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MODEL REDUCTION AND OUTER APPROXIMATION FOR OPTIMISING THE PLACEMENT OF CONTROL VALVES IN COMPLEX WATER NETWORKS

Filippo Pecci[1], Edo Abraham[2], and Ivan Stoianov[3]

[1]Dept. of Civil and Environmental Engineering (InfraSense Labs), Imperial College London, London, UK. Email: f.pecci14@imperial.ac.uk

[2]Department of Water Management, Faculty of Civil Engineering and Geosciences, TU Delft, Stevinweg 1, 2628 CN Delft, the Netherlands. Email: e.abraham@tudelft.nl

[3]Dept. of Civil and Environmental Engineering (InfraSense Labs), Imperial College London, London, UK. Email: ivan.stoianov@imperial.ac.uk

ABSTRACT

The optimal placement and operation of pressure control valves in water distribution networks is a challenging engineering problem. When formulated in a mathematical optimisation framework, this problem results in a nonconvex mixed integer nonlinear program (MINLP), which has combinatorial computational complexity. As a result, the considered MINLP becomes particularly difficult to solve for large-scale looped operational networks. We extend and combine network model reduction techniques with the proposed optimisation framework in order to lower the computational burden and enable the optimal placement and operation of control valves in these complex water distribution networks. An outer approximation algorithm is used to solve the considered MINLPs on reduced hydraulic models. We demonstrate that the restriction of the considered optimisation problem on a reduced hydraulic model is not equivalent to solving the original larger MINLP, and its solution is therefore sub-optimal. Consequently, we investigate the trade-off between reducing computational complexity and the potential sub-optimality of the solutions that

can be controlled with a parameter of the model reduction routine. The efficacy of the proposed method is evaluated using two large scale water distribution network models.

INTRODUCTION

Ageing infrastructure, growing water demand and more stringent environmental standards pose unprecedented challenges to the management of water distribution networks (WDNs). Significant benefits can be achieved through an efficient pressure control that results in the reduction of leakage (Lambert 2000; Wright et al. 2015) and risk of pipe failure (Lambert and Thornton 2011). Traditionally, pressure control in WDNs is actuated by pressure reducing valves (PRVs), which regulate pressure at their downstream node. The optimal placement and operation of control valves are complex tasks, and the locations of such control devices are usually determined based on engineering judgement. When formulated into a mathematical framework, these tasks result in a difficult co-design optimisation problem, which combines continuous and discrete decision variables. Continuous variables include nodal hydraulic heads and pipe flow rates, while discrete decision variables are used to represent control valve locations. Energy and mass conservation laws are enforced across each pipe and at each node, respectively, resulting in nonconvex optimisation constraints. A faithful representation of WDN daily operation requires the consideration of multiple water demand conditions and associated pumps control profiles, thus further increasing the number of continuous optimisation variables and constraints. The network models presented in this paper do not include pumps. However, pumps operation can be modelled by adding suitable optimisation constraints - e.g. see Equation (10) in D'Ambrosio et al. (2015). The resulting optimisation problem is analogous to the one considered here and it can be solved using the methods discussed in the following sections.

In the present manuscript, we consider multiple demand conditions and build upon the problem formulation introduced and briefly discussed in Pecci et al. (2017a). The proposed problem reformulation reduces the degree of nonlinearity of the constraints and the overall problem size in comparison to previous literature (Eck and Mevissen 2012; Dai and Li 2014; Pecci et al. 2017b).

The resulting problem is a nonconvex Mixed Integer Nonlinear Program (MINLP) that is difficult to solve, and it is usually dealt with using meta-heuristic approaches (Nicolini and Zovatto 2009; Creaco et al. 2015; Ali 2015; De Paola et al. 2017) or local optimisation methods (Eck and Mevissen 2012; Dai and Li 2014; Pecci et al. 2017b). As a consequence, the quality of the generated solution will depend on the algorithmic initialisation. It is sometimes convenient to start the optimisation process with different initial conditions, selecting *a posteriori* the best objective function performance. In addition, when multiple objectives need to be minimised at the same time, typical mathematical optimisation methods rely on the solution of sequences of MINLPs - see examples shown in Pecci et al. (2017d). Consequently, it is important to take into account the computational effort required to generate a solution. Solving a MINLP requires a substantial computational effort when the number of discrete variables is large. This is the case when we study operational water distribution networks. Additional problem-specific computational challenges can be posed by the structure of a water distribution network considered for the optimal placement and operation of control valves. In the case of a highly inter-connected network, there exist multiple control valve configurations with similar objective function performances. The high degree of symmetry in the solution space results in an increased computational effort (Margot 2010).

In the present study, we investigate the application of alternative network reduction approaches to decrease the dimension of the search space and the computational load associated with solving the problem of optimal placement and operation of control valves within complex water distribution networks. The considered model-reduction techniques have already been demonstrated to improve the computational performance of hydraulic simulation tools (Deuerlein et al. 2016; Deuerlein 2008; Simpson et al. 2014) and for operational optimisation of large water networks (Burgschweiger et al. 2005). However, their use within a framework for the optimal placement of control valves (i.e. design problems) in water distribution networks has not been previously investigated. In particular, we first consider the forest-core decomposition proposed by Elhay et al. (2014), and pose reduced size MINLP using only the core of the network (i.e. the part of a network that is not contained in the forest, where the forest is the union of all trees of the network). In addition, we implement the contraction of links, which are connected in series, through a zero demand node as proposed by Burgschweiger et al. (2005) to reduce network size before operational optimisation. The resulting model reduction procedure is then expanded by introducing the elimination of *trivial loops*, "leafy loops", which include nodes with zero demand.

We investigate the integration of these model reduction routines with optimisation methods for solving the co-design problem of optimal placement and operation of control valves. The two problem formulations, when applied upon full-scale and reduced network models, result in nonconvex MINLPs with a similar structure. Hence, the optimal valve placement problems for the different network models are solved using the same optimisation tools. We utilise the Outer Approximation with Equality Relaxation (OA/ER) algorithm for the solution of the considered MINLPs. This solution approach was initially proposed by Kocis and Grossmann (1987). The OA/ER algorithm solves an alternating sequence of nonlinear programs (primal problems) and mixed integer linear programs (master problems). Under certain convexity assumptions on the optimisation constraints, OA/ER converges to global optimal solutions (Floudas 1995, Section 6.5). When the problem is nonconvex, like the one considered here, OA/ER does not provide theoretical guarantees of global optimality. Nonetheless, OA/ER was shown to find near-optimal solutions when previous applied to problems in process synthesis optimisation by Kocis and Grossmann (1987) and Viswanathan and Grossmann (1990).

The main contributions of this paper are as follows. Firstly, we evaluate strengths and limitations of the application of the OA/ER method in complex and operational water distribution networks. Secondly, we numerically investigate the coupling of model reduction and outer approximation for solving the problem of optimal placement and operation of control valves in complex water distribution networks. In particular, we observe that the restriction of the considered optimisation problem on a reduced network can result in sub-optimal solutions. This is due to the exclusion of links/sequences of links with significant elevation differences within the reduced network model. Therefore, we propose a heuristic that preserves those links connected to nodes with elevation differences larger than a certain threshold parameter; the elevation difference threshold. Thirdly, the trade-off between the model size reduction and potential sub-optimality is numerically investigated using two complex water distribution networks as case studies.

PROBLEM FORMULATION

A water distribution network with n_0 water sources (eg. reservoirs or tanks), n_n nodes and n_p pipes, is modelled as a graph with $n_n + n_0$ vertices and n_p links. We define the two edge-node incidence matrices $\mathbf{A_{12}} \in \mathbb{R}^{n_p \times n_n}$ and $\mathbf{A_{10}} \in \mathbb{R}^{n_p \times n_0}$, respectively, for the n_n junction nodes and the n_0 water sources, respectively. Moreover, we include in the formulation n_l different demand conditions - e.g. describing daily water demand profiles. Let $t \in \{1, ..., n_l\}$ be a time step and let $\mathbf{d}^t \in \mathbb{R}^{n_n}$ be the assigned vector of nodal demands. Vectors of unknown hydraulic heads and flows are defined as $\mathbf{h}^t := [h_1^t \dots h_{n_n}^t]^T$ and $\mathbf{q}^t := [q_1^t \dots q_{n_p}^t]^T$, respectively. Hydraulic heads at the water sources are known and denoted by $h_{0_i}^t$ for each $i = 1, ..., n_0$. Moreover, the vector of nodal elevation is represented by $\boldsymbol{\xi} \in \mathbb{R}^{n_n}$. Finally, for every link j we have maximum allowed flow though j defined by $q_j^{\max}$.

The frictional energy losses across network pipes can be modelled by either the Hazen-Williams (HW) or Darcy-Weisbach (DW) formulae. However, these are not suitable for being used in a mathematical optimisation framework, since they involve non-smooth terms. Consequently, it is necessary to consider smooth approximations for both friction head loss formulae. Here we apply a quadratic approximation minimising the integral of relative errors - see Eck and Mevissen (2015) and Pecci et al. (2017c). For a pipe j and time t, the resulting quadratic function can be written as $\phi_j(q_j^t) := (a_j|q_j^t| + b_j)q_j^t$, where $a_j \geq 0$, $b_j \geq 0$ are positive coefficients. Let $\mathbf{\Phi}(\mathbf{q^t}) := [\phi_1(q_1^t), \dots, \phi_{n_p}(q_{n_p}^t)]^T$, for each $t \in \{1, \dots, n_l\}$.

In this manuscript we consider an optimisation problem for placement and operation of control valves, and so we introduce the vectors of unknown binary variable $\mathbf{z}^+ \in \{0,1\}^{n_p}$ and $\mathbf{z}^- \in \{0,1\}^{n_p}$ to model the possible placement of control valves on n_p links, with the following permutations :

- $z_j^+ = 1 \Leftrightarrow$ there is a valve on link j in the assigned positive flow direction,
- $z_j^- = 1 \Leftrightarrow$ there is a valve on link j in the assigned negative flow direction,
- $z_j^+ = z_j^- = 0 \Leftrightarrow$ no valve is placed on link j,

and the constraints

- $z_j^+ + z_j^- \leq 1$ to preclude the placement of two valves on a single link j,

for each $j = 1, \ldots, n_p$.

The objective to be minimised is average zone pressure (AZP), which is used as a surrogate measure for pressure-driven leakage (Wright et al. 2015) and is defined as:

$$\frac{1}{n_l W} \sum_{t=1}^{n_l} \mathbf{w}^T (\mathbf{h}^t - \boldsymbol{\xi}) \tag{1}$$

where L_j is the length of link j, $w_i = \sum_{j \in I(i)} L_j/2$ with $I(i)$ set of indices for links incident at node i, and $W = \sum_{i=1}^{n_n} w_i$ is a normalisation factor.

The optimisation problem is subject to physical constraints in the form of energy and mass conservation laws:

$$\boldsymbol{\Phi}(\mathbf{q^t}) + \mathbf{A_{12}} \mathbf{h^t} + \mathbf{A_{10}} \mathbf{h_0^t} + \boldsymbol{\eta^t} = 0, \quad t = 1, \ldots, n_l, \tag{2}$$

$$\mathbf{A_{12}}^T \mathbf{q^t} - \mathbf{d^t} = 0. \quad t = 1, \ldots, n_l, \tag{3}$$

where the vector $\boldsymbol{\eta^t} := [\eta_1^t \ldots \eta_{n_p}^t]^T$ in equation (2) represents the unknown additional head losses introduced by the action of control valves. In order to formulate linear constraints modelling the placement of a valve or otherwise on network links, we introduce diagonal matrices of large positive constants $\mathbf{M}^+ := \operatorname{diag}({M^+}_1, \ldots, {M^+}_{n_p}) \in \mathbb{R}^{n_p \times n_p}$ and $\mathbf{M}^- := \operatorname{diag}({M^-}_1, \ldots, {M^-}_{n_p}) \in \mathbb{R}^{n_p \times n_p}$, and define $\mathbf{Q}^{\max} := \operatorname{diag}(q_1^{\max}, \ldots, q_{n_p}^{\max}) \in \mathbb{R}^{n_p \times n_p}$. Then, we formulate the inequality constraints:

$$\boldsymbol{\eta}^t - \mathbf{M}^+ \mathbf{z}^+ \leq 0, \quad t = 1, \ldots, n_l, \tag{4}$$

$$-\mathbf{q}^t + \mathbf{Q}^{\max} \mathbf{z}^+ \leq \mathbf{q}^{\max}, \quad t = 1, \ldots, n_l, \tag{5}$$

$$-\boldsymbol{\eta}^t - \mathbf{M}^- \mathbf{z}^- \leq 0, \quad t = 1, \ldots, n_l, \tag{6}$$

$$\mathbf{q}^t + \mathbf{Q}^{\max} \mathbf{z}^- \leq \mathbf{q}^{\max}, \quad t = 1, \ldots, n_l. \tag{7}$$

In the following, we clarify the role of these linear constraints. Assume that $z_j^+ = z_j^- = 0$ for a particular link j. Constraints (4)-(5) imply that $\eta_j^t = 0$, while the sign of q_j^t is not constrained and $-q_j^{\max} \leq q_j^t \leq q_j^{\max}$ for all $t \in \{1, \ldots, n_l\}$. Therefore, (2) represents the standard Bernoulli equation for energy conservation across link j. Now let $z_j^+ = 1$, which implies $z_j^- = 0$. Constraints (4) - (7) yield $0 \leq \eta_j^t \leq M_j^+$ and $0 \leq q_j^t \leq q_j^{\max}$, $\forall t \in \{1, \ldots, n_l\}$. Note that M_j^+ has to be larger then any feasible value for η_j^t. Analogously, if $z_j^- = 1$, we have $-M_j^- \leq \eta_j^t \leq 0$ and $-q_j^{\max} \leq q_j^t \leq 0$, for all time steps $t \in \{1, \ldots, n_l\}$. Consequently, in our problem formulation, once the direction of operation of a valve is chosen, we do not allow the flow direction to change during the control period - e.g. 24 hours. This assumption is not restrictive from an engineering point of view, as it represents the standard operation of pressure reducing valves, which regulate pressure at their downstream node with no or negligible backflow. Finally, we include in the formulation additional operational, physical and economic constraints:

$$\mathbf{h}^t \leq \mathbf{h}^t_{\max}, \quad t = 1, \ldots, n_l, \tag{8}$$

$$-\mathbf{h}^t \leq -\mathbf{h}^t_{\min}, \quad t = 1, \ldots, n_l, \tag{9}$$

$$\mathbf{z}^+ + \mathbf{z}^- \leq \mathbf{1}, \tag{10}$$

$$\sum_{j=1}^{n_p} (z_j^+ + z_j^-) = n_v, \tag{11}$$

where $\mathbf{h}^t_{\max}$ and $\mathbf{h}^t_{min}$ are the vectors of maximum and minimum allowed pressure head, respectively, $\mathbf{1} := [1,\ldots,1]^T \in \mathbb{R}^{n_p}$, and n_v is the number of PRVs to be installed, based on financial constraints.

In summary, the problem formulation assumes known hydraulic heads at water sources, nodal demands, elevations, and bounds on allowed hydraulic heads and flow rates. Optimisation variables include hydraulic heads, flows, additional head losses introduced by the action of control valves, and valve locations. The resulting optimal valve placement problem is formulated as:

$$\begin{aligned} &\text{minimise} && \frac{1}{n_l W}\sum_{t=1}^{n_l} \mathbf{w}^T(\mathbf{h}^t - \boldsymbol{\xi}) \\ &\text{subject to} && (\mathbf{q}^t)_t, (\mathbf{h}^t)_t, (\boldsymbol{\eta}^t)_t, \mathbf{z}^+, \mathbf{z}^- \text{satisfy (2)-(11)} \\ & && \mathbf{z}^+, \mathbf{z}^- \in \{0,1\}^{n_p}. \end{aligned} \tag{12}$$

Note that the Problem (12) has multiple sources of nonconvexity. Firstly, it includes binary constraints which result in a nonconvex disconnected feasible set, requiring the application of branch and bound procedures. In addition, the nonlinear equality constraints in (2) can not be relaxed as convex inequality constraints and so they can not be efficiently handled by convex optimisation tools. Finally, the components of function $\mathbf{\Phi}(\cdot)$ are nonconvex, because their second order derivatives involve the $\text{sign}(\cdot)$ function.

The number of linear constraints in Problem (12) is $n_l(3n_n + 4n_p) + n_p + 1$ while the nonlinear equations involved in the problem formulation are $n_l n_p$. In addition, only the $n_l n_p$ flow variables appear within nonlinear expressions, while the optimisation constraints are linear with respect to the remaining variables. The formulation used in previous literature (Pecci et al. 2017b; Dai and Li 2014; Eck and Mevissen 2012) includes more constraints with higher degree of nonlinearity involving both flows and hydraulic heads as unknowns. The main difference between the solution spaces resulting from the two formulations is represented by the behaviour of a fully open valve. The model used in (Pecci et al. 2017b; Dai and Li 2014; Eck and Mevissen 2012) allows flow in both directions when a valve is fully open. On the other hand, in the present work, a solution is feasible only if the flow across a valve never changes sign during the control period - e.g. 24

hours. This assumption is not restrictive from the engineering point of view while resulting in a simplification of the optimisation constraints.

When the number of binary variables is large, the solution of Problem (12) poses significant computational challenges for standard MINLP solvers. To mitigate this challenge, in the next section we investigate possible approaches for (considerably) reducing the size of (12), without (considerably) affecting the quality of the solutions.

MODEL REDUCTION

The complexity of Problem (12) grows combinatorially as the size of the considered network increases. In the literature, various model-reduction approaches have been used for improving the computational performance of hydraulic simulation tools (Deuerlein 2008; Deuerlein et al. 2016; Simpson et al. 2014) and optimising the operation of large operational water networks (Ulanicki et al. 1996; Burgschweiger et al. 2005; Paluszczyszyn et al. 2013). However, the application of these simplification schemes to the co-design problem of optimal placement and operation of control valves in WDNs has not been investigated. In this work, we study the implementation of model-reduction as a pre-processing routine for optimal co-design problems in WDNs and discuss its benefit and limitations. In particular, we investigate whether a reduction in the number of binary variables is achievable while preserving equivalence between the optimisation problems for the reduced and original models. To do so, we first give some essential definitions for the applied graph decomposition.

Definition 3.1 *A non-fixed head node $V(j)$ belonging to the graph of a WDN is called a* leaf *if it has cardinality one.*

The following definition of a tree in a WDN is introduced in Deuerlein (2008) and Simpson et al. (2014)

Definition 3.2 A tree *in a WDN graph is an acyclic connected subgraph such that at least one of its nodes is a leaf, and only one of its nodes is connected to either a looped part of the network or to a fixed head node. Such a unique node is called* root.

Definition 3.3 *(Deuerlein 2008; Simpson et al. 2014) The* forest *of a water network is defined as the disjoint union of all trees in the network. The part of the network which is not contained in the forest but includes the roots of all the trees is called* core.

We now introduce the definition of *trivial loops*, i.e. "leafy loops" involving only nodes with zero demand. In hydraulic models of operational water networks, such loops can be found where some nodal demands have been set to zero to account for disconnected customer connections or where the driver for near real time hydraulic models has resulted in the alignment between hydraulic models and GIS information.

Definition 3.4 *For a WDN graph, we define a loop as a* trivial loop *if:*

- *all nodes in the loop have demands equal to zero;*
- *all nodes except one have cardinality two; the unique node with cardinality greater than two is referred to as* root of the loop.

In order to describe the model-reduction algorithm and illustrate the challenges posed by its application to co-design optimisation problems in WDNs, we devise and present an example network (appropriately named "ToyNet"), whose layout is reported in Figure 1. The details for the pipes and nodes are listed on the left and right columns of Table 1, respectively. For this model, the H-W friction head loss formula is used. All nodes with non-zero demand have a required minimum pressure of 15 m while the maximum velocity in each pipe is 2 $\frac{m}{s}$, hence we set $q_{P_j}^{max} := \frac{\pi D_{P_j}^2}{4} \cdot 2$. The maximum allowed hydraulic head at each node is equal to the head at the reservoir, $H_0 = 120\, m$.

Given the small size of this example network, it is possible to compute the global minimiser of Problem (12) for ToyNet using the global MINLP solver `SCIP` (Gamrath et al. 2016), implemented here via the Matlab interface provided by the `OPTI TOOLBOX` (Currie and Wilson 2012). The globally optimal solution for the placement of 3 valves is on links P_4, P_5, P_7 and results in an average zone pressure of 39.53 m.

Now consider the index sets for the links and non-fixed head nodes of the full network model $P := \{P_1, \ldots, P_7\}$ and $V := \{V_1, \ldots, V_6\}$, respectively. At the current stage, the unique leaf node is V_6 and the corresponding link is P_7. The conservation of mass and energy equations at V_6 and across P_7, respectively, are:

$$q_{P_7} = d_{V_6} \tag{13}$$

$$h_{V_6} = h_{V_5} - d_{V_6} \cdot (a_{P_7} \cdot d_{V_6} + b_{P_7}) - \eta_{P_7} \tag{14}$$

Therefore, q_{P_7} is known *a priori* while h_{V_6} can be expressed as a linear function of the head h_{V_5} and the additional head loss introduced by a possible valve placed on P_7, denoted by η_{P_7}. We update demand at V_5 with $d_{V_5} \leftarrow d_{V_5} + d_{V_6} = 0.01 + 0.01 = 0.02\,(m^3/s)$ and now we get the reduced model $P \leftarrow \{P_1, \ldots, P_6\}$, $V \leftarrow \{V_1, \ldots, V_5\}$. In the network described by (P, V), we identify V_5 as a leaf node whose corresponding link is P_6. As before, we can discard the variables q_{P_6} and h_{V_5} as we can evaluate them from the formulae

$$q_{P_6} = d_{V_5}, \tag{15}$$

$$h_{V_5} = h_{V_3} - d_{V_5} \cdot (a_{P_6} \cdot d_{V_5} + b_{P_6}) - \eta_{P_6}, \tag{16}$$

and perform the update $d_{V_3} \leftarrow d_{V_3} + d_{V_5} + d_{V_6} = 0.02$. We now express the head at V_6 with

$$h_{V_6} = h_{V_3} - d_{V_6} \cdot (a_{P_7} \cdot d_{V_6} + b_{P_7}) - d_{V_5} \cdot (a_{P_6} \cdot d_{V_5} + b_{P_6}) - \eta_{P_6} - \eta_{P_7}. \tag{17}$$

After this second reduction, we have $P \leftarrow \{P_1, P_2, P_3, P_4, P_5\}$ and $V \leftarrow \{V_1, V_2, V_3, V_4\}$. At this stage, all leaf nodes have been removed from (P, V). We observe that links P_2, P_3 are connected in series to V_2, which has demand equal to zero. The corresponding conservation laws are:

$$q_{P_4} - q_{P_5} = d_{V_4} \tag{18}$$

$$q_{P_1} - q_{P_2} = d_{V_1} \tag{19}$$

$$q_{P_2} - q_{P_4} = 0 \tag{20}$$

$$h_{V_1} - h_{V_2} = q_{P_2}(a_{P_2}|q_{P_2}| + b_{P_2}) + \eta_{P_2} \tag{21}$$

$$h_{V_2} - h_{V_4} = q_{P_4}(a_{P_4}|q_{P_4}| + b_{P_4}) + \eta_{P_4} \tag{22}$$

As shown in Pecci et al. (2017c), in the case of H-W friction models, the quadratic approximation coefficients are defined such that $a_{P_2} = r_{P_2}\alpha(q_{P_2}^{max})$, $b_{P_2} = r_{P_2}\beta(q_{P_2}^{max})$ and $a_{P_4} = r_{P_4}\alpha(q_{P_4}^{max})$, $b_{P_4} = r_{P_4}\beta(q_{P_4}^{max})$. Equation (20) implies that $q_{P_2} = q_{P_4}$. Hence, $q_{P_2}^{max} = q_{P_4}^{max}$ and we have that $\alpha(q_{P_2}^{max}) = \alpha(q_{P_4}^{max})$ and $\beta(q_{P_2}^{max}) = \beta(q_{P_4}^{max})$. We can introduce a pseudo-link P_8 connecting V_1 and V_4 with flow q_{P_8} and quadratic approximation coefficients $a_{P_8} := a_{P_2} + a_{P_4}$ and $b_{P_8} := b_{P_2} + b_{P_4}$. The conservation laws (18)-(22) are equivalent to:

$$q_{P_8} - q_{P_5} = d_{V_4} \tag{23}$$

$$q_{P_1} - q_{P_8} = d_{V_1} \tag{24}$$

$$h_{V_1} - h_{V_4} = q_{P_8}(a_{P_8}|q_{P_8}| + b_{P_8}) + \eta_{P_2} + \eta_{P_4} \tag{25}$$

$$h_{V_2} = \frac{r_{P_4}}{r_{P_2} + r_{P_4}} h_{V_1} + \frac{r_{P_2}}{r_{P_2} + r_{P_4}} h_{P_4} - \frac{r_{P_4}}{r_{P_2} + r_{P_4}} \eta_{P_2} + \frac{r_{P_2}}{r_{P_2} + r_{P_4}} \eta_{P_4} \tag{26}$$

Constraints (23)-(25) are added to the original problem formulation, while removing (13)-(16) and (18)-(22). As a consequence, variables q_{P_7}, q_{P_6}, q_{P_2}, q_{P_4}, h_{V_6}, h_{V_5} and h_{V_2} can be discarded from the optimisation together with the corresponding constraints. We set $P \leftarrow \{P_1, P_3, P_5, P_8\}$ and $V \leftarrow \{V_1, V_3, V_4\}$. In order to preserve the feasible set of the original problem, all binary variables related to discarded links have to be included within the problem formulation. Moreover, it is necessary to add linear constraints to enforce physical and operational constraints at discarded nodes and links. As a result, the graph simplification does not result in a substantial reduction of the combinatorial complexity: while the overall number of continuous variables and nonlinear constraints is reduced, the set of of binary variables and the number of linear constraints involving the binary variables is preserved. With the aim of reducing the number of binary variables, we assume that no valve has to be placed on forest links P_6 and P_7. In this case, it is possible to set $z^-_{P_6} = z^+_{P_6} = z^-_{P_7} = z^+_{P_7} = 0$ and enforce constraints at nodes h_{V_5} and h_{V_6} by appropriately modifying minimum and maximum allowed hydraulic heads at the root node V_3, taking into account the head losses occurring across forest links:

$$h_{\min}(V_3) \leftarrow \max\left\{h_{\min}(V_3), h_{\min}(V_5) + \phi_{P_6}(d_{V_5}), h_{\min}(V_6) + \phi_{P_7}(d_{V_6}) + \phi_{P_6}(d_{V_5})\right\} \quad (27)$$

$$h_{\max}(V_3) \leftarrow \min\left\{h_{\max}(V_3), h_{\max}(V_5) + \phi_{P_6}(d_{V_5}), h_{\max}(V_6) + \phi_{P_7}(d_{V_6}) + \phi_{P_6}(d_{V_5})\right\} \quad (28)$$

It is therefore possible to ignore all variables and constraints related to forest nodes and links while preserving the feasibility of the solution. However, as we see in the remainder of this section, the computed valve configuration can be sub-optimal, since we discard links P_6 and P_7 from the set of candidate locations. In comparison, the elimination of binary variables related to links P_2 and P_4 while enforcing feasibility at node V_2 requires the inclusion of the pseudo-link P_8 as candidate valve location. In fact, the simple exclusion of both links P_2 and P_4 from the set of candidate locations would inevitably result in sub-optimal solutions.

Therefore, we propose the following two stage algorithm. Firstly, we introduce additional variables η_{P_8}, $z^+_{P_8}$, $z^-_{P_8}$, and solve Problem (12) on the simplified network defined by (P, V) - see Figure 2, with updated minimum and maximum allowed hydraulic heads at node V_3. At this first stage, the optimisation process is ignoring the existence of node V_2 and the changes in elevation occurring along the path composed of links P_2 and P_4. The resulting optimal locations are used to determine a set of candidate locations for the second stage, where Problem (12) is solved on the original full network model, with binary variables restricted to the set defined in the first stage.

We solved Problem (12) on the reduced network using SCIP and found the global optimum with valve placements on P_1, P_5, P_8. The set of candidate locations is then restricted to $\{P_1, P_5, P_2, P_4\}$ and Problem (12) is solved for the full network model with SCIP. The optimal solution has a corresponding AZP of $42.65\,m$ and valves on links P_1, P_4, P_5; compare with the global optima of 39.53 with valves placed on links $P_4, P5, P_7$.

The implemented two-stage algorithm has resulted in a sub-optimal solution. The reason for such an outcome is the exclusion of forest links from the set of possible valve locations. In fact, the significant changes in elevation occurring at nodes V_5 and V_6 requires the installation of a control valve on link P_7. Analogously, it is possible to define examples where the sub-optimality is caused by ignoring changes in elevations occurring across a sequence of demand nodes discarded by contraction. In order to limit the level of sub-optimality, we include a simple heuristic in the model-reduction algorithm to preserve those links that connect nodes with elevation differentials bigger than some constant $\varepsilon_{\text{thres}} > 0$; we discuss how to choose appropriate $\varepsilon_{\text{thres}}$ values in the Numerical Results section. We then apply the two-stage approach outlined using ToyNet.

In general terms, the model reduction algorithm proceeds as follows - for a detailed description see Appendix I. A procedure for computing network forest and core is presented in Simpson et al. (2014), with the aim of improving computational efficiency of hydraulic simulation. We extend the approach by Simpson et al. (2014) in order to enforce the satisfaction of minimum and maximum pressure constraints (8) and (9) at forest nodes. The second stage of our algorithm involves the elimination of all *trivial loops*. These can be collapsed into a single node, the *root of the loop*, whose hydraulic head is equal to the hydraulic heads of every other node. Because all the links involved in the *trivial loops* have zero flow, such links cannot be candidates for valve placement. Consequently, *trivial loops* are considered as member of the forest. Finally, we operate the contraction of sequences of links connecting nodes with zero demand by introducing hydraulically equivalent pseudo-links.

Let P and V be the index sets of all network links and nodes, respectively, resulting from the model reduction routine. Let $\mathbf{\Phi}_P(\mathbf{q}^t(P)) := \text{diag}(\phi_{P(1)}(q^t_{P(1)}), \ldots, \phi_{P(|P|)}(q^t_{P(|P|)}))$. The restriction of Problem (12) to the network defined by (P,V) can be formulated as follows:

$$
\begin{aligned}
\text{minimise} \quad & \frac{1}{n_l \hat{W}} \sum_{t=1}^{n_l} \hat{\mathbf{w}}^T (\hat{\mathbf{h}}^t - \boldsymbol{\xi}(V)) \\
\text{subject to} \quad & \boldsymbol{\Phi}_P(\hat{\mathbf{q}}^t) + \mathbf{A_{12}}(P,V)\hat{\mathbf{h}}^t + \mathbf{A_{10}}(P,:)\mathbf{h_0}^t + \hat{\boldsymbol{\eta}}^t = 0, \quad t = 1,\ldots,n_l \\
& \mathbf{A_{12}}(P,V)^T \hat{\mathbf{q}}^t - \mathbf{d}(\mathbf{V})^t = 0, \quad t = 1,\ldots,n_l \\
& (\hat{\mathbf{q}}^t)_t, (\hat{\mathbf{h}}^t)_t, (\hat{\boldsymbol{\eta}}^t)_t, \hat{\mathbf{z}}^+ \hat{\mathbf{z}}^- \text{satisfy (4)-(11) restricted to } (P,V) \\
& \hat{\mathbf{z}}^+, \hat{\mathbf{z}}^- \in \{0,1\}^{|P|},
\end{aligned}
\tag{29}
$$

where the following notation is adopted: given a matrix $\mathbf{B}$, the expression $\mathbf{B}(I,J)$ denotes the sub-matrix composed by rows and columns of $\mathbf{B}$ whose indices are in I and J, respectively. The above formulation includes a smaller number of variables and constraints with respect to Problem (12). In particular, Problem (29) has less nonlinear constraints, thus reducing the total nonconvexities, and a smaller number of binary variables.

After solving Problem (29), let $\hat{\mathbf{z}}^+$ and $\hat{\mathbf{z}}^-$ define optimal valve placements for the reduced model, which we shall use to define candidate valve locations for the original full network. If a valve is placed on a pseudo link, then all links contracted in making it become candidate locations. Similarly, if a valve is placed on a real link of the reduced model, then that link also becomes a candidate valve location. This can be implemented using binary cuts as follows, where z_j^+ and z_j^- are set to zero for non-candidate links j. Let $\hat{\mathbf{z}}_\mathbf{b} = \mathbf{0} \in \mathbb{R}^{n_p}$, then:

- if $\hat{z}_l^+ + \hat{z}_l^- = 1$ and $P(l)$ is not a pseudo-link, we set $\hat{\mathbf{z}}_\mathbf{b}(P(l)) = 1$.
- if $\hat{z}_u^+ + \hat{z}_u^- = 1$ and $P(u)$ is a pseudo-link, let $P(l_0),\ldots,P(l_N)$ be the sequence of links that have been contracted in $P(u)$. We set $\hat{\mathbf{z}}_\mathbf{b}(P(l_j)) = 1$, $\forall j \in \{0,\ldots,N\}$.

Using $\hat{\mathbf{z}}_{\mathbf{b}}$, we add binary cuts to the original Problem in (12) to form the MINLP:

$$\begin{aligned}
\text{minimise} \quad & \frac{1}{n_l W}\sum_{t=1}^{n_l} \mathbf{w}^T(\mathbf{h}^t - \boldsymbol{\xi}) \\
\text{subject to} \quad & (\mathbf{q}^t)_t, (\mathbf{h}^t)_t, (\boldsymbol{\eta}^t)_t, \mathbf{z}^+, \mathbf{z}^- \text{satisfy (2)-(10)} \\
& \mathbf{z}^+ \leq \hat{\mathbf{z}}_{\mathbf{b}} \\
& \mathbf{z}^- \leq \hat{\mathbf{z}}_{\mathbf{b}} \\
& \mathbf{z}^+, \mathbf{z}^- \in \{0,1\}^{n_p}.
\end{aligned} \tag{30}$$

The binary cuts introduced in Problem (30) considerably reduce the combinatorial complexity with respect to Problem (12) and make the problem easier to solve. In fact, as a consequence of the binary cuts, many binary variables in Problem (30) are fixed. The proposed two-stage method is characterised by the subsequent solution of Problems (29) and (30) and is summarised in Algorithm 1 and Figure 3.

As observed before, the constraints in Problem (29) do not include information about discarded nodes involved in elevation changes smaller than $\varepsilon_{\text{thres}}$. Therefore, Problem (29) represents an approximation of the original Problem (12), which was formulated on the full network model. The reduction in accuracy of such approximation becomes higher for larger $\varepsilon_{\text{thres}}$. A computational evaluation of the exact level of sub-optimality caused by a particular value of $\varepsilon_{\text{thres}}$ would be possible only by applying a global MINLP solver, which is not practical in problem instances for complex water networks. Nonetheless, based on the illustrative example ToyNet and the results reported in the Numerical Results section, we conjecture that the larger the value of $\varepsilon_{\text{thres}}$, the greater the possibility of obtaining a severely sub-optimal solution from Algorithm 1 and demonstrate that physically reasonable values can be derived by solving the problem for larger values and gradually decreasing $\varepsilon_{\text{thres}}$ until no improvements can be shown or the problem becomes intractable.

SOLUTION METHOD

We observe that Problems (12), (29), and (30) are mixed integer nonlinear programs (MINLPs) with similar structure, involving nonlinear equality constraints and a number of linear constraints.

Algorithm 1 Two-stage method for optimal placement and operation of control valves

1: **Input:**Network properties and an elevation threshold ε_{thres}
2: Apply the network reduction and compute index sets P, V
3: **Stage 1**: solve Problem (29) and obtain $\hat{\mathbf{z}}^+$ and $\hat{\mathbf{z}}^-$
4: Define vector $\hat{\mathbf{z}}_\mathbf{b}$
5: **Stage 2**: solve Problem (30)

As a consequence, we apply the same solution method to all three problems. We implement the Outer Approximation with Equality-Relaxation (OA/ER), which was initially employed by Kocis and Grossmann (1987) for problems in process synthesis optimisation. OA/ER relies on the solution of an alternating sequence of *master* mixed integer linear programs (MILPs) and *primal* nonlinear programs (NLPs), until a termination criteria is met. Master MILPs are defined by linearisations of the nonlinear equality constraints. In the case considered here, at each iteration, the solution of the master MILP results in a set of candidate valve locations. On the other hand, the primal NLP corresponds to the problem of optimising valves control settings, while their locations are fixed. A detailed description of the OA/ER algorithm can be found in Appendix II.

Under suitable convexity assumptions OA/ER converges to the globally optimal solution, see Floudas (1995, Section 6.5). However, the functions involved in the nonlinear equality constraints within Problems (12), (29), and (30) are nonconvex, hence OA/ER is applied only as a local optimisation method. In this work, we terminate OA/ER if the master MILP is infeasible or the best objective function values are not decreasing in consecutive iterations.

The nonconvexity of the equality constraints has two main effects on the application of OA/ER to Problems (12), (29), and (30). Firstly, the corresponding primal NLPs are nonconvex and the application of gradient-based NLP solvers results in local optima, with no theoretical guarantee of global optimality. Secondly, the linearised constraints within the master MILP may cut out portions of the feasible set, discarding the globally optimal choice of binary variables. As shown in the next section, this can result in early termination of the OA/ER algorithm, due the infeasibility of the master MILP caused by inconsistent linearised constraints.

Consequently, the quality of the solutions computed by OA/ER depends on the initialisation.

We initialise OA/ER using the solution of Problem (12) with $n_v = 0$, which is feasible provided that hydraulic heads and flows satisfy constraints (4)-(9) when no valve is installed. We observe that solving Problem (12) with $n_v = 0$ is equivalent to simulating the network model without valves. Alternatively, the authors in Viswanathan and Grossmann (1990) have proposed to initialise OA/ER with the solution of the NLP relaxation of Problem (12), where the binary constraints in (12) are ignored and variables z_j^+ and z_j^- are allowed to assume any value between 0 and 1, for all $j \in \{1, \dots, n_p\}$. The numerical results reported in the next section show that good quality solutions can be achieved by applying one of these two initialisation strategies.

NUMERICAL RESULTS

The developed model reduction and OA/ER methods for the solution of Problem (12) have been evaluated using two large operational network models. The solver `IPOPT` (v3.12.6) (Waechter and Biegler 2006) is used to solve the primal NLP problems within OA/ER as well as any NLP needed to initialise OA/ER. `IPOPT` is implemented in MATLAB through the interface provided by the `OPTI TOOLBOX` (Currie and Wilson 2012). Moreover, in the implementation of `IPOPT` we directly supply the solver with sparse gradients and Jacobians, in order to take advantage of the very sparse structure of our problem. The master MILP within OA/ER is solved using the commercial solver `GUROBI` (v7.0) (Gurobi Optimization 2017), and implemented in MATLAB using the supplied interface with tolerance for the relative MIP optimality gap set to 0.01. All other `GUROBI` options were set to their default values. In particular, these include the presolving routines, that are applied before starting the linear programming based branch and bound algorithm implemented in `GUROBI`. In order to provide a fair comparison between the different instances, we report the total CPU time employed by OA/ER to reach a solution as well as the number of `IPOPT` iterations, the amount of simplex iterations, and the number of nodes visited by the branch and bound algorithm within `GUROBI` - these are referred to as "BB Nodes" in Tables 4, 6, 7, 8, and 10. All computations were executed within MATLAB 2016b-64 bit for Windows 7, installed on a 2.40GHz Intel® Xeon(R) CPU E5-2665 0 with 16 Cores and 32 GB of RAM.

Case study 1

We first consider BWFLnet, network model of the Smart Water Network Demonstrator, a "Field Lab" operated by Bristol Water, InfraSense Labs at Imperial College London and Cla-Val presented in Wright et al. (2015). This water supply network consists of 2310 nodes, 2369 pipes and 2 inlets (with fixed known hydraulic heads) - see also Table 2, where the quantities $\frac{n_p - n_n}{n_p}$ and $\frac{2n_p}{n_n}$ correspond to the loopiness of network topology and the average degree of connectivity per node, respectively. We observe that BWFLnet represents a typical network in urban area in United Kingdom, which is characterised by a *tree-like* structure with few loops. In addition, since its average degree of connectivity per node is close to 2, the network model includes a large number of link sequences (possibly involving non-zero demand nodes). As a consequence, we expect the proposed model reduction procedure to result in considerable computational savings. Following the work by (Wright et al. 2015), the network operator has already installed 3 PRVs, currently operated in order to minimise AZP as a surrogate measure for leakage. For the purpose of this numerical experiment, the presence of the PRVs is ignored and their corresponding links are modelled without PRVs. This is useful also because we want to analyse the degree of sub-optimality of the current locations. The network graph is presented in Figure 4. The frictional head losses are modelled in BWFLnet using the HW formula. In this study, we use the quadratic approximation of the H-W formula proposed in (Eck and Mevissen 2015), where the maximum velocity in each pipe is set to $3\,\frac{m}{s}$.

In the present formulation we consider 24 different demand conditions, one for each hour of the day. The minimum allowed pressure head at demand nodes is 18 m, while this value is relaxed to zero for nodes with no demand. We formulate Problem (12) for the optimal placement and operation of 1 to 5 control valves, addressing the minimisation of AZP, for the full network model. The number of continuous variables, binary variables and constraints is reported in Table 3.

We initialise OA/ER using the solution of Problem (12) with $n_v = 0$. With this initial point, the OA/ER algorithm has successfully converged after two iterations to (local) solutions in all instances. The number of iterations taken from OA/ER is limited because of the nonconvexity of the constraints; once the first iteration is completed and a vector of binary variables has been identified, the set of linearised constraints becomes inconsistent and so the master MILP at the second iteration is infeasible.

If we fix the locations of PRVs to those currently installed by the network operator in BWFLnet, we obtain an optimised AZP value of 37.48 m. Therefore, the application of OA/ER for the placement of 3 control valves has resulted in a good quality configuration with a slightly lower value of the objective function - see Table 4. This is in agreement with the numerical results reported in Kocis and Grossmann (1987) and Viswanathan and Grossmann (1990), where OA/ER has resulted in near-optimal solutions for problems in process synthesis optimisation. Finally, the overall computational performance is summarised in Table 4.

The number of nodes explored in the branch and bound procedure grows rapidly with n_v and so does the CPU time. However, for the considered case study, the computational effort required for OA/ER to converge is limited to a few hours, on the desktop machine used for the numerical tests reported in Table 4. When the considered network model is larger, the combinatorial problem could become intractable and the implementation of MINLP solution algorithms that efficiently exploit multiple available CPU cores is subject of ongoing research (Ralphs et al. 2018). In addition, in order to improve the quality of the solutions, it is sometimes convenient to implement a multi-start optimisation strategy, where OA/ER is executed with many different initial points. Furthermore, it is possible to seek the minimisation of additional objective functions together with AZP. In this case, standard approaches require the solution of a parametrised sequence of MINLPs with the same structure as Problem (12) - see Pecci et al. (2017d) for an example. Under such circumstances, the computational burden could easily become impractical.

In order to reduce the computational effort, we investigate the application of the two stage approach outlined in Algorithm 1. Firstly, we focus on the choice of $\varepsilon_{\text{thres}}$. In the following, the ratio $|P|/n_p$ is used as surrogate measure of the reduction in computational burden, as the number of binary variables is $2|P|$. In addition, we conjecture that the larger value of $\varepsilon_{\text{thres}}$, the higher the possibility of generating a sub-optimal solution - see the example ToyNet in the Model Reduction section.

Numerical tests show that, for this case study, very small/negligible model reduction is achieved for $\varepsilon_{\text{thres}} > 5$ and no further reduction is achieved when $\varepsilon_{\text{thres}} > 28$. Therefore, we report in Figure 5 the values of $|P|/n_p$ corresponding to $\varepsilon_{\text{thres}} \in \{0, 1, 2, \ldots, 28\}$. Figure 5 shows that the most significant reductions in problem size occur for $\varepsilon_{\text{thres}} \leq 3$. Elevation differences of such magnitude are analogous to the order of uncertainty usually experienced in WDN models. In particular, pressure control in operational water networks is subject to multiple sources of data and modelling errors. These include stochastic nature of customer demand, dynamic hydraulic conditions, uncertainty affecting the hydraulic model and the data, and failures of the control pilots and equipment - see the experimental study reported in (Wright et al. 2015).

In the following, we investigate the computational performance of Algorithm 1 with $\varepsilon_{\text{thres}} \in \{1, 2\}$.

The size of the simplified network after the different stages of the reduction algorithm is summarised in Table 5. When $\varepsilon_{\text{thres}} = 1$, the final reduced network is composed of roughly 45% of the links and nodes of the full order model. In comparison, if $\varepsilon_{\text{thres}} = 2$, the network size is reduced by roughly 65%. In both cases, the formulation of Problem (29) results in a considerably smaller nonconvex MINLP than the one formulated for the full network model, with the number of binary variables reduced by roughly 45% and 65%, respectively.

Following Algorithm 1, OA/ER is applied to solve Problem (29) and then Problem (30), for each choice of $\varepsilon_{\text{thres}} \in \{1, 2\}$. The performance of Algorithm 1 with $\varepsilon_{\text{thres}} = 1$ is reported in Table 6. In all instances, it results in the same solutions computed with the full network model. However, we observe that both computational time and number of nodes visited by the branch and bound algorithm are reduced by an order of magnitude. In addition, Table 6 shows that the number of nodes visited during the second stage of Algorithm 1 is either zero or very small (< 10). This is because, at this stage, OA/ER is applied to solve Problem (30), where binary cuts have been added to restrict the set of feasible binary variables according to the solution computed at the previous stage.

When a larger threshold is considered, the computational performance is further improved. However, as observed in the previous sections, Algorithm 1 is more likely to converge to sub-optimal solutions. In the case considered here, the use of $\varepsilon_{\text{thres}} = 2$ results in slightly worse solutions in the case of $n_v = 3,4,5$ - see Table 7. Nonetheless, the differences between AZP values from Tables 6 and 7 are smaller than the level of hydraulic head uncertainties for models of operational water networks. The computational time reported in Table 7 is reduced with respect to Table 6. However, number of iterations, CPU time and amount of visited nodes reported in Tables 6 and 7 are of the same order of magnitude in all instances. Less conservative choices of $\varepsilon_{\text{thres}}$ would result in small reductions of network dimension and hence of computational effort, possibly with more severely sub-optimal solutions. Therefore, we limited our analysis to the computational performance corresponding to $\varepsilon_{\text{thres}} \in \{1,2\}$.

Case study 2

In this section, we evaluate the developed methods on a network model with different size and level of connectivity from BWFLnet. We consider NYnet (Ostfeld et al. 2008), which represents an highly looped city network from USA- see Figure 6. This network model has 12523 nodes, 14830 pipes and 7 inlets (modelled as nodes with fixed hydraulic heads) and has been previously presented in the framework of optimal sensor placement (Ostfeld et al. 2008). To the best of our knowledge, this network model has not been previously used to evaluate solution methods for optimal valve placement and operation problems, and the present study is the only example where the considered problem is solved for a network as complex as NYnet. The network topological properties are reported in Table 2. Since NYnet is highly looped and it has a larger average degree of connectivity per node than BWFLnet, we expect the model reduction algorithm to have a less significant impact on the size of the network and hence on the corresponding combinatorial complexity of Problem (12) - see also Figure 7. The NYnet hydraulic model considers a single demand condition, by setting $n_l = 1$. As a result, the number of continuous variables and constraints in the problem formulation is reduced in comparison to BWFLnet (see Table 3). This results in a smaller computational load for the solution of the primal NLP problem for NYnet within OA/ER by the solver IPOPT. However, computing optimal valve locations for NYnet is more challenging in comparison to the case of BWFLnet. This is due to the larger number of binary variables (i.e. candidate valve locations, see Table 3) included in the problem formulation and the highly looped topology of NYnet, which increases the degree of symmetry of the resulting MINLP. The presence of multiple demand conditions does not affect the combinatorial difficulty of the problem, since the number of binary variables remains the same. Some nodes experience low pressure, thus we set the minimum pressure at demand nodes to $6\,m$, relaxing this value to zero for those nodes with no demand. The friction head loss model used in NYnet is the DW formula, which we approximate using smooth quadratic function as described by Eck and Mevissen (2015). For the purpose of computing the approximation, we consider values of the Reynolds number between 4000 and the value corresponding to a velocity of $3\,\frac{m}{s}$. However, during the optimisation process, the maximum allowed velocity is set to $12\,\frac{m}{s}$, as few network pipes are subject to very high velocities. We formulate and solve Problem (12) on NYnet.

As observed in the previous sections, in the case of nonconvex constraints OA/ER is applied as a heuristic, hence the quality of the computed solutions depends significantly on algorithmic initialisation. OA/ER results in poor quality solutions for $n_v = 2,3,4,5$ when it is initialised using the solution of Problem (12) with $n_v = 0$. Therefore, we initialise OA/ER by means of the solution of the NLP relaxation of Problem (12), obtained by ignoring the binary constraints in (12) and allowing variables z_j^+ and z_j^- to assume any value between 0 and 1, for all $j \in \{1,\ldots,n_p\}$. With such initial point, in instances with $n_v = 1,2,3$, the algorithm converges to good quality solutions, which are reported in Table 8 together with the computational performance. Table 8 shows that the solution of the continuous relaxation of Problem (12) requires a substantial computational effort from IPOPT - this is expected, as continuous relaxations of MINLPs are known to be difficult to solve. However, we observe that the solution of the primal NLP problem at iteration 1 requires a reduced number of IPOPT iterations with respect to what reported for BWFLnet - see also Table 4. On the contrary, the number of simplex iterations and nodes visited by GUROBI is larger than what reported in Table 4 for BWFLnet.

The cases of $n_v = 4,5$ show the limitations of the application of OA/ER to the network in study. In particular, after two iterations of OA/ER no feasible solutions for $n_v = 4$ was generated and the optimisation process was manually terminated. At the same time, the reported solution of the master MILPs is computationally expensive, with a large number of nodes visited by the branch and bound procedure. During an outer approximation algorithm, the generation of infeasible binary choices is not unexpected. Binary cuts are included in the formulation of the master MILP to prevent the algorithm from generating the same infeasible binary assignments more than once. As a consequence, it is possible that OA/ER would eventually produce a feasible solution, in a sufficiently large number of iterations. However, for the purpose of the present study, we decided to interrupt the iterative search after two consecutive infeasible binary solutions, because of time constraints. The complexity of the considered problem is further amplified for $n_v = 5$. In this case, the optimisation process was manually interrupted during the first iteration of the OA/ER algorithm, with `GUROBI` experiencing very slow progress towards the solution of the master MILP. In fact, after a longer CPU time than what reported for the entire run with $n_v = 4$, the relative optimality gap is still equal to 7.90%.

We investigate the effect of the presented model reduction routine on the dimension of NYnet and hence on the size of the corresponding combinatorial problem for optimal placement and operation of control valves. Numerical tests on NYnet show that no further reduction is possible when $\varepsilon_{\text{thres}} > 19$ and that the maximum decrease in the number of pipes is around 25% - see Figure 7. In addition, Table 9 shows the reductions in model size achieved by the simplification procedure, when $\varepsilon_{\text{thres}} = 3$.

We implement Algorithm 1 for solving Problem (12) on NYnet, with $\varepsilon_{\text{thres}} = 3$. As we can see from Table 10, in the cases of $n_v = 1,2,3$, the two-stage approach results in the same solutions as those reported in Table 8, when OA/ER was directly applied to the full network model. In addition, as expected, the time required to generate a solution is smaller when the model is reduced. In particular, in the first stage of Algorithm 1, the number of nodes visited by the branch and bound procedure is reduced by up to a factor of 3.7, compared to what reported in Table 8. Nonetheless, the gains in computational burden are not as significant as for the case of the BWFLnet model. The application of the model reduction algorithm did not enhance the ability of OA/ER to solve the considered problem for $n_v = 4,5$. In particular, for $n_v = 4$, no feasible solution was found after two iterations of OA/ER and the algorithm was interrupted. Furthermore, the method was manually terminated in the case $n_v = 5$, as `GUROBI` showed a slow progress towards the solution of the master MILP. This limitation in impact of the model reduction algorithm is explained by the high density of the NYnet network model, where the forest and pipe sequences for contraction constitute a smaller fraction of the network.

The challenging computational experience of the solver `GUROBI` is caused by the characteristics of the case study. Firstly, the number of binary variables involved in the formulation of Problem (12) for NYnet is an order larger than the number of binary variables corresponding to BWFLnet - see Figure 3. In addition, as observed at the beginning of this section, NYnet is highly looped and presents an higher level of connectivity than BWFLnet. As a result, the solution space for NYnet is characterised by an increased degree of symmetry, with multiple valve configurations resulting in similar AZP performances. It is well known that symmetry of an integer program results in the generation of a large enumeration tree within the branch and bound procedure and therefore should be detected and removed (Liberti 2012; Margot 2010). Therefore, in the case of networks that are not highly looped (i.e. $n_p - n_n \ll n_p$) with $\frac{2n_p}{n_n} \ll 3$, we expect the model reduction to considerably reduce the computational cost associated with the solution of the optimal valve placement and operation problem, as reported for the case of BWFLnet. In comparison, further investigation is needed on symmetry-breaking techniques to reduce the computational load required to optimally locate control valves in highly looped water networks with an high level of connectivity.

CONCLUSIONS

In this paper, we have proposed and investigated the application of model reduction and outer approximation with equality relaxation (OA/ER) algorithms for generating good quality solutions for the problem of optimal valve placement and operation in water distribution networks. The numerical results reported in the manuscript suggest that OA/ER has enabled the convergence to good quality solutions when large operational water networks with a relatively low number of loops are considered. The numerical experience also indicates that OA/ER can fail to generate a solution for highly meshed network instances. Since the computational load of solving the considered optimisation problem grows combinatorially with the network dimensions, we have proposed the application of model reduction techniques for water distribution networks. The reformulation of the considered optimisation problem on a reduced network model does not result in an equivalent MINLP and its solution can be severely sub-optimal. As a consequence, we have introduced an arbitrary parameter of the model reduction algorithm in order to regulate the trade-off between reducing computational complexity and potential sub-optimality of the solutions. The numerical results reported in the manuscript show that, when networks with a relatively lower number of loops are considered (e.g. more branched systems common in United Kingdom), significant computational gains can be made by integrating model reduction approaches and OA/ER algorithm, without affecting the quality of the solutions. Furthermore, we have demonstrated that the proposed model reduction routines have limited effect on highly looped, dense water networks where the problem presents high degree of symmetry (e.g. networks from United States). Future work will investigate the application of symmetry-breaking techniques for solving the problem of optimal placement and operation of control valves in complex and highly looped water distribution networks.

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NOTATION

The following symbols are used in this paper:

n_0	number of water sources;
n_p, n_n	number of pipes and nodes, respectively;
n_l	number of loading conditions;
n_v	number of valves to be installed;
$\mathbf{A_{12}}$, $\mathbf{A_{10}}$	edge-node incidence matrices for the n_n nodes and n_0 water sources, respectively;
$\mathbf{d}^t$	nodal demands at time t;
$\boldsymbol{\xi}$	vector of nodal elevations;
$\mathbf{h}^t_{\max}$, $\mathbf{h}^t_{\min}$	vectors of maximum and minimum hydraulic heads at nodes, respectively;
$\mathbf{w}$, $\hat{\mathbf{w}}$	full scale and reduced vectors of weights, respectively;
L_j	Length of pipe j;
$q_j^{\max}$	maximum flow allowed across pipe j;
$\mathbf{\Phi}(\cdot)$, $\mathbf{\Phi}_P(\cdot)$	friction head loss functions for full scale and reduced network models, respectively;
a_j, b_j	positive coefficients of the friction head loss function for link j;
$\mathbf{Q}^{\max}$	diagonal matrix with diagonal elements equal to $q_1^{\max}, \ldots, q_{n_p}^{\max}$;
$\mathbf{e}$	vector composed of ones;
$\mathbf{M}^+, \mathbf{M}^-$	diagonal matrices of large positive constants;
$\mathbf{h}^t$, $\hat{\mathbf{h}}^t$	full scale and reduced vectors of unknown hydraulic heads at time t, respectively;
$\mathbf{q}^t$, $\hat{\mathbf{q}}^t$	full scale and reduced vectors of unknown flows at time t, respectively;
$\mathbf{z}^+$, $\mathbf{z}^-$	vectors of binary variables for the full scale network model;
$\hat{\mathbf{z}}^+$, $\hat{\mathbf{z}}^-$	vectors of binary variables for the reduced network model;
$\boldsymbol{\eta}^t$, $\hat{\boldsymbol{\eta}}$	full scale and reduced vectors of unknown additional head losses, respectively;
P, V	index sets of pipes and nodes in the reduced network model, respectively;
$\varepsilon_{\text{thres}}$	parameter used within the model reduction routine;
$\hat{\mathbf{z}}_{\mathbf{b}}$	vector used to define binary cuts.

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List of Tables

TABLE 1. ToyNet data

Link	D (m)	L (m)	C_{HW}	Node	d (m^3/s)	ξ (m)
P_1	0.40	1000	70	V_1	0.03	50
P_2	0.30	1000	100	V_2	0	100
P_3	0.25	1000	100	V_3	0	35
P_4	0.30	1000	100	V_4	0.05	30
P_5	0.25	1000	100	V_5	0.01	90
P_6	0.25	1000	100	V_6	0.01	5
P_7	0.25	1000	100			

TABLE 2. Network topological characteristics for the two case studies

Name	n_p	n_n	n_0	n_l	$\frac{n_p - n_n}{n_p}$	$\frac{2n_p}{n_n}$
BWFLnet	2369	2310	2	24	0.025	2.051
NYnet	14830	12523	7	1	0.156	2.368

TABLE 3. Problem size for the two case studies

Name	No. cont. var.	No. bin. var.	No. lin. const.	No. nonlin. const.
BWFLnet	169152	4738	285234	56856
NYnet	42183	29660	86674	14830

TABLE 4. Overall performance of OA/ER applied to the full network model BWFLnet

	AZP	CPU time	OA/ER iter	Simplex iter	BB nodes	IPOPT iter
$n_v = 1$	44.84 m	315 s	0	-	-	2
			1	147336	47	19
			2	0	0	-
$n_v = 2$	39.61 m	680 s	0	-	-	2
			1	1017019	1090	43
			2	68159	0	-
$n_v = 3$	36.43 m	4527 s	0	-	-	2
			1	4765154	5428	49
			2	95564	0	-
$n_v = 4$	34.49 m	31987 s	0	-	-	2
			1	25428435	42738	86
			2	0	0	-
$n_v = 5$	33.40 m	87667 s	0	-	-	2
			1	44096088	78042	57
			2	0	0	-

TABLE 5. Subsequent reductions of BWFLnet dimensions, with $\varepsilon_{\text{thres}} = 1, 2$.

	$\varepsilon_{\text{thres}} = 1$		$\varepsilon_{\text{thres}} = 2$	
	$\|P\|/n_p$	$\|V\|/n_n$	$\|P\|/n_p$	$\|V\|/n_n$
Initial	1	1	1	1
Forest-Core decomposition	0.72	0.72	0.61	0.60
Final	0.46	0.44	0.35	0.34

TABLE 6. Computational performance of Algorithm 1 applied to BWFLnet with $\varepsilon_{\text{thres}} = 1$.

	AZP	CPU time		OA/ER iter	Simplex iter	BB nodes	IPOPT iter
$n_v = 1$	44.84 m	68 s	Stage 1	0	-	-	2
				1	62729	19	26
				2	0	0	-
			Stage 2	0	-	-	2
				1	34881	0	19
				2	0	0	-
$n_v = 2$	39.61 m	206 s	Stage 1	0	-	-	2
				1	213185	235	42
				2	0	0	-
			Stage 2	0	-	-	2
				1	37946	0	43
				2	86836	0	-
$n_v = 3$	36.43 m	599 s	Stage 1	0	-	-	2
				1	925233	703	28
				2	0	0	-
			Stage 2	0	-	-	2
				1	42009	6	49
				2	41815	0	-
$n_v = 4$	34.49 m	3289 s	Stage 1	0	-	-	2
				1	4948463	9022	35
				2	0	0	-
			Stage 2	0	-	-	2
				1	41745	3	86
				2	0	0	-
$n_v = 5$	33.40 m	8856 s	Stage 1	0	-	-	2
				1	11499816	18133	46
				2	0	0	-
			Stage 2	0	-	-	2
				1	51172	7	57
				2	46693	0	-

TABLE 7. Computational performance of Algorithm 1 applied to BWFLnet with $\varepsilon_{\text{thres}} = 2$.

	AZP	CPU time		OA/ER iter	Simplex iter	BB nodes	IPOPT iter
$n_v = 1$	44.84 m	57 s	Stage 1	0	-	-	2
				1	52616	21	21
				2	0	0	-
			Stage 2	0	2	-	-
				1	34881	0	19
				2	0	0	-
$n_v = 2$	39.61 m	141 s	Stage 1	0	-	-	2
				1	121604	137	32
				2	0	0	-
			Stage 2	0	-	-	2
				1	37946	0	43
				2	86836	0	-
$n_v = 3$	36.50 m	370 s	Stage 1	0	-	-	2
				1	538511	518	20
				2	0	0	-
			Stage 2	0	-	-	2
				1	41547	5	47
				2	40774	0	-
$n_v = 4$	34.55 m	1781 s	Stage 1	0	-	-	2
				1	2121801	6159	27
				2	74406	0	-
			Stage 2	0	-	-	2
				1	42466	3	79
				2	0	0	-
$n_v = 5$	33.46 m	7401 s	Stage 1	0	-	-	2
				1	11189820	22695	74
				2	0	0	-
			Stage 2	0	-	-	2
				1	50593	7	39
				2	45438	0	-

TABLE 8. Overall performance of OA/ER applied to the full network model NYnet

	AZP	CPU time	OA/ER iter	Simplex iter	BB nodes	IPOPT iter
$n_v = 1$	30.80 m	610 s	0	-	-	235
			1	94485	41	11
			2	73872	0	–
$n_v = 2$	30.49 m	2112 s	0	-	-	581
			1	983186	6177	18
			2	66746	0	-
$n_v = 3$	26.68 m	7601 s	0	-	-	1084
			1	7618460	43185	18
			2	0	0	-
$n_v = 4$	-	819189 s	0	-	-	978
			1	273950103	1173708	Infeasible
			2	202464015	970874	Infeasible
$n_v = 5$	-	1032790 s	0	-	-	1168
			1	173250345	4299016	-
			2	-	-	-

TABLE 9. Subsequent reductions of NYnet dimensions, with $\varepsilon_{\text{thres}} = 3$.

	$\varepsilon_{\text{thres}} = 3$	
	$\|P\|/n_p$	$\|V\|/n_n$
Initial	1	1
Forest-Core decomposition	0.81	0.78
Final	0.76	0.71

TABLE 10. Computational performance of Algorithm 1 applied to NYnet with $\varepsilon_{\text{thres}} = 3$.

	AZP	CPU time		OA/ER iter	Simplex iter	BB nodes	`IPOPT` iter
$n_v = 1$	30.80 m	573 s	Stage 1	0	-	-	237
				1	85557	42	12
				2	66823	0	-
			Stage 2	0	-	-	27
				1	30284	3	11
				2	30697	0	13
$n_v = 2$	30.80 m	1513 s	Stage 1	0	-	-	746
				1	400713	3078	14
				2	55245	0	-
			Stage 2	0	-	-	29
				1	31120	11	`Infeasible`
				2	31949	7	14
				3	72626	0	-
$n_v = 3$	26.68 m	2379 s	Stage 1	0	-	-	644
				1	2231130	17193	20
				2	57614	0	-
			Stage 2	0	-	-	32
				1	29088	11	18
				2	29383	0	-
$n_v = 4$	-	36584 s	Stage 1	0	-	-	882
				1	21942579	290218	`Infeasible`
				2	23802048	334473	`Infeasible`
$n_v = 5$	-	83857 s	Stage 1	0	-	-	1334
				1	53282719	1455812	-
				2	-	-	-

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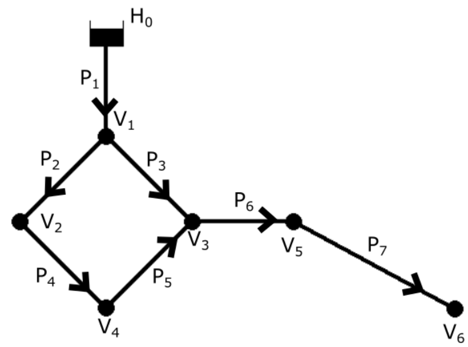

Fig. 1. ToyNet layout

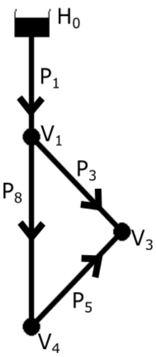

Fig. 2. ToyNet reduced model

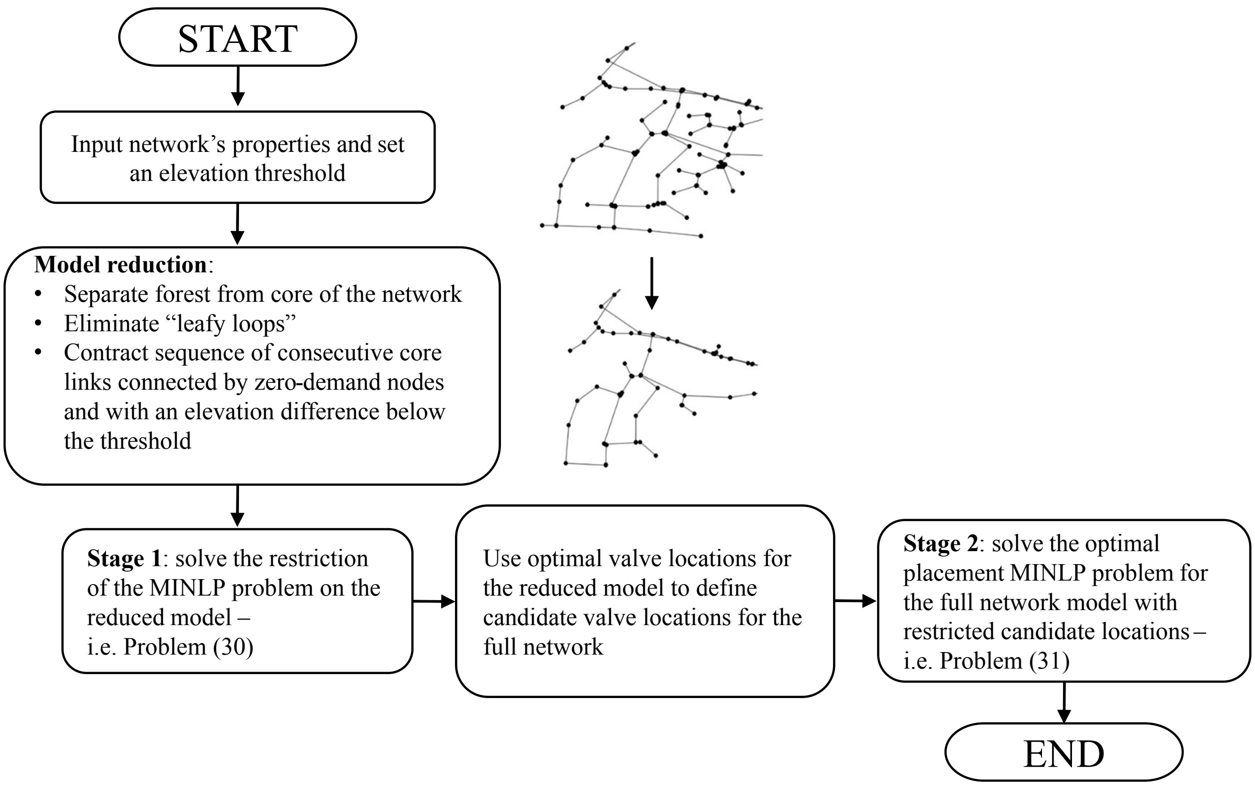

Fig. 3. Flowchart of Algorithm 1

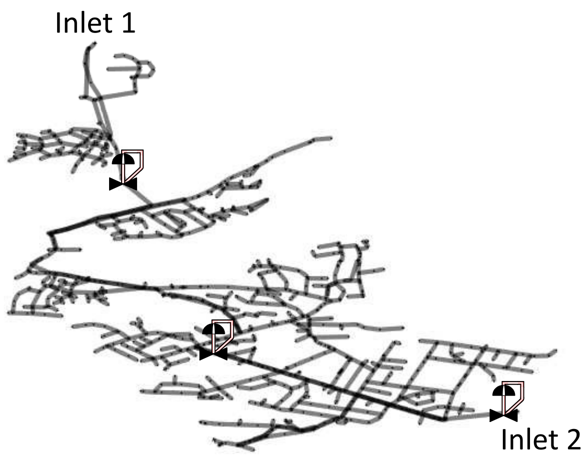

Fig. 4. BWFLnet with current valve configuration

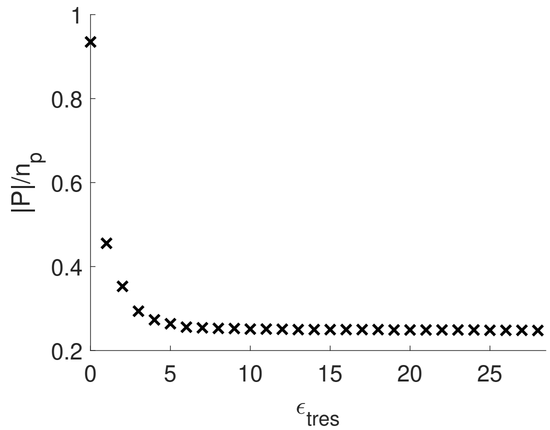

Fig. 5. Values of $|P|/n_p$ corresponding to $\varepsilon_{\text{thres}} \in \{0, 1, 2, \ldots, 28\}$

Fig. 6. NYnet

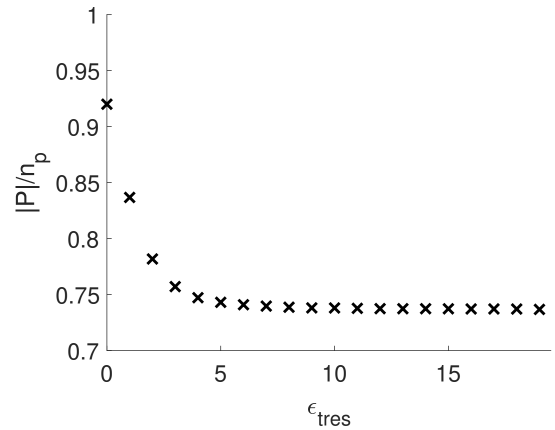

Fig. 7. Values of $|P|/n_p$ corresponding to $\varepsilon_{\text{thres}} \in \{0, 1, 2, \ldots, 19\}$