limiting Reagent methods. Both the Limiting Reagent and Neutralization methods are included in EPA's Water Security Toolkit (WST), a suite of software tools designed to help evaluate and plan response strategies in the case of a contamination incident. Additional information on these methods and on human health impact models used to compute the population dosed can be found in the WST User Manual (EPA 2014).

2.1. *Neutralization method*

The Neutralization method assumes that the chlorine completely and instantaneously inactivates all of the contaminant on contact. The Neutralization method takes advantage of several simplifying assumptions to address uncertainty related to the contaminant-chlorine reaction. The first assumption is that the interaction between the contaminant and chlorine does not impact the transport of chlorine throughout the water distribution system. The second assumption is that the hydraulics are not

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altered by the injection of either species, and that both the contaminant and chlorine behave like tracers, meaning they do not undergo any decay. Third, the Neutralization method assumes that a sufficient concentration of chlorine is injected to completely and instantaneously inactivate the contaminant if they come into contact. Finally, this method assumes that only chlorine injected at a booster station reacts with the contaminant; residual chlorine from the treatment plant or other booster stations is ignored. These assumptions remove the need to embed a reaction model within the problem formulation. The Neutralization formulation relies on data from independent simulations of chlorine and the contaminant based on a water distribution network model. These assumptions allow the booster station placement problem to be written as an MILP, with hydraulic and water quality simulations performed outside the optimization routine. The Neutralization method is equivalent to a weighted maximal set coverage problem. The formulation is described in Seth et al. (2017) and is included below for completeness:

$$\min \quad \sum_{s \in S} P(s) \sum_{n \in N} z_{ns} pop_n \tag{1}$$

$$s.t. \quad \delta_{nts} \geq 1 - \sum_{b \in D_{nts}} y_b \qquad \forall n \in N, t \in T, s \in S \tag{2}$$

$$d_{ns} = \sum_{t \in T} \delta_{nts} I_{nts} \qquad \forall n \in N, s \in S \tag{3}$$

$$d_{ns} \leq z_{ns}(M - \tau) + \tau \qquad \forall n \in N, s \in S \tag{4}$$

$$\sum_{b \in B} y_b \leq B_{max} \tag{5}$$

$$0 \leq \delta_{nts} \leq 1 \qquad \forall n \in N, t \in T, s \in S \tag{6}$$

$$y_b \in \{0, 1\} \qquad \forall b \in B \tag{7}$$

$$z_{ns} \in \{0, 1\} \qquad \forall n \in N, s \in S \tag{8}$$

where S, N, T, and B represent the sets of contamination scenarios, network nodes, time steps, and potential booster locations, respectively. The objective function in Equation 1 is set to minimize the population dosed across all nodes and for every

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scenario in the simulation. Each scenario s has probability $P(s)$. Binary variable z_{ns} is used to indicate whether the total dosage at node n for scenario s is above a user specified dose threshold τ. The total population at a node is represented by pop_n. For simplicity, it is assumed that every person at a node receives the same dose. The continuous variable δ_{nts} indicates whether or not contaminant is consumed at node n over time step t for scenario s. Equation 2 ensures that δ_{nts} equals 0 if at least one selected booster station location provides neutralization of node n over time step t for scenario s, otherwise, δ_{nts} equals 1. The set D_{nts} contains the booster station locations that neutralize node n over time step t for scenario s. D_{nts} is determined from the precomputed booster station simulations. These simulations determine the node-time pairs that are neutralized based on the specific contaminant scenario and feasible booster station locations. The binary variable y_b is 1 if node b is selected as a booster station location and 0 otherwise. Equation 3 calculates the mass dose, d_{ns}, received by the population at node n for scenario s. The parameter I_{nts} represents the mass ingested by the population at node n over the time step t for scenario s. This parameter is calculated from precomputed injection scenario simulations. Equation 4 is the big-M constraint used to switch the binary variable z_{ns} to 1 when the total mass dosed at node n for scenario s is above the threshold τ. Equation 5 restricts the number of booster stations to be less than or equal to B_{max}. Equations 6, 7, and 8 limit the range for δ_{nts} and state that booster placement, y_b, and dose above threshold, z_{ns}, are binary decision variables.

2.2. *Limiting reagent method*

The Limiting Reagent method assumes instantaneous reaction of the contaminant and chlorine according to a stoichiometric ratio, which is defined as the mass of chlorine removed per the mass (mg, if chemical) or colony-forming units (CFU, if biological) of contaminant rendered harmless by its reaction with chlorine. While this is more realistic than the Neutralization method, this is still a simplification of complex reaction dynamics. While specific contaminant-chlorine reactions can be modeled using multi-species dynamics, for example using EPANET-MSX (Shang, Uber, and Rossman 2008), these models cannot be imbedded into MILP formulations. To illustrate

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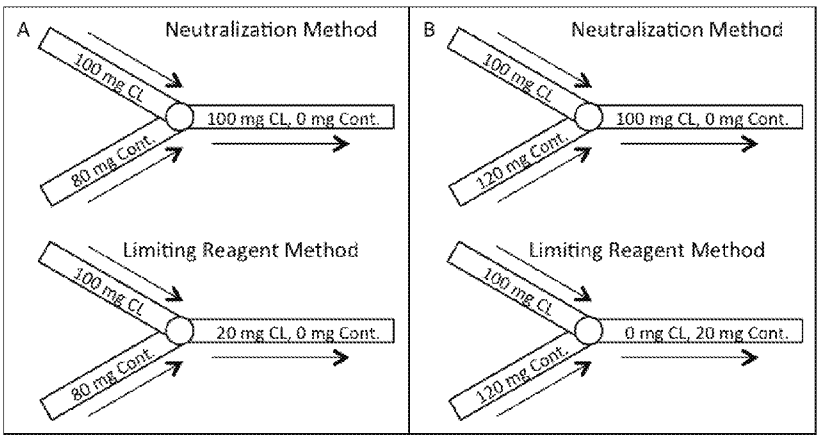

Figure 1.: Neutralization and Limiting Reagent method examples. Both examples assume a stoichiometric ratio of 1 mg chlorine (CL) per mg contaminant (Cont)

the difference between the Limiting Reagent and Neutralization method, two examples (A and B) are shown in Figure 1. For both examples, a stoichiometric ratio of 1 mg chlorine/mg contaminant is used for the Limiting Reagent method. In Example A, 100 mg of chlorine comes in contact with 80 mg of contaminant at a pipe junction. Using the Neutralization method, all of the contaminant is inactivated and the amount of chlorine remains unchanged. Using the Limiting Reagent method, 80 mg of chlorine is used to inactivate all of the contaminant. In this case, the contaminant is the limiting reagent and 20 mg of chlorine remains. Example B illustrates a case where chlorine is the limiting reagent. In this case, 100 mg of chlorine comes in contact with 120 mg of contaminant. Results using the Neutralization method are unchanged. Using the Limiting Reagent method, 100 mg of chlorine can inactivate 100 mg of the contaminant with 20 mg of contaminant remaining.

The Limiting Reagent method assumes that the reaction between chlorine and the contaminant is fast compared to the time of the simulation and that the reaction proceeds until the limiting reagent is fully utilized. As the stoichiometric ratio approaches zero, the Limiting Reagent method is equivalent to the Neutralization method. The Limiting Reagent method also assumes that the water distribution hydraulics are not altered by the injection of chlorine, and that only chlorine injected from booster stations affects contaminant concentration. However, unlike the Neutralization method, the concentrations of the contaminant and chlorine are explicitly included in the optimization. The Limiting Reagent method can be written as an MILP that embeds a

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linear water quality model for the contaminant and chlorine. The Limiting Reagent method is defined as:

$$
\begin{aligned}
\min \quad & \sum_{s \in S} P(s) \sum_{n \in N} z_{ns} pop_n & & (9)\\
s.t. \quad & \mathbf{G}\mathbf{c}_s^{con} = \mathbf{D}(\mathbf{m}_s^{con} - \mathbf{r}_s^{con}) & \forall s \in S & (10)\\
& \mathbf{G}\mathbf{c}_s^{dis} = \mathbf{D}(\mathbf{m}_s^{dis} - \rho \mathbf{r}_s^{con}) & \forall s \in S & (11)\\
& m_{bts}^{dis} = y_b L_{bts} & \forall b \in B, t \in T, s \in S & (12)\\
& m_{nts}^{dis} = 0 & \forall n \in N \backslash B, t \in T, s \in S & (13)\\
& d_{ns} = \sum_{t \in T} c_{nst}^{con} v_{nst} & \forall n \in N, s \in S & (14)\\
& d_{ns} \leq z_{ns}(M - \tau) + \tau & \forall n \in N, s \in S & (15)\\
& \sum_{b \in B} y_b \leq B_{max} & & (16)\\
& y_b \in \{0, 1\} & \forall b \in B & (17)\\
& z_{ns} \in \{0, 1\} & \forall n \in N, s \in S & (18)\\
& c_{nts}^{con}, c_{nts}^{dis}, r_{nts}^{con} \geq 0 & \forall n \in N, t \in T, s \in S & (19)\\
& & & (20)
\end{aligned}
$$

where S, N, T and B represent the sets of contamination scenarios, network nodes, time steps, and potential booster station locations, respectively. The objective function in Equation 9 minimizes the population dosed at all nodes for every contamination scenario in the simulation. Each scenario s has probability $P(s)$. Binary variable z_{ns} is used to indicate whether the total dosage at node n for scenario s is above a user specified dose threshold τ. The total population at a node is represented by pop_n. These definitions are the same as defined in the Neutralization method above.

In the Linear Reagent method, the water quality model is formulated as a set of linear equations and the forward tracing simulations can be included directly within the MILP. The concentration of the contaminant and chlorine, c_{nts}^{con} and c_{nts}^{dis}, respectively, are defined for each node n, time step t, and contamination scenario s. The variables

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m_{nts}^{con} and m_{nts}^{dis} are the mass injections for the contaminant and chlorine, respectively, at node n and time step t for contamination scenario s. Equations 10 and 11 include the embedded linear water quality model, Merlion, as stored in the $\mathbf{G}$ and $\mathbf{D}$ matrices. The $\mathbf{G}$ and $\mathbf{D}$ matrices map the contaminant and chlorine mass injected at all nodes and time steps for a scenario s (vectors $\mathbf{m}_s^{con}$ and $\mathbf{m}_s^{dis}$) to contaminant and chlorine concentration at all nodes and time steps for each scenario s (vectors $\mathbf{c}_s^{con}$ and $\mathbf{c}_s^{dis}$). The contaminant mass removed at all nodes and time steps for contamination scenario s, based on the reaction between the contaminant and chlorine, is given by the vector $\mathbf{r}_s^{con}$. The stoichiometric ratio, ρ, defines the mass of chlorine removed per mass of contaminant removed. Equations 12 and 13 set the booster injection amount. The amount is L_{bts} if a booster station is placed at node b, otherwise the injection amount is zero. The binary variable y_b is 1 if node b is selected as a booster station location and 0 otherwise. Equation 14 calculates the mass dosed by the population,d_{ns}, at node n for scenario s. The parameter v_{nst} represents the volume of water ingested by the population at node n for scenario s, over the time step t. Equation 15 is the big-M constraint used to switch the binary variable z_{ns} to 1 when the total mass dosed at node n for scenario s is above the threshold τ. Equation 16 restricts the number of booster stations to be less than or equal to B_{max}. Equation 17 and 18 define y_b and z_{ns} as a binary variable respectively. Equation 19 indicates that the contaminant and chlorine concentrations and the contaminant mass removed are greater than or equal to zero.

3. Case study design

A case study was designed to evaluate the effectiveness of chlorine injection at booster stations as a response to water contamination incidents, and compare the results from the Neutralization and Limiting Reagent methods. This section includes a description of the water distribution network models, the sensor placement layout used to detect contamination and initiate a response action, the ensemble of possible contamination scenarios, and a description of how the booster stations operate.

Two example water distribution network models are used in this case study. The

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first network, referred to as 'Network 1,' is the Example Network 3 distributed with EPANET 2.0 (Figure 2). This network contains 92 junctions, 3 tanks, and 2 reservoirs. Network 1 provides drinking water to approximately 79,000 customers, assuming an average usage rate per person of 200 gallons per day. A more complex network, referred to as 'Network 2,' contains 407 junctions, 2 tanks, and 1 reservoir (Watson, Murray, and Hart 2009) (Figure 3). Network 2 serves approximately 6,400 customers.

The sensor placement layout can have a large impact on the effectiveness of response action plans. The time it takes to detect contamination and the time it takes to respond using boosted chlorination greatly affects the ability of boosters to reduce the impacts of contamination incidents. If the boosters are initiated too late, most of the contaminant has already been consumed by customers, and the impacts cannot be reduced. For that reason, several sensor placement layouts were used in this study to examine the influence of detection time. For Network 1, three sensor placement layouts were optimized to place 2, 5, and 10 sensors. For Network 2, the studies were performed using one sensor placement layout with 5 optimally placed sensors. Examples of the sensor locations are shown in Figures 2 and 3.

A set of possible contamination scenarios must be defined for the optimal placement of sensors and booster stations. The set of scenarios does not have to be the same for the two independent optimization problems. For simplicity, the same set of scenarios was used for the optimum placement of sensors and booster stations in this case study. Sensor placement optimization used detection time as the objective metric to minimize, while booster placement used population dosed. One contamination scenario was simulated from each non-zero demand (NZD) node in the network. NZD nodes are defined as nodes with positive customer demands. Network 1 has 59 NZD nodes and Network 2 has 105 NZD nodes. Injection characteristics and dosage threshold values from Davis, Janke, and Magnuson (2014) were used to provide representative results. For each scenario, 0.5 kg of contaminant was injected into the network, starting at midnight on the second day of the simulation and ending an hour later. The impact of each contamination scenario was calculated for 8 hours following the detection time. To calculate population dosed, it was assumed that each person ingested 2 liters of water uniformly throughout the day. Two dosage thresholds (τ) were used to evaluate

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the population dosed metric: 0.0001 and 0.1 mg. Although these threshold values can be lower for certain contaminants, for the purposes of this article, a dose threshold of 0.0001 mg represents high toxicity, while a dose threshold of 0.1 mg represents low toxicity. It should be noted that the mass injection rate and the dose threshold are relative and can be scaled as described in Davis, Janke, and Magnuson (2014); Davis and Janke (2011).

After detection (and possibly additional response delay time), booster stations could start injecting additional chlorine into the network. Booster stations were assumed to inject chlorine at a concentration of 4 mg/L (the MCL for chlorine) and continue for 8 hours. The optimization methods did not account for residual chlorine levels but only for the chlorine supplied by the booster stations after the response action started. For both networks, the set of feasible booster station locations was limited to NZD nodes. The Neutralization method and the Limiting Reagent method were used to identify optimal booster station locations in both networks. The stoichiometric ratio, ρ, in the Limiting Reagent method approximates the contaminant inactivation by chlorine. In order to cover a wide range of contaminants, the following stoichiometric ratios were used to approximate a strong to weak reaction with chlorine: 0 mg CL/mg contaminant, 1 mg CL/mg contaminant, 10 mg CL/mg contaminant, and 100 mg CL/mg contaminant. When the stoichiometric ratio is set to 0 mg CL/mg contaminant, the Neutralization method is used to place boosters in the network. This case study utilizes several modules from the WST software, including hydraulic and water quality simulation, impact assessment using population dosed, sensor placement optimization, and booster placement optimization.

4. Case study results

The following results compare the effectiveness of booster station response to a set of possible contamination scenarios in two networks given a range of detection times (i.e., range of sensor layouts), contaminant toxicities, and stoichiometric ratios. Since booster stations would not be turned on until after detection, it is important to understand how a particular sensor layout impacts the population dosed at the time

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of detection. For Network 1, three sensor layouts (2, 5, and 10 sensors) were used to detect the possible contamination scenarios, while for Network 2 a single network design with 5 sensors was tested. Ideally, all scenarios would be detected by a given sensor placement layout, but this is not the case (unless a sensor can be placed at every node). The number of detected scenarios in Network 1 increased from 72% with a 2-sensor layout to 85% with a 5-sensor layout to 93% with a 10-sensor layout. For the detected scenarios, the corresponding average detection time decreased from 8.0 hours to 1.9 hours to 1.6 hour. The average population dosed at the time of detection was 16,537, using a 2-sensor layout, 2,999 using a 5-sensor layout and 1,123 using a 10-sensor layout, assuming a highly toxic contaminant (dose threshold of 0.0001 mg). This impact cannot be reduced by adding chlorine at booster stations because the boosters are not initiated until after detection. The percent of scenarios detected in Network 2 was lower than Network 1, the average detection time and population dosed at detection was also higher in Network 2. Based on a 5-sensor layout, 78% of contamination scenarios was detected, the average detection time was 4.6 hours, and the population dosed at time of detection was 162 assuming a highly toxic contaminant (dose threshold of 0.0001 mg). Using a 10-sensor layout, 86% of contamination scenarios was detected, the average detection time was 2.9 hours, and the population dosed at time of detection was 132, assuming a highly toxic contaminant (dose threshold of 0.0001 mg).

The Neutralization and Limiting Reagent methods were used to optimally locate 1 to 10 booster station locations in both networks. Figures 2 and 3 illustrate five optimally placed booster stations in Network 1 and Network 2 using two different sets of parameters that include the number of sensors, the stoichiometric ratio (Neutralization = 0, Limiting Reagent = 100), and the dose threshold. Both figures show significant variability in the optimal booster station locations depending on these parameters. Figures 2a and 2b show that going from 2 sensors to 5 sensors can result in very different booster placements for both Neutralization and Limiting Reagent methods. However, the Neutralization method shows very little or no sensitivity to dose threshold as evident from comparing Figures 2c and 2d or Figures 3a and 3b. In general, the Neutralization method resulted in placements that were closer to the upstream

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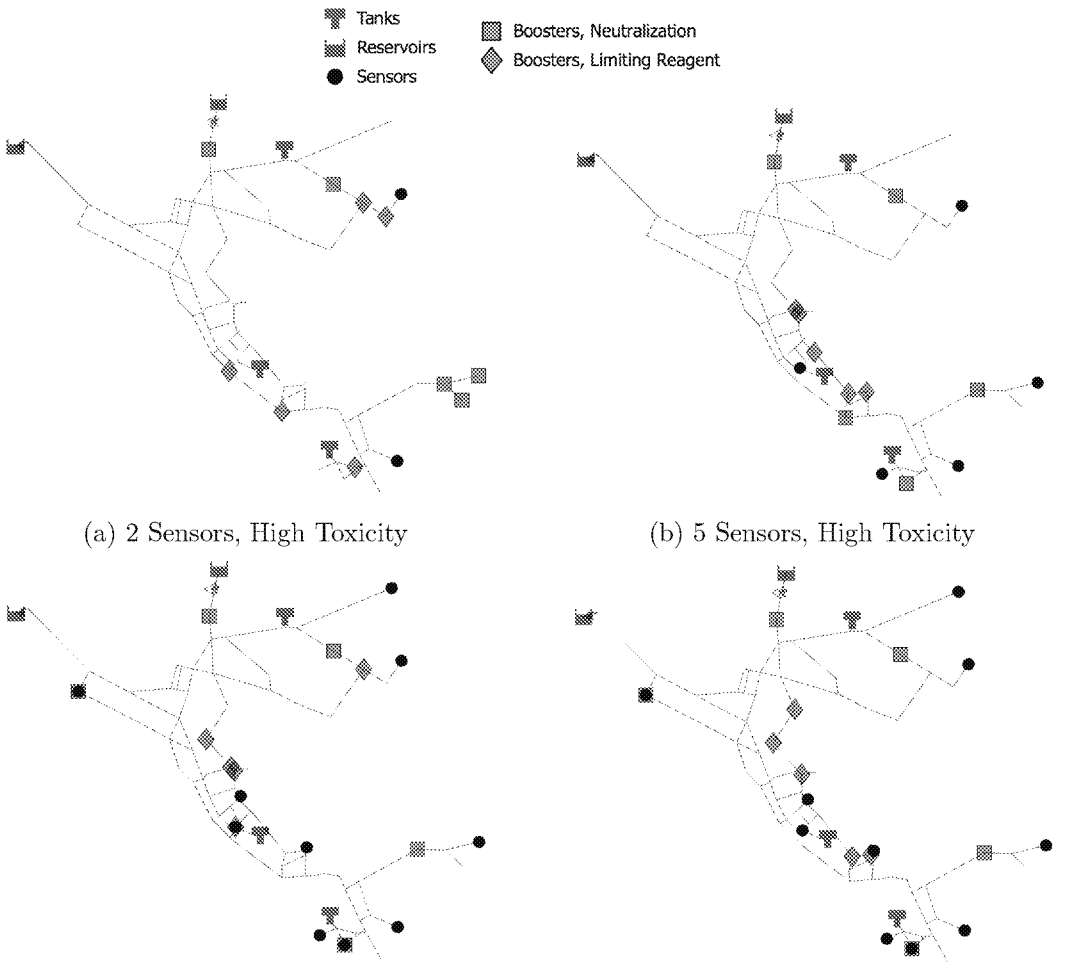

(a) 2 Sensors, High Toxicity

(b) 5 Sensors, High Toxicity

(c) 10 Sensors, Low Toxicity

(d) 10 Sensors, High Toxicity

Figure 2.: Booster station placements for Network 1 with different sensor designs and contaminant toxicity using the Neutralization and Limiting Reagent methods.

and downstream edges of the network while the Limiting Reagent method (with a high stoichiometric ratio) resulted in more central placements. With the Neutralization method, the disinfectant has more impact further downstream and can reduce contaminant to a larger number of nodes.

A series of optimization problems were solved to quantify the population dosed given variable number of boosters and sensors, stoichiometric ratios, and contaminant toxicities. Results for Network 1 are shown in Figure 4. Results for Network 2 are shown in Figure 5 and include only one sensor design. For Network 2, the effect of contaminant toxicity was not as significant as observed in Network 1. It is conjectured that this behavior is due to the fact that Network 2 has a much smaller population that

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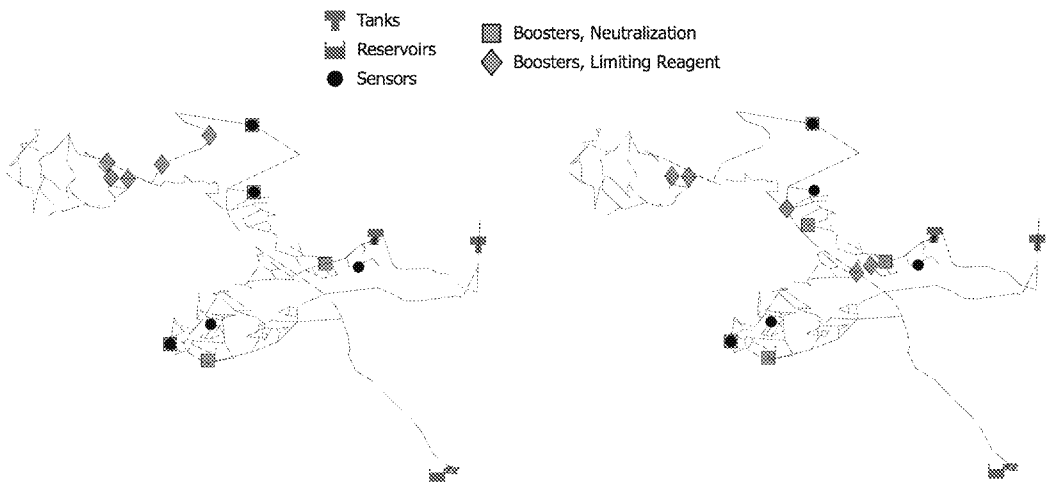

(a) Low Toxicity (b) High Toxicity

Figure 3.: Booster station placements for Network 2 with a 5 sensor layout and different contaminant toxicity using the Neutralization and Limiting Reagent methods.

is spread out over a larger number of nodes, and, therefore the expected population dosed did not show a big variation with respect to the contaminant toxicity even in the absence of booster stations. Based on this analysis, the following set of observations can be made:

(1) With an increase in the number of booster stations, the population dosed asymptotically approached a minimum value.

(2) This minimum value was a function of the number of sensors, the stoichiometric ratio, and the contaminant toxicity.

(3) A three orders of magnitude difference in the dose threshold resulted in about an order of magnitude difference in the number of population dosed. For example, the population dosed for the 10 optimally placed booster obtained using the Neutralization method (ρ=0) with 2 sensors and a dose threshold of 0.0001 mg (high toxicity) was 17,498, while the population dosed for the same set of parameters using a dose threshold of 0.1 mg (low toxicity) was 1,224.

(4) Going from 2 sensors to 5 sensors had a bigger impact in the performance of the booster stations as compared to going from 5 sensors to 10 sensors. This was because of a larger reduction in mean detection time going from 2 sensors to 5 sensors (8.0 hours to 1.9 hours) as compared to the reduction in mean detection time going from 5 sensors to 10 sensors (1.9 hours to 1.6 hours).

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(5) The effect of the stoichiometric ratio on the expected population dosed was more significant in the presence of higher number of sensors. For example, in Figure 4f (10 sensors, high toxicity), placing 10 boosters resulted in the population dosed going from 1,433 for a stochiometric ratio of 1 to 7,021 for a stochiometric ratio of 100. On the other hand, in Figure 4d (5 sensors, high toxicity), placing 10 boosters resulted in the population dosed going from 3,467 for a stochiometric ratio of 1 to 7,239 for a stochiometric ratio of 100.

If booster stations are to be used as a part of water utilities response action plan, then a single booster station placement would be used without knowing the specific contaminant toxicity or its reaction with chlorine. The physical locations of booster stations placed using the Neutralization and Limiting Reagent methods can be evaluated given contamination scenarios with different toxicities and stoichiometric ratios of reaction with chlorine. For example, if the water utility assumes the worst, and places booster stations assuming that the contaminant is of high toxicity and does not react strongly with chlorine, then the booster stations placed using the Limiting Reagent method with a high stoichiometric ratio and low population dosed threshold (high toxicity) can be used to evaluate other types of scenarios. Tables 1 list the expected population dosed given the optimal placement of 10 booster stations for each toxicity level and stoichiometric ratio using Networks 1 and 2. The optimal placement was then used to evaluate the population dosed under a range of contaminant toxicities and stoichiometric ratios. Each case used the 5-sensor layout to detect contamination in the network. The last column in each table is the mean of the expected population dosed over each row; the mean describes the expected number of people dosed assuming all 8 of the scenarios were uniformly distributed and the specific set of booster stations were installed.

As expected, for a particular contaminant toxicity and stoichiometric ratio, the optimal placement always gave a lowest objective (shown in bold) as compared to the evaluation of all other placements on the same contaminant toxicity and stoichiometric ratio. For instance, for Network 1, the expected population dosed for the optimal placement considering high contaminant toxicity and a stoichiometric ratio of 1 was 3,455. This value was lower than all the evaluated objective values for high contaminant

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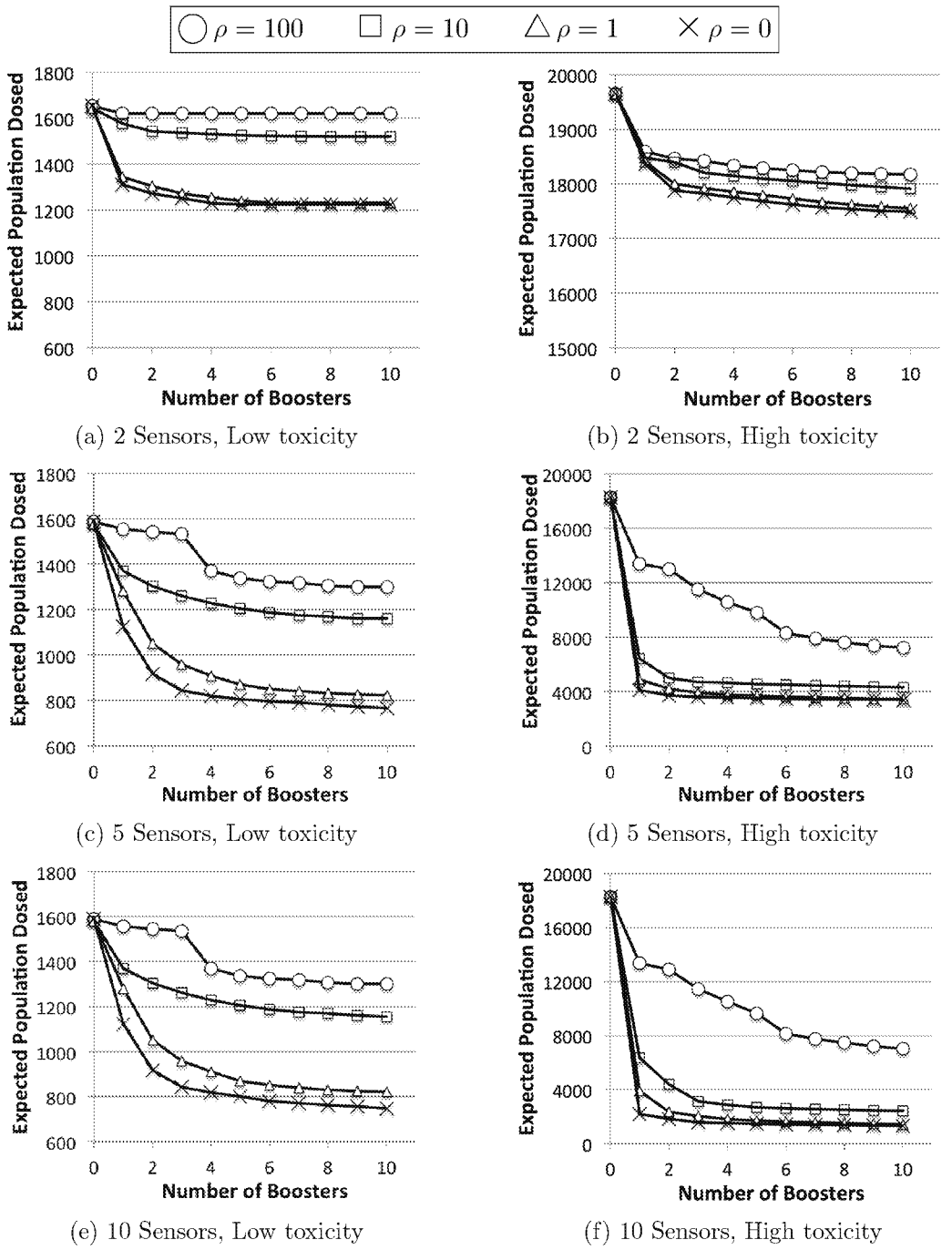

Figure 4.: Reduction in expected population dosed on Network 1 using high and low toxicity and variable number of sensors. ρ=0 represents Neutralization method.

toxicity and stoichiometric ratio of 1 (3rd column). This evaluation also show that the overall performance of a booster placement, represented as the mean of population dosed values over different levels of contaminant toxicity and stoichiometric ratio (last column), improved as the stoichiometric ratio and the contaminant toxicity increased.

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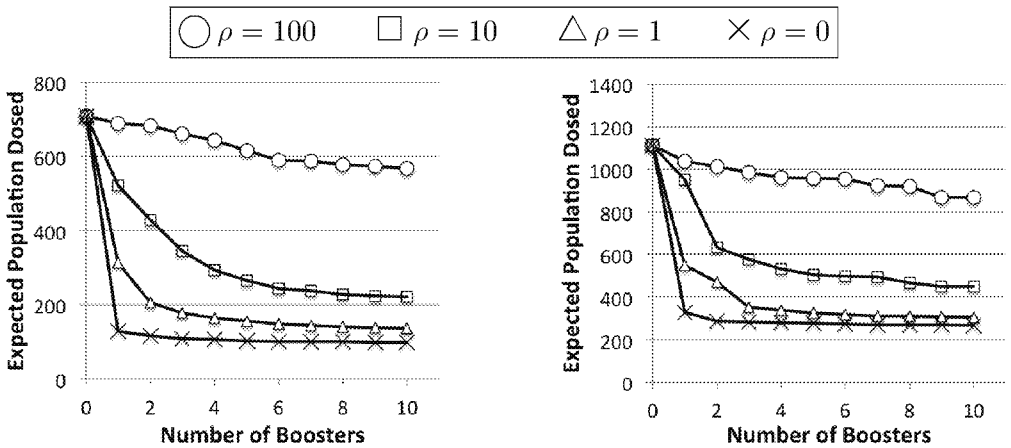

(a) Low toxicity (b) High toxicity

Figure 5.: Reduction in expected population dosed on Network 2 with high and low toxicity and 5 sensors. ρ=0 represents Neutralization method.

For Network 1, the lowest mean expected population dosed was evaluated at 3,061 using contamination scenarios of high toxicity and high stoichiometric ratio (ρ=100). On the other hand, the largest mean expected population dosed was evaluated at 4,320 using contamination scenarios of high toxicity and ρ=0 (Neutralization method). Comparing these two numbers (minimum and maximum mean) resulted in a difference of 1,251 in the mean expected population dosed on Network 1. Similarly, for Network 2, the lowest mean expected population dosed was evaluated at 366 using contamination scenarios of high toxicity and high stoichiometric ratio (ρ=100). These results imply that under the assumption that all eight contaminant toxicity and dose threshold scenarios are uniformly distributed, performing optimal booster placement for the worst case scenario (high contaminant toxicity and high stoichiometric ratio) resulted in a booster station placement that gave the best overall performance measured in terms of expected population dosed.

Given that water distribution system models can be very large, problem size and solution time is of interest to practitioners. Table 2 provides mean number of variables and solution time statistics for all the optimization problems solved using the Neutralization and Limiting Reagent methods. These results highlight the advantage of the Neutralization method. While the Limiting Reagent formulation can take several hours to solve for Network 2, the Neutralization formulation solves within seconds. Instead of embedding the water quality model into the formulation, the Neutralization method

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Table 1.: Evaluation of optimal booster placements for Network 1 (top) and Network 2 (bottom) in terms of population dosed. Each row represents the evaluation of 10 optimally placed booster stations based on a particular stoichiometric ratio (ρ) and contaminant toxicity (first column) against seven other contamination scenarios with different ratios and toxicities (column 2-9). The optimal objective value for the evaluated booster placement is provided in bold. ρ=0 represents Neutralization method.

Network 1	Evaluation Scenarios								
Toxicity, ρ	High	High	High	High	Low	Low	Low	Low	
	ρ=0	ρ=1	ρ=10	ρ=100	ρ=0	ρ=1	ρ=10	ρ=100	Mean
High, $\rho = 0$	**3,397**	4,884	8,522	12,897	792	1,061	1,465	1,540	4,320
High, $\rho = 1$	3,445	**3,455**	4,529	12,670	821	868	1,199	1,540	3,566
High, $\rho = 10$	3,510	3,615	**4,319**	10,711	822	899	1,204	1,537	3,327
High, $\rho = 100$	3,555	4,147	4,666	**7,239**	892	1,290	1,327	1,370	3,061
Low, $\rho = 0$	3,611	4,365	8,739	12,879	**767**	1,067	1,480	1,547	4,307
Low, $\rho = 1$	3,692	4,166	8,569	12,287	820	**823**	1,396	1,531	4,161
Low, $\rho = 10$	3,821	4,273	5,378	12,248	912	949	**1,161**	1,528	3,784
Low, $\rho = 100$	3,838	3,919	4,717	10,694	919	974	1,244	**1,300**	3,451

Network 2	Evaluation Scenarios								
Toxicity, ρ	High	High	High	High	Low	Low	Low	Low	
	ρ=0	ρ=1	ρ=10	ρ=100	ρ=0	ρ=1	ρ=10	ρ=100	Mean
High, $\rho = 0$	**268**	374	787	1,041	100	209	461	694	492
High, $\rho = 1$	290	**297**	632	1021	117	168	386	683	449
High, $\rho = 10$	285	337	**351**	924	118	161	238	587	375
High, $\rho = 100$	325	363	416	**667**	131	183	255	586	366
Low, $\rho = 0$	274	571	1,036	1,080	**99**	257	561	702	573
Low, $\rho = 1$	281	310	481	968	111	**137**	311	651	406
Low, $\rho = 10$	284	336	404	929	115	167	**221**	585	380
Low, $\rho = 100$	284	336	399	868	115	167	222	**568**	370

benefits from performing simulations outside of the optimization that take less than a 10 seconds to solve for both networks. However, as seen from the analysis above, performing optimal booster placement for the worst case scenario using the Limiting Reagent method can result in better performance over a wide range of scenarios.

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Table 2.: Mean number of variables and solution times for the Neutralization and Limiting Reagent formulations on Network 1 and Network 2.

		Neutralization Method		Limiting Reagent Method	
Network	Junctions	Variables	Solve Time (Hrs)	Variables	Solve Time (Hrs)
Network 1	92	6,114	0.002	461,928	1.23
Network 2	407	18,253	0.01	3,583,786	7.32

5. Discussion

In the event of a contamination incident in a water distribution system, booster stations could be used to inject additional chlorine to reduce the impact of the incident. Once contamination has been detected by a an online sensor, booster stations could be initiated to inject chlorine into the system to inactivate the contaminant. The effectiveness of booster stations used in this way depends largely on the sensor placement layout used to detect contamination and the reaction dynamics between chlorine and the contaminant. Given that the contaminant and injection location are likely unknown at the time of detection, fixed booster stations would have to be effective for a wide range of contamination incidents. In this article, two booster station placement optimization methods were compared: the Neutralization and Limiting Reagent methods. Each method is formulated as a MILP and uses simplifying assumptions about the contaminant and chlorine reaction dynamics. The major differences between these two methods is that the Neutralization method assumes that chlorine remains in stoichiometric excess as it neutralizes the contaminant through the network, while the Limiting Reagent method lets the user provide a stoichiometric ratio as a parameter to approximate different kinds of contaminant-chlorine reactions. This article provides a comparison between these two methods and shows how these two methods can result in significantly different booster station placements on two different water distribution network models.

This article also compares the performance of these two methods in terms of expected population dosed. Since the population dosed depends on the dose level of a

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contaminant, two dosage thresholds were studied along with a range of stoichiometric ratios. The results show that the effect of contaminant toxicity on the performance of booster stations can be very significant for some networks (about an order of magnitude for Network 1). Furthermore, each optimal booster station placement obtained using different levels of contaminant toxicity and stoichiometric ratios was evaluated over the same range of toxicities and stoichiometric ratios. The results show that under the assumption that the probability of contaminant toxicities and stoichiometric ratios are uniformly distributed, the optimal booster station placement obtained assuming the worst case scenario of high contaminant toxicity and high chlorine to contaminant stoichiometric ratio, resulted in the lowest overall expected population dosed. Additionally, this article studies the impact of the number of water quality sensors used to detect potential contamination incidents on the performance of booster stations. The results show that reducing incident detection times by placing more sensors can significantly improve the effectiveness of booster stations. To improve emergency response plans using boosted chlorine, future research should consider: (1) the combined placement of sensors and booster stations, (2) combine booster stations with other response options (e.g., flushing or isolation) in order to minimize health risk to the population, and (3) evaluation using multi-species reaction models for a range of specific contaminants.

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describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

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