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- Mixed integer programming for optimal design and control of water networks
- Optimal placement and operation of pressure control valves and chlorine boosters
- New heuristic enables joint optimization of pressure and disinfectant dosage

Relax-Tighten-Round Algorithm for Optimal Placement and Control of Valves and Chlorine Boosters in Water Networks

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Abstract

In this paper, a new mixed integer nonlinear programming formulation is proposed for optimally placing and operating pressure reducing valves and chlorine booster stations in water distribution networks. The objective is the minimization of average zone pressure, while penalizing deviations from a target chlorine concentration. We propose a relax-tighten-round algorithm based on tightened polyhedral relaxations and a rounding scheme to compute feasible solutions, with bounds on their optimality gaps. This is because off-the-shelf global optimization solvers failed to compute feasible solutions for the considered non-convex mixed integer nonlinear program. The implemented algorithm is evaluated using three benchmarking water networks, and they are shown to outperform off-the-shelf solvers, for these case studies. The proposed heuristic has enabled the computation of good quality feasible solutions in most instances, with bounds on the optimality gaps that are comparable to the order of uncertainty observed in operational water network models.

Keywords: Global optimization, Mixed integer nonlinear programming, Water networks, Pressure management, Water quality.

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1. Introduction

The main operational objectives for water utilities include the reduction of water leaks, and management of drinking-water quality. Leakage reduction is achieved by controlling average zone pressure (AZP) within water distribution networks (WDNs), while satisfying minimum service requirements (Wright et al., 2015). Pressure control schemes are implemented through pressure reducing valves (PRVs), which reduce pressure at their downstream node. The problem of optimal placement and operation of PRVs in WDNs has been formulated in previous literature, and solved using both evolutionary algorithms (Araujo et al., 2006; Nicolini & Zovatto, 2009) and mathematical optimization methods (Eck & Mevissen, 2012; Pecci et al., 2019).

Monitoring and control of disinfectant residuals in drinking water distribution networks is critical to maintain the water quality and eliminate the risks of contamination with pathogens such as bacteria and viruses in distribution (Aisopou et al., 2014; Sakomoto et al., 2020). This is particularly critical during the current COVID-19 pandemic as leaking sewage from sewer networks could allow potentially harmful contaminants into drinking water networks (Quilliam et al., 2020). In order to deactivate any pathogens that might exist in distribution networks, disinfectant is typically added at water sources (e.g. water treatment plants), with chlorine being a commonly used water disinfectant. Because chlorine is reactive, it is depleted over time as it travels across the pipe networks, causing a reduction in the ability to prevent microbial contamination. Water utilities aim to maintain a target chlorine concentration, which is sufficient to safeguard public health, while avoiding excessive chlorination, resulting in taste and odor problems, as well as the growth of disinfection by-products. In addition, the objective is to maintain optimal and constant chlorine concentrations, as variations in chlorine concentration are perceived as water quality problems by customers. Chlorine booster stations are used to deal with this challenge (Boccelli et al., 1998; Propato & Uber, 2004). Using booster chlorination, disinfectant is re-applied at selected locations within the network, leading to a more uniform spatial and temporal distribution of chlorine residuals. Previous literature has modeled the operation of booster stations assuming known flow velocities across network pipes - see as examples Boccelli et al. (1998); Propato & Uber (2004). However, this can lead to sub-optimal design and operation of WDNs. In fact, in order to mitigate disinfectant decay reactions, network operators should aim to reduce travel time from water sources to demand nodes. This may result in sub-optimal pressure management schemes, where minimum pressure constraints are not satisfied, as observed in Kang & Lansey (2010). Therefore, we consider the joint optimization of hydraulic pressure and flows, together with chlorine residual concentrations in WDNs.

We investigate the problem of minimizing average zone pressure, while penalizing deviations from chlorine target concentrations, and satisfying regulatory constraints on pressure and chlorine concentration levels. Ostfeld (2005) and Kang & Lansey (2010) implemented genetic algorithms to solve problems of optimal operation of WDNs, where optimization unknowns include network flows and chlorine concentrations, while locations of PRVs and chlorine booster stations are fixed. However, pressure reducing valves and booster stations should be optimally placed for a more effective pressure control and management of chlorine residual concentrations.

In this manuscript, we propose a new mathematical framework for the optimal placement and operation of pressure reducing valves and chlorine booster stations. The considered objective is the minimization of average zone pressure, while penalizing deviations from target chlorine concentrations at demand nodes. The transport of chlorine through each pipe is modeled by a one dimensional first-order advection PDE (Rossman & Boulos, 1996), where flow velocity corresponds to the one-dimensional velocity field, and a linear function is used to represent chlorine decay (Hallam et al., 2002). We implement an implicit upwind scheme to discretize the considered PDE. Optimization constraints include quadratic equations modelling head loss due to pipe friction (Eck & Mevissen, 2015; Pecci et al., 2017), and bilinear terms due to the presence of unknown flow velocities within the discretized advection PDE. In addition, binary variables are used to model the direction of flow across pipes, and the placement of valves and booster stations. The resulting optimization problem is a non-convex mixed integer nonlinear program.

In comparison to previous literature (Ostfeld, 2005; Kang & Lansey, 2010), which relied on genetic algorithms, we investigate the application of mathematical optimization methods to compute feasible solutions for the considered problem, with guaranteed bounds on their optimality gaps. We propose a relax-tighen-round (RTR) algorithm based on polyhedral relaxations of the non-convex terms, an optimization-based-bound-tightening scheme, and a rounding heuristic. The developed RTR algorithm computes a feasible solution for the considered non-convex MINLP, with bounds on its optimality gap. In comparison, we show that off-the-shelf global optimization solvers failed to generate feasible solutions for the considered problem. The performance of the RTR algorithm is investigated using multiple problem instances for different WDN case studies.

2. Problem formulation

We formulate the problem of optimal placement and operation of pressure reducing valves and chlorine booster stations, with the objective of minimizing average zone pressure, while penalizing deviations from target chlorine concentrations at demand nodes. A WDN with n_n demand nodes, n_0 source nodes (e.g. water sources, water treatment plants), and n_p links is modelled as a directed graph with $n_n + n_0$ vertices and n_p edges. Define $\mathcal{P} := \{1, \dots, n_p\}$ and $\mathcal{N} := \{1, \dots, n_n\}$, $\mathcal{N}^0 := \{1, \dots, n_0\}$. Given a node $i \in \mathcal{N}$, let I_i^{in} and I_i^{out} be the index sets corresponding to links with assigned direction entering and leaving the node, respectively. We consider network operation within a discretized time interval $\mathcal{T} = 1, \dots, n_t$. The objective of this study is to minimize average zone pressure in water distribution networks, while penalizing deviation from target chlorine concentrations. Average Zone Pressure (AZP) is defined as the following weighted sum of nodal pressures (Wright et al., 2015):

$$\sum_{k\in\mathcal{T}}\sum_{i\in\mathcal{N}} \omega_i (h_{i,k} - h_i^{\mathrm{elev}}) \tag{1}$$

where $h_{i,k}$ is the unknown hydraulic head at node $i \in \mathcal{N}$ and time $k \in \mathcal{T}$, while $\boldsymbol{h}^{\mathrm{elev}} \in \mathbb{R}^{n_n}$ is the vector of known nodal elevations. Weights are defined as follows:

$$\omega_i := \frac{\sum_{l\in I_i^{\mathrm{in}}\cup I_i^{\mathrm{out}}} L_l}{n_t \sum_{j\in\mathcal{N}} \sum_{l\in I_j^{\mathrm{in}}\cup I_j^{\mathrm{out}}} L_l}, \quad \forall i \in \mathcal{N} \tag{2}$$

Let $\boldsymbol{c}^* \in \mathbb{R}^{n_n}$ be a vector of target chlorine concentration at network nodes. Moreover, set

$$\hat{d}_{i,k} = \frac{d_{i,k}}{\sum_{k\in\mathcal{T}}\sum_{j\in\mathcal{N}} d_{j,k}}, \quad \forall i \in \mathcal{N},\ k \in \mathcal{T} \tag{3}$$

where $d_{i,k}$ is the known demand at node $i \in \mathcal{N}$ and time $k \in \mathcal{T}$. Denote by $c_{i,k}$ the unknown chlorine concentration at node $i \in \mathcal{N} \cup \mathcal{N}^0$ and time $k \in \mathcal{T}$. We define the Average Target Deviation (ATD) as

$$\sum_{k\in\mathcal{T}}\sum_{i\in\mathcal{N}} \hat{d}_{i,k} |c_{i,k} - c_i^*| \tag{4}$$

The formula for ATD can be reformulated as a linear function by introducing auxiliary variables $\mu_{i,k}$, which satisfy the following linear constraints:

$$c_{i,k} - c_i^* \leq \mu_{i,k}, \quad \forall i \in \mathcal{N},\ k \in \mathcal{T} \tag{5a}$$

$$-c_{i,k} + c_i^* \leq \mu_{i,k}, \quad \forall i \in \mathcal{N},\ k \in \mathcal{T}. \tag{5b}$$

The objective function to be minimized is written as:

$$\sum_{k\in\mathcal{T}}\sum_{i\in\mathcal{N}} \omega_i h_{i,k} + \sum_{k\in\mathcal{T}}\sum_{i\in\mathcal{N}} \hat{d}_{i,k}\mu_{i,k} \tag{6}$$

Since the considered problem aims to optimize both hydraulic pressure and water quality, its formulation is based on hydraulics and water quality modelling.

2.1. Hydraulic variables and constraints

First, we introduce optimization variables and constraints related to network hydraulic properties. Source nodes are assumed to have known hydraulic heads

$h^0_{i,k}$, $i \in \mathcal{N}^0$, $k \in \mathcal{T}$. We denote by $q_{l,k}$ the unknown flow in link $l \in \mathcal{P}$ at time $k \in \mathcal{T}$. The unknown frictional head loss across link l at time k is denoted by $\theta_{l,k}$. Pressure control valves reduce pressure at their downstream node, introducing additional head losses, which are represented by variable $\eta_{l,k}$, $l \in \mathcal{P}$, $k \in \mathcal{T}$. Vector of binary variables $\mathbf{v} \in \{0,1\}^{2n_p}$ models the placement of control valves. We have:

$$v_l = \begin{cases} 1 & \text{a valve is placed on link } l \text{ in the positive flow direction} \\ 0 & \text{otherwise,} \end{cases} \tag{7}$$

and

$$v_{n_p+l} = \begin{cases} 1 & \text{a valve is placed on link } l \text{ in the negative flow direction} \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

These binary variables are subject to the following physical and economical constraints:

$$v_l + v_{n_p+l} \leq 1, \quad l \in \mathcal{P} \tag{9a}$$

$$\sum_{l \in \mathcal{P}} (v_l + v_{n_p+l}) = n_v \tag{9b}$$

The following constraints formulate energy and mass conservation laws, and the placement of pressure reducing valves on network links:

$$h_{i_1,k} - h_{i_2,k} = \theta_{l,k} + \eta_{l,k}, \quad i_1 \xrightarrow{l} i_2, l \in \mathcal{P}, i_1 \in \mathcal{N}, i_2 \in \mathcal{N}, k \in \mathcal{T} \tag{10a}$$

$$h^0_{i_1,k} - h_{i_2,k} = \theta_{l,k} + \eta_{l,k}, \quad i_1 \xrightarrow{l} i_2, l \in \mathcal{P}, i_1 \in \mathcal{N}^0, i_2 \in \mathcal{N}, k \in \mathcal{T} \tag{10b}$$

$$\sum_{l \in I_i^{\text{in}}} q_{l,k} - \sum_{l \in \in I_i^{\text{out}}} q_{l,k} = d_{i,k}, \quad i \in \mathcal{N}, k \in \mathcal{T} \tag{10c}$$

$$\eta_{l,k} - \eta^{\max}_{l,k} v_l \leq 0, \quad l \in \mathcal{P}, k \in \mathcal{T} \tag{10d}$$

$$-\eta_{l,k} + \eta^{\min}_{l,k} v_{n_p+l} \leq 0, \quad l \in \mathcal{P}, k \in \mathcal{T} \tag{10e}$$

$$-q_{l,k} - q^{\min}_{l,k} v_l \leq -q^{\min}_{l,k}, \quad l \in \mathcal{P}, k \in \mathcal{T} \tag{10f}$$

$$q_{l,k} + q^{\max}_{l,k} v_{n_p+l} \leq q^{\max}_{l,k}, \quad l \in \mathcal{P}, k \in \mathcal{T} \tag{10g}$$

In order to model the transport of chlorine constituent, it is required to explicitly consider the flow direction across network links as a decision variable. Therefore, we introduce auxiliary variables $q^+_{l,k}$, $q^-_{l,k}$, $\theta^+_{l,k}$, $\theta^-_{l,k}$, $s_{l,k}$, and binary variable $z_{l,k} \quad \{0,1\}$ such that

$$q_{l,k} = q^+_{l,k} - q^-_{l,k}, \quad l \quad P, \; k \quad T \tag{11a}$$

$$s_{l,k} = q^+_{l,k} + q^-_{l,k}, \quad l \quad P, \; k \quad T \tag{11b}$$

$$\theta_{l,k} = \theta^+_{l,k} - \theta^-_{l,k}, \quad l \quad P, \; k \quad T \tag{11c}$$

$$0 \leq q^+_{l,k} \leq (q^+)^{\max}_{l,k} z_{l,k}, \quad l \quad P, \; k \quad T \tag{11d}$$

$$0 \leq q^-_{l,k} \leq (q^-)^{\max}_{l,k}(1 - z_{l,k}), \quad l \quad P, \; k \quad T \tag{11e}$$

$$0 \leq \theta^+_{l,k} \leq (\theta^+)^{\max}_{l,k} z_{l,k}, \quad l \quad P, \; k \quad T \tag{11f}$$

$$0 \leq \theta^-_{l,k} \leq (\theta^-)^{\max}_{l,k}(1 - z_{l,k}), \quad l \quad P, \; k \quad T \tag{11g}$$

Frictional head losses are often represented by either the Hazen-Williams (H-W) or the Darcy-Weisbach (D-W) equations (D'Ambrosio et al., 2015). Since both formulae involve non-smooth terms, quadratic approximations have been proposed and used in previous literature (Eck & Mevissen, 2015; Pecci et al., 2017). Let $\boldsymbol{a} \quad \mathbb{R}^{n_p}$ and $\boldsymbol{b} \quad \mathbb{R}^{n_p}$ be vector of coefficients of these approximations. We enforce the following constraints on variables $\theta^+_{l,k}$ and $\theta^-_{l,k}$:

$$\theta^+_{l,k} = a_l (q^+_{l,k})^2 + b_l q^+_{l,k}, \quad l \quad P, \; k \quad T \tag{12a}$$

$$\theta^-_{l,k} = a_l (q^-_{l,k})^2 + b_l q^-_{l,k}, \quad l \quad P, \; k \quad T. \tag{12b}$$

Constraints $z_{l,k} \quad \{0,1\}$, (11), and (12) are equivalent to the non-linear equations:

$$s_{l,k} = |q_{l,k}|, \quad l \quad P, \; k \quad T \tag{13a}$$

$$q^+_{l,k} = \max(q_{l,k}, 0), \quad l \quad P, \; k \quad T \tag{13b}$$

$$q^-_{l,k} = -\min(q_{l,k}, 0), \quad l \quad P, \; k \quad T \tag{13c}$$

$$\theta^+_{l,k} = \max(\theta_{l,k}, 0), \quad l \quad P, \; k \quad T \tag{13d}$$

$$\theta^-_{l,k} = -\min(\theta_{l,k}, 0), \quad l \quad P, \; k \quad T, \tag{13e}$$

$$z_{l,k} = \frac{1 + \operatorname{sign}(q_{l,k})}{2}, \quad l \quad P, \; k \quad T, \tag{13f}$$

and

$$\theta_{l,k} = a_l |q_{l,k}| q_{l,k} + b_l q_{l,k}, \quad l \quad P, \; k \quad T, \tag{14}$$

where $\mathrm{sign}(q_{l,k}) = 1$ if $q_{l,k} > 0$, and $\mathrm{sign}(q_{l,k}) = -1$ otherwise. Lower and upper bounds on hydraulic variables are given by

$$q_{l,k}^{\min} \le q_{l,k} \le q_{l,k}^{\max}, \quad l \in \mathcal{P},\ k \in \mathcal{T} \tag{15a}$$

$$h_{i,k}^{\min} \le h_{i,k} \le h_{i,k}^{\max}, \quad i \in \mathcal{N},\ k \in \mathcal{T} \tag{15b}$$

$$\eta_{l,k}^{\min} \le \eta_{l,k} \le \eta_{l,k}^{\max}, \quad l \in \mathcal{P},\ k \in \mathcal{T} \tag{15c}$$

$$\theta_{l,k}^{\min} \le \theta_{l,k} \le \theta_{l,k}^{\max}, \quad l \in \mathcal{P},\ k \in \mathcal{T} \tag{15d}$$

and

$$(q^+)_{l,k}^{\min} \le q_{l,k}^+ \le (q^+)_{l,k}^{\max}, \quad l \in \mathcal{P},\ k \in \mathcal{T} \tag{16a}$$

$$(q^-)_{l,k}^{\min} \le q_{l,k}^- \le (q^-)_{l,k}^{\max}, \quad l \in \mathcal{P},\ k \in \mathcal{T} \tag{16b}$$

$$(\theta^+)_{l,k}^{\min} \le \theta_{l,k}^+ \le (\theta^+)_{l,k}^{\max}, \quad l \in \mathcal{P},\ k \in \mathcal{T} \tag{16c}$$

$$(\theta^-)_{l,k}^{\min} \le \theta_{l,k}^- \le (\theta^-)_{l,k}^{\max}, \quad l \in \mathcal{P},\ k \in \mathcal{T} \tag{16d}$$

$$s_{l,k}^{\min} \le s_{l,k} \le s_{l,k}^{\max}, \quad l \in \mathcal{P},\ k \in \mathcal{T}. \tag{16e}$$

2.2. Water quality variables and constraints

Next, we describe variables and constraints associated with water quality. Let $c_{i,k}^{\max}$ be the maximum allowed chlorine concentration at network node $i \in \mathcal{N} \setminus \mathcal{N}^0$ and time $k \in \mathcal{T}$. The evolution of chlorine concentration along a given link $l \in \mathcal{P}$ is governed by a PDE modelling advective transport of constituent with first order decay Rossman & Boulos (1996). We implement an Eulerian implicit upwind discretization scheme, where backward differences are used to approximate both temporal and spatial derivatives (Islam et al., 1999). For each link $l \in \mathcal{P}$, we introduce a space discretization $j\Delta x_l$, $j \in \{0, \ldots, J_l\}$, with $\Delta x_l = \frac{L_l}{J_l}$, where L_l is the length of link l. We denote by $r_{j,l,k}$ the chlorine concentration at $j\Delta x_l$ and time k, for all $j \in \{0, \ldots, J_l\}$ and $k \in \{0, \ldots, n_t\}$. We also have auxiliary variables $w_{j,l,k}$ such that:

$$w_{j,l,k} = s_{l,k} r_{j,l,k}, \quad j = 0, \ldots, J_l,\ l \in \mathcal{P},\ k \in \mathcal{T}, \tag{17}$$

For all $j \in \{1, \ldots, J_l\}$, $l \in \mathcal{P}$, and $k \in \mathcal{T}$, the discretized PDE yields:

$$(1 + \alpha_l \Delta t) r_{j,l,k} - r_{j,l,k-1} + \gamma_l (w_{j,l,k} - w_{j-1,l,k}) = 0, \tag{18}$$

where $\gamma_l = (4\Delta t)/(10^3 \pi D_l^2 \Delta x_l)$, with L_l and D_l length and diameter of link l, respectively, and $\alpha_l > 0$ is the first order decay coefficient associated with pipe l (Hallam et al., 2002). Initial concentrations in pipes are defined as

$$r_{j,l,0} = c^0_{i_2}, \quad \forall j \in \{0, \ldots, J_l\}, \quad \forall l \in \mathcal{P}, \quad i_1 \xrightarrow{l} i_2 \tag{19}$$

with given initial concentration c_i^0 at node $i \in \mathcal{N} \cup \mathcal{N}^0$. Furthermore, $r_{0,l,k}$ is assumed to be equal to the concentration of the upstream node, depending on the flow direction:

$$r_{0,l,k} - c_{i_1,k} + c^{\max}_{i_2} z_{l,k} \leq c^{\max}_{i_2} \tag{20a}$$

$$-r_{0,l,k} + c_{i_1,k} + c^{\max}_{i_1} z_{l,k} \leq c^{\max}_{i_1} \tag{20b}$$

$$r_{0,l,k} - c_{i_2,k} - c^{\max}_{i_1} z_{l,k} \leq 0 \tag{20c}$$

$$-r_{0,l,k} + c_{i_2,k} - c^{\max}_{i_2} z_{l,k} \leq 0, \tag{20d}$$

Our problem formulation considers as free decision variables concentrations at source nodes $c_{i,k}$, $i \in \mathcal{N}^0$. Moreover, let $\mathbf{v}^b \in \{0,1\}^{n_n}$ be a vector of binary decision variables, modelling the placement of a chlorine booster station at network nodes, i.e. $v_i^b = 1$ if a chlorine booster station is placed at node i, $v_i^b = 0$, otherwise. The number of boosters considered for installation is enforced by the linear constraint:

$$\mathbf{1}^T \mathbf{v}^b = n_b \tag{21}$$

Chlorine concentration at unknown head node $i \in \mathcal{N}$ and time $k \in \mathcal{T}$ is governed by the following mixing equations:

$$c_{i,k} d_{i,k} + \sum_{l \in I_i^{\text{in}}} (w_{0,l,k} - \rho_{l,k}) + \sum_{l \in I_i^{\text{out}}} (\rho_{l,k} - w_{N_l,l,k}) - \xi_{i,k} = 0 \tag{22a}$$

$$0 \leq \xi_{i,k} \leq \xi^{\max}_{i,k} v_i^b, \tag{22b}$$

where slack variable $\xi_{i,k} \geq 0$ is introduced to model the additional constituent mass injected by a booster, and $\xi^{\max}_{i,k}$ are sufficiently large positive constants, for all $i \in \mathcal{N}$, and $k \in \mathcal{T}$. In addition, auxiliary variables $\rho_{l,k}$ are subject to the following linear constraints:

$$0 \leq \rho_{l,k} \leq \rho_{l,k}^{\max} z_{l,k} \tag{23a}$$

$$w_{0,l,k} + w_{N_l,l,k} - \rho_{l,k} - \rho_{l,k}^{\max} z_{l,k} \leq \rho_{l,k}^{\max} \tag{23b}$$

$$- w_{0,l,k} - w_{N_l,l,k} + \rho_{l,k} \leq 0 \tag{23c}$$

Finally, we include the following lower and upper bounds:

$$0 \leq c_{i,k} \leq c_i^{\max}, \quad i \in \mathcal{N} \setminus \mathcal{N}^0,\ k \in \mathcal{T}, \tag{24a}$$

$$0 \leq r_{j,l,k} \leq r_{j,l}^{\max}, \quad j = 0, \ldots, J_l,\ l \in \mathcal{P},\ k \in \mathcal{T}, \tag{24b}$$

$$0 \leq w_{j,l,k} \leq w_{j,l,k}^{\max} \quad j = 0, \ldots, J_l,\ l \in \mathcal{P},\ k \in \mathcal{T}, \tag{24c}$$

$$0 \leq \rho_{l,k} \leq \rho_{l,k}^{\max} \quad l \in \mathcal{P},\ k \in \mathcal{T}, \tag{24d}$$

$$0 \leq \xi_{i,k} \leq \xi_{i,k}^{\max}, \quad i \in \mathcal{N},\ k \in \mathcal{T}. \tag{24e}$$

2.3. Mixed Integer Non-linear Program

The problem of optimal placement and control of valves and chlorine boosters aims to minimize (6), subject to non-convex quadratic constraints (12) and (17), and linear constraints (5), (9), (10), (11), (15), (16), (18), (20), (21), (22), (23), (24). The optimization problem considers both continuous and binary variables. We write the problem in compact form, defining vectors $\boldsymbol{x} := [\boldsymbol{q}\, \boldsymbol{h}\, \boldsymbol{\eta}\, \boldsymbol{\theta}]^T$, $\boldsymbol{u} := [\boldsymbol{s}\, \boldsymbol{q}^+\, \boldsymbol{q}^-\, \boldsymbol{\theta}^+\, \boldsymbol{\theta}^-]^T$, and $\boldsymbol{y} := [\boldsymbol{c}\, \boldsymbol{r}\, \boldsymbol{w}\, \boldsymbol{\rho}\, \boldsymbol{\xi}\, \boldsymbol{\mu}]^T$. Consider the following Mixed Integer Non-linear Program (MINLP):

$$\min_{\substack{\boldsymbol{x},\boldsymbol{u},\boldsymbol{z}\\ \boldsymbol{y},\boldsymbol{v},\boldsymbol{v}^b}} \quad f_{\text{AZP}}(\boldsymbol{x}) + f_{\text{ATD}}(\boldsymbol{y}) \tag{25a}$$

$$\text{s.t.} \quad \boldsymbol{F}\boldsymbol{u} = \operatorname{diag}(\boldsymbol{A}\boldsymbol{u})\boldsymbol{A}\boldsymbol{u} + \boldsymbol{B}\boldsymbol{u} \tag{25b}$$

$$\boldsymbol{W}\boldsymbol{y} = \operatorname{diag}(\boldsymbol{S}\boldsymbol{u})\boldsymbol{R}\boldsymbol{y} \tag{25c}$$

$$\boldsymbol{M}\boldsymbol{x} + \boldsymbol{N}\boldsymbol{u} + \boldsymbol{P}\boldsymbol{z} \leq \boldsymbol{p} \tag{25d}$$

$$\boldsymbol{x} \in X(\boldsymbol{v}), \boldsymbol{v} \in V \tag{25e}$$

$$\boldsymbol{y} \in Y(\boldsymbol{z}, \boldsymbol{v}^b) \tag{25f}$$

$$\boldsymbol{1}^T\boldsymbol{v}^b = n_b \tag{25g}$$

$$\boldsymbol{z} \in \{0,1\}^{n_t n_p}, \boldsymbol{v} \in \{0,1\}^{2n_p}, \boldsymbol{v}^b \in \{0,1\}^{n_n}, \tag{25h}$$

where, given a vector $\boldsymbol{e} \in \mathbb{R}^N$, $\mathrm{diag}(\boldsymbol{e}) \in \mathbb{R}^{N\times N}$ is the diagonal matrix with diagonal entries equal to the components of vector $\boldsymbol{e}$. Linear functions $f_{\mathrm{AZP}}(\cdot)$ and $f_{\mathrm{ATD}}(\cdot)$ are such that (25a) corresponds to (6). Matrices $\boldsymbol{F}$, $\boldsymbol{A}$, and $\boldsymbol{B}$ are defined so that the rows of (25b) correspond to the non-convex quadratic constraints (12). Matrices $\boldsymbol{W}$, $\boldsymbol{S}$, and $\boldsymbol{R}$ are opportunely defined so that the rows of (25c) correspond to (17). The set V is defined by linear constraints (9). Given $\boldsymbol{v} \in V$, we denote by $X(\boldsymbol{v})$ the polyhedral set defined by constraints (10) and (15). Moreover, $\boldsymbol{M}$, $\boldsymbol{N}$, $\boldsymbol{P}$, and $\boldsymbol{p}$ are defined so that the rows of (25d) correspond to constraints (11) and (16). Finally, given vectors $\boldsymbol{v}^b$ and $\boldsymbol{z}$, we define $Y(\boldsymbol{v}^b, \boldsymbol{z})$ as the polyhedral set defined by constraints (5), (18), (20), (22), (23), (24). Problem (25) has $n_t(8n_p + 4n_n + 2\bar{J} + n_0)$ continuous variables, $n_t n_p + 2n_p + n_n$ binary variables, and $n_t(2n_p + \bar{J})$ non-convex quadratic constraints, where $\bar{J} = \sum_{l\in\mathcal{P}}(1 + J_l)$. Therefore, even for small water networks, it results in large non-convex MINLPs, which are difficult to solve - see Table 1.

3. Solution algorithm

The considered MINLP (25) combines difficulties in handling non-convex constraints with the presence of integer decision variables. In addition, the formulation of Problem (25) includes a discretized PDE for each network link, resulting in a large number of continuous variables and non-convex constraints, even for small size WDNs - see Table 1.

We investigate the performance of off-the-shelf solvers to compute solutions for Problem (25), considering two case study network models, namely `2loopsNet` and `pescara` - see Section 4 for network properties and layouts. We formulate Problem (25) in `2loopsNet` for $n_v \in \{1, 2, 3\}$ and $n_b = n_v$, and `pescara` for $n_v \in \{1, 2, 3, 4, 5\}$ and $n_b = n_v$ - a total of 8 experiments. This study considers the global optimization solvers `BARON` (Tawarmalani & Sahinidis, 2002), `scip` (Gleixner et al., 2017), `LINDOGlobal` (Lindo Systems, Inc., 2020), and `Couenne` (Belotti et al., 2009). Moreover, we investigate the ability of solvers `Bonmin` (Bonami et al., 2008), `Knitro` (Artelys, 2020), `Ipopt` (Waechter

& Biegler, 2006), and `AlphaECP` (Westerlund & Prn, 2002) to compute feasible solutions to Problem (25). We refer to these as local solvers, because they do not provide guarantees of global optimality when considering non-convex MINLPs like Problem (25). All experiments are performed on NEOS Server for Optimization (Czyzyk et al., 1998), with a time limit of 6 hours. Since `Ipopt` does not directly handle problems with binary constraints, we have substituted them with the following complementary constraints:

$$\begin{aligned} \operatorname{diag}(\boldsymbol{z})(\mathbf{1} - \boldsymbol{z}) &= \mathbf{0} \\ \operatorname{diag}(\boldsymbol{v})(\mathbf{1} - \boldsymbol{v}) &= \mathbf{0} \\ \operatorname{diag}(\boldsymbol{v}^b)(\mathbf{1} - \boldsymbol{v}^b) &= \mathbf{0} \end{aligned} \tag{26}$$

The results of these experiments are summarized in Tables A1 - A16 of Appendix 2. When considering the small case study `2loopsNet`, `BARON` and `SCIP` were able to compute feasible solutions for $n_v \in \{2,3\}$. Moreover, local solvers `AlphaECP` and `Bonmin` have computed feasible solutions only when $n_v = 2$. In comparison, `LINDOGlobal`, `Couenne`, `Knitro` and `Ipopt` failed to compute feasible solutions for all problem instances considering `2loopsNet`. Furthermore, none of the tested solvers was able to compute feasible solutions for problem instances considering `pescara`. As off-the-shelf solvers were not able to compute feasible solutions in most tested instances, we propose an algorithm to compute feasible solutions for Problem (25), together with bounds on their optimality gaps.

We propose the relax-tighten-round (RTR) algorithm, which combines a rounding heuristic with the solution of a continuous polyhedral relaxation of the non-convex MINLP in Problem (25), tightened using an optimization-based bound-tightening (OBBT) scheme. If successful, the algorithm computes a lower bound LB and an upper bound UB to the optimal value of Problem (25). A worst-case estimate on optimality gap of the computed solution is given by:

$$\text{Gap} := 100\frac{\text{UB} - \text{LB}}{\text{LB}} \tag{27}$$

In order to evaluate the obtained bounds on the optimality gaps, it is important to take into account the range of uncertainties that are inherent in hydraulic and water quality modelling of water networks. For example, Wright et al. (2015) and Waldron et al. (2020) showed that uncertainties affecting pressure control of operational water networks can result in up to 20% relative difference between simulated and measured pressure at network nodes. We expect the uncertainty range to be of the same magnitude and possibly higher for chlorine residuals.

The steps necessary to derive the RTR algorithm are detailed in the following sub-sections. Section 3.1 presents a rounding heuristic to compute feasible solutions of Problem (25). In Section 3.2, we introduce polyhedral relaxations of the non-convex constraints in Problem (25). Then, Section 3.3 describes the OBBT procedure to tighten the relaxation, and Section 3.4 presents the overall RTR algorithm.

3.1. Rounding heuristic

Firstly, we describe a heuristic to compute a feasible solution of Problem (25), given a vector of fractional values $\mathbf{v} \in [0,1]^{2n_p} \cap V$. Let $J_{n_v} \subseteq \{1,\dots,2n_p\}$ be the set of indices corresponding to the n_v largest elements in $\mathbf{v}$, where only the largest value between v_l and v_{n_p+l} is considered for each link $l = 1,\dots,n_p$. For all $l = 1,\dots,2n_p$, define:

$$\hat{v}_l = \begin{cases} 1 & \text{if } l \in J_{n_v} \\ 0 & \text{otherwise.} \end{cases} \tag{28}$$

This rounding scheme yields a vector $\hat{\mathbf{v}} \in V \cap \{0,1\}^{2n_p}$. Next, we obtain a feasible solution of Problem (25). Observe that only constraints (25c) and (25f) couple vectors of hydraulic variables $\mathbf{x}, \mathbf{u}, \mathbf{z}$ with water quality vectors $\mathbf{y}, \mathbf{v}^b$. We implement a two-stage approach, where hydraulic and water quality quantities are optimized in sequence. We consider the following MINLP:

$$\min_{\boldsymbol{x},\boldsymbol{u},\boldsymbol{z}} \; f_{\mathrm{AZP}}(\boldsymbol{x}) \tag{29a}$$

$$\text{s.t.} \quad \boldsymbol{F}\boldsymbol{u} = \operatorname{diag}(\boldsymbol{A}\boldsymbol{u})\boldsymbol{A}\boldsymbol{u} + \boldsymbol{B}\boldsymbol{u} \tag{29b}$$

$$\boldsymbol{M}\boldsymbol{x} + \boldsymbol{N}\boldsymbol{u} + \boldsymbol{P}\boldsymbol{z} \leq \boldsymbol{p} \tag{29c}$$

$$\boldsymbol{x} \quad X(\hat{\boldsymbol{v}}), \boldsymbol{z} \quad \{0,1\}^{n_t n_p}. \tag{29d}$$

Problem (29) includes $n_t n_p$ integer variables, and it is difficult to solve even for small/medium water networks. We have observed that $\boldsymbol{z} \quad \{0,1\}^{n_t n_p}$, (11), and (12) are equivalent to non-linear equations (13) and (14). Since (29b) and (29c) correspond to constraints (12) and (11), respectively, Problem (29) is equivalent to the following non-linear program:

$$\min_{\boldsymbol{x}} \; f_{\mathrm{AZP}}(\boldsymbol{x}) \tag{30a}$$

$$\text{s.t.} \quad \boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{0} \tag{30b}$$

$$\boldsymbol{x} \quad X(\hat{\boldsymbol{v}}) \tag{30c}$$

where $\boldsymbol{g}(\cdot)$ is a non-linear function such that $\boldsymbol{g}(\boldsymbol{x})$ is the vector whose components are the rows of equalities (14). Let $\hat{\boldsymbol{x}} = [\hat{\boldsymbol{q}}\,\hat{\boldsymbol{h}}\,\hat{\boldsymbol{\eta}}\,\hat{\boldsymbol{\theta}}]^T$ be a locally optimal solution of Problem (30) computed by a NLP solver. We recover a feasible solution of Problem (29) by defining vectors $\hat{\boldsymbol{u}} = [\hat{\boldsymbol{s}}\,\hat{\boldsymbol{q}}^+\,\hat{\boldsymbol{q}}^-\,\hat{\boldsymbol{\theta}}^+\,\hat{\boldsymbol{\theta}}^-]^T$ and $\hat{\boldsymbol{z}}$ using (13). Finally, let $(\hat{\boldsymbol{y}}, \hat{\boldsymbol{v}}^b)$ be solution of the mixed integer linear program (MILP):

$$\begin{aligned} \min_{\boldsymbol{y},\boldsymbol{v}^b} \;& f_{\mathrm{ATD}}(\boldsymbol{y}) \\ \text{s.t.} \;& \boldsymbol{W}\boldsymbol{y} = \operatorname{diag}(\boldsymbol{S}\hat{\boldsymbol{u}})\boldsymbol{R}\boldsymbol{y} \\ & \boldsymbol{y} \quad Y(\hat{\boldsymbol{z}}, \boldsymbol{v}^b) \\ & \boldsymbol{1}^T\boldsymbol{v}^b = n_b \\ & \boldsymbol{v}^b \quad \{0,1\}^{n_n}. \end{aligned} \tag{31}$$

Since constraints in Problems (29) and (31) correspond to constraints in Problem (25), we conclude that $(\hat{\boldsymbol{x}}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{z}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{v}}, \hat{\boldsymbol{v}}^b)$ is a feasible solution for Problem (25).

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