# Water network design and operation optimization: Leveraging linear approximations for solving challenging MINLPs

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**Abstract**

This study addresses water network design and operational problems, such as managing produced water in the oil and gas industry and urban water network design. We specifically address a key challenge in solving these: the representation of frictional pressure changes across network nodes using nonlinear constraints, typically modeled by the Hazen-Williams equation. For the optimization of produced water networks, we demonstrate the effectiveness of using a standard piecewise linear approximation to generate near-optimal solutions for the original problem. Computational results with real-world problems confirm the success of this approach. However, in the context of urban water network design problems, we recognize the limitations of this approximation and propose an alternative solution. We develop a general-purpose primal heuristic to handle MINLPs with nonlinearities in continuous variables, leveraging linear approximations and bound-reduction techniques. This heuristic consistently produces high quality primal solutions, even outperforming the best-known solutions in three urban water network design case studies.

*Keywords:* PARETO; Produced water; Hazen-William equation; Urban water design.

## 1. Introduction and literature review

Optimization of fresh and waste water networks is important due to high infrastructure costs, water scarcity in certain parts of the world and environmental considerations. Depending on the application, the optimization can be of solely of the network design, solely of the operation of devices like pumps, or simultaneous design and operation. Our paper discusses two specific applications of water network optimization: first in produced water management in the oil and gas industry and second in urban water supply network design. Both these problems share a common feature that the frictional pressure loss is governed by nonlinear expressions of volumetric flow rate of water, giving rise to nonconvexities in the resulting formulations. Such nonconvexities make these optimization problem challenging.

Produced water, a highly saline byproduct of crude oil drilling, necessitates careful disposal to mitigate ecological risks. Dedicated disposal sites have been established to manage it responsibly (US Geological Survey (2024); PARETO (2024). Disposal offers a cost-effective way of handling produced water and typically involves injecting it to an underground formation. Produced water can also be reused within the oil and gas industry itself for drilling. It also has potential for being treated and put to secondary use such as in mining or agriculture. Building a network for produced water management is vital to ensure management in a cost-effective and environmentally responsible manner. This network should aim to minimize infrastructure and operational costs while enforcing all physical and resource constraints. Worth mentioning in this context is the project PARETO which is an initiative by the U.S. Department of Energy that aims to develop an open-source optimization framework for the management of produced water (Drouven et al., 2023).

Finding high-quality primal solutions for these types of problems presents a considerable challenge, even for the most advanced Mixed Integer Nonlinear Programming (MINLP) solvers (Li et al., 2024). The nonlinear constraints of frictional pressure drop in the problem formulations, according to the Hazen-Williams equation (Williams & Hazen, 1905), hinder the solution of water network design problems. The pressure drop is directly proportional to flow raised to the power of 1.85 and inversely proportional to the diameter raised to the power of 4.87. The electricity consumption of an electric pump is directly proportional to the pressure increase from the pump and the volumetric flow rate of water, leading to another nonlinearity. In such a context, we analytically show that a standard piecewise linear approximation can produce near-optimal solutions and confirm experimentally for several real-world case studies. For another example demonstrating global guarantees of a linear approximation in MINLP for pooling problem, refer to Dey & Gupte (2015).

Our paper also considers urban water network design problems. Unlike the produced water network management, in this application setting, the demands at the customer locations are known and assumed to be fixed across time. Additionally, these problems involve optimization of only network design, whereas produced water network optimization incorporates the optimization of both design and operation decisions. The objective is to determine pipeline diameters and flows that minimize infrastructure costs while meeting demand requirements and hydraulic constraints within a fixed network topology, as described in Bragalli et al. (2012). As with the produced water network management, a primary difficulty is the nonlinear constraints involving frictional pressure drops. These MINLP problems pose significant challenges for nonlinear solvers, particularly in finding good feasible solutions. Here, we aim to find high-quality primal solutions to optimize these water network designs. As is extensively discussed in (Bragalli et al., 2012), a direct use of piecewise linear approximation in urban water network problems, such as the Hanoi water distribution network design problem (MINLPLib, 2024), may result in Mixed Integer Linear Programs (MILPs) whose solutions are infeasible for the MINLP unless a very fine grid is used. When a fine grid is used, the resulting MILPs become intractable for modern MILP solvers. This is due to the presence of hard nonlinear equality constraints that model the Hazen-Williams relation and contain no slacks.

To address this challenge in the urban water network design problem, we have developed a new general-purpose primal heuristic to produce high-quality, feasible solutions. Our approach involves iteratively solving linear approximations of nonlinear constraints and systematically reducing bounds on continuous variables around the solution. While the initial linear approximation solutions may be infeasible for the MINLP problem, as the bounds tighten, feasibility is achieved within a desired tolerance.

A significant amount of research has been conducted in the area of water distribution network optimization. Awe et al. (2019) provide valuable insights into this field, while Mala-Jetmarova et al. (2018) provide a comprehensive review of water distribution systems. Additionally, several works have explored heuristics and metaheuristics for water distribution networks, such as Cunha & Sousa (1999).

The literature shows a growing interest in the utilization of MILPs to either approximate or relax optimization problems related to water networks. Several studies have demonstrated the advantages of using MILP formulations, particularly by developing suitable piecewise linear approximations or multi-parametric dis-aggregation of variables in nonlinear expressions. In their recent and a general study, Braun & Burlacu (2023) conducted experiments that compare different piecewise linearization formulations when applied to over 300 MINLPLib benchmark instances. Their work emphasizes the advantages of incremental models for piecewise linear formulations.

Bragalli et al. (2012) propose a MINLP approach to solve the water distribution network problem. They demonstrate how the solutions they obtained are easily implementable due to the accurate modeling of frictional pressure drop, which ensures correct hydraulics functioning. They note that MILP approximations of these problems are typically intractable for any meaningful feasibility tolerance. Additionally, Morsi et al. (2012) and Geißler et al. (2011) successfully apply a piecewise linear approximation to solve water supply operation problems on tested networks. Similarly, Vieira et al. (2020) provide a piecewise linearization technique along with a correction scheme to obtain solutions to operational planning problem of water distribution networks. Notably, the technique outperforms all previous best results for three benchmark problems in the literature. However, existing research primarily explores MILP approximations for operation planning of water distribution networks. In contrast, our paper focuses on MILP approximations for produced water network design and operation problems and for design of urban water networks.

Alperovits & Shamir (1977) present a heuristic approach to the water network design problem, which involves iteratively fixing flows, solving the linear program (LP) for the design problem, and using duals to update the flows. However, the solutions derived from this method do not guarantee closeness to the globally optimal solution. Similarly, Samani & Zanganeh (2010) propose a heuristic for the municipal water distribution network problem, which involves iteratively solving the MILP problem to determine diameter choices and pumpheads. They then conduct hydraulic analysis to obtain flow and pressure values.

In the context of water treatment network design, MILP approximation techniques have proven to be successful. Teles et al. (2012) and Ting et al. (2016) apply these techniques to solve a water treatment network design problem. The main challenge in water treatment network design lies in the nonconvexity due to the bilinear terms comprising flow and concentrations. Faria & Bagajewicz (2011) address this challenge by proposing a bound contraction procedure for variables appearing in bilinear terms and applying it to water management problems. These water network optimization models are different from the ones considered in this work in the sense that they do not account for the nonlinearities arising from the Hazen-William equations.

The contributions of our work to linear approximations of MINLPs are twofold:

- We demonstrate through analytical results and real-world case studies that a standard piecewise linear approximation identifies near-global optimal solutions for the produced water network optimization problems.

- Conversely, for the urban water network design problems, such an approximation is not efficient and fails to produce feasible solutions. To address this limitation, we develop a general-purpose primal heuristic to tackle MINLPs with nonlinearities in continuous variables. We test our heuristic against the solutions obtained by the BARON global optimization solver. Our primal heuristic consistently delivers near-optimal solutions for all our water network design instances, including standard urban water network design problems and produced water management. Notably, our heuristic produces feasible solutions with superior objective values for three of the standard urban water network design instances compared to the best-known solutions in the existing literature.

Based on the literature, our heuristic can be compared to the mesh refinement algorithm presented in Burlacu et al. (2020), which focuses on making discretizations finer in successive iterations. In contrast to traditional mesh refinement at a region, our heuristic restricts the domain to a smaller interval centered around the previous approximation solution. Furthermore, similarities can be drawn between our approach and diving heuristics for discrete variables, as discussed in Berthold (2008) and Bonami & Gonçalves (2012). In diving heuristics, the values of integer variables are fixed from the solution of a relaxation. However, our approach distinguishes itself by restricting the domain of a continuous variable to a smaller interval centered at the solution to an approximation.

The remainder of this paper is structured as follows. Section 2 describes the produced water network optimization problem and provides a basic mathematical formulation for it. Section 3 details the proposed piecewise linear approximation to the nonlinear constraints. This section also presents analytical results guaranteeing near optimality of the solutions to the MINLP that are obtained using the proposed approximation scheme. Section 4 describes the continuous-variable-diving (CVD) heuristic. Finally, experimental results are presented in section 5 followed by conclusions in Section 6.

## 2. Problem formulation for the produced water network optimization problem

We present a basic problem setting and the corresponding mathematical formulation to enhance the readability and clarity of our approach. We refer to PARETO (2024) for the comprehensive formulation, to which we will apply the proposed method.

### *2.1. Problem setting*

We consider the problem of determining pipeline diameters for new installations or replacing existing pipelines. We have three sets of nodes: demand nodes $D$, which process produced water; supply nodes $S$, which are the source of the produced water; and intermediate nodes $N$ of the pipeline. The flow possibilities between nodes are represented by a set of arcs $\mathcal{A}$. This set has one arc for each pair of nodes where flow can occur in a single direction, and two arcs for each pair of nodes where flow can occur in either direction.

Another set we consider is the set of extension pipeline diameters, $K$. When extending the current pipeline, the new diameter is the sum of the current diameter and a selected diameter from the set $K$. A cost is associated with installing a new diameter pipeline, and each diameter value determines the maximum volumetric flow rate through the pipe. Additionally, the set $K$ includes a diameter of 0, representing the option not to extend and keep the current pipeline between the locations.

The pressure values at the supply nodes are known, as are the elevations of all the nodes. The frictional pressure loss in the direction of the flow is calculated using the Hazen-William equation. We can install a pump between any pair of nodes to increase the pressure in the direction of the flow or install a relief valve to reduce the pressure in the direction of the flow. Pumps have a fixed installation cost and a variable electricity cost, which is directly proportional to the product of the volumetric flow rate of water and the pressure increase due to the pump. The pressure values at each node must be within the limits (minimum pressure limit and maximum tolerance limit) set by the pipe.

The objective is to identify minimum cost decisions for pipeline diameters and pump locations while ensuring flow conservation, hydraulics pressure constraints, and flow capacities. Furthermore, all produced water from the supply nodes must be properly managed, and the processing capacities at the nodes processing produced water must be adhered to.

### *2.2. Mathematical formulation*

All sets, parameters, and variables are reported in Table 1.

We formulate the problem as follows:

$$\min \sum_{k\in K} \sum_{(i,j)\in\mathcal{A}} c_{ij}^k y_{ij}^k + \sum_{(i,j)\in\mathcal{A}} \mathcal{C}_{ij} \tag{1}$$

s.t.

$$\sum_{j:(i,j)\in\mathcal{A}} q_{ij}^t = b_i^t \qquad i\in S, t\in T \tag{2}$$

$$\sum_{j:(ji)\in\mathcal{A}} q_{ji}^t \le -b_i^t \qquad i\in D, t\in T \tag{3}$$

$$\sum_{j:(ji)\in\mathcal{A}} q_{ji}^t = \sum_{j:(ij)\in\mathcal{A}} q_{ij}^t \qquad i\in N, t\in T \tag{4}$$

$$q_{ij}^t \le \sum_{k\in K} F_{ij}^k y_{ij}^k \qquad (i,j)\in\mathcal{A}, t\in T \tag{5}$$

$$q_{ij}^t \le M_1 z_{ij}^t \qquad (i,j)\in\mathcal{A}, t\in T \tag{6}$$

$$z_{ij}^t + z_{ji}^t = 1 \qquad (i,j)\in\mathcal{A}, t\in T \text{ s.t. } (j,i)\in\mathcal{A} \tag{7}$$

$$\sum_{k\in K} y_{ij}^k = 1 \qquad (i,j)\in\mathcal{A} \tag{8}$$

$$y_{ij}^k = y_{ji}^k \qquad (i,j)\in\mathcal{A}, k\in K \text{ s.t. } (j,i)\in\mathcal{A} \tag{9}$$

$$p_i^t = P_{i,t} \qquad i\in S, t\in T \tag{10}$$

$$(d_{ij} + \sum_{k\in K} k y_{ij}^k)^{4.87} H_{ij}^{\text{Friction},t} = \gamma_{ij}(q_{ij}^t)^{1.85} \qquad (i,j)\in\mathcal{A}, t\in T \tag{11}$$

$$\begin{aligned} p_i^t + \rho g E_i \ge p_j^t + \rho g E_j + H_{ij}^{\text{Friction},t} - \Delta_{ij}^{\text{Pump},t} \\ + \Delta_{ij}^{\text{Valve},t} - M_2(1 - z_{ij}^t) \end{aligned} \qquad (i,j)\in\mathcal{A}, t\in T \tag{12}$$

$$\begin{aligned} p_i^t + \rho g E_i \le p_j^t + \rho g E_j + H_{ij}^{\text{Friction},t} - \Delta_{ij}^{\text{Pump},t} \\ + \Delta_{ij}^{\text{Valve},t} + M_2(1 - z_{ij}^t) \end{aligned} \qquad (i,j)\in\mathcal{A}, t\in T \tag{13}$$

$$p_{\min} \le p_i^t \le p_{\max} \qquad i\in N, t\in T \tag{14}$$

$$\Delta_{ij}^{\text{Pump},t} \le M_2 v_{ij} \qquad (i,j)\in\mathcal{A}, t\in T \tag{15}$$

$$\mathcal{C}_{ij} = C_1 v_{ij} + C_2 \sum_{t\in T} \Delta_{ij}^{\text{Pump},t} q_{ij}^t \qquad (i,j)\in\mathcal{A} \tag{16}$$

$$q_{ij}^t \ge 0, \quad \Delta_{ij}^{\text{Pump},t} \ge 0, \quad \Delta_{ij}^{\text{Valve},t} \ge 0 \qquad (i,j)\in\mathcal{A}, t\in T \tag{17}$$

***Table 1:*** *Sets, parameters, and variables*

| | |
|---|---|
| Sets | |
| $S$ | Set of supply nodes |
| $D$ | Set of demand nodes |
| $N$ | Set of intermediate nodes |
| $\mathcal{A}$ | Set of arcs |
| $K$ | Set of pipeline diameters for extension, includes 0 diameter case |
| $T$ | Set of time periods |
| Indices | |
| $i, j$ | Indices for the nodes of the network |
| $t$ | Index for time |
| $k$ | Index for diameter choice |
| Parameters | |
| $c_{ij}^k$ | Cost of installing pipeline from $i$ to $j$ with diameter selection $k$ |
| $F_{ij}^k$ | Flow capacity of pipeline from $i$ to $j$ if the extension diameter selected is $k$ |
| $b_i^t$ | Supply (if positive) or capacity at demand node (if negative) at node $i$ at time period $t$. |
| $p_{\max}$ | Maximum tolerable pressure at an intermediate node |
| $p_{\min}$ | Minimum required pressure at an intermediate node |
| $P_{i,t}$ | Fixed pressures at the supply node $i$ in period $t$ |
| $E_i$ | Elevation of node $i$ |
| $\rho$ | Density of water |
| $g$ | Accelaration due to gravity |
| $\gamma_{ij}$ | Constant dependent on length of pipe, material of pipe and unit conversion |
| $C_1$ | Fixed cost of installing a pump |
| $C_2$ | Variable cost of using a pump |
| $M_1$ | A large value (maximum flow) |
| $M_2$ | A large value (maximum pressure) |
| Variables | |
| $y_{i,j}^k$ | Binary variable equals to 1 if diameter $k$ is selected for extension $i$ to $j$, 0 otherwise |
| $v_{i,j}$ | Binary variable equals to 1 if pump is installed between nodes $i$ and $j$, 0 otherwise |
| $z_{i,j}^t$ | Binary variable equals to 1 if flow is from node $i$ to node $j$ at time period $t$, 0 otherwise |
| $q_{ij}^t$ | Volumetric flow rate of water from node $i$ to node $j$ at period $t$ |
| $p_t^t$ | Pressure at node $i$ at period $t$ |
| $\Delta_{ij}^{\text{Pump},t}$ | Pump head from node $i$ to node $j$ at period $t$ |
| $\Delta_{ij}^{\text{Valve},t}$ | Pressure release via valve from node $i$ to node $j$ at period $t$ |
| $H_{ij}^{\text{Friction},t}$ | Pressure loss due to friction from node $i$ to node $j$ at period $t$ |
| $\mathcal{C}_{ij}$ | Total pump cost, fixed and variable, from node $i$ to node $j$ |

The objective function (1) minimizes the overall cost of pumps and pipe installations. Constraints (2) and (3) model the flows from supply nodes and flows into the demand nodes, respectively. The equalities at supply nodes indicate that all produced water must be discharged, while the inequalities at the demand nodes reflect the maximum processing capacities at these locations. Flow conservation equations are enforced by Constraints (4). Additionally, Constraints (5) define the flow capacities based on the selected diameter. Constraints (6) dictate that the flow through an arc at a particular time period will be zero if the corresponding binary indicator variable is zero. Constraints (7) ensure that flow occurs in a single direction. Exactly one diameter is to be selected (8) and the diameter of the pipe in the reverse arc must match that of the forward arc (9). Constraints (10) establish pressure values at the supply nodes. Constraints (11) are the Hazen-Williams equations to calculate frictional pressure loss. Combining Constraints (12) and (13) provides a rule for calculating node pressures. This rule does not apply if there is no flow along an arc. Therefore, this rule is modeled as two inequalities with big-M instead of an equality. Constraints (14) set the maximum tolerable pressure at the intermediate nodes. Constraints (15) ensure the pump head is set to zero if no pump is installed. Constraints (16) define the cost of using a pump, which consists of a fixed component and a variable component depending on usage. Finally, Constraints (17) ensure the nonnegativity of the flow, pump-head, and valve-head variables.

## 3. A piecewise linear approximation to produced water management problem and analysis

The Hazen-William frictional pressure loss (11) and the pump cost rule (16) are the sources of nonlinearities in the MINLP formulation. Here, we develop a linear approximation for these constraints. In Lemma 1, we show that any solution to the linear approximation can be made feasible to the original MINLP formulation with minor adjustments.

### *3.1. A piecewise linear approximation*

#### *3.1.1. Hazen-William equation*

We use a piecewise linear approximation to approximate $f(q_{ij}^t) = (q_{ij}^t)^{1.85}$ appearing in the right-hand side of the Hazen-Williams equation (11).

Suppose the values of flows range from 0 to $Q_{\max}$. Divide this range of flow into intervals of length $\Delta_Q$ where $Q_{\max}$ is an integer multiple of $\Delta_Q$. Introduce convex combination multipliers $\lambda_{i,j}^{t,1}$, $\lambda_{i,j}^{t,2}$, ..., $\lambda_{i,j}^{t,1+Q_{\max}/\Delta_Q}$. The flows will be a convex combination of $1 + Q_{\max}/\Delta_Q$ equally spaced points in the range. Let $\zeta_{ij}^t$ denote the piecewise linear approximation of $f(q_{ij}^t)$. The following system of equations and inequalities yield $\zeta_{ij}^t$.

$$q_{ij}^t = \sum_{s=1}^{1+Q_{\max}/\Delta_Q} (s-1)\Delta_Q \lambda_{i,j}^{t,s} \qquad (i,j) \in \mathcal{A}, t \in T \tag{18}$$

$$\zeta_{ij}^t = \sum_{s=1}^{1+Q_{\max}/\Delta_Q} ((s-1)\Delta_Q)^{1.85} \lambda_{i,j}^{t,s} \qquad (i,j) \in \mathcal{A}, t \in T \tag{19}$$

$$\sum_{s=1}^{1+Q_{\max}/\Delta_Q} \lambda_{i,j}^{t,s} = 1 \qquad (i,j) \in \mathcal{A}, t \in T \tag{20}$$

$$\lambda_{i,j}^{t,1} \leq u_{ij}^{t,1} \qquad (i,j) \in \mathcal{A}, t \in T \tag{21}$$

$$\lambda_{i,j}^{t,s} \leq u_{ij}^{t,s} + u_{ij}^{t,s-1} \qquad (i,j) \in \mathcal{A}, t \in T, s \in \{2, 3, ..., Q_{\max}/\Delta_Q\} \tag{22}$$

$$\lambda_{i,j}^{t,1+Q_{\max}/\Delta_Q} \leq u_{ij}^{t,Q_{\max}/\Delta_Q} \qquad (i,j) \in \mathcal{A}, t \in T \tag{23}$$

$$\sum_{s=1}^{Q_{\max}/\Delta_Q} u_{i,j}^{t,s} = 1 \qquad (i,j) \in \mathcal{A}, t \in T \tag{24}$$

Here, Equation (18) represents flows as a convex combination of uniformly located points in the range 0 to $Q_{\max}$. Equation (19) uses the same convex combination multipliers to approximate $f(q_{ij}^t)$ by expressing it as a convex combination of function values at these uniformly located points. Equation (20) ensures that the convex combination multipliers equals 1. Finally, Constraints (21) to (23) impose a condition on the convex combination multipliers, specifying that a maximum of two can be nonzero, depending on which interval of the piecewise linear graph is selected. Here, $u_{ij}^{t,s}$ are auxiliary binary variables that take a value of one for the interval of the piecewise linear function that is selected. Equation (24) enforces that exactly one interval is chosen.

The Hazen-William equation can be transformed into the following equation by rewriting the expression for effective diameter on the LHS:

$$\sum_{k \in K} (d_{ij} + k)^{4.87} y_{ij}^k H_{ij}^{\text{Friction},t} = \kappa_{ij} \zeta_{ij}^t \quad (i,j) \in \mathcal{A}, t \in T$$

Note that this approach involves a product of binary diameter selection variables with the frictional pressure loss. This product can be easily linearized using McCormick inequalities. We know that when one of two variables in a bilinear product is binary, these McCormick inequalities accurately model the product. Thus, by introducing a new variable $\mathcal{P}_{ij}^{tk}$ for the product, we can enforce the above Hazen-William equation as:

$$\sum_{k \in K} (d_{ij} + k)^{4.87} \mathcal{P}_{ij}^{tk} = \kappa_{ij} \zeta_{ij}^t \quad (i,j) \in \mathcal{A}, t \in T \tag{25}$$

$$\mathcal{P}_{ij}^{tk} \geq 0 \quad (i,j) \in \mathcal{A}, t \in T, k \in K \tag{26}$$

$$\mathcal{P}_{ij}^{tk} \leq H_{ij}^{\text{Friction},t} \quad (i,j) \in \mathcal{A}, t \in T, k \in K \tag{27}$$

$$\mathcal{P}_{ij}^{tk} \leq M_2 y_{ij}^k \quad (i,j) \in \mathcal{A}, t \in T, k \in K \tag{28}$$

$$\mathcal{P}_{ij}^{tk} \geq H_{ij}^{\text{Friction},t} + M_2 y_{ij}^k - M_2 \quad (i,j) \in \mathcal{A}, t \in T, k \in K \tag{29}$$

Instead of using Constraints (11), we use Constraints (18) to (24) and (25) to (29) to create a linear approximation. The approximation error may be caused by modeling $f(q_{ij}^t)$ as a piecewise linear function. Increasing the number of points for piecewise linear approximation improves accuracy but reduces the solution process efficiency. In our current setup, we found that a somewhat coarse point selection still led to a near-optimal solution. This observation is supported by the propositions in Subsection 3.2.

*3.1.2. Electricity (variable) cost of operating pumps*

The variable cost, which is the electricity cost of using a water pump, depends on the product of the pressure change induced by the pump and the volumetric flow rate of water through the pump. Specifically, the variable cost at any given time period is calculated using the formula $\mathcal{V}_{ij}^t = C_2 \Delta_{ij}^{\text{Pump},t} q_{ij}^t$, for all $(i,j) \in \mathcal{A}$. After expressing the flow as a convex combination of discrete points in its range, we can linearize the variable cost using the following inequality.

$$\mathcal{V}_{ij}^t \geq C_2(s\Delta_Q)\Delta_{ij}^{\text{Pump},t} - M(1 - u_{ij}^{t,s}) \qquad s \in \{1, 2, ..., Q_{\max}/\Delta_Q\} \tag{30}$$

The variable cost $\mathcal{V}_{ij}^t$ in the system of inequalities is set based on the cost calculated using the minimum point of the respective flow. When the respective flow does not fall within the range of intervals, the constraints are deactivated using the big-M term. Since the overall problem is a minimization problem, optimality ensures that $\mathcal{V}_{ij}^t$ is equal to the largest of the terms on the right-hand side of (30).

For the sake of conciseness, we provide the complete formulation for the piecewise linear approximation in Appendix A.

### *3.2. Analytical results*

Let $z_{MINLP}$ be the optimal objective cost of the MINLP and $z_{PL}$ be the optimal objective cost of the piecewise linear formulation.

**Proposition 3.1** (Approximate equivalance between piecewise linearization and MINLP)**.** *Assume the loops present in the network are chordless, and the source nodes have only one neighbor. Let $\epsilon$ be the maximum error of approximation of the nonlinear frictional pressure drops with piecewise linear approximation, let $L$ be the set of loops in the network, and let $E$ be the set of edges of the network. Suppose the optimal solution of the MINLP ($\bar{y}_{ij}^k$, $\bar{z}_{ij}^t$, $\bar{v}_{ij}$, $\bar{q}_{ij}^t$, $\bar{\Delta}_{ij}^{Pump,t}$, $\bar{\Delta}_{ij}^{Valve,t}$, $\bar{H}_{ij}^{Friction,t}$, $\bar{p}_i^t$, $\bar{\mathcal{C}}_{ij}$) satisfies the condition that the operating pressure at each node is at least $|E|\epsilon + |L||E|\epsilon$ more than the minimum allowable pressure and at least $|L||E|\epsilon$ less than the maximum allowable pressure. Then, $0 \leq z_{PL} - z_{MINLP} \leq C_2 Q_{\max}\epsilon|E| + C_2 \sum_{t\in T}\sum_{(i,j)\in\mathcal{A}} \Delta_{ij}^{Pump,t}\Delta_Q$.*

The following two lemmas lead to the proposition.

**Lemma 1.** *For every solution to the piecewise linear approximation, there is a corresponding solution to the MINLP with no higher cost.*

*Proof.* Consider a solution to the piecewise linear approximation ($\hat{y}_{ij}^k$, $\hat{z}_{ij}^t$, $\hat{v}_{ij}$, $\hat{q}_{ij}^t$, $\hat{\Delta}_{ij}^{\text{Pump},t}$, $\hat{\Delta}_{ij}^{\text{Valve},t}$, $\hat{H}_{ij}^{\text{Friction},t}$, $\hat{\mathcal{C}}_{ij}$). Construct a solution to the original MINLP as follows.

Set $\bar{y}_{ij}^k = \hat{y}_{ij}^k$, $\bar{z}_{ij}^t = \hat{z}_{ij}^t$, $v_{ij} = \hat{v}_{ij}$, $q_{ij}^t = \hat{q}_{ij}^t$, $\bar{\Delta}_{ij}^{\text{Pump},t} = \hat{\Delta}_{ij}^{\text{Pump},t}$. The value of $\bar{H}_{ij}^{\text{Friction},t}$ will be set by the nonlinear equation (11) to $\bar{H}_{ij}^{\text{Friction},t} = \kappa_{ij}(\hat{q}_{ij}^t)^{1.85}/((d_{ij} + \sum_{k\in K} k\hat{y}_{ij}^k)^{4.87})$. Further, set $\bar{\Delta}_{ij}^{\text{Valve},t} = \hat{\Delta}_{ij}^{\text{Valve},t} + \hat{H}_{ij}^{\text{Friction},t} - \bar{H}_{ij}^{\text{Friction},t}$. Then, the defined solution ($\bar{y}_{ij}^k$, $\bar{z}_{ij}^t$, $\bar{v}_{ij}$, $\bar{q}_{ij}^t$, $\bar{\Delta}_{ij}^{\text{Pump},t}$, $\bar{\Delta}_{ij}^{\text{Valve},t}$, $\bar{H}_{ij}^{\text{Friction},t}$, $\bar{p}_i^t$, $\bar{\mathcal{C}}_{ij}$) satisfies all the constraints of the original MINLP.

The cost of diameter extension in the constructed MINLP solution $\sum_{k\in K}\sum_{(ij)\in\mathcal{A}} c_{ij}^k \bar{y}_{ij}^k = \sum_{k\in K}\sum_{(ij)\in\mathcal{A}} c_{ij}^k \hat{y}_{ij}^k$ is the same as the piecewise linear approximation formulation. Furthermore, the pump cost $\hat{\mathcal{C}}_{ij}$ in the piecewise linear approximation overestimates $\bar{\mathcal{C}}_{ij}$ in the MINLP because the flow in an interval is at its maximum in the piecewise linear approximation. Therefore, the objective cost of the constructed MINLP solution is less than or equal to the objective cost of the piecewise linear solution. □

**Remark** (Upper Bound). *Lemma 1 provides an effective method for obtaining good feasible solutions to the MINLP. By leveraging the efficient solving capabilities of modern MILP solvers, we can obtain a valid upper bound.*

**Remark** (Optimal objectives). *A corollary to the above proposition is that $z_{MINLP} \leq z_{PL}$.*

The next lemma gives guarantees on qualities of such solutions under mild assumptions.

**Lemma 2.** *Assume that the loops present in the network are chordless and the source nodes have only one neighbor. Let $\epsilon$ be the maximum error of approximation for the nonlinear frictional pressure drops with piecewise linear approximation, let $L$ be the set of loops in the network, and let $E$ be the set of edges of the network. Consider any solution of the MINLP ($\bar{y}^k_{ij}$, $\bar{z}^t_{ij}$, $\bar{v}_{ij}$, $\bar{q}^t_{ij}$, $\bar{\Delta}^{Pump,t}_{ij}$, $\bar{\Delta}^{Valve,t}_{ij}$, $\bar{H}^{Friction,t}_{ij}$, $\bar{p}^t_i$, $\bar{C}_{ij}$) satisfying the condition that the operating pressure at each node is at least $|E|\epsilon + |L||E|\epsilon$ more than the minimum allowable pressure and at least $|L||E|\epsilon$ less than the maximum allowable pressure. Then, there exists a corresponding solution to the piecewise linear approximation with a cost increase of at most $C_2\epsilon Q_{\max}|E|$ $+C_2 \sum_{t\in T}\sum_{(i,j)\in\mathcal{A}} \Delta^{Pump,t}_{ij}\Delta_Q$ from the MINLP cost, where $Q_{\max}$ is an upper bound on the flow capacities.*

*Proof.* We construct a solution feasible for the piecewise linear formulation ($\hat{y}^k_{ij}$, $\hat{z}^t_{ij}$, $\hat{v}_{ij}$, $\hat{q}^t_{ij}$, $\hat{\Delta}^{\text{Pump},t}_{ij}$, $\hat{\Delta}^{\text{Valve},t}_{ij}$, $\hat{H}^{\text{Friction},t}_{ij}$, $\hat{p}^t_i$) whose objective function is at most $C_2\epsilon Q_{\max}|E|+$ $C_2 \sum_{t\in T}\sum_{(i,j)\in\mathcal{A}} \Delta^{\text{Pump},t}_{ij}\Delta_Q$ higher than the known feasible solution of the MINLP. In order to construct this solution, we perturb the solution of the MINLP. Specifically, we keep the variable values ($\bar{y}^k_{ij}$, $\bar{z}^t_{ij}$, $\bar{v}_{ij}$, $\bar{q}^t_{ij}$) from the MINLP solution fixed and adjust the variables $\bar{\Delta}^{\text{Pump},t}_{ij}$, $\bar{\Delta}^{\text{Valve},t}_{ij}$, $\bar{H}^{\text{Friction},t}_{ij}$, $\bar{p}^t_i$ in order to be feasible for the piecewise linear formulation. In the beginning, we set ($\hat{\Delta}^{\text{Pump},t}_{ij}$, $\hat{\Delta}^{\text{Valve},t}_{ij}$) $=$ ($\bar{\Delta}^{\text{Pump},t}_{ij}$,$\bar{\Delta}^{\text{Valve},t}_{ij}$). Furthermore, we set $\hat{H}^{\text{Friction},t}_{ij}$ as the piecewise linear approximation of the frictional pressure loss.

We need to construct a pressure profile feasible for the piecewise linear formulation at any time $t$. The piecewise linear approximation of frictional pressure drops tends to overestimate the MINLP frictional pressure drops for the same flow. To offset this effect, we will first adjust the $\hat{\Delta}^{\text{Pump},t}_{ij}$ and $\hat{\Delta}^{\text{Valve},t}_{ij}$ variables in the piecewise linear formulation.

We begin by adjusting the variables ($\hat{\Delta}^{\text{Pump},t}_{ij}$ and $\hat{\Delta}^{\text{Valve},t}_{ij}$) so that the total pressure drop around a loop is 0. In the network, there are two types of loops. The first type involves all water flows in a single direction in the MINLP solution and, therefore, in the constructed piecewise linear approximation solution, such as clockwise. Such a loop must contain a pump. This can be seen by adding the pressure change constraints (12) and (13) over the arcs in the loop. Let $l$ be the set of arcs in the clockwise direction. Since the pressure values and the changes in elevation cancel out, we obtain the following equation:

$$\sum_{(ij)\in l} \bar{\Delta}^{\text{Pump},t}_{ij} = \sum_{(ij)\in l} \bar{\Delta}^{\text{Valve},t}_{ij} + \sum_{(ij)\in l} \bar{H}^{\text{Friction},t}_{ij}$$

Since the right hand side of the above equation is strictly positive, there must be a nonzero pumphead in the loop. Next, the piecewise linear approximation overestimates the pressure drop across every edge in the loop, resulting in a net positive pressure drop around the loop in a clockwise direction. We can calculate the magnitude of this net pressure drop as $R_l$, considering that none of the flows are altered. To counterbalance this effect, we increase the pump head variable as $\hat{\Delta}^{\text{Pump}}_{i(l),j(l)} = \hat{\Delta}^{\text{Pump}}_{i(l),j(l)} + R_l$. This ensures total pressure drops around such loops are 0. The maximum possible value for $R_l$ is $\epsilon|l|$.

In the second type of loop, the flows are not all in the same direction. Without loss of generality, let the net pressure drop across the loop with frictional drops calculated with piecewise linear function be positive in the clockwise direction as $R_l$. Then, select an arc $(i, j)$ where the flow $\bar{q}_{ij}^t$ is in the counterclockwise direction. Set $\hat{\Delta}_{ij}^{\text{Valve},t} = \hat{\Delta}_{ij}^{\text{Valve},t} + R_l$. This adjustment ensures that the total pressure drop across the loop is 0, thus achieving a net pressure drop of zero across each loop in the piecewise linear formulation.

Henceforth, for arcs where both $i$ and $j$ are not source nodes, the values of $\hat{\Delta}_{ij}^{\text{Valve},t}$ and $\hat{\Delta}_{ij}^{\text{Pump},t}$ are fixed according to the assigned values. The value of $\hat{H}_{ij}^{\text{Friction},t}$ is also fixed for all arcs. Thus, we already know the value of $\hat{p_i^t} - \hat{p_j^t}$ for these arcs based on inequalities (12) and (13).

Next, we need to adjust the values of $\hat{\Delta}_{ij}^{\text{Valve},t}$ and $\hat{\Delta}_{ij}^{\text{Pump},t}$ for arcs where either $i$ or $j$ is a source node. We also need to assign the value of $\hat{p}_i^t$ for all nodes in order to produce a feasible solution.

To assign operating pressures at each node, we define $S$ as the set of source nodes with known and fixed pressure values. For each $s \in S$, let $n(s)$ be the immediate neighbor of the source nodes $s$. Let $V$ represent the set of all nodes. Then assign the node pressures in the piecewise linear formulation according to the following steps:

1. For each $s \in S$, set the source node pressures $\hat{p}_s^t$ with the known fixed pressures.

2. Select an arbitrary starting source node $s_0 \in S$. Compute a tentative value for pressure at $n(s_0)$, say $\widetilde{p^t}_{n(s_0)}$, using the values of $\bar{\Delta}_{s_0,n(s_0)}^{\text{Valve},t}$, $\bar{\Delta}_{s_0,n(s_0)}^{\text{Pump},t}$ and $\bar{H}_{s_0,n(s_0)}^{\text{Friction},t}$ via inequalities (12) and (13).

3. Since $\hat{p_i^t} - \hat{p_j^t}$ is fixed for all arcs $(i, j)$ such that $i, j \in V \setminus S$, starting with $n(s_0)$, assign tentative pressure values $\widetilde{p^t}_i$ for all nodes $i$ in $V \setminus S$. In other words, $\widetilde{p^t}_i - \widetilde{p^t}_j = \hat{p_i^t} - \hat{p_j^t}$ for all $i, j \in V \setminus S$.

   Loops have zero pressure drops around them, so there should be no conflict associated with them.

4. The above tentative pressure values may not be feasible since $\hat{p}_s^t - \widetilde{p}_{n(s)}^t$ may not be equal to

$$-\rho g E_s + \rho g E_{n(s)} + H_{s,n(s)}^{\text{Friction},t} - \bar{\Delta}_{s,n(s)}^{\text{Pump},t} + \bar{\Delta}_{s,n(s)}^{\text{Valve},t}$$

   for some $s \in S \setminus \{s_0\}$. If the value of $\hat{p}_s^t - \widetilde{p^t}_{n(s)}$ is larger than the above expression, then we can fix the solution by appropriately increasing the value of $\hat{\Delta}_{s,n(s)}^{\text{Valve},t}$. If $\hat{p}_s^t - \widetilde{p^t}_{n(s)}$ is smaller than the above expression, then we will globally reduce the value of the node pressures at all nodes in set $V \setminus S$ to attain feasibility. We do this by calculating the following quantity for all source nodes $s \in S$:

$$D(s) = \max \left\{ (-\rho g E_s + \rho g E_{n(s)} + \hat{H}_{s,n(s)}^{\text{Friction},t} - \hat{\Delta}_{s,n(s)}^{\text{Pump},t} + \hat{\Delta}_{s,n(s)}^{\text{Valve},t}) - (\hat{p}_s^t - \widetilde{p^t}_{n(s)}), 0 \right\}, \quad s \in S.$$

   Then, we proceed in three steps:

   (a) Let D $= \max_{s \in S}(D(s))$.

   (b) Decrease the pressures of all the nodes in $V \setminus S$ by D. That is, set $\hat{p}_i^t = \widetilde{p}_i^t - D$, for all $i \in V \setminus S$.

   (c) Finally, for all $s \in S$ set $\hat{\Delta}_{s,n(s)}^{\text{Valve},t} = (\hat{p}_s^t - (-\rho g E_s + \rho g E_{n(s)} + \hat{H}_{s,n(s)}^{\text{Friction},t} - \hat{\Delta}_{s,n(s)}^{\text{Pump},t} + \hat{\Delta}_{s,n(s)}^{\text{Valve},t})) - \hat{p}_{n(s)}^t$.

The pressure assignment is feasible because of the given assumptions. The increase in cost from the MINLP solution is due to the increase in pump head variables and the error in approximating the pump costs. The cost increase due to pump head increase can be bounded for each loop with the unidirectional flow as $C_2\bar{q}^t_{i_l,j_l}R_l \leq C_2\bar{q}^t_{i_l,j_l}\epsilon|l|$. Therefore, the total cost increase due to pump head increase can be bounded as $\sum_{l\in L_p} C_2\bar{q}^t_{i_l,j_l}\epsilon|l| \leq C_2Q_{\max}\epsilon\sum_{l\in L_p}|l| \leq C_2Q_{\max}\epsilon|E|$. The increase in cost due to the approximation error of the pump operating cost can also be quantified as $C_2\sum_{t\in T}\sum_{(i,j)\in\mathcal{A}}\Delta^{\text{Pump},t}_{ij}\Delta_Q$.
□

**Remark.** *The relationship between $\Delta_Q$ and $\epsilon$ is as follows: for each interval $[s\Delta_Q,(s+1)\Delta_Q]$, we define $\zeta_s(x)$ as the value of the line segment that connects $(s\Delta_Q,(s\Delta_Q)^{1.85})$ and $((s+1)\Delta_Q,((s+1)\Delta_Q)^{1.85})$. This gives us a piecewise linear approximation. Our goal is to maximize the concave function $\zeta_s(x)-x^{1.85}$ by taking the derivative with respect to $x$. We denote this maximum value as $\epsilon_s$. Then, $\epsilon=\kappa\max_{s\in\{1,2,\ldots,1+Q_{\max}/\Delta_Q\}}\epsilon_s$, where $\kappa$ is the pipeline specific constant.*

**Remark.** *A corollary to the above lemma is $z_{PL}-z_{MINLP}\leq C_2Q_{\max}\epsilon|E|+C_2\sum_{t\in T}\sum_{(i,j)\in\mathcal{A}}\Delta^{Pump,t}_{ij}\Delta_Q$. Combining it with the previous corollary, that is $z_{PL}-z_{MINLP}\geq 0$ leads to Proposition 3.1.*

## 4. The continuous-variable-diving heuristic: combining linear approximation and domain reduction

According to Bragalli et al. (2012), the direct use of piecewise-linear approximation for urban water network design is ineffective and inefficient. This formulation is slow to solve using modern MILP solvers, and feasible solutions obtained from the approximation are often infeasible for the original MINLP problem. Based on these challenges and the effectiveness of global solvers in providing dual bounds for network design problems, our focus is on designing a general-purpose primal heuristic to generate high-quality feasible solutions for all water network design instances we tested.

We propose the Continuous-Variable-Diving (CVD) algorithm, which solves mixed-integer linear approximations of the MINLP problem followed by domain reduction. We assume that all continuous variables appearing in nonlinear expressions are bounded. The steps of the CVD algorithm are as follows:

1. To approximate the nonlinear terms in the constraints and objective, we approximate them as linear functions using methods such as sampling points within variable bounds and fitting a linear function using standard linear regression. In our experiments, we uniformly select sample points within the current bounds to perform the regression. We refer to the resulting linear function as a least squares fit.

2. Substitute the nonlinear expressions in the objective and constraints with the linear expressions obtained previously. The resulting problem will then be an MILP. Solve the MILP, but not necessarily optimally. In our experiments, we provide the MILP solvers with a fixed amount of time as the stopping criterion. If the MILP is infeasible, then the heuristic fails and is terminated.

3. If the difference between the linear expressions and the original nonlinear function at the obtained solution is within the desired tolerance, then terminate the algorithm. Otherwise, reduce the domains of continuous variables to a smaller sized interval centered around the current MILP

solution. This reduction is achieved in the following way: denote the reduction factor as $\eta$, which is a pre-specified constant greater than 2; let $\bar{x}$ be the MILP solution to a continuous variable and the current length of the domain of the variable be $l$; then, update the bounds of this variable to

$$[\bar{x} - l/\eta,\ \bar{x} + l/\eta]\,,$$

and return to Step 1.

The gap between the upper and lower bounds of each continuous variable shrinks exponentially with each iteration. However, the domains of these continuous variables may not be nested. This means that the domain of a variable in one iteration might not be a subset of the domain of the same variable in the previous iteration.

Algorithm 1 is a pseudo-code for the CVD algorithm applied to the water network design problem. The urban network design problem also excludes operational components (Bragalli et al., 2012). In this context, flow variables may have positive or negative values based on the flow direction. The pressure drop from node 'a' to node 'b' is proportional to the flow from 'a' to 'b' raised to the power of 1.85. When the flow is from 'b' to 'a', the pressure drop is negative. To represent this relationship in the model, we use a nonlinear expression of the form signpower$(q, 1.85)$, which evaluates to $|q|^{1.85}$ for positive flow $q$, and $-|q|^{1.85}$ for negative flow $q$.

**Algorithm 1** Continuous variable diving heuristic for water network design

**Require:** Error tolerance $\tau$, reduction factor $\eta > 0$, number of sample points $P$

Calculate initial upper and lower bounds $q_i^{L,0}, q_i^{U,0}$ for all the flow variables by minimizing and maximizing them over a relaxation formed by relaxing the nonlinear constraints of the formulation.
$j \leftarrow 0$
**while** true **do**
    Sample $P$ uniformly spaced points $(\bar{q}_i^k, \text{signpower}(\bar{q}_i^k, 1.85))$, $k \in \{1, 2, ..., P\}$, $i \in A$, where $\bar{q}_i^k = q_i^{L,j} + (k-1)(q_i^{U,j} - q_i^{L,j})/(P-1)$.
    For every $i \in A$, find the least squares fit $m_i q_i + c_i$ by fitting the sampled points $\{(\bar{q}_i^k, \text{signpower}(\bar{q}_i^k, 1.85)) : k \in \{1, 2, ..., P\}\}$.
    Solve the MILP resulting from replacing each signpower$(q_i, 1.85)$ with the least squares fit $m_i q_i + c_i$. ▷ The process in Section 4 is used for the linearization of the diameter terms.
    Let $\tilde{q}_i$, $i \in A$ denote the solution to flows for the above MILP after a fixed amount of time.
    $l_i \leftarrow q_i^{U,j} - q_i^{L,j}$. ▷ Current box sizes
    If for each flow, the discrepancies $|\text{signpower}(\tilde{q}_i) - (m_i \tilde{q}_i + c_i)| \leq \tau$ break.
    $q_i^{L,j+1} \leftarrow \tilde{q}_i - l_i/\eta$. ▷ Reducing the domain
    $q_i^{U,j+1} \leftarrow \tilde{q}_i + l_i/\eta$.
    $j \leftarrow j + 1$.
**end while**
Return the solution of the last MILP solved.

**Proposition 4.1.** *When using the CVD algorithm, if the nonlinearities that are linearized are unidimensional and Lipschitz continuous with Lipschitz constant $\gamma$, then the maximum number of MILPs solved by the CVD algorithm can be bounded from above by $\lceil log(2D_0\gamma/\epsilon)/log(\eta) \rceil$ where $\epsilon$ is the feasibility tolerance of the constraints, $\eta$ is the reduction factor defined above, and $D_0$ is the maximum length of the intervals containing the continuous variables that appear in any of the nonlinearities.*

*Proof.* When a nonlinear expression $f(x)$ of a single variable is replaced with the least squares fit, there will be a point $x_0$ in the domain of $f$ where the least squares fit value ($L(x_0)$) equals the value of the nonlinear function ($f(x_0)$). To observe this, since $L(x)$ is the least squares fit, there are two sampled points $x_0'$ and $x_0''$ such that $L(x_0') \geq f(x_0')$ and $L(x_0'') \leq f(x_0'')$. Else, $L(x)$ could be perturbed by adding or subracting a small constant to fit the sampled points better. If $L(x_0') = f(x_0')$ or $L(x_0'') = f(x_0'')$, then we select $x_0 = x_0'$ or $x_0 = x_0''$ respectively. If not, then we have $L(x_0') > f(x_0')$ and $L(x_0'') < f(x_0'')$. Then, the continuity of $f(x)$ and $L(x)$ implies the existence of a point $x_0$ on the line segment joining $x_0'$ and $x_0''$ such that $L(x_0) = f(x_0)$.

The maximum magnitude of the slope of $L(x)$ is upper bounded by $\gamma$ because the linear fit helps explain the variability in the data points. For a more detailed explanation, refer to Lemma 3 in the Appendix.

In the current iteration, let the maximum length of the intervals of the continuous variables be denoted as $l$. Thus, we have the following two inequalities for a nonlinearity $f(x)$, its linear fit $L(x)$, and a general point $x$ in the domain: $|f(x) - f(x_0)| \leq l\gamma$ and $|L(x) - L(x_0)| \leq l\gamma$. Combining the two equations, we find the error of approximation $|f(x) - L(x)| \leq 2\gamma l$. In order for all errors to be less than a tolerance $\epsilon$, it must hold that $2\gamma l \leq \epsilon$, which implies $l \leq \epsilon/(2\gamma)$. By recalling that the reduction factor in each step is $\eta$, the maximum length of the intervals containing the continuous variables after $N$ iterations of the algorithm can be expressed as $D_0/\eta^N$. Therefore, it is necessary that $D_0/\eta^N \leq \epsilon/(2\gamma)$. This condition leads to the expression $N \geq \log(2D_0\gamma/\epsilon)/\log(\eta)$. $\square$

## 5. Numerical experiments

### 5.1. Hardware and software

The computational experiments were conducted using an Intel i7 CPU with 16 GB RAM. Gurobi 11.0 was used as the MILP solver for linear approximation, and BARON 24.3 was used to solve the MINLP models. We tried Gurobi 11 for the MINLP models but observed that it was reporting primal solutions which violated some of the constraints for a small instance of produced water network optimization. Furthermore, for one of the larger case studies (Permian case study), Gurobi 11 falsely concludes infeasibility, whereas BARON comes up with a feasible solution.

### 5.2. Instances

#### 5.2.1. Produced water network optimization problems

We used the four networks as part of the PARETO case studies (PARETO, 2024) for the produced water optimization problem.

- Toy: nine intermediate nodes, four production nodes, six demand nodes (including one completion pad, two disposal sites, one storage site, two water treatment facilities).

- Small: 28 intermediate nodes, 15 production nodes, 11 demand nodes (including four completion pads, three disposal sites, two storage sites, and two water treatment facilities). Pipeline diameters are fixed.

- Permian: 28 intermediate nodes, 15 production nodes, 17 demand nodes (including three completion pads, five disposal sites, three storage sites, and six water treatment facilities).

- Treatment: Same components as the Permian case study but with more arcs offering diameter expansion flexibility.

We created more instances by modifying the amounts of produced water at the production nodes. For each time period, we increased the produced water amount at the production pads by a stress factor. We also increased the intake capacity at the completion pads using the same stress factor. The stress factors used were 0.8, 1.2, and 1.6.

#### *5.2.2. Urban water network design instances*

We evaluated our CVD algorithm by testing it with standard instances of urban water network design problems, which are widely used as benchmark problems for testing optimization techniques (MINLPLib website, (MINLPLib, 2024)). The smallest instance, Shamir, consists of 112 binary variables for diameter choices, 46 constraints, and a total of 135 variables. The largest instance, Modena, consists of 4121 binary variables for diameter choices, 1853 constraints, and a total of 5027 variables.

### *5.3. Results*

#### *5.3.1. Piecewise-linearization results*

Tables 2 and 3 display the results for the optimization of the produced water network using piecewise linear approximation. Table 2 presents results for four case studies, while Table 3 shows the results for variations to these case studies.

The piecewise linear approximation method provided nearly optimal solutions within reasonable time frames, while the nonlinear solvers struggled to produce good bounds within the same time frames, even with a coarse grid and a small number of intervals for piecewise-linearization (in this case, four). The time required to solve the approximations ranged from a few seconds for the smallest instance to around 12 minutes for the largest instance.

In all tested instances, except the strategic small case study, the nonlinear solver BARON failed to provide a good upper bound within 1 hour. Moreover, multiplying the produced water quantities by 1.2 or more at all periods made the strategic small case study problem infeasible. The lower bounds provided by BARON were generally not good, except for a strategic small case study. However, by removing the nonlinear constraints and solving the resulting MILP, a relaxation is created that gives a tight lower bound for these instances. This is due to the relatively low pump costs in the objective, and reducing the hydraulic component of the formulation provides a very close estimate of the objective cost.

In the cases we tested, we found that the optimal solutions had relatively low frictional pressure drops. Therefore, when making decisions related to pump installations, changes in elevation were the primary, if not the sole, determining factor. This clarifies why approximating frictional pressure loss is appropriate for these specific instances. Nonetheless, as discussed in Section 3, we anticipate achieving near-optimal results for networks and instances where the frictional pressure drop is substantial.

#### *5.3.2. CVD results*

We tested the CVD algorithm on both produced water network optimization and standard urban water network design instances. The results can be found in Table 4 for the produced water network

**Table 2:** PARETO instances (We use $m$, $n$, and $d$ to denote the numbers of constraints, variables and binary variables, respectively)

| Instance | MINLP | | | | Piecewise linearization | | |
|---|---|---|---|---|---|---|---|
| | Size | Time (s) | UB | LB | Time (s) | Objective | Gap |
| Toy | $m = 22,218$<br>$n = 15,652$<br>$d = 5,884$ | 3,600 | - | $-12,844$ | 28 | 6,126 | <0.1% |
| Small | $m = 44,902$<br>$n = 35,287$<br>$d = 6,323$ | 3,600 | 88,250 | 88,207 | 3 | 88,214 | <0.1% |
| Permian | $m = 49,986$<br>$n = 39,622$<br>$d = 13,662$ | 3,600 | 60,487 | 7,656 | 67 | 14,024 | <0.1% |
| Treatment | $m = 53,640$<br>$n = 40,670$<br>$d = 21,860$ | 3,600 | - | 9,649 | 832 | 17,329 | <0.1% |

**Table 3:** Varying stress levels (lower bound obtained by removing the nonlinear constraints and solving the resulting MILP)

| Instance | Stress | MILP | | Lower bound | Gap | BARON UB (1 hr) |
|---|---|---|---|---|---|---|
| | | Time (s) | Objective | | | |
| Toy | 0.8 | 8 | 4,903 | 4,900 | <0.1% | 19,760 |
| | 1.2 | 6 | 7,511 | 7,508 | <0.1% | N/A |
| | 1.6 | 5 | 10,195 | 10,192 | <0.1% | N/A |
| Small | 0.8 | 13 | 53,422 | 53,407 | <0.1% | 58,380 |
| | 1.2 | 0.2 | Infeasible | | | Infeasible |
| | 1.6 | 0.2 | Infeasible | | | Infeasible |
| Permian | 0.8 | 85 | 12,076 | 12,066 | <0.1% | 79,388 |
| | 1.2 | 94 | 18,588 | 18,578 | <0.1% | 81,381 |
| | 1.6 | 87 | 28,781 | 28,759 | <0.1% | N/A |
| Treatment | 0.8 | 173 | 14,224 | 14,215 | <0.1% | N/A |
| | 1.2 | 425 | 21,769 | 21,757 | <0.1% | N/A |
| | 1.6 | 425 | 32,029 | 32,020 | <0.1% | N/A |

and Table 5 for the urban water network. The best known upper bounds in Table 5 were obtained from Grossmann & Lee (2024). We used a reduction factor of $\eta = 3$ and a feasibility tolerance of $10^{-5}$. All MILPs solved in the iterations of the algorithm were feasible with these settings. The maximum time limit for each MILP approximation was set to 120 seconds, except for the Pescara and Modena instances. We improved the best known feasible solutions for Fosspoly1, Pescara, and Modena. For the Pescara problem, we increased the runtime of each MILP to around 20 minutes and obtained a solution with an objective of $1,812,564$ within approximately two hours. For the Modena instance, we increased the maximum time limit to three hours for each MILP approximation and obtained a solution with the objective value of $2,539,446$ within approximately two days.

**Table 4:** CVD algorithm on PARETO instances (lower bound obtained by removing the nonlinear constraints and solving the resulting MILP)

| Instance | Stress | CVD UB | Time (s) | LB | Gap (%) |
|---|---|---|---|---|---|
| Toy | 0.8 | 4,903 | 15 | 4,900 | 0.06 |
| | 1 | 6,126 | 11 | 6,123 | 0.05 |
| | 1.2 | 7,512 | 14 | 7,508 | 0.05 |
| | 1.6 | 10,196 | 8 | 10,192 | 0.04 |
| Small | 0.8 | 53,421 | 6 | 53,407 | 0.03 |
| | 1 | 88,214 | 3 | 88,200 | 0.02 |
| | 1.2 | Infeasible | | | |
| | 1.6 | Infeasible | | | |
| Permian | 0.8 | 12,077 | 37 | 12,066 | 0.09 |
| | 1 | 14,025 | 59 | 14,015 | 0.07 |
| | 1.2 | 18,588 | 78 | 18,578 | 0.05 |
| | 1.6 | 28,769 | 126 | 28,759 | 0.03 |
| Treatment | 0.8 | 14,225 | 332 | 14,215 | 0.07 |
| | 1 | 17,320 | 537 | 17,311 | 0.05 |
| | 1.2 | 21,769 | 574 | 21,757 | 0.06 |
| | 1.6 | 32,031 | 413 | 32,020 | 0.03 |

**Table 5:** CVD algorithm: benchmark instances ($\Delta_1$: Improvement over best known solution, $\Delta_2$: Optimality gap compared to LB obtained from BARON)

| Name | CVD | | BARON | | | Best known | $\Delta_1$ | $\Delta_2$ |
|---|---|---|---|---|---|---|---|---|
| | Time | UB | Time | UB | LB | | | |
| blacksburg | 44 s | 118,461 | 1.5 h | 121,393 | 116,625 | 116,945 | −1.3% | 1.5% |
| fossiron | 1,237 s | 178,282 | 1.5 h | 438,858 | 175,905 | 175,922 | −1.3% | 1.3% |
| fosspoly1 | 1,528 s | 27,051 | 1.5 h | 30,406 | 25,709 | 27,851 | 2.9% | 5.0% |
| fosspoly0 | 885 s | 72,888,489 | 1.5 h | 79,520,517 | 67,557,672 | 67,559,218 | −7.9% | 7.3% |
| hanoi | 131 s | 6,125,369 | 1,575 s | 6,109,620 | 6,109,620 | 6,109,620 | −0.25% | 0.2% |
| pescara | 2.1 h | 1,812,564 | 3 h | N/A | 1,663,840 | 1,820,264 | 0.42% | 8.2% |
| modena | 2 d | 2,539,446 | 2 d | N/A | 2,130,040 | 2,576,589 | 1.4% | 16.1% |
| shamir | 10 s | 419,000 | 62 s | 419,000 | 419,000 | 419,000 | 0 | 0 |

## 6. Conclusions

This paper proposes a new approach to the optimization of produced water networks in the oil and gas industry. Our approximate MILP formulation uses a coarse piecewise linear fitting of the nonlinear terms and consistently delivers optimal results. The piecewise linear approximation code has been integrated into the PARETO open source software, benefiting the broader research community. Additionally, we introduce the Continuous Variable Diving heuristic, which not only improves known upper bounds for standard urban water network instances but also generates near-optimal results for produced water network optimization problems. Future research could explore the performance of this heuristic in addressing various other MINLP problems with nonlinearity in continuous variables, extending the impact of this work within the field of optimization.


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## Appendix A. Piecewise linear formulation for produced water network optimization

$$\min \sum_{k\in K}\sum_{(i,j)\in\mathcal{A}} c_{ij}^k y_{ij}^k + \sum_{(i,j)\in\mathcal{A}} \mathcal{C}_{ij} \tag{A.1}$$

s.t.

$$\sum_{j:(i,j)\in\mathcal{A}} q_{ij}^t = b_i^t \qquad i\in S, t\in T \tag{A.2}$$

$$\sum_{j:(ji)\in\mathcal{A}} q_{ji}^t \leq -b_i^t \qquad i\in D, t\in T \tag{A.3}$$

$$\sum_{j:(ji)\in\mathcal{A}} q_{ji}^t = \sum_{j:(ij)\in\mathcal{A}} q_{ij}^t \qquad i\in N, t\in T \tag{A.4}$$

$$q_{ij}^t \leq \sum_{k\in K} F_{ij}^k y_{ij}^k \qquad (i,j)\in\mathcal{A}, t\in T \tag{A.5}$$

$$q_{ij}^t \leq M_1 z_{ij}^t \qquad (i,j)\in\mathcal{A}, t\in T \tag{A.6}$$

$$z_{ij}^t + z_{ji}^t = 1 \qquad (i,j)\in\mathcal{A}, t\in T s.t. (j,i)\in\mathcal{A} \tag{A.7}$$

$$\sum_{k\in K} y_{ij}^k = 1 \qquad (i,j)\in\mathcal{A} \tag{A.8}$$

$$y_{ij}^k = y_{ji}^k \qquad (i,j)\in\mathcal{A}, k\in K s.t. (j,i)\in\mathcal{A} \tag{A.9}$$

$$p_i^t = P_{i,t} \qquad i\in S, t\in T \tag{A.10}$$

$$q_{ij}^t = \sum_{s=1}^{1+Q_{\max}/\Delta_Q} (s-1)\Delta_Q \lambda_{i,j}^{t,s} \qquad (i,j)\in\mathcal{A}, t\in T \tag{A.11}$$

$$\zeta_{ij}^t = \sum_{s=1}^{1+Q_{\max}/\Delta_Q} ((s-1)\Delta_Q)^{1.85} \lambda_{i,j}^{t,s} \qquad (i,j)\in\mathcal{A}, t\in T \tag{A.12}$$

$$\sum_{s=1}^{1+Q_{\max}/\Delta_Q} \lambda_{i,j}^{t,s} = 1 \qquad (i,j)\in\mathcal{A}, t\in T \tag{A.13}$$

$$\lambda_{i,j}^{t,1} \leq u_{ij}^{t,1} \qquad (i,j)\in\mathcal{A}, t\in T \tag{A.14}$$

$$\lambda_{i,j}^{t,s} \leq u_{ij}^{t,s} + u_{ij}^{t,s-1} \qquad (i,j) \in \mathcal{A}, t \in T, s \in \{2,3,...,Q_{\max}/\Delta_Q\} \tag{A.15}$$

$$\lambda_{i,j}^{t,1+Q_{\max}/\Delta_Q} \leq u_{ij}^{t,Q_{\max}/\Delta_Q} \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.16}$$

$$\sum_{s=1}^{Q_{\max}/\Delta_Q} u_{i,j}^{t,s} = 1 \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.17}$$

$$\sum_{k \in K} (d_{ij} + k)^{4.87} \mathcal{P}_{ij}^{tk} = \kappa_{ij} \zeta_{ij}^{t} \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.18}$$

$$\mathcal{P}_{ij}^{tk} \geq 0 \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.19}$$

$$\mathcal{P}_{ij}^{tk} \leq H_{ij}^{\text{Friction},t} \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.20}$$

$$\mathcal{P}_{ij}^{tk} \leq M_2 y_{ij}^{k} \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.21}$$

$$\mathcal{P}_{ij}^{tk} \geq H_{ij}^{\text{Friction},t} + M_2 y_{ij}^{k} - M_2 \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.22}$$

$$\begin{aligned} p_i^t + \rho g E_i \geq p_j^t + \rho g E_j + H_{ij}^{\text{Friction},t} - \Delta_{ij}^{\text{Pump},t} \\ + \Delta_{ij}^{\text{Valve},t} - M_2(1 - z_{ij}^t) \qquad (i,j) \in \mathcal{A}, t \in T \end{aligned} \tag{A.23}$$

$$\begin{aligned} p_i^t + \rho g E_i \leq p_j^t + \rho g E_j + H_{ij}^{\text{Friction},t} - \Delta_{ij}^{\text{Pump},t} \\ + \Delta_{ij}^{\text{Valve},t} + M_2(1 - z_{ij}^t) \qquad (i,j) \in \mathcal{A}, t \in T \end{aligned} \tag{A.24}$$

$$p_{\min} \leq p_i^t \leq p_{\max} \qquad i \in N, t \in T \tag{A.25}$$

$$\Delta_{ij}^{\text{Pump},t} \leq M_2 v_{ij} \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.26}$$

$$\mathcal{C}_{ij} = C_1 v_{ij} + C_2 \sum_{t \in T} \Delta_{ij}^{\text{Pump},t} q_{ij}^t \qquad (i,j) \in \mathcal{A} \tag{A.27}$$

$$q_{ij}^t \geq 0, \quad \Delta_{ij}^{\text{Pump},t} \geq 0, \quad \Delta_{ij}^{\text{Valve},t} \geq 0 \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.28}$$

## Appendix B. Lemma

**Lemma 3.** *Suppose the nonlinear function $f(x)$ that is linearized in the CVD algorithm is unidimensional and Lipschitz continuous with Lipschitz constant $\gamma$. Then, the least squares fit $x$ has a Lipschitz constant $L(x)$ that is upper bounded by $\gamma$.*

*Proof.* We will prove that an upper bound on the magnitude of the slope of $L(x)$ is $\gamma$ by the method of contradiction. Let the magnitude of the slope of $L(x)$ be $M > \gamma$. Without loss of generality, let $L(x) = Mx + c$. There is a point $x_0$ where $L(x_0) = f(x_0)$. From $M > \gamma$, it follows that for $x > x_0$, $L(x) > f(x_0)$ and for $x < x_0$, $L(x) < f(x_0)$. Next, consider a very small rotation of to $L(x)$ about $(x_0, L(x_0))$ which reduces the slope magnitude $M$ to $M - \epsilon$ where $\epsilon = \frac{M-\gamma}{2} > 0$. Then for any $x > x_0$, the error of approximation reduces by $\epsilon(x - x_0)$ whereas for any $x < x_0$ the error of approximation reduces by $\epsilon(x_0 - x)$. Further, for $x_0$, the error of approximation remains the same, that is 0. Thus, the rotated plane reduces the error of approximation everywhere in the domain and particularly at the sampled points. Hence, the rotated plane is a better fit than $L(x)$ leading to a contradiction.

□