Water network design and operation optimization: Leveraging approximations

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Abstract

This study concerns the optimal design and operation of produced water and urban water networks. The optimization formulations of these problems have inherent nonconvexity, making them hard to solve. We address a key source of nonconvexity and difficulty in solving these problems: 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 analytically show the effectiveness of using a standard piecewise linear approximation to generate near-optimal solutions for the original problem for a general network. Computational results with real-world problems confirm the success of this approach in terms solution quality and runtime. However, in the context of urban water network design problems, we recognize the limitations of a direct piecewise-linear approximation and propose an alternative solution. In particular, we develop a general-purpose primal heuristic to handle MINLPs with nonlinearities in continuous variables. The heuristic solves a sequence of approximations, with successively smaller domains of continuous variables appearing in nonlinearities. High-quality primal solutions for problems from the literature are obtained, even outperforming the best-known solutions in three of the nine problem instances.

Keywords: Produced water; Hazen-Williams equation; Urban water network design.

1. Introduction and background

Optimization of fresh and waste water networks is essential due to high infrastructure costs, water scarcity in certain parts of the world, and environmental considerations. Applications in which optimizing network parameters is important include drinking water distribution networks (Mala-Jetmarova et al., 2018), wastewater treatment networks (Koleva et al., 2017), wastewater collection networks (Zhao et al., 2015), produced water management networks in the context of oil and gas drilling (Drouven et al., 2023), and irrigation networks (Wang et al., 2023). Depending on the application, the optimization can be performed solely for the design of the network, solely for the operation of devices such as pumps, or simultaneously for design and operational decisions. In this work, we consider two 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 of these problems have inherent nonconvexities and are challenging to solve by global solvers. These two problems share a common feature in that the frictional pressure loss is governed by nonlinear expressions of the volumetric flow rate of water, giving rise to nonconvexities in the resulting formulations.

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 different types of heuristics and metaheuristics for water distribution networks have been explored, see the review papers Parvaze et al. (2023), Sarbu (2021). Here, we focus on works that use approximations of relaxations in order to obtain MILPs that are computationally more tractable than MINLPs. 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.

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 disaggregation of variables in nonlinear expressions. In a more 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. 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 pump heads (pressure change due to pumps). They then conduct hydraulic analysis to obtain flow and pressure values. Recently, Shao et al. (2024) provide a piecewise linearization approach for pump schedule optimization. The authors adaptively adjust the location of breakpoints based on the desired accuracy. Advantage over genetic algorithm-based scheduling is observed in the case studies. Thomas & Sela (2024) provide an optimization framework “MILPnet” which applies MILPs to model hydraulics in water distribution networks. Application of the framework was demonstrated in examples of pump scheduling optimization. These works do not present theoretical guarantees on the performance of approximations. For an example demonstrating global guarantees of a linear approximation in MINLP for the pooling problem, refer to Dey & Gupte (2015). In this work, we present analytical and experimental results for the effectiveness of using a standard piecewise linear approximation for a general produced water network optimization problem instance.

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. Similarly, in water supply networks, Housh (2023) shows computational efficiency of using MILP approximating MINLP on a tested case study. These water network optimization models are different from the ones considered in this paper because they do not account for the nonlinearities arising from the Hazen-Williams equations.

Produced water, a highly saline byproduct of oil and gas development, 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 into an underground formation. It can also be reused within the oil and gas industry itself for fracturing. Further, produced water has potential for being treated and put to secondary beneficial use, such as in mining or agriculture. With all these considerations, building a network for produced water management becomes vital to ensure cost-effective and environmentally responsible handling. The network should aim to minimize infrastructure and operational costs while enforcing physical and resource constraints.

Finding high-quality primal solutions for produced water optimization problems presents a considerable challenge, even for the most advanced Mixed Integer Nonlinear Programming (MINLP) solvers (Li et al., 2024). The nonlinear constraints representing the frictional pressure drop in the problem formulation, according to the Hazen-Williams equation (Williams & Hazen, 1905), make it challenging to find good solutions for water network design problems. 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 show analytically and confirm experimentally for several real-world case studies that a standard piecewise linear approximation can produce near-optimal solutions for a general network setting. Thus, the approach provides an efficient and effective method for solving the produced water optimization problem.

Our paper also considers urban water network design problems. Unlike produced water network management, in this application setting, the demands at the customer locations are known and assumed to be fixed across time, while a reservoir supplies an unlimited quantity of water. Additionally, these problems only involve the optimization of 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 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 Bragalli et al. (2012) discussed extensively, 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. To address infeasibility, a very dense set of breakpoints for the flow variables needs to be used for the piecewise linear approximation of pressure loss. However, when fine intervals are chosen in the piecewise linear approximation, the resulting MILPs become intractable for modern MILP solvers. 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.

The contributions of our work are twofold:

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

- Standard piecewise linear approximations are inefficient for urban water network design problems 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.

Our primal heuristic can be compared to the mesh refinement algorithms presented in Burlacu et al. (2020) and Nagarajan et al. (2019), which focus on refining the intervals for the piecewise linear approximation of nonlinear functions of continuous variables in successive iterations. In contrast to traditional mesh refinement at a region, our approach 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 quantity of produced water varies with time across the source nodes, whereas the processing capacity (demand nodes) is fixed with time. 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.

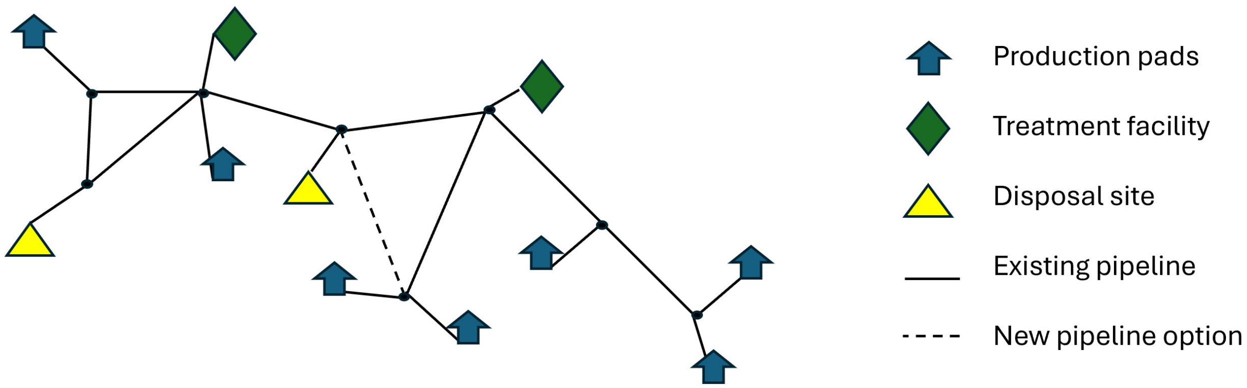

Figure 1: *An example network*

Another set we consider is the set of upgrade diameters, K. When upgrading from the current pipeline, the new diameter is the sum of the current diameter and a selected length 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 an upgrade choice of 0, representing the option not to upgrade and keep the current pipeline intact 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-Williams 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:

$$\min \sum_{k \in K} \sum_{(i,j) \in \mathcal{A}} c_{ijk} y_{ijk} + \sum_{(i,j) \in \mathcal{A}} \mathcal{C}_{ij} + \sum_{i \in D} c_i^{proc} (\sum_{t \in T} \sum_{j:(i,j) \in \mathcal{A}} q_{jit}) \tag{1}$$

s.t.

$$\sum_{j:(i,j) \in \mathcal{A}} q_{ijt} = b_{it} \qquad i \in S, t \in T \tag{2}$$

$$\sum_{j:(j,i) \in \mathcal{A}} q_{jit} \leq -b_{it} \qquad i \in D, t \in T \tag{3}$$

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_{ijk}	Cost of installing pipeline from i to j with diameter selection k
c_i^{proc}	Unit cost of processing produced water at location i
d_{ij}	Current diameter value from i to j
σ_{ijk}	Diameter increase length for a choice $k \in K$ of enlargement of pipeline from i to j
F_{ijk}	Flow capacity of pipeline from i to j if the extension diameter selected is k
b_{it}	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_{it}	Fixed pressures at the supply node i in period t
E_i	Elevation of node i
ρ	Density of water
g	Acceleration due to gravity
γ_{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
Q_{max}	Maximum possible flow
M_1	A large value (maximum flow)
M_2	A large value (maximum pressure)
Variables	
y_{ijk}	Binary variable equals 1 if diameter k is selected for extension for arc (i, j), 0 otherwise
v_{ij}	Binary variable equals 1 if pump is installed between nodes i and j, 0 otherwise
z_{ijt}	Binary variable equals 1 if flow is from node i to node j at time period t, 0 otherwise
q_{ijt}	Volumetric flow rate of water from node i to node j at period t
p_{it}	Pressure at node i at period t
$\Delta_{ijt}^{\text{Pump}}$	Pump head from node i to node j at period t
$\Delta_{ijt}^{\text{Valve}}$	Pressure release via valve from node i to node j at period t
$H_{ijt}^{\text{Friction}}$	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

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

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

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

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

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

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

$$p_{it} = P_{it} \qquad i \in S, t \in T \tag{10}$$

$$(d_{ij} + \sum_{k\in K} \sigma_{ijk} y_{ijk})^{4.87} H^{\text{Friction}}_{ijt} = \gamma_{ij} q^{1.85}_{ijt} \qquad (i,j) \in \mathcal{A}, t \in T \tag{11}$$

$$p_{it} + \rho g E_i \ge p_{jt} + \rho g E_j + H^{\text{Friction}}_{ijt} - \Delta^{\text{Pump}}_{ijt} + \Delta^{\text{Valve}}_{ijt} - M_2(1 - z_{ijt}) \qquad (i,j) \in \mathcal{A}, t \in T \tag{12}$$

$$p_{it} + \rho g E_i \le p_{jt} + \rho g E_j + H^{\text{Friction}}_{ijt} - \Delta^{\text{Pump}}_{ijt} + \Delta^{\text{Valve}}_{ijt} + M_2(1 - z_{ijt}) \qquad (i,j) \in \mathcal{A}, t \in T \tag{13}$$

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

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

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

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

$$y_{ijk} \in \{0,1\} \qquad (i,j) \in \mathcal{A}, k \in K \tag{18}$$

$$v_{ij} \in \{0,1\}, z_{ij} \in \{0,1\} \qquad (i,j) \in \mathcal{A} \tag{19}$$

The objective function (1) minimizes the overall cost of pumps, pipe installations, and processing produced water. 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 during time period t. 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 equality constraints. Constraints (14) set the minimum and 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, while Constraints (18)–(19)

enforce binary conditions.

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

The Hazen-Williams frictional pressure loss (11) and the pump cost rule (16) are the sources of nonlinearities in the MINLP formulation. Here, we first present a standard linear approximation for these constraints and then present analytical guarantees that they are effective for a general network.

3.1. A piecewise linear approximation

3.1.1. Hazen-Williams equation

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

Suppose the values of flows range from 0 to an upper bound $Q_{\max}$. Choose intervals of length Δ_Q such that $Q_{\max}$ is an integer multiple of Δ_Q. Introduce convex combination multipliers λ_{ijt1}, λ_{ijt2}, ..., $\lambda_{ijt1+Q_{\max}/\Delta_Q} \in [0,1]$. The flows will be a convex combination of $1+Q_{\max}/\Delta_Q$ equally spaced points in the range $[0, Q_{max}]$. Let ζ_{ijt} denote the piecewise linear approximation of $f(q_{ijt})$. The following system of equations and inequalities yields ζ_{ijt}.

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

$$\zeta_{ijt} = \sum_{s=1}^{1+Q_{\max}/\Delta_Q} ((s-1)\Delta_Q)^{1.85} \lambda_{ijts} \qquad (i,j) \in \mathcal{A}, t \in T \tag{21}$$

$$\sum_{s=1}^{1+Q_{\max}/\Delta_Q} \lambda_{ijts} = 1 \qquad (i,j) \in \mathcal{A}, t \in T \tag{22}$$

$$\lambda_{ijt1} \leq u_{ijt1} \qquad (i,j) \in \mathcal{A}, t \in T \tag{23}$$

$$\lambda_{ijts} \leq u_{ijts} + u_{ijt(s-1)} \qquad (i,j) \in \mathcal{A}, t \in T, s \in \{2, \ldots, Q_{\max}/\Delta_Q\} \tag{24}$$

$$\lambda_{ijt1+Q_{\max}/\Delta_Q} \leq u_{ijt(Q_{\max}/\Delta_Q)} \qquad (i,j) \in \mathcal{A}, t \in T \tag{25}$$

$$\sum_{s=1}^{Q_{\max}/\Delta_Q} u_{ijts} = 1 \qquad (i,j) \in \mathcal{A}, t \in T \tag{26}$$

$$u_{ijts} \in \{0,1\} \qquad (i,j) \in \mathcal{A}, t \in T, s \in \{1, \ldots, Q_{\max}/\Delta_Q\} \tag{27}$$

Here, equation (20) represents flows as a convex combination of uniformly located points in the range 0 to $Q_{\max}$. Equation (21) uses the same convex combination multipliers to approximate $f(q_{ijt})$ by expressing it as a convex combination of function values at these uniformly located points. Equation (22) ensures that the convex combination multipliers equals 1. Finally, Constraints (23) to (25) impose a condition on the convex combination multipliers, specifying that a maximum of two can be nonzero and that the nonzero multipliers have to be consecutive; Here, u_{ijts} are auxiliary binary variables that take a value of one for the interval of the piecewise linear function that is selected. Equation (26) enforces that exactly one interval is chosen.

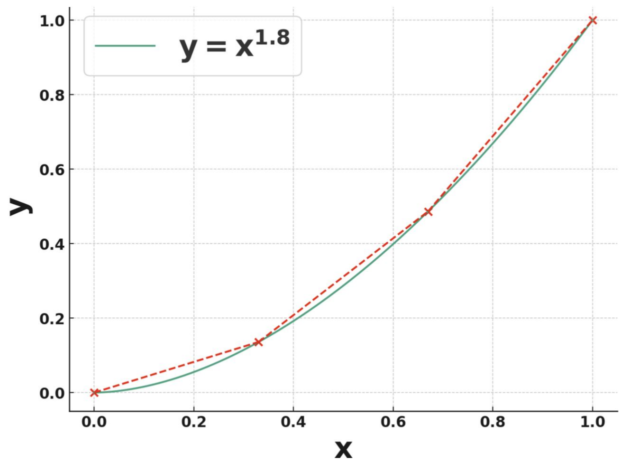

Figure 2: *Piecewise linear approximation for the RHS of the Hazen-Williams constraint*

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

$$\sum_{k\in K}(d_{ij}+\sigma_{ijk})^{4.87} y_{ijk} H^{\text{Friction}}_{ijt} = \gamma_{ij}\zeta_{ijt} \qquad (i,j)\in\mathcal{A}, t\in T$$

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 $\mathcal{P}_{ijtk}$ for the product, we can enforce the above Hazen-Williams equation as:

$$\sum_{k\in K}(d_{ij}+\sigma_{ijk})^{4.87}\mathcal{P}_{ijtk} = \gamma_{ij}\zeta_{ijt} \qquad (i,j)\in\mathcal{A}, t\in T \tag{28}$$

$$\mathcal{P}_{ijtk} \geq 0 \qquad (i,j)\in\mathcal{A}, t\in T, k\in K \tag{29}$$

$$\mathcal{P}_{ijtk} \leq H^{\text{Friction}}_{ijt} \qquad (i,j)\in\mathcal{A}, t\in T, k\in K \tag{30}$$

$$\mathcal{P}_{ijtk} \leq M_2 y_{ijk} \qquad (i,j)\in\mathcal{A}, t\in T, k\in K \tag{31}$$

$$\mathcal{P}_{ijtk} \geq H^{\text{Friction}}_{ijt} + M_2 y_{ijk} - M_2 \qquad (i,j)\in\mathcal{A}, t\in T, k\in K \tag{32}$$

Instead of using Constraints (11), we use Constraints (20) to (32) to create a linear approximation. The approximation error is caused by modeling $f(q_{ijt})$ as a piecewise linear function. Increasing the number of points of the piecewise linear approximation improves accuracy but reduces the solution process efficiency. In our current setup, we found that a somewhat coarse point selection (with four intervals) 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 $\mathcal{V}_{ijt} = C_2\Delta_{ijt}^{\text{Pump}} q_{ijt}$, 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.

$$\mathcal{V}_{ijt} \geq C_2(s\Delta_Q)\Delta_{ijt}^{\text{Pump}} - M(1 - u_{ijts}) \qquad s \in \{1, \ldots, Q_{\max}/\Delta_Q\} \tag{33}$$

The variable cost $\mathcal{V}_{ijt}$ in the system of inequalities is set based on the cost calculated using the maximum point of the respective flow interval. 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 $\mathcal{V}_{ijt}$ is equal to the largest of the terms on the right-hand side of (33).

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 described above.

The next set of propositions provides a way to generate and assess the quality of a solution to the MINLP using a solution to the piecewise linear approximation.

The first proposition proves that one can produce a feasible solution of the MINLP using an optimal solution of the piecewise linear approximation. In particular, one can find a feasible solution of the MINLP by fixing the flow values, diameter choices, and pump locations of the optimal solution of the piecewise linear approximation and only perturbing the relief valve pressure differences. The proof of the proposition shows how to make these perturbations. The obtained solution of the MINLP has at least as good objective value as the piecewise linear approximation's objective. As a result, the piecewise linear approximation always leads to a feasible solution of the MINLP.

Proposition 3.1. *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 ($\hat{y}_{ijk}$, $\hat{z}_{ijt}$, $\hat{v}_{ij}$, $\hat{q}_{ijt}$, $\hat{\Delta}_{ijt}^{\text{Pump}}$, $\hat{\Delta}_{ijt}^{\text{Valve}}$, $\hat{H}_{ijt}^{\text{Friction}}$, $\hat{\mathcal{C}}_{ij}$). Construct a solution to the original MINLP as follows.

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

The cost of diameter extension in the constructed MINLP solution $\sum_{k\in K}\sum_{(ij)\in\mathcal{A}} c_{ijk}\bar{y}_{ijk} = \sum_{k\in K}\sum_{(ij)\in\mathcal{A}} c_{ijk}\hat{y}_{ijk}$ is the same as the piecewise linear approximation formulation. Similarly, the cost of processing remains the same because the flows into the processing sites are kept the same. 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)**.** *Proposition 3.1 provides an efficient method for obtaining good feasible solutions to the MINLP. By leveraging the efficient solving capabilities of modern MILP solvers, one can* *obtain a valid feasible solution to an instance of the produced water network problem. Additionally,* $z_{\text{MINLP}} \leq z_{\text{PL}}$.

As we have shown above, the solution of the piecewise linear approximation can always be converted to a feasible solution of the MINLP with an objective value that is at least as good as that of the piecewise linear approximation. We next ask the question how good are the solutions produced using this approach. In order to study this question, we will take the optimal solution of the MINLP and show that there is a feasible solution in the piecewise linear approximation which is nearly as good.

We present two such results. The first result makes an assumption about the structure of the network and a minor assumption about the MINLP optimal solution. We note here that these assumptions hold true for all instances we solved in this work. The second result makes no such assumptions but comes at the cost of weaker bounds.

Before we present our results, we present the following relationship between the horizontal grid size and the error of the approximation of the frictional pressure loss, which enhances the understanding of the bounds obtained.

Remark. *Let* ϵ *be the maximum approximation error for the nonlinear frictional pressure drops with a piecewise linear approximation. The relationship between* Δ_Q *and* ϵ *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* ϵ_s*. Then,* $\epsilon = \gamma \max_{s\in\{1,\ldots,1+Q_{\max}/\Delta_Q\}} \epsilon_s$*, where* γ *is the pipeline-specific constant.*

Proposition 3.2. *Suppose the cycles in the network are chordless. Let* L, E *denote the set of cycles and arcs, respectively. Suppose there exists an optimal solution to the MINLP where the operating pressures are at least* $2|L||E|\epsilon$ *more than the minimum allowable pressure and at least* $|L||E|\epsilon$ *less than the maximum allowable pressure. Then there is a feasible solution to the piecewise-linear approximation with a maximum cost deterioration of* $C_2 Q_{\max}\epsilon|E|T + C_2(p_{max} - p_{min})\Delta_Q|E|T$*.*

Proof. Consider any solution of the MINLP ($\bar{y}_{ijk}$, $\bar{z}_{ijt}$, $\bar{v}_{ij}$, $\bar{q}_{ijt}$, $\bar{\Delta}^{\text{Pump}}_{ijt}$, $\bar{\Delta}^{\text{Valve}}_{ijt}$, $\bar{H}^{\text{Friction}}_{ijt}$, $\bar{p}_{it}$, $\bar{\mathcal{C}}_{ij}$). We construct a solution feasible for the piecewise linear formulation ($\hat{y}_{ijk}$, $\hat{z}_{ijt}$, $\hat{v}_{ij}$, $\hat{q}_{ijt}$, $\hat{\Delta}^{\text{Pump}}_{ijt}$, $\hat{\Delta}^{\text{Valve}}_{ijt}$, $\hat{H}^{\text{Friction}}_{ijt}$, $\hat{p}_{it}$) whose objective function is at most $C_2 Q_{\max}\epsilon|E|T + C_2(p_{max} - p_{min})\Delta_Q|E|T$ 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 ($\bar{y}_{ijk}$, $\bar{z}_{ijt}$, $\bar{v}_{ij}$, $\bar{q}_{ijt}$) from the MINLP solution fixed and adjust the variables $\bar{\Delta}^{\text{Pump}}_{ijt}$, $\bar{\Delta}^{\text{Valve}}_{ijt}$, $\bar{H}^{\text{Friction}}_{ijt}$, $\bar{p}_{it}$ in order to be feasible for the piecewise linear formulation. In the beginning, we set ($\hat{\Delta}^{\text{Pump}}_{ijt}$, $\hat{\Delta}^{\text{Valve}}_{ijt}$) = ($\bar{\Delta}^{\text{Pump}}_{ijt}$,$\bar{\Delta}^{\text{Valve}}_{ijt}$). Furthermore, we set $\hat{H}^{\text{Friction}}_{ijt}$ 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 the frictional pressure drops tends to overestimate the frictional pressure drops of MINLP for the same flow. To offset this effect, we will first adjust the $\hat{\Delta}^{\text{Pump}}_{ijt}$ and $\hat{\Delta}^{\text{Valve}}_{ijt}$ variables in the piecewise linear formulation.

We begin by adjusting the variables ($\hat{\Delta}^{\text{Pump}}_{ijt}$ and $\hat{\Delta}^{\text{Valve}}_{ijt}$) so that the total pressure drop around a cycle is 0. In the network, there are two types of cycles. The first type involves all water flows in a single direction, such as clockwise, in the MINLP solution and, therefore, in the constructed piecewise linear approximation solution. Such a cycle must contain a pump. This can be seen by adding the pressure change constraints (12) and (13) over the arcs in the cycles. Let L_c 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:

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

Since the right-hand side of the above equation is strictly positive, there must be a nonzero pumphead in the cycle. The piecewise linear approximation overestimates the pressure drop across every edge in the cycle, resulting in a net positive pressure drop around the cycle 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 of the arc containing a pump to $\hat{\Delta}^{\text{Pump}}_{ij} = \hat{\Delta}^{\text{Pump}}_{ij} + R_l$. This ensures that total pressure drops around such cycles are 0. The maximum possible value for R_l is $\epsilon|L_c|$.

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

Henceforth, for arcs where both i and j are not source nodes, the values of $\hat{\Delta}^{\text{Valve}}_{ijt}$ and $\hat{\Delta}^{\text{Pump}}_{ijt}$ are fixed according to the assigned values. The value of $\hat{H}^{\text{Friction}}_{ijt}$ is also fixed for all arcs. Thus, the values of $\hat{p}_{it} - \hat{p}_{jt}$ for the arcs in which neither i nor j is source from the inequalities (12) and (13) is fixed.

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

To assign operating pressures to each node, we define S as the set of source nodes with known and fixed pressure values. For each $s \in S$, let $\mathcal{N}(s)$ be the set of all neighbors of the source node 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 known fixed pressures.

2. Select an arbitrary starting source node $s_0 \in S$. Compute a tentative value for the pressure in a neighbor n, say $\widetilde{p}_{nt}$, using the values of $\bar{\Delta}^{\text{Valve}}_{s_0nt}$, $\bar{\Delta}^{\text{Pump}}_{s_0nt}$ and $\bar{H}^{\text{Friction}}_{s_0nt}$ through inequalities (12) and (13).

3. Since $\hat{p}_{it} - \hat{p}_{jt}$ is fixed for all arcs (i,j) such that $i,j \in V \setminus S$, starting with n, assign tentative pressure values $\widetilde{p}_{it}$ for all nodes i in $V \setminus S$. In other words, $\widetilde{p}_{it} - \widetilde{p}_{jt} = \hat{p}_{it} - \hat{p}_{jt}$ for all $i,j \in V \setminus S$. cycles 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 for some $s \in S, n1 \in \mathcal{N}(s)$ $\hat{p}^t_s - \widetilde{p}^t_{n1}$ may not be equal to

$$-\rho g E_s + \rho g E_{n1} + H^{\text{Friction}}_{s,n1,t} - \bar{\Delta}^{\text{Pump}}_{sn1t} + \bar{\Delta}^{\text{Valve}}_{sn1t}$$

. If the value of $\hat{p}_{st} - \widetilde{p}_{n1t}$ is larger than the above expression, then we find a feasible solution by appropriately increasing the value of $\hat{\Delta}^{\text{Valve},t}_{s,n1}$. If $\hat{p}_{st} - \widetilde{p}_{n1t}$ 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 $s \in S, n1 \in \mathcal{N}(s)$:

$$D(s, n1) = \max\left\{(-\rho g E_s + \rho g E_{n1} + \hat{H}^{\text{Friction},t}_{s,n1} - \hat{\Delta}^{\text{Pump},t}_{s,n1} + \hat{\Delta}^{\text{Valve},t}_{s,n1}) - (\hat{p}^t_s - \widetilde{p}_{n1t}), 0\right\}$$

Then, we proceed in three steps:

(a) Let D $= \max_{s \in S, n1 \in \mathcal{N}(s)}(D(s, n1)$.

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

(c) Finally, for all $s \in S, n1 \in \mathcal{N}(s)$, set $\hat{\Delta}^{\text{Valve}}_{sn1t} = (\hat{p}_{st} - (-\rho g E_s + \rho g E_{n1} + \hat{H}^{\text{Friction}}_{sn1t} - \hat{\Delta}^{\text{Pump}}_{sn1t} + \hat{\Delta}^{\text{Valve}}_{s,n1t})) - \hat{p}_{n1t}$.

At the end of such assignment, we obtain feasible pressure profiles due to the following reason. After adjusting the pump and valve pressure differences to address residuals around the loops, pressure assignments can deviate from the MINLP solution by a maximum magnitude of $|L||E|\epsilon$. Further, after adjusting the valves of source and neighbors of the source, the pressure assignments can further show a reduction from MINLP pressure assignments by a maximum $|L||E|\epsilon$. Thus, the assumptions of the proposition ensure the feasibility of the constructed pressure profile.

Objective value of the constructed solution: 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 cycles with unidirectional flow as $C_2 \bar{q}_{i_l j_l t} R_l \leq C_2 \bar{q}_{i_l j_l t} \epsilon |L_c|$ where i_l and j_l are the nodes where the pump operates. Therefore, the total cost increase due to pump head increase at any period can be bounded as $\sum_{l \in L_p} C_2 \bar{q}_{i_l j_l t} \epsilon |L_c| \leq C_2 Q_{\max} \epsilon \sum_{l \in L_p} |L_c| \leq C_2 Q_{\max} \epsilon |E|$. The increase in cost due to the approximation error of the pump operating cost can also be quantified as $C_2 \sum_{t \in T} \sum_{(i,j) \in \mathcal{A}} \hat{\Delta}^{\text{Pump}}_{ijt} \Delta_Q$. Upper bounding $\hat{\Delta}^{\text{Pump}}_{ijt}$ with $p_{max} - p_{min}$ results in the mentioned bound.

□

Proposition 3.1 allows us to compute a feasible solution to the MINLP for any problem instance described in Section 2. However, Proposition 3.2, which provides near-optimality guarantees of such a solution, requires assumptions of chordless cycles and a structure on the optimal solution of the pressures in the MINLP. Although the assumptions are mild and satisfied in all our case studies, it is conceivable that there exist networks where the loops have chords. Next, we prove a weaker bound on the feasible solution obtained via Proposition 3.1 for a general network. Since the cost of installing pumps is a fraction of the overall cost of building the network and processing the produced water, the bounds proved next become meaningful.

Proposition 3.3. *For every solution to the MINLP, there is a corresponding solution to the piecewise linear approximation with cost that is no worse than* $C_1|E| + C_2 \epsilon T Q_{max}|E|$.

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

Set $\hat{y}_{ijk} \leftarrow \bar{y}_{ijk}$, $\hat{z}_{ijt} \leftarrow \bar{z}_{ijt}$, $\hat{v}_{ij} \leftarrow 1$, $\hat{q}_{ijt} \leftarrow \bar{q}_{ijt}$, $\hat{\Delta}^{\text{Valve}}_{ijt} \leftarrow \bar{\Delta}^{\text{Valve}}_{ijt}$. The value of $\hat{H}^{\text{Friction}}_{ijt}$ will be set using the piecewise linear approximation of the $\bar{q}^{1.85}_{ijt}$ term. Set $\hat{\Delta}^{\text{Pump}}_{ijt} \leftarrow \bar{\Delta}^{\text{Pump}}_{ijt} + \hat{H}^{\text{Friction}}_{ijt} -$

$\bar{H}_{ijt}^{\text{Friction}}$. Then, the defined solution ($\hat{y}_{ijk}$, $\hat{z}_{ijt}$, $\hat{v}_{ij}$, $\hat{q}_{ijt}$, $\hat{\Delta}_{ijt}^{\text{Pump}}$, $\hat{\Delta}_{ijt}^{\text{Valve}}$, $\hat{H}_{ijt}^{\text{Friction}}$, $\hat{p}_{it}$, $\hat{\mathcal{C}}_{ij}$) satisfies all the constraints of the original MINLP.

The cost increase is due to the installation of an electric pump and operating at a higher power can be bounded from above by $C_1|E| + C_2\epsilon TQ_{max}|E|$ where the first term corresponds to the fixed cost and the second term is the electricity cost. □

Remark. *For Proposition 3.2, the terms $C_2Q_{\max}\epsilon|E|T + C_2(p_{max} - p_{min})\Delta_Q|E|T$ can be interpreted as the cost incurred if $|E|$ pumps were to operate over all the time periods at a small pressure difference ϵ but with a maximum flow (first term) as well as the cost incurred if $|E|$ pumps were to operate over all the time periods at a maximum pressure difference $p_{max} - p_{min}$ but with a small flow Δ_Q. Similar intuition can be derived for the second term of Proposition 3.3. That is, the second term $C_2\epsilon TQ_{max}|E|$ is the electricity cost incurred if the pumps were to operate at maximum flow but a tiny pressure difference of ϵ.*

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.

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 use linear functions obtained via 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 is said to have failed 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 accept the solution and stop the algorithm. Otherwise, reduce the domains of all nonlinear continuous variables to smaller intervals centered around the current MILP solution. This reduction is achieved in the following way. Denote the reduction factor as η, 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 τ, reduction factor $\eta > 2$, number of sample points P

- $q^L_{i0}, q^U_{i0} \leftarrow$ initial upper and lower bounds of flows [1]
- $j \leftarrow 0$
- $\delta \leftarrow \tau + 0.01$ ▷ Maximum discrepency between nonlinear terms and the approximations, initially more than τ
- **while** $\delta > \tau$ **do**
  - For each $i \in A$, sample P uniformly spaced points $(\bar{q}^k_i, \text{signpower}(\bar{q}^k_i, 1.85))$, $k \in \{1, \ldots, P\}$ between q^L_{ij} and q^U_{ij}.
  - Let $m_i q_i + c_i$ is the least square fit of the sampled points $\{(\bar{q}^k_i, \text{signpower}(\bar{q}^k_i, 1.85)) : k \in \{1, \ldots, P\}\}, i \in A$.
  - For each $i \in A$, replace signpower$(q_i, 1.85)$ in the original formulation with the least squares fit $m_i q_i + c_i$. This gives an approximation MILP. ▷ The process in Section 3 is used for the linearization of the diameter terms.
  - Let $\tilde{q}_i$, $i \in \mathcal{A}$ denote the solution to flows for the above MILP after a fixed time.
  - $\delta \leftarrow \max_{i \in \mathcal{A}}(|\text{signpower}(\tilde{q}_i) - (m_i \tilde{q}_i + c_i)|)$
  - $l_i \leftarrow q^U_{ij} - q^L_{ij}$. ▷ Current box sizes
  - $q^L_{i,j+1} \leftarrow \tilde{q}_i - l_i/\eta$. ▷ Reducing the domain
  - $q^U_{i,j+1} \leftarrow \tilde{q}_i + l_i/\eta$.
  - $j \leftarrow j + 1$.
- **end while**
- Return the solution of the last MILP solved in the above while loop.

For the following proposition, assume ϵ is the feasibility tolerance of the constraints, η 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.

[1] UB and LB obtained by minimizing and maximizing the flow variables over a relaxation formed by relaxing the nonlinear constraints of the formulation.

Proposition 4.1. *If the nonlinearities that are linearized are unidimensional and Lipschitz continuous with Lipschitz constant γ, then the maximum number of MILPs solved by the CVD algorithm can be bounded from above by $\lceil log(2D_0\gamma/\epsilon)/log(\eta/2)\rceil$.*

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 γ because the linear fit helps explain the variability in the data points. For a more detailed explanation, refer to Lemma 1 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 ϵ, 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 $\eta/2$, the maximum length of the intervals containing the continuous variables after N iterations of the algorithm can be expressed as $D_0/(\eta/2)^N$. Therefore, it is necessary that $D_0/(\eta/2)^N \leq \epsilon/(2\gamma)$. This condition leads to the expression $N \geq \log(2D_0\gamma/\epsilon)/\log(\eta/2)$. □

5. Numerical experiments

5.1. Hardware and software

The computational experiments were conducted using an Intel i7-1165G7 CPU with 16 GB RAM. Gurobi 12.0 was used as the MILP solver for linear approximation, and BARON 25.2 was used to solve the MINLP models.

5.2. Instances

5.2.1. Produced water network optimization problems

We used the four networks as part of the PARETO case studies for the produced water optimization problem (PARETO, 2024). These include some of the real-world water networks in the Permian Basin hosting several shale oil wells (Drouven et al., 2023). The sizes of these networks are shown in Table 2. The networks for " Permian Case Study" and " Treatment Case Study" are identical but there are more arcs with options to enlarge the diameters in the " Treatment Case Study."

We created additional 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. Additionally, to test the limits of the piecewise linear approximation to solve the case studies, we increase the costs of the pumps by multiplying with a factor of 5, 10, and 15.

Table 2: *Instance sizes*

Case study	Production nodes	Intermediate nodes	Completion pad	Disposal sites	Storage sites	Water treatment sites
Toy	4	9	1	2	1	2
Small	15	28	4	3	2	2
Permian	15	28	3	5	3	6
Treatment	15	28	3	5	3	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, 2024). The smallest instance, Shamir, contains 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 3 and 4 display the results for the optimization of the produced water network using piecewise linear approximation. Table 3 presents results for four case studies, while Table 4 shows the results for variations to these case studies. The piecewise linear approximation method provided near-optimal solutions within reasonable times, while the nonlinear solvers struggled to produce good feasible solutions within the same time frames, even with a coarse grid and a small number of intervals for piecewise linearization (in this case, four). The stopping criterion for solving the piecewise linear approximation was set to be an optimality gap of 4%. The time required to solve the approximations ranged from a few seconds for the smallest instance to around 20 minutes for the largest instance.

In all instances tested, except for the small case study, the nonlinear solver BARON failed to provide a good upper bound within 3 hours. The lower bounds provided by BARON were generally good, except for the treatment case study. We observed that dropping the nonlinear constraints and solving the resulting MILP, a relaxation is created that gives a tight lower bound for these instances.

With regards to the stress experiments presented in Table 4, multiplying the produced water quantities by 1.2 or more at all periods made the small case study problem infeasible. For the remaining feasible instances, the performance of BARON and piecewise linearization were similar to the trends mentioned above.

Next, we tested the sensitivity of the piecewise linearization approach with respect to the electric pump costs. The propositions in Section 3 show that the optimality gap can be sensitive to the relative magnitude of the pump cost. Thus, we tested the proposed approach on the same case studies but with the pump cost multiplied by the factors of 5, 10, and 15. Table 5 presents the results obtained. As expected, the optimality gap of the solutions obtained is an increasing function of the cost of the electric pumps, with all the optimality gaps less than 5%.

Table 3: PARETO instances (m, n, and d denote the numbers of constraints, variables and binary variables, respectively)

Case study	MINLP (BARON)				Piecewise linearization		
	Size	Time (s)	UB	LB	Time (s)	UB[1]	Gap[2]
Toy	$m = 22,218$ $n = 15,652$ $d = 5,884$	10,800	7,438	$6,126$	89	6,136	0.2%
Small	$m = 44,902$ $n = 35,287$ $d = 6,323$	10,800	90,103	88,243	7	88,278	0.1%
Permian	$m = 49,986$ $n = 39,622$ $d = 13,662$	10,800	-	14,035	215	14,059	0.3%
Treatment	$m = 53,640$ $n = 40,670$ $d = 21,860$	10,800	-	9,649	1,267	17,364	0.25%

Table 4: Results with varying stress levels

Case study	Stress	BARON UB (3 hr)	Piecewise Linearization		LB[3]	Gap[2]
			Time (s)	UB		
Toy	0.8	5854	56	4,913	4,900	0.3%
	1.2	8021	129	7,522	7,508	0.2%
	1.6	10,236	47	10,206	10,192	0.1%
Small	0.8	67,983	18	53,461	53,407	0.4%
	1.2	Infeasible	0.2	Infeasible		
	1.6	Infeasible	0.2	Infeasible		
Permian	0.8	N/A	186	12,112	12,066	0.4%
	1.2	N/A	299	18,627	18,578	0.3%
	1.6	N/A	333	28,807	28,759	0.2%
Treatment	0.8	N/A	642	14,259	14,215	0.3%
	1.2	N/A	2,054	21,805	21,757	0.3%
	1.6	N/A	2127	32,068	32,020	0.2%

Table 5: Piecewise Linearization results for varying pump costs

Case study	Pump cost factor	UB	LB[3]	Time (s)	Gap[2] (%)
Toy	5	6,188	6,122	136	1.1
	10	6,252	6,122	272	2.1
	15	6,302	6,122	254	2.8
Small	5	88,566	88,199	10	0.4
	10	91,187	88,199	11	3.3
	15	92,335	88,199	16	4.5
Permian	5	14,239	14,014	141	1.6
	10	14,484	14,014	128	3.2
Treatment	5	17,541	17,320	488	1.2
	10	17,760	17,320	501	2.4
	15	17,981	17,320	442	3.6

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 6 for the urban water network and Table 8 for the produced water network. To the best of our knowledge, Grossmann & Lee (2024) and the dissertation Rajagopalan (2018) provide the current best-known solutions for the benchmark instances of urban water network instances. We compare the objective our solutions to the best-knowns. Concerning the parameters of the algorithm, we used a reduction factor of $\eta = 3$ and a feasibility tolerance of 10^{-5}. The maximum time limit for each MILP approximation was set to 120 seconds if the root node time for the first LP relaxation was less than 30 seconds, 20 minutes if the root node time for the LP relaxation was between 30 seconds to 2 minutes, otherwise 3 hours. All MILPs, except for the 'New York' benchmark instance, solved in the iterations of the algorithm were feasible with these settings. Additionally, the time taken to calculate the initial upper and lower bounds on the flow variables in the CVD algorithm was insignificant compared to the total time of the algorithm. These bounds were obtained by dropping nonlinearities and minimizing and maximizing the flow variables subject to the remaining linear constraints. We have omitted reporting these times.

As can be seen from Tables 6 and 8, the CVD algorithm is successful in finding good feasible solutions much faster than BARON. Moreover, for three of the benchmark urban water network instances, the CVD algorithm found better solutions than the best-known solutions. CVD algorithm did not succeed in finding solutions to the 'New York' instance. However, we observed that modifying the linear approximation from one line segment to a piecewise linear approximation with two pieces, yielded optimal solution of the instance in about 25 minutes. Table 7 presents the best of the two versions of CVD, with time as the sum of the two runtimes.

Table 6: CVD algorithm: benchmark instances (Δ_1: CVD's improvement over best known solution, Δ_2: Optimality gap compared to LB obtained from BARON)

Name	BARON			CVD		Best known	Δ_1	Δ_2
	Time	UB	LB	Time	UB			
blacksburg	1.5 h	121,393	116,625	44 s	118,461	116,945	−1.3%	1.5%
fossiron	1.5 h	438,858	175,905	1,237 s	178,282	175,922	−1.3%	1.3%
fosspoly1	1.5 h	30,406	25,709	1,528 s	27,051	27,851	2.9%	5.0%
fosspoly0	1.5 h	79,520,517	67,557,672	885 s	72,888,489	67,559,218	−7.9%	7.3%
hanoi	1,575 s	6,109,620	6,109,620	131 s	6,125,369	6,109,620	−0.25%	0.2%
pescara	3 h	N/A	1,663,840	2.1 h	1,812,564	1,820,264	0.42%	8.2%
modena	2 d	N/A	2,130,040	2 d	2,539,446	2,576,589	1.4%	16.1%
shamir	62 s	419,000	419,000	10 s	419,000	419,000	0	0
new york	2 h	45,361,900	28,044,300	120	N/A	39,307,800	N/A	N/A

[1] UB to MINLP obtained starting from piecewise linear approximation's optimal solution and then applying Proposition 3.1.

[2] "Gap" in the tables refers to the gap of the feasible MINLP solution with respect to the lower bounds obtained by dropping nonlinear constraints and solving the resulting MILP.

[3] Lower bounds obtained by dropping nonlinear constraints and solving the resulting MILP.

Table 7: CVD algorithm (best of two): benchmark instances (Δ_1: CVD's percent improvement over best known solution, Δ_2: Optimality gap in percent compared to LB obtained from BARON)

Name	CVD		Best known	Δ_1	Δ_2
	Time	UB			
blacksburg	37 s	118,461	116,945	−1.3%	1.5%
fossiron	2,474 s	178,282	175,922	−1.3%	1.3%
fosspoly1	1,759 s	27,051	27,851	2.9%	5.0%
fosspoly0	2,250 s	72,888,489	67,559,218	−7.9%	7.3%
hanoi [4]	258 s	6,109,620	6,109,620	0%	0%
pescara	4.6 h	1,812,564	1,820,264	0.42%	8.2%
modena	2 d	2,539,446	2,576,589	1.4%	16.1%
shamir	26 s	419,000	419,000	0	0
new york [4]	1,643 s	39,307,800	39,307,800	0	0

Table 8: CVD algorithm on PARETO instances (lower bound obtained by removing the nonlinear constraints and solving the resulting MILP)

Case study	Stress	CVD UB	Time (s)	LB	Gap (%)
Toy	0.8	4,921	71	4,900	0.4
	1	6,144	80	6,123	0.3
	1.2	7,530	43	7,508	0.3
	1.6	10,209	54	10,192	0.2
Small	0.8	74,921	14	53,407	30
	1	115,724	15	88,200	24
	1.2	Infeasible			
	1.6	Infeasible			
Permian	0.8	12,203	55	12,066	1.1
	1	14,223	197	14,015	1.4
	1.2	19,002	350	18,578	2.2
	1.6	29,049	70	28,759	1.0
Treatment	0.8	14,269	709	14,215	0.4
	1	17,375	540	17,311	0.4
	1.2	21,848	709	21,757	0.4
	1.6	32,083	714	32,020	0.2

Table 9: CVD algorithm on PARETO instances for varying pump costs

Instance	Pump cost factor	UB	LB[3]	Time (s)	Gap[2] (%)
Toy	5	6,228	6,122	56	1.7
	10	6,333	6,122	34	3.3
	15	6,490	6,122	70	5.7
Small	5	111,515	88,199	14	21
	10	113,469	88,199	21	23
	15	114,172	88,199	23	23
Permian	5	14,437	14,014	18	2.9
	10	14,731	14,014	88	4.9
	15	15,007	14,014	118	6.7
Treatment	5	17,590	17,320	603	1.5
	10	17,880	17,320	558	3.1
	15	18,167	17,320	295	4.7

Table 10: CVD algorithm: sensitivity with respect to reduction factor

Name	$\eta = 2.5$		$\eta = 3.0$		$\eta = 4.0$	
	Time	UB	Time	UB	Time	UB
blacksburg	121 s	Infeasible	44 s	118,461	67 s	125,128
fossiron	2,079 s	180,688	1237 s	178,282	653 s	181,056
fosspoly1	2,980 s	29,470	1528 s	27,051	1067 s	28,033
fosspoly0	1,490 s	70,680,508	885 s	72,888,489	552 s	71,345,012
hanoi	305 s	6,125,369	131 s	6,125,369	173 s	Infeasible
pescara	7.5 hours	1,820,843	2.1 hours	1,812,564	2.9 hours	Infeasible
modena	3 d	2,694,276	2 d	2,539,446	30 hours	Infeasible
shamir	27 s	419,000	10 s	419,000	16 s	423,000

5.3.3. CVD sensitivity analysis

For the next set of experiments, we experimented with variations in the reduction factor and time limit given for each MILP approximation. Table 10 shows the performance of the algorithm for three different sets of reduction factor, namely $\eta = 2.5$, $\eta = 3$ and $\eta = 4.0$. It can be observed from this table that $\eta = 3$ is optimal value of the reduction factor. A lower reduction factor of $\eta = 2.5$ leads to a slower convergence of the algorithm and a slight deterioration in the solution quality for most instances. An exception of this is the fosspoly0 instance, for which, the solution quality improves with the lower reduction factor. Similarly, and as one can expect, with a higher reduction factor of $\eta = 4$, the convergence becomes faster but the solution quality deteriorates. With such a higher reduction factor, three of the instances show infeasibility at some point of the CVD algorithm. A recommended approach to find the optimal value of the reduction factor for a given problem is to adjust it for a smaller problem instance and then use the tuned parameter for the larger instances. See Figure 3 for the reduction in nonlinear constraint violations as a result of approximations plotted against iterations of CVD for the Shamir instance. Next, Table 11 shows the performance of the algorithm relative to different time settings. In the first time setting, the MILP timeout is set to be 80 seconds for the problems where the root node relaxation can be solved within 30 seconds, 800 seconds for the problems with root node time between 30 seconds to 2 minutes and 2 hours if the root node time is beyond 2 minutes. In the second time setting, the MILP timeout is set to be 120 seconds for the problems where

Table 11: CVD algorithm: sensitivity with respect to MILP time ($\eta = 3$)

Name	Time setting 1		Time setting 2		Time setting 3	
	Time	UB	Time	UB	Time	UB
blacksburg	41 s	Infeasible	44 s	118,461	51 s	Infeasible
fossiron	888 s	180,381	1237 s	178,282	1639 s	180,688
fosspoly1	1242 s	28,157	1528 s	27,051	2552 s	27,767
fosspoly0	613 s	72,821,347	885 s	72,888,489	1275 s	72,759,146
hanoi	80 s	6,125,369	131 s	6,125,369	130 s	6,125,369
pescara	3.3 hours	1,851,378	2.1 hours	1,812,564	6 hours	1,816,745
modena	1.5d	2,580,684	2 d	2,539,446	3d	2,529,012
shamir	9 s	419,000	10 s	419,000	11 s	419,000

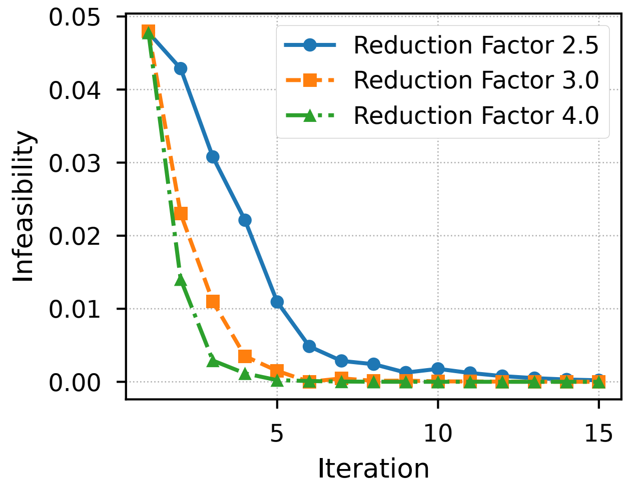

Figure 3: *Reduction of maximum violations of nonlinear constraints with iteration (Shamir instance)*

the root node relaxation can be solved within 30 seconds, 20 minutes for the problems with root node time between 30 seconds to 2 minutes and 3 hours if the root node time is beyond 2 minutes. Finally, in the third time setting, the MILP timeout is set to be 180 seconds for the problems where the root node relaxation can be solved within 30 seconds, 30 minutes for the problems with root node time between 30 seconds to 2 minutes and 4 hours if the root node time is beyond 2 minutes. It can be observed that the second time is more or less optimal, barring two of the instances which showed a better solution quality with the third time setting.

The second time setting was the default setting of the parameter in the previous experiments.

[4] Optimal solution found using CVD with two pieces to approximate the nonlinear function $x^{1.85}$.

6. Conclusions

We analytically and empirically establish the usefulness of piecewise-linear approximation for produced water networks in the oil and gas industry. 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 broader range of practically relevant MINLPs.

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Appendix A. Piecewise linear formulation for produced water network optimization

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

s.t.

$$\sum_{j:(i,j)\in\mathcal{A}} q_{ijt} = b_{it} \qquad i\in S, t\in T \tag{A.2}$$

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

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

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

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

$$z_{ijt} + z_{jit} = 1 \qquad (i,j) \in \mathcal{A} \text{ with } (j,i) \in \mathcal{A}, t \in T \tag{A.7}$$

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

$$y_{ijk} = y_{jik} \qquad (i,j) \in \mathcal{A} \text{ with } (j,i) \in \mathcal{A} k \in K \tag{A.9}$$

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

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

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

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

$$\lambda_{ijt1} \leq u_{ijt1} \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.14}$$

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

$$\lambda_{ijt1+Q_{\max}/\Delta_Q} \leq u_{ijtQ_{\max}/\Delta_Q} \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.16}$$

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

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

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

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

$$\mathcal{P}_{ijtk} \leq M_2 y_{ijk} \qquad (i,j) \in \mathcal{A}, t \in T \tag{A.21}$$

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

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

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

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

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

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

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

Appendix B. Lemma

Lemma 1. *Suppose the nonlinear function $f(x)$ that is linearized in the CVD algorithm is uni-dimensional and Lipschitz continuous with Lipschitz constant γ. Then, the least squares fit x has a Lipschitz constant $L(x)$ that is upper bounded by γ.*

Proof. We will prove that an upper bound on the magnitude of the slope of $L(x)$ is γ 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.

□