Optimizing the design and operation of water networks: Two decomposition approaches

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Abstract

We consider the design and operation of water networks simultaneously. Water network problems can be divided into two categories: the design problem and the operation problem. The design problem involves determining the appropriate pipe sizing and placements of pump stations, while the operation problem involves scheduling pump stations over multiple time periods to account for changes in supply and demand. Our focus is on networks that involve water co-produced with oil and gas. While solving the optimization formulation for such networks, we found that obtaining a primal (feasible) solution is more challenging than obtaining dual bounds using off-the-shelf mixed-integer nonlinear programming solvers. Therefore, we propose two methods to obtain good primal solutions. One method involves a decomposition framework that utilizes a convex reformulation, while the other is based on time decomposition. To test our proposed methods, we conduct computational experiments on a network derived from the PARETO case study.

Keywords: Mixed-Integer Nonlinear Optimization, Time decomposition, Network Design, Produced Water

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1. Introduction

Water is a crucial resource for both residential and industrial usage around the world. It is extracted from various natural sources and requires a distribution network for its transportation. The type of water network used depends on the characteristics of the water sources. In 2019, approximately $48 billion was spent on water infrastructure. However, it is predicted that a total of $129 billion will be needed to ensure continued access to sufficient water in the future (ASCE, 2023). Our research explores the challenges associated with managing the so-called "produced water" that is co-produced when oil and gas are extracted from reservoirs. Reports indicate that while the volume of produced water continues to increase, disposal capacities are decreasing (Caputo, 2020). This situation necessitates better treatment and reuse options, as well as more efficient designs and operational schedules for water networks.

We begin by considering several important characteristics when dealing with produced-water networks. Firstly, the volume of water produced typically decreases over time, meaning that we need to model this change over a multiple time period formulation. A realistic example of this trend can be seen in Section 5 of Drouven et al. (2023). Secondly, the elevations of the nodes of the network play a significant role in the behavior of the network, since produced water is usually co-produced in a basin. Elevation differences between two nodes in the network cause a change in pressure that needs to be accounted for when formulating the problem. Lastly, pump stations can be installed at certain locations in the network to boost the water pressure and prevent pressure from violating desired limits. However, there is usually an upper limit on the number of pump stations that can be installed. Therefore, the location of each pump station must be carefully considered when making design decisions.

In this work, we examine the design and operation of water networks simultaneously. Typically, the design problem involves determining pipe sizes and the placement of pump stations, while the operation scheduling problem takes into account the changes in supply and demand over time, as well as scheduling the installed pump stations.

Our paper provides two main contributions. First, it presents a unified model that combines the water network design and operation problems. This model enables the optimization of decisions related to pipe diameter choices and the operational status of the pumps and relief valves. These two problems are often considered separately, but our model integrates them into one problem to obtain solutions with better objective values, commonly in terms of the combined cost of construction and operation. From the practical point of view, the network operators in many cases are also the network designers and can, therefore, benefit from the co-optimization. Second, we propose two time decomposition frameworks to solve our model. Our numerical experiments demonstrate the effectiveness of both decomposition frameworks. Among the two frameworks, the time decomposition approach is more effective in obtaining high-quality feasible solutions for real-world produced-water network instances. Time decomposition can effectively reduce the size and complexity of the problems solved in each step of which smaller and simpler problems provide solutions that lead to high-quality feasible solutions to the original problem. Moreover, our results show that state-of-the-art solvers struggle to find a feasible solution within the same amount of computational time.

The remainder of this paper is organized into several sections. Section 2 reviews the literature related to the problem. Section 3 provides a compact formulation and the technical background for the problem. Section 4 discusses the two algorithms used to obtain feasible solutions. Section 4.1 presents a decomposition framework similar to that proposed in the work of Li et al. (2024) for gas networks. Section 4.2 is based on a time decomposition of the compact formulation. Section 5 presents the computational experiments and discusses the results. Lastly, Section 6 concludes the paper and provides directions for further research.

2. Literature review

Water network design is a popular topic in the literature. For instance, in their paper, Mala-Jetmarova et al. (2017) give a comprehensive overview of the different types of water system design problems. Two common types of water system design problems are considered in the literature. The first is the Water Using Network (WUN) design, which considers freshwater usage for both industrial and residential purposes. This type of problem often involves studying the distribution of contaminants and water quality. A review of this type of problem can be found in Castro and Teles (2013). Other notable works include Teles et al. (2008, 2012, 2009). These works utilize linear programming or mixed-integer linear programming techniques to reformulate the nonlinear problem and propose algorithms to solve the resulting reformulation. The other type of water system design problem focuses on the hydraulic effect of water flow in pipes. Since our work belongs to the latter type, we provide a detailed review of relevant works in this area.

We start by reviewing some relevant literature on the design problem and the operation problem. Bragalli et al. (2012) investigate a design problem that involves selecting the diameters of pipes in a purely gravity-fed network with no pump stations or relief valves. They present a mixed-integer nonlinear programming (MINLP) formulation and focus on reformulations and implementation considerations to optimize the performance of `Bonmin` (Bonami and Lee, 2006; Bonami et al., 2008). Their numerical experiments are conducted using common benchmark networks found in MIPLIB (Gleixner et al., 2021). Similarly, Raghunathan (2013) also examines a design problem on pipe diameter selections without pump stations or relief valves, and presents a similar MINLP model, in which the nonlinear constraints governing the water flow are linearized. The author then uses a linearization-based branch-and-bound framework to solve the model and also proposes a new leaf-node problem for the framework to correct the discrepancies introduced by linearization. The study uses the same set of benchmark networks as a previous study by Bragalli et al. (2012) for numerical experiments. Later, Rajagopalan (2018) produces a follow-up study, proposing a new formulation for the leaf-node problem from the earlier study by Raghunathan (2013). Numerical results from the new formulation show improvements for several networks. In a slightly different design problem of optimal placements of relief valves to minimize the average zone pressure, Pecci et al. (2019) use an MINLP model. They investigate other linear relaxation schemes using a tailored domain reduction procedure to strengthen the relaxations. Computational experiments are performed using benchmark networks including a real-world network from the UK. In Ghaddar et al. (2015), the authors explore the problem of pump scheduling in a fixed topology. They use a Lagrangian decomposition approach to decouple the constraints of a MINLP formulation into smaller subproblems that can be solved separately. To account for additional operation constraints on the pump stations, the authors also propose a simulation-based heuristic. Numerical results are obtained on two networks with up to 47 nodes. In Bonvin et al. (2021), the authors study the pump scheduling problem using an LP/NLP-based branch-and-bound framework. They propose a linear relaxation of the original nonconvex formulation for use in a branch-and-bound framework. Additionally, they suggest a specialized primal heuristic to repair near-feasible integer solutions from the linear relaxation and improve computational efficiency.

It is common in operation problems to have so-called minimum-up and minimum-down constraints that model the technical requirements of pump stations. The minimum-up constraints require that once a pump station is turned on or off, it must remain on or off for a specific minimum number of periods. The polytope formed by these constraints has been studied in detail in the area of power system design. The study by Ostrowski et al. (2012) provides a detailed exploration of this topic. Other studies have proposed several sets of minimum-up and minimum-down constraints while changing the number of variables employed. Lee et al. (2004) studies the "one-variable" variant of the polytope, while Rajan and Takriti (2005) explore the "two-variables" variant. More information about the discussion and comparison across the variants can be found in Ostrowski et al. (2012).

Time decomposition is a technique that can be used to simplify problems that involve multiple time periods. This approach involves breaking down the original problem into smaller problems, with each problem only considering a subset of the time periods. One of the most popular time decomposition schemes is rolling horizon. In a recent study by Glomb et al. (2022), rolling horizon is used for multiple time period optimization.

3. Problem description

3.1. Technical background

In this section, we provide background information on how to model a water network using only the components present in our setting. We consider T time periods, denoted by $\{1, \ldots, T\}$. To represent the water network, we use a directed graph $G = (\mathcal{V}, \mathcal{A})$. Each vertex $v \in \mathcal{V}$ can be a customer with demand, a reservoir with supply, or an in-node with neither demand nor supply. In each time period $t \in \{1, \ldots, T\}$, there is a pressure variable $p_{v,t}$ associated with each vertex. This variable is lower and upper bounded by $p_v^{\min}$ and $p_v^{\max}$. Each pipe in the network is represented by an arc $a \in \mathcal{A}$.

Pipes: The characteristics of a pipe $a = (v, w)$ are defined by its length l_a, diameter D_a, and material properties. We use $q_{a,t}$ to denote the volumetric flowrate for the pipe in period $t \in \{1, \ldots, T\}$. The maximum flowrate, $q_a^{\max}$, is proportional to the pipe's cross-sectional area $A = \pi D_a^2/4$. The pipe allows water to flow in both directions, and the constraint reflecting the maximum flowrate and bi-directional flow is given by

$$-q_a^{\max} \leq q_{a,t} \leq q_a^{\max}, \quad t \in \{1, \ldots, T\}. \tag{1}$$

The locations of pump stations are design decisions and each pipe is assumed to have a relief valve. Therefore, a pressure increase or relief can be incurred in addition to pressure change due to friction and elevation. We begin by addressing pressure loss due to friction. Water flow in a pipe is governed by a set of partial differential equations. Under steady-state flow and other technical assumptions, we can simplify the partial differential equations to a set of nonlinear equations. Two variants of nonlinear equations have been proposed. First, the Hazen-Williams equation is given as

$$p_{v,t} - p_{w,t} = \frac{10.704 l_a}{C^{1.852} D_a^{4.87}} \rho g |q_{a,t}| q_{a,t}^{0.852}, \quad t \in \{1, \ldots, T\}, \tag{2}$$

where C is the Hazen-Williams constant, which is dependent on the material properties of the pipe, ρ is the density of water, and g is the gravitational acceleration constant. Second, the Darcy equation is given as

$$p_{v,t} - p_{w,t} = f_D \frac{8 l_a}{\pi^2 g D_a^5} \rho g |q_{a,t}| q_{a,t}, \quad t \in \{1, \ldots, T\}, \tag{3}$$

where f_D is the friction coefficient that depends on the Reynolds number of water flow and other properties of the pipe's material. We can represent both equations as

$$p_{v,t} - p_{w,t} = \alpha_a |q_{a,t}| q_{a,t}^{\eta}, \quad t \in \{1, \ldots, T\}, \tag{4}$$

where α_a is the pressure loss coefficient and η is 0.852 or 1. Additionally, elevation changes across a pipe result in a pressure change that is proportional to the elevation change. If we denote the elevation at v and w by e_v and e_w, we can calculate the pressure change induced by the elevation change using the following equation:

$$\delta_a = (e_v - e_w)\rho g. \tag{5}$$

It is important to note that δ_a remains constant and can be computed beforehand when solving the design problem.

Now, we can use a binary variable, $z_{I,a}$, to model the decision of whether to place a pump station on the pipe. If a pump station is placed, then $z_{I,a} = 1$; otherwise, it is 0. We also need to introduce two additional continuous variables, $\Delta_{I,a,t}$ and $\Delta_{R,a,t}$, which indicate the amount of pressure increase induced by a pump station and the amount of pressure relief induced by a relief valve in period $t \in \{1, \dots, T\}$, respectively. We place an upper bound on the pressure increase that the pump station can induce, which is denoted by $\overline{\Delta}_{I,a}$. On the other hand, an upper bound on pressure relief that a relief valve can induce can be very large, so we do not set any upper bound on $\Delta_{R,a,t}$.

As a result, the total pressure change across a pipe due to friction, elevation, and additional pressure increase or relief is given by

$$p_{v,t} - p_{w,t} = \alpha_a |q_{a,t}| q_{a,t}^{\eta} + \delta_a - \Delta_{I,a,t} + \Delta_{R,a,t}, \quad t \in \{1, \dots, T\}. \tag{6}$$

Additional constraints on pump stations: We assume that there is an upper bound on the number of pump stations for the entire network, denoted by N. We write a constraint as follows:

$$\sum_{a \in A_p} z_{I,a} \leq N. \tag{7}$$

Next, we write the so-called minimum-up and minimum-down constraints for a pump $a \in A_p$. Specifically, once a pump station is turned on or off, it must remain in that state for a total of τ_o (resp. τ_f) periods. We decide to use the "one-variable" variant of the constraints (see Section 2), as we do not take start-up costs into account. To represent the status of the pump station in each time period, we use binary variables $\xi_{a,t}$, where $\xi_{a,t}$ is equal to 1 if the pump station is on in period t and 0 otherwise. The minimum-up and minimum-down constraints are given by

$$\xi_{a,t} \leq z_{I,a}, \qquad t \in \{1, \dots, T\}, \tag{8}$$

$$\xi_{a,t} - \xi_{a,t-1} \leq \xi_{a,\tau}, \qquad t \in \{2, \dots, T\}, \tau \in \{t+1, \dots, \min\{t+\tau_o, T\}\}, \tag{9}$$

$$\xi_{a,t-1} - \xi_{a,t} \leq 1 - \xi_{a,\tau}, \quad t \in \{2, \dots, T\}, \tau \in \{t+1, \dots, \min\{t+\tau_f, T\}\}. \tag{10}$$

Additionally, we place an upper bound, M_a, on the number of periods a pump station $a \in A_p$ is on to simulate operational cost constraints. Formally, we have the following

$$\sum_{t \in \{1,\dots,T\}} \xi_{a,t} \leq M_a. \tag{11}$$

Note that the upper bounds, M_a and $M_{a'}$, can differ for two pipes $a, a' \in A_p$.

Reservoirs: Reservoirs are typically used as the primary sources for supplying water to the network. It is common practice to assume that the pressures at these reservoirs are fixed. Therefore, if we denote the set of source nodes as $V^{\text{src}} \subset \mathcal{V}$, we can write constraints:

$$p_{v,t} = p^{\text{src}}_{v,t}, \quad v \in V^{\text{src}},\ t \in \{1, \dots, T\}. \tag{12}$$

3.2. A summary on problem formulation

We use A_p to represent a set of pipes. In our setting, this means $\mathcal{A} = A_p$. We consider discrete diameter choices for the pipes by the set $[n] := \{1, 2, \dots, n\}$. We use binary variables $z_{a,i}$ for $a \in A_p$ and $i \in [n]$ to indicate the diameter choices. The diameter value for $z_{a,i}$ is denoted by $D_{a,i}$. We denote the fixed cost of constructing a pipe with a diameter $D_{a,i}$ by $f_{a,i}$. Additionally, we create copies of flow variables $q_{a,t}$ for different diameters as $q_{a,t,i}$. The maximum flowrate for each diameter choice is denoted by $q^{\max}_{a,i}$. Since pipes allow bi-directional water flows, we introduce a binary flow direction variable $x^{\text{dir}}_{a,t}$ to indicate the flow direction for $a \in \mathcal{A}$ and decompose the flow into a positive and negative flow. As a result, the flow variables are $q^+_{a,t,i}$ and $q^-_{a,t,i}$ for a pipe. For each vertex $v \in \mathcal{V}$, we denote the set of incoming and outgoing arcs by $A_{in}(v)$ and $A_{out}(v)$, respectively, i.e., $A_{in}(v) = \{a \in \mathcal{A} | a = (w, v)\}$ and $A_{out}(v) = \{a \in \mathcal{A} | a = (v, w)\}$. Lastly, we use $d_{v,t}$ to denote the demand (a supply can be reflected by a negative demand value) at a vertex $v \in \mathcal{V}$ in period t. With these additional notations, we can now present the formulation of the problem.

`Objective`
$$\min_{z,q^+,q^-,p,x^{\text{dir}},z_I,\Delta_I,\Delta_R,\xi} \sum_{a\in A_p} \sum_{i\in[n]} f_{a,i} z_{a,i}, \tag{13}$$

s.t.

`Flow conservation`
$$\sum_{i\in[n]} \sum_{a\in A_{in}(v)} (q^+_{a,t,i} - q^-_{a,t,i}) - \sum_{i\in[n]} \sum_{a\in A_{out}(v)} (q^+_{a,t,i} - q^-_{a,t,i}) = d_{v,t},$$
$$v \in \mathcal{V}, t \in \{1, \dots, T\}, \tag{14}$$

`Pressures`
$$p^{\min}_v \le p_{v,t} \le p^{\max}_v, \quad v \in \mathcal{V} \backslash V^{\text{src}}, t \in \{1, \dots, T\}, \tag{15}$$
$$p_{v,t} = p^{\text{src}}_{v,t}, \quad v \in V^{\text{src}}, t \in \{1, \dots, T\}, \tag{16}$$

`Pipes`
$$0 \le q^-_{a,t,i},\ q^+_{a,t,i} \le q^{\max}_{a,i} z_{a,i}, \quad a \in A_p, i \in [n], t \in \{1, \dots, T\}, \tag{17}$$
$$p_{v,t} - p_{w,t} = \sum_{i\in[n]} \alpha_{a,i} (q^+_{a,t,i})^{1+\eta} - \sum_{i\in[n]} \alpha_{a,i} (q^-_{a,t,i})^{1+\eta}$$
$$+ \delta_a - \Delta_{I,a,t} + \Delta_{R,a,t}, \quad a \in A_p, t \in \{1, \dots, T\}, \tag{18}$$
$$0 \le q^+_{a,t,i} \le q^{\max}_{a,i} x^{\text{dir}}_{a,t}, \qquad a \in A_p, i \in [n], t \in \{1, \dots, T\} \tag{19}$$
$$0 \le q^-_{a,t,i} \le q^{\max}_{a,i} (1 - x^{\text{dir}}_{a,t}), \qquad a \in A_p, i \in [n], t \in \{1, \dots, T\} \tag{20}$$
$$\sum_{i\in[n]} z_{a,i} = 1, \qquad a \in A_p \tag{21}$$

`Pump stations`
$$\Delta_{I,a,t} \le \overline{\Delta}_{I,a} \xi_{a,t}, \quad a \in A_p, t \in \{1, \dots, T\}, \tag{22}$$
$$\xi_{a,t} \le z_{I,a}, \quad a \in A_p, t \in \{1, \dots, T\}, \tag{23}$$
$$\sum_{a\in A_p} z_{I,a} \le N, \tag{24}$$

$$\sum_{t\in\{1,\dots,T\}} \xi_{a,t} \le M_a, \quad a \in A_p, \tag{25}$$

$$\xi_{a,t} - \xi_{a,t-1} \le \xi_{a,\tau}, \quad t \in \{2,\dots,T\},$$
$$\tau \in \{t+1,\dots,\min\{t+\tau_o, T\}\}, \tag{26}$$

$$\xi_{a,t-1} - \xi_{a,t} \le 1 - \xi_{a,\tau}, \quad t \in \{2,\dots,T\},$$
$$\tau \in \{t+1,\dots,\min\{t+\tau_f, T\}\}. \tag{27}$$

Note that η is 0.852 or 1 depending on whether we use the Hazen-Williams or Darcy equation. In the remainder of this paper, we use the Hazen-Williams equation as it is more commonly used in both literature and in practice; therefore, we use $\eta = 0.852$. This equation results in a general nonlinear and nonconvex formulation. We also group the objective function and the constraints into blocks. A summary of these blocks is given in Table 1.

We used the solvers BARON (Tawarmalani and Sahinidis, 2005) and SCIP (Achterberg, 2009) in our preliminary study to understand the performances of the formulation (13) - (27). In the preliminary study, we noticed that both solvers are able to improve the dual bounds consistently but have trouble obtaining primal (feasible) solutions. This motivates us to investigate other means to obtain primal solutions and provide them to the solver.

4. Primal solutions

This section presents the two algorithms to obtain primal solutions. The first algorithm is adapted from the decomposition algorithm presented in Li et al. (2024) and is based on the CVXNLP reformulation that is described in Raghunathan (2013) and Li et al. (2024). The main components in this algorithm are a primal bound loop and an initial budget search. The second algorithm is based on time decomposition.

Table 1: Constraint blocks

References	Block names	Explanations
(13)	`Objective`	Objective function to minimize the total cost of constructions (the budget)
(14)	`Flow_conservation`	Flow conservation
(15)-(16)	`Pressures`	Non-source node pressure bounds (15); source node pressures (16)
(17)-(21)	`Pipes`	Flow limits on diameter choices (17); pressure drop (18); flow limits on directions (19)-(20); diameter selection (21)
(22)-(27)	`Pump stations`	Pressure increase limit (22); Pump station can be on only when installed (23); Resource limit on number of pump stations (24); Resource limit on number of periods a pump station is on (25); minimum-up (26); minimum-down (27)

4.1. CVXNLP-based decomposition

4.1.1. Primal bound loop

The primal bound loop is an iterative procedure that involves a master problem and a subproblem. It checks whether there exists a feasible set of flows and pressures that can satisfy the demand and supply within a given budget C. This set of feasible flows and pressures also corresponds to a set of diameter choices, pump station locations, and schedules for the pump stations and relief valves.

The master problem is formulated using CVXNLP and is given as

$$
\begin{aligned}
(P_m) \quad \min_{z,q^+,q^-} \quad & \sum_{t\in\{1,\dots,T\}} \sum_{i\in[n]} \sum_{a\in A_p} \left[\frac{\alpha_{a,i}}{1+\eta} (q^+_{a,t,i})^{1+\eta} + \delta_a q^+_{a,t,i} + \right. \\
& \qquad \left. \frac{\alpha_{a,i}}{1+\eta} (q^-_{a,t,i})^{1+\eta} + \delta_a q^-_{a,t,i} \right] \\
& - \sum_{t\in\{1,\dots,T\}} \sum_{v\in V^{\text{src}}} p^{\text{src}}_{v,t} \left[\sum_{i\in[n]} \sum_{a\in A_{in}(v)} (q^+_{a,t,i} - q^-_{a,t,i}) - \right. \\
& \qquad \left. \sum_{i\in[n]} \sum_{a\in A_{out}(v)} (q^+_{a,t,i} - q^-_{a,t,i}) \right], \qquad (28)
\end{aligned}
$$

$$
\begin{aligned}
\text{s.t.} \quad & \sum_{i\in[n]} \sum_{a\in A_{in}(v)} (q^+_{a,t,i} - q^-_{a,t,i}) - \sum_{i\in[n]} \sum_{a\in A_{out}(v)} (q^+_{a,t,i} - q^-_{a,t,i}) = d_{v,t}, \\
& \qquad v \in \mathcal{V}\backslash V^{\text{src}}, t \in \{1,\dots,T\} \qquad (29) \\
& 0 \le q^-_{a,t,i}, q^+_{a,t,i} \le q^{\max}_{a,i} z_{a,i}, \quad a \in A_p, i \in [n], t \in \{1,\dots,T\}, \qquad (30) \\
& \sum_{i\in[n]} z_{a,i} = 1, \ \forall a \in A_p, \qquad (31) \\
& \sum_{a\in A_p} \sum_{i\in[n]} f_{a,i} z_{a,i} \le C. \qquad (32)
\end{aligned}
$$

Note that in the objective function (28), we have not included the additional pressure increase $\Delta_{I,a,t}$ or additional pressure relief $\Delta_{R,a,t}$. The reasons are two-fold. First, we have not considered the decisions regarding the locations of pump stations in the master problem (P_m). Secondly, we can rewrite the pressure change equation (17) as

$$p_{v,t} - p_{w,t} + \Delta_{I,a,t} - \Delta_{R,a,t} = \sum_{i\in[n]} \alpha_{a,i}(q^+_{a,t,i})^{1+\eta} - \sum_{i\in[n]} \alpha_{a,i}(q^-_{a,t,i})^{1+\eta} + \delta_a. \quad (33)$$

As a result, we can consider the values of $\Delta_{I,a,t}$ and $\Delta_{R,a,t}$ as part of the pressure $p_{v,t}$ or $p_{w,t}$.

From (P_m), we can obtain a set of binary solutions for diameter choices, $z^*_{a,i}$, for $a \in A_p$ and $i \in [n]$. Consequently, we can compute the pressure loss coefficient and the max flowrate for each pipe $a \in A_p$ by

$$\alpha_a = \sum_{i\in[n]} \alpha_{a,i} z^*_{a,i}, \quad (34)$$

$$q^{\max}_a = \sum_{i\in[n]} q^{\max}_{a,i} z^*_{a,i}. \quad (35)$$

Then, we can fix the corresponding binary variables and obtain a subproblem (P_s) that differs only from the compact formulation (13)–(27) in a few constraint blocks. Formally, we describe the changes in each of the blocks.

- `Objective.` Instead of minimizing the total cost on pipes, we have a feasibility problem as

$$\text{Find} \quad q^+_{a,t}, q^-_{a,t}, x^{\text{dir}}_{a,t}, p_{v,t}, z_{I,a}, \xi_{a,t}, \Delta_{I,a,t}, \Delta_{R,a,t}. \quad (36)$$

- `Flow conservation.` Once we obtain the diameter choices, we only have one set of the flowrate variables for each pipe $a \in A_p$ in each time period $t \in \{1, \dots, T\}$, denoted by $q^+_{a,t}$ and $q^-_{a,t}$. We can then write the flow conservation constraint as

$$\sum_{a\in A_{in}(v)} (q^+_{a,t} - q^-_{a,t}) - \sum_{a\in A_{out}(v)} (q^+_{a,t} - q^-_{a,t}) = d_{v,t}, \quad v \in \mathcal{V}, t \in \{1, \dots, T\}. \quad (37)$$

- `Pressures.` This block remains unchanged.
- `Pipes.` Similar to the `Flow conservation` block, we only need one set of the flowrate variables, $q^+_{a,t}$ and $q^-_{a,t}$, for $a \in A_p$ and $t \in \{1, \dots, T\}$. We simplify the `Pipes` block as follows:

$$p_{v,t} - p_{w,t} = \alpha_a (q^+_{a,t})^{1+\eta} - \alpha_a (q^-_{a,t})^{1+\eta} + \delta_a - \Delta_{I,a,t} + \Delta_{R,a,t}, \quad a \in A_p, t \in \{1, \dots, T\}, \tag{38}$$

$$0 \le q^+_{a,t} \le q^{\max}_a x^{\text{dir}}_{a,t}, \qquad a \in A_p, i \in [n], t \in \{1, \dots, T\}, \tag{39}$$

$$0 \le q^-_{a,t} \le q^{\max}_a (1 - x^{\text{dir}}_{a,t}), \qquad a \in A_p, i \in [n], t \in \{1, \dots, T\}. \tag{40}$$

- `Pump stations.` This block remains unchanged.

If the subproblem (P_s) is infeasible, we can add an integer no-good cut to the master problem (P_m) of the form,

$$\sum_{i \in [n]} \sum_{a \in A_p, z^*_{a,i}=0} z_{a,i} + \sum_{i \in [n]} \sum_{a \in A_p, z^*_{a,i}=1} (1 - z_{a,i}) \ge 1, \tag{41}$$

and re-solve the master problem (P_m). If (P_s) is feasible, we can then obtain a set of primal solutions to the original formulation that have an objective value of C. The primal bound loop terminates when we obtain a feasible budget or when it reaches a pre-set time limit. If the time limit is reached, we double the budget C and re-run the primal bound loop.

4.1.2. Initial budget search

To obtain an initial starting budget for the primal bound loop, we propose a budget search procedure, which is a loop consisting of a master problem and subproblem. The master problem (I_m) is given as follows:

$$(I_m) \quad \min_z \sum_{a \in A_p} \sum_{i \in [n]} f_{a,i} z_{a,i}, \tag{42}$$

$$\text{s.t.} \sum_{i\in[n]} z_{a,i} = 1, \; \forall a \in A_p, \tag{43}$$

$$z_{a,i} \in \{0,1\}, \qquad a \in A_p, i \in [n]. \tag{44}$$

We only consider the available diameter choices in (I_m) and select the least cost option. This problem can be solved quickly compared to (P_m). After obtaining a set of solutions $z^*_{a,i}$ for $a \in A_p$ and $i \in [n]$, we use (34) and (35) to compute the pressure loss coefficients and maximum flowrates, respectively. The resulting subproblem is the same as (P_s). If (P_s) is feasible, we conclude that the original problem has been solved, and the optimal cost is the objective value of problem (I_m). Otherwise, we add the integer no-good cut of the form (41) and resolve (I_m).

4.1.3. Summary of the algorithm

Algorithm 1 presents the overall procedure with both components from the previous sections.

Algorithm 1: CVXNLP-based decomposition

Initial budget search is run for 10 min.
if *a feasible budget is obtained* **then**
    terminate with the optimal cost of constructions for this set of demand and supply
end
else
    Set starting budget based on the returned value from initial budget search;
    Primal bound loop is run for 45 min for each budget.
end
return *Primal solutions or no primal solution found*

4.2. Time decomposition

In this section, we discuss the time decomposition framework. Let us consider a subset of time periods denoted by $\tilde{T} < T$. If we restrict the original problem to $\{1,\ldots,\tilde{T}\}$, we can solve it to a target accuracy ε relatively efficiently. As we mentioned in Section 1, one characteristic of the problem is that the amount of water produced is typically high at the beginning, and it gradually decreases over time. This means that the diameter choices from solving the problem with restricted time periods $\{1,\ldots,\tilde{T}\}$ are very likely to be feasible with respect to the volume of water produced in $\{\tilde{T}+1,\ldots,T\}$. Additionally, we argue that a pump station is more likely to be needed when the amount of water produced is high. Consider a pipe $a=(v,w)$ and the pressure change equation for a single diameter choice case in a particular time period t, along with the bounds on the pressure variables,

$$p_{v,t} - p_{w,t} = \alpha_a {q^+_{a,t}}^{1+\eta} - \alpha_a {q^-_{a,t}}^{1+\eta}, \tag{45}$$

$$p_v^{\min} \le p_{v,t} \le p_v^{\max}, \tag{46}$$

$$p_w^{\min} \le p_{w,t} \le p_w^{\max}. \tag{47}$$

When a larger amount of water is produced, it results in a higher frictional pressure loss, which can lead to either a higher pressure value at w or a smaller pressure value at v. As a result, the upper bound at w or the lower bound at v may be violated. The only solution to this problem is to install a pump station on this pipe, which reduces the frictional pressure loss at the same flowrate and ensures that the pressure values at v and w remain feasible.

Based on our observations, we present the time decomposition algorithm. First, we modify the constraint (25) to the following form

$$\sum_{t\in\{1,\ldots,\tilde{T}\}} \xi_{a,t} \le M_a \frac{\tilde{T}}{T}, \quad a \in A_p, \tag{48}$$

and after that, solve the resulting restricted problem for the time periods $\{1,\ldots,\tilde{T}\}$ to a target accuracy ε. This will give us a set of binary solutions for the diameter choices $z^*_{a,i}$, locations of pump stations $z^*_{I,a}$ for $a \in A_p$ and

$i \in [n]$, and a set of binary solutions for the status of the pump stations $\xi^*_{a,t}$ for $a \in A_p$ and $t \in \{1, \ldots, \tilde{T}\}$. Once we fix the diameter choices and locations of the pump stations, we can obtain a feasibility problem (P_r) for the remaining time periods $t \in \{\tilde{T}+1, \ldots, T\}$ by modifying the objective and constraint blocks as follows,

- `Objective.` Instead of minimizing the total cost of pipes, we have a feasibility problem as

$$\text{Find} \quad q^+_{a,t}, q^-_{a,t}, x^{\text{dir}}_{a,t}, p_{v,t}, z_{I,a}, \xi_{a,t}, \Delta_{I,a,t}, \Delta_{R,a,t}. \tag{49}$$

- `Pressures.` Block remains unchanged.

- `Flow conservation.` Once we obtain the diameter choices, we only have one set of the flowrate variables for each pipe $a \in A_p$ in each time period $t \in \{\tilde{T}+1, \ldots, T\}$, denoted by $q^+_{a,t}$ and $q^-_{a,t}$. We can then write the flow conservation constraint as

$$\sum_{a \in A_{in}(v)} (q^+_{a,t} - q^-_{a,t}) - \sum_{a \in A_{out}(v)} (q^+_{a,t} - q^-_{a,t}) = d_{v,t}, \quad v \in \mathcal{V}, t \in \{\tilde{T}+1, \ldots, T\}. \tag{50}$$

- `Pipes.` Similar to the `Flow conservation` block, we only need one set of the flowrate variables, $q^+_{a,t}$ and $q^-_{a,t}$, for $a \in A_p$ and $t \in \{1, \ldots, T\}$. We simplify the `Pipes` block as follows:

$$p_{v,t} - p_{w,t} = \alpha_a (q^+_{a,t})^{1+\eta} - \alpha_a (q^-_{a,t})^{1+\eta} + \delta_a - \Delta_{I,a,t} + \Delta_{R,a,t}, \quad a \in A_p, t \in \{\tilde{T}+1, \ldots, T\}, \tag{51}$$

$$0 \le q^+_{a,t} \le q^{\max}_a x^{\text{dir}}_{a,t}, \quad a \in A_p, i \in [n], t \in \{\tilde{T}+1, \ldots, T\}, \tag{52}$$

$$0 \le q^-_{a,t} \le q^{\max}_a (1 - x^{\text{dir}}_{a,t}), \quad a \in A_p, i \in [n], t \in \{\tilde{T}+1, \ldots, T\}. \tag{53}$$

- `Pump stations.` Once we fix the locations of the pump stations, we simplify this block to be as follows,

$$\Delta_{I,a,t} \leq \overline{\Delta}_{I,a}\xi_{a,t}, \quad a \in A_p, t \in \{\tilde{T}+1,\ldots,T\}, \tag{54}$$

$$\xi_{a,t} \leq z^*_{I,a}, \quad a \in A_p, t \in \{\tilde{T}+1,\ldots,T\}, \tag{55}$$

$$\sum_{t\in\{\tilde{T}+1,\ldots,T\}} \xi_{a,t} \leq M_a(1-\frac{\tilde{T}}{T}), \quad a \in A_p, \tag{56}$$

$$\begin{aligned} \xi_{a,t} - \xi_{a,t-1} \leq \xi_{a,\tau}, \quad & t \in \{\pi_{a,\tilde{T},o},\ldots,T\}, \\ & \tau \in \{t+1,\ldots,\min\{t+\tau_o,T\}\}, \end{aligned} \tag{57}$$

$$\begin{aligned} \xi_{a,t-1} - \xi_{a,t} \leq 1-\xi_{a,\tau}, \quad & t \in \{\pi_{a,\tilde{T},f},\ldots,T\}, \\ & \tau \in \{t+1,\ldots,\min\{t+\tau_f,T\}\}, \end{aligned} \tag{58}$$

where $\pi_{a,\tilde{T},o}$ and $\pi_{a,\tilde{T},f}$ are two parameters that depend on the values of $\xi^*_{a,t}$ for $a \in A_p$ and $t \in \{1,\ldots,\tilde{T}\}$, and we may need to fix the variables $\xi_{a,t}$ for $t \in \{\tilde{T}+1,\ldots,T\}$ due to constraints (26) and (27). Formally, if we denote the set of pipes where the pump stations are installed by $\tilde{A}$, we have the procedure in Algorithm 2.

If the problem (P_r) is feasible, we can obtain a set of primal solutions for the original problem by combining the variable values from the restricted problem for time periods $\{1,\ldots,\tilde{T}\}$ and (P_r). This set of primal solutions would have the same objective value as the restricted problem. However, if (P_r) is not feasible, we need to choose a different $\tilde{T}$ or target accuracy ε and repeat the algorithm.

Note that we can adapt this algorithm to handle non-monotonic changes in the amount of water produced across the time periods by constructing a restricted problem for a total of $\tilde{T}$ periods with the highest water production and then solving a similar feasibility problem for the remaining periods. However, the fixing procedure in Algorithm 2 will require modifications.

Algorithm 2: Fixing procedure

for $a \in \tilde{A}$ **do**
    Initialize $t_o = \tilde{T}$
    while $t_o \geq \tilde{T} - \tau_o + 1$ *and* $t_o \geq 2$ **do**
        if $\xi_{a,t_o} - \xi_{a,t_o-1} = 1$ **then**
            Fix $\xi_{a,\tau} = 1$ for $\tau \in \{\tilde{T}+1, \ldots, t_o + \tau_o\}$
            Set $\pi_{a,\tilde{T},o} = t_o + \tau_o + 1$
        end
        $t_o = t_o - 1$
    end
    Initialize $t_f = \tilde{T}$
    while $t_f \geq \tilde{T} - \tau_f + 1$ *and* $t_f \geq 2$ **do**
        if $\xi_{a,t_f-1} - \xi_{a,t_f} = 1$ **then**
            Fix $\xi_{a,\tau} = 0$ for $\tau \in \{\tilde{T}+1, \ldots, t_f + \tau_f\}$
            Set $\pi_{a,\tilde{T},f} = t_f + \tau_f + 1$
        end
        $t_f = t_f - 1$
    end
    if $\pi_{a,\tilde{T},o}$ *has not been set* **then** Set $\pi_{a,\tilde{T},o} = \tilde{T} + 2$;
    if $\pi_{a,\tilde{T},f}$ *has not been set* **then** Set $\pi_{a,\tilde{T},f} = \tilde{T} + 2$;
end

4.2.1. Summary of the algorithm

In this section, we provide a summary of the algorithm. It is important to note that there is a trade-off to consider when selecting $\tilde{T}$ and ε. A small $\tilde{T}$ and a large ε lead to a restricted problem that can be solved quickly. However, the diameter choices and locations of pump stations obtained from such a restricted problem may not result in a feasible (P_r). To address this, we can select $\tilde{T}$ from a set $\mathcal{T}$ and ε from a set $\mathcal{E}$. This will allow us to obtain a set of primal solutions. The algorithm is presented in Algorithm 3.

Algorithm 3: Time decomposition

Initialize $Sol = \emptyset$
for $\tilde{T} \in \mathcal{T}$ **do**
    for $\varepsilon \in \mathcal{E}$ **do**
        Solve the restricted problem with time periods $\{1, \ldots, \tilde{T}\}$ to a target accuracy of ε by SCIP
        Solve the problem (P_r) for time periods $\{\tilde{T}+1, \ldots, T\}$ after the fixing procedure (Algorithm 2)
        if (P_r) *is feasible* **then**
            Add the primal solution to Sol with the objective value of the restricted problem
        end
    end
end
if $Sol \neq \emptyset$ **then return** *The primal solution with smallest objective value*;
else return *No primal solution found*;

5. Numerical experiments

5.1. Instances

Our numerical experiments were conducted on a network derived from the Produced Water Application for Beneficial Reuse, Environmental Impact and Treatment Optimization (PARETO) strategic case study (Drouven et al., 2023). An illustration of a PARETO network is given in Figure 8 of Drouven et al. (2023). The characteristics of the network are listed in Table 2, and for more details, we refer readers to the Project PARETO website. We considered two values of T with $T = 24$ and $T = 53$. The base demand and supply scenario follows the same trend as the one given in the Project PARETO strategic case study. Additionally, we used stress factors to create more demand and supply scenarios, as done in the numerical experiments of Li et al. (2024). Specifically, we used stress factors from the set $\{0.1, 0.5, 1.5, 2.0\}$, which are directly multiplied by the base demand and supply values of each individual node to create new demand and supply scenarios. We considered four different diameter choices and assumed that the fixed cost of construction is proportional to the circumferences of the pipe.

Table 2: Characteristics of the networks

Sources	Sinks	In-nodes	Pipes
19	7	29	58

5.2. Implementation settings

We conducted our experiments on a computer with an Intel i9 CPU (3.70GHz) with 64GB RAM. Our formulation is coded in Python using Pyomo. After testing BARON (Tawarmalani and Sahinidis, 2005) and SCIP (Achterberg, 2009), we found that SCIP performs slightly better and decided to use SCIP in the experiments, including solving the formulation (13)–(27) as a baseline comparison. In particular, we use SCIP through GAMS. We follow Algorithm 4 to solve the problem, starting by obtaining the first primal solution and providing it as an initial point to SCIP, which then proceeds to improve the dual bounds, and in some cases, generates better primal solutions. For a comparison, we also use SCIP to solve the problem directly for five hours.

Algorithm 4: Overall procedure

Run CVXNLP-based decomposition (Algorithm 1) or Time decomposition (Algorithm 3)
if *a primal solution is obtained* **then**
  Record the time taken to obtain the primal solution;
  Provide the primal solution to SCIP;
  Run SCIP for the remainder of 5 hours
end
return *Primal bound* $\overline{C}$ *and dual bound* $\underline{C}$

5.3. Results

In this section, we present our computational results. We compare the performance of solving the compact formulation by SCIP directly, running Algorithm 4 with CVXNLP-based composition, and running Algorithm 4 with time decomposition. We report the primal bound $\overline{C}$, lower bound $\underline{C}$, and percentage gap, which is computed by

$$\text{gap} = \frac{\overline{C} - \underline{C}}{\underline{C}}. \tag{59}$$

The first set of results for $T = 24$ is in Table 3, where $\overline{C}$ and $\underline{C}$ are reported in 10^4. We see that SCIP is only able to find primal solutions for stress factors 1.0 and 2.0. While running Algorithm 4 with either CVXNLP-based decomposition or time decomposition, we are able to find primal solutions for all stress factors with the largest optimality gap of about 25%. We observe further improvement when running Algorithm 4 with time decomposition instead of CVXNLP-based decomposition. Additionally, we report that the SCIP solver obtained new primal solutions for stress factors 0.5 and 1.0 when running Algorithm 4 with CVXNLP-based decomposition. The final primal solution reported has about 37.6% and 38.5% improvements from the primal solutions provided to SCIP for the two stress factors, respectively. For all other demand and supply scenarios, the final primal solutions were obtained from Algorithm 4. Furthermore, in comparing the dual bounds $\underline{C}$, we see that SCIP has the best dual bounds as Algorithm 4 takes time to obtain the primal solutions. The dual bounds from Algorithm 4 with time decomposition are slightly better than those from Algorithm 4 with CVXNLP-based decomposition. This observation suggests that Algorithm 4 with time decomposition takes less time to find a primal solution than Algorithm 4 with CVXNLP-based decomposition does, thus allowing more time to SCIP to improve the dual bound. Generally, increasing the stress factor makes the demand and supply scenario more challenging to solve. However, this trend is not evident in running SCIP directly as SCIP is able to find feasible primal solutions for stress factors 1.0 and 2.0. In both instances, SCIP obtained the primal solutions via heuristics. We believe that certain problem structures may trigger heuristics in SCIP for some stress factors, while in general, it remains very challenging to obtain primal solutions when running SCIP directly.

Table 3: Computational results for $T = 24$

Stress	SCIP			Algorithm 4; CVXNLP			Algorithm 4; Time decomp		
	$\overline{C}$	$\underline{C}$	gap(%)	$\overline{C}$	$\underline{C}$	gap (%)	$\overline{C}$	$\underline{C}$	gap (%)
0.1	-	2443.39	-	2443.39	2443.39	0.00	2443.39	2443.39	0.00
0.5	-	2498.78	-	2682.88	2493.39	7.60	2616.23	2496.77	4.78
1.0	3070.02	2632.23	16.63	2892.44	2627.61	10.08	2789.74	2631.38	6.02
1.5	-	2805.03	-	3219.64	2793.41	15.26	3023.93	2804.21	7.84
2.0	3276.69	2937.63	11.54	3683.82	2918.45	26.23	3199.12	2937.07	8.92

The next set of results for $T = 53$ can be found in Table 4. The values for $\overline{C}$ and $\underline{C}$ are reported in 10^4. As the number of time period increases, the problems become more challenging to solve. Currently, SCIP is unable to obtain a primal solution for any of the stress factors. However, Algorithm 4 with CVXNLP-based decomposition is able to obtain primal solutions for all stress factors except for 2.0. Algorithm 4 with time decomposition is able to obtain primal solutions for all stress factors, with the largest optimality gap of less than 15%.

The results for $T = 53$ confirm that, as the stress factor increases, the problem becomes more challenging to solve. Unlike a few instances for $T = 24$, all the primal solutions reported in this table are obtained from Algorithm 4. The variant of Algorithm 4 that uses CVXNLP-based decomposition struggles to find good primal solutions for stress factors 1.0 and 1.5, terminating with large optimality gaps. Moreover, the dual bounds for Algorithm 4 with both CVXNLP-based decomposition and time decomposition are comparable, indicating it now takes longer to obtain primal solutions with time decomposition. If we consider a larger network or more time periods, solving the restricted problem for $\{1, \ldots, \tilde{T}\}$ (Step 4 of Algorithm 3) may not be ideal for the computation time needed. Instead, we can consider using the CVXNLP-based decomposition to solve the restricted problem.

Table 4: Computational results for $T = 53$

Stress	SCIP			Algorithm 4; CVXNLP			Algorithm 4; Time decomp		
	$\overline{C}$	$\underline{C}$	gap(%)	$\overline{C}$	$\underline{C}$	gap (%)	$\overline{C}$	$\underline{C}$	gap (%)
0.1	-	2443.39	-	2443.39	2443.39	0.00	2443.39	2443.39	0.00
0.5	-	2493.29	-	2721.64	2493.29	9.16	2645.06	2493.29	6.09
1.0	-	2599.72	-	4822.70	2583.69	86.66	2828.82	2582.85	9.52
1.5	-	2748.69	-	5288.98	2715.45	94.77	3054.41	2711.14	12.66
2.0	-	2857.61	-	-	-	-	3212.51	2829.65	13.53

6. Conclusions

Our study explores a water network problem that considers design and operation aspects simultaneously. Our formulation results in a nonconvex mixed-integer nonlinear program. We observe that off-the-shelf solvers consistently provide good dual bounds of the formulation, but struggle to find primal solutions. To obtain primal solutions, we proposed two algorithms. One algorithm uses the CVXNLP reformulation and is similar to the framework proposed in Li et al. (2024), while the other is based on time decomposition. Our computational studies, which use a network derived from the

PARETO strategic case study, show that our algorithms can obtain good primal solutions for most of the demand and supply scenarios. The algorithm based on time decomposition outperforms the algorithm based on CVXNLP.

We propose a possible future direction for our work. It involves factoring in the costs of pump stations and relief valves into the proposed algorithms. Both algorithms can be adapted to handle these additional cost components.

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