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Outer approximation methods for the solution of co-design optimisation problems in water distribution networks ⋆

Filippo Pecci * **Edo Abraham** ** **Ivan Stoianov** ***

* *Dept. of Civil and Environmental Engineering (InfraSense Labs), Imperial College London, London, UK, (f.pecci14@imperial.ac.uk).*
** *Faculty of Civil Engineering and Geosciences, TU Delft, Stevinweg 1, 2628 CN Delft, the Netherlands, (e.abraham@tudelft.nl)*
*** *Dept. of Civil and Environmental Engineering (InfraSense Labs), Imperial College London, London, UK ,(ivan.stoianov@imperial.ac.uk)*

Abstract: In the present manuscript, we investigate and demonstrate the use of outer approximation methods for simultaneously optimising the placement and operation of control valves in water distribution networks. The problem definition results in a mixed-integer nonlinear program with nonconvex constraints. We simplify the formulation, compared to previous literature, in order to reduce the degree of nonlinearity in the constraints and decrease the total problem size. We then formulate the application of outer approximation based methods for the generation of good quality local optimal solutions for the considered co-design problem. Finally, we present the results of applying the developed techniques to two case studies, and also comparing the performances of the outer approximation approaches with those of other local mixed integer nonlinear programming solution methods.

Keywords: Optimization and control of large-scale network systems, Water supply and distribution systems, Optimal operation of water resources systems.

1. INTRODUCTION

The management of water distribution networks (WDNs) faces increasing operational challenges due to growing water demand, ageing infrastructure and more stringent environmental standards. Efficient operation of WDNs requires the satisfaction of multiple objectives, ranging from reduction of leakage to the improvement of network resilience and water quality. Consequently, advances in optimisation and control strategies are needed to support the design and operation of WDNs. Significant reduction in leakage can be achieved when the network pressure is maintained as close as possible to a minimum service level. For example, the UK water regulator Ofwat defines this service level as a minimum pressure of 10m that must be maintained at the boundary of a property in order to deliver 9 l/minute flow. In addition, optimal pressure management can be used to improve resilience and water quality, see Pecci et al. (2016c) and Abraham et al. (2016), respectively. In the present work, we consider pressure management that is actuated by control valves. These network controllers can be operated to reduce pressure at their downstream node or they can be closed. We consider the co-design problem of optimising both the valve locations and control settings, simultaneously.

The mathematical formulation for optimal valve placement and operation presents significant challenges as it requires the solution of a nonlinear optimisation problem with both continuous and discrete variables – a mixed integer nonlinear program (MINLP). In particular, nodal pressures and pipe flows are considered as continuous decision variables, while binary variables are introduced to model the placement of valves. Mass and energy conservation laws are enforced as optimisation constraints at each node and pipe of the network, respectively. The bidirectional nature of flow across pipes complicates the mathematical formulation of energy conservation laws, resulting in nonconvex constraints Eck and Mevissen (2012); Dai and Li (2014); Pecci et al. (2016a). An additional physical constraint from the control valves enforces the pressure differential across the control valves to be in the same direction as the flow through the valve. This constraint has so far been modelled by introducing highly nonlinear nonconvex equations and two links with unidirectional flows to model each physical pipe - see Eck and Mevissen (2012); Dai and Li (2014); Pecci et al. (2016a). This problem formulation includes high-order nonconvex constraints and it is difficult to solve.

In this paper, a new problem formulation is proposed that reduces the degree of nonlinearity in the constraints and, in addition, it reduces the total problem size. The reformulated problem is a nonconvex mixed integer nonlinear program where only bidirectional flow variables are involved in nonlinear expressions, while the other variables appear linearly in the optimisation constraints. Global solution approaches for nonconvex MINLP problems couple the generation of convex envelopes to formulate lower bounding convex MINLP problems with computationally expensive global optimisation techniques. For a complete review, please refer to Belotti et al. (2013). In comparison, the direct application of convex optimisation tools generally requires less computational effort it but does not guarantee global optimality for nonconvex MINLP problems. Nonetheless, the practical implementation of such mathemat-

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ical programming approaches can generate good quality local solutions, without theoretical guarantees for global optimality (Grossmann, 2002).

Since outer approximation (OA) algorithms are known to perform well on "mostly linear" MINLP problems (Grossmann, 2002), we investigative their use to solve the mixed integer program considered here, where the vast majority of optimisation variables appear linearly within the optimisation constraints of our reformulation. Using case studies, we show that the new method has much smaller computational complexity compared to other approaches used in literature for the solution of optimal valve placement and operation in water distribution networks (Eck and Mevissen, 2012; Dai and Li, 2014; Pecci et al., 2016a). Furthermore, the application of OA to the new problem formulation for the co-design control optimisation in WDNs has enabled the convergence to a (local) solution in large scale networks. To our best knowledge, the presented case study is the first example of a solution for the optimal valve placement and operation problem for a network of this size and number of time steps. We also show that the method generates good quality local solutions compared to the best known solutions for these problems. Although no theoretical guarantees can be given, this result is in line with expectation for outer approximation to find near optimal solution for nonconvex MINLPs.

2. PROBLEM FORMULATION

In the present formulation we model a water distribution network with n_0 water sources (eg. reservoirs or tanks), n_n nodes and n_p pipes, as an undirected graph (V,E), with n_n+n_0 vertices and n_p links. Moreover, we consider control over a typical 24 hour horizon and we include in the formulation $n_l = 24$ different demand scenarios. Let $t \in \{1,...,n_l\}$ be a time step. We define the vectors of unknown hydraulic heads and flows as $h^t := [h^t_1 \dots h^t_{n_n}]^T$ and $q^t := [q^t_1 \dots q^t_{n_p}]^T$, respectively. Each node i has known elevation e_i and demand d^t_i. Hydraulic heads at the water sources are known and denoted by h^t_{0i} for each $i = 1,...,n_0$. Finally, let link j have flow q^t_j going from node i_1 to node i_2 and maximum allowed flow defined by q^{max}_j, $\forall i_1 \xrightarrow{j} i_2$, $j = 1,\dots,n_p$. The friction head loss across a pipe j at time t can be represented by either the Hazen-Williams (HW) or Darcy-Weisbach (DW) formulae. In DW models the relation between friction head loss and flow is defined by an implicit semi-empirical equation, which involves non-smooth terms, and it can be numerically calculated through an iterative process. Similarly, HW formula is semi-empirical and non-smooth, since the second derivative of HW formula is unbounded around the origin (Larock et al., 1999, Sections 2.2.2 and 2.2.3) for details on these friction head loss formulae. For both DW and HW models, Eck and Mevissen (2015) propose the use of a quadratic approximation for head losses minimising the relative errors. In addition, Pecci et al. (2016b) proposed an alternative approximation scheme which minimises absolute errors. Both approaches can be used to determine a quadratic approximation for friction head losses. Once such quadratic approximation is identified, this can be represented as $\phi_j(q^t_j) := (a_j|q^t_j| + b_j)q^t_j$. Let $\Phi(q^t) := [\phi_1(q^t_1),\dots,\phi_{n_p}(q^t_{n_p})]^T$, for each $t \in \{1,\dots,n_l\}$. In addition, we have the node-edge incidence matrices $A^T_{12} \in \mathbb{R}^{n_n \times n_p}$ and $A^T_{10} \in \mathbb{R}^{n_0 \times n_p}$ for the n_n nodes and the n_0 water sources, respectively. Finally, since we aim to solve a co-design problem for optimal valve placement and control we introduce the vectors of unknown binary variable $v^+ \in \{0,1\}^{n_p}$ and $v^- \in \{0,1\}^{n_p}$, where for each $k = 1,\dots,n_p$ we have

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

Now let t be a time step in $\{1,\dots,n_l\}$ and $j \in \{1,\dots,n_p\}$ with $i_1 \xrightarrow{j} i_2$. We define the positive constants ${N^+}^t_j := (h^t_{max})_{i_1} - (h^t_{min})_{i_2}$ and ${N^-}^t_j := (h^t_{max})_{i_2} - (h^t_{min})_{i_1}$, where $(h^t_{max})_i$ and $(h^t_{min})_i$ are the maximum and minimum possible hydraulic head at node i and time t, respectively.

Let ${N^+}^t := \mathtt{diag}({N^+}^t_1,\dots,{N^+}^t_{n_p}) \in \mathbb{R}^{n_p \times n_p}$, and ${N^-}^t := \mathtt{diag}({N^-}^t_1,\dots,{N^-}^t_{n_p}) \in \mathbb{R}^{n_p \times n_p}$ be the diagonal matrices of big-N's while $Q^{max} := \mathtt{diag}(q^{max}_1,\dots,q^{max}_{n_p}) \in \mathbb{R}^{n_p \times n_p}$ is the diagonal matrix of maximum allowed flows.

Wright et al. (2015) have considered the problem of optimising control settings of pressure reducing valves whose locations are known. The action of each valve is modelled by an additional variable representing the head loss introduced by the controller. In the present manuscript, we take a similar approach for representing the head loss and consider a vector of unknown additional head losses $\eta^t := [\eta^t_1 \dots \eta^t_{n_p}]^T$. However, since the locations of the valves are themselves unknown, linear constraints are introduced to model the presence of a valve for a particular link. We can define the following vector of continuous unknowns:

$$x := [{q^1}^T \, {h^1}^T \, {\eta^1}^T \cdots {q^{n_l}}^T \, {h^{n_l}}^T \, {\eta^{n_l}}^T]^T$$

Assume the objective to be minimised is a convex C^2 function $f : (x, v^+, v^-) \longmapsto f(x, v^+, v^-)$.

The optimisation problem for valve placement and operation can be formulated as:

$$\begin{aligned}
&\min f(x, v^+, v^-) \\
&\text{s.t. } \Phi(q^t) + A_{12}h^t + \eta^t + A_{10}h^t_0 = 0, \quad t = 1,\dots,n_l, && \text{(1a)}\\
&\quad A^T_{12}q^t - d^t = 0, \quad t = 1,\dots,n_l, && \text{(1b)}\\
&\quad \eta^t - {N^+}^t v^+ \leq 0, \quad t = 1,\dots,n_l, && \text{(1c)}\\
&\quad -\eta^t - {N^-}^t v^- \leq 0, \quad t = 1,\dots,n_l, && \text{(1d)}\\
&\quad -q^t + Q^{max}v^+ \leq q^{max}, \quad t = 1,\dots,n_l, && \text{(1e)}\\
&\quad q^t + Q^{max}v^- \leq q^{max}, \quad t = 1,\dots,n_l, && \text{(1f)}\\
&\quad h^t \leq h^t_{max}, \quad t = 1,\dots,n_l, && \text{(1g)}\\
&\quad -h^t \leq -h^t_{min}, \quad t = 1,\dots,n_l, && \text{(1h)}\\
&\quad v^+ + v^- \leq \mathbf{e}, && \text{(1i)}\\
&\quad \sum_{k=1}^{n_p}(v^+_k + v^-_k) = n_v, && \text{(1j)}\\
&\quad v^+, v^- \in \{0,1\}^{n_p}. && \text{(1k)}
\end{aligned}$$

where $\mathbf{e} := [1 \dots 1]^T \in \mathbb{R}^{n_p}$. Constraints (1a) and (1b) represent hydraulic energy and mass conservation laws, respectively. Additionally, the linear constraints (1c)-(1f) are used to ensure that the direction of the flow through the valve is in accordance with the direction of the induced additional head loss, as we show in the following. Let $v^+_j = v^-_j = 0$. From (1c) and (1d) we have that $\eta_j^t = 0, \forall t$; in addition, (1e) and (1f) ensure that the direction of the flow through the link j is not constrained. On the other had, $v_j^+ = 1$, $v_j^- = 0$ imply $\eta_j^t \geq 0, q_j^t \geq 0$, $\forall t$. Similarly, $v_j^+ = 0$, $v_j^- = 1$ enforce that $\eta_j^t \leq 0, q_j^t \leq 0$, $\forall t$. As a result, in our problem formulation, once the direction of operation of a control valve is chosen, we do not allow such direction to change during the day. This assumption is not too restrictive, as it represents the standard operation of pressure reducing valves, which regulate pressure at their downstream node. Finally, linear bounds (1g) - (1j) represent physical, operational and economical constraints on the range of possible nodal hydraulic heads and number of installed valves.

We conclude this section by writing Problem (1) is a more compact form. Let $c^t : \mathbb{R}^{n_l(n_n+2n_p)} \to \mathbb{R}^{n_p}$ be the function whose components correspond to the rows of constraints in (1a), for every t. In addition, define the following compact polyhedral set:

$$V := \left\{(v^+, v^-) \in \{0,1\}^{n_p} \times \{0,1\}^{n_p} \,|\, (v^+, v^-) \text{ satisfies (1i),(1j)}\right\}.$$

In addition, given $(v^+, v^-) \in V$, we consider the compact polyhedral set :

$$X(v^+, v^-) := \left\{x \in \mathbb{R}^{n_l(n_n+2n_p)} \,|\, x \text{ satisfies (1b)-(1h)}\right\}.$$

Problem (1) can be rewritten as:

$$\begin{aligned} &\min f(x, v^+, v^-) \\ &\quad \text{s.t. } c^t(x) = 0, \quad t = 1, \ldots, n_l, \\ &\qquad x \in X(v^+, v^-), \\ &\qquad (v^+, v^-) \in V. \end{aligned} \tag{P}$$

Given binary vectors $\hat{v}^+, \hat{v}^- \in V$, we can define the following nonlinear program:

$$\begin{aligned} &\min \tilde{f}(x) \\ &\quad \text{s.t } c^t(x) = 0, \quad t = 1, \ldots, n_l, \\ &\qquad x \in X(\hat{v}^+, \hat{v}^-). \end{aligned} \tag{NLP($\hat{v}^+, \hat{v}^-$)}$$

where $\tilde{f}(\cdot) := f(\cdot, \hat{v}^+, \hat{v}^-)$. Note that the solution of (NLP($\hat{v}^+, \hat{v}^-$)) yields an upper bound to (P), provided it has at least one feasible solution.

Since their nonlinear constraints are nonconvex, both problems (P) and (NLP($\hat{v}^+, \hat{v}^-$)) are nonconvex. Note that the nonconvexity is due to the presence of the friction head loss terms, whose second order derivatives involves the sign($\cdot$) function.

Problem (P) has $n_l(3n_n + 4n_p) + n_p + 1$ linear constraints and $n_l n_p$ nonlinear constraints. Moreover, only $n_l n_p$ variables are involved in nonlinear functions, while the remaining $n_l(n_n + n_p) + 2n_p$ unknowns appear linearly in all the constraints. This is the main difference between the problem formulation for optimal valve placement proposed in the present work and the one considered in Eck and Mevissen (2012); Dai and Li (2014); Pecci et al. (2016a). In fact, energy conservation across pipes and valves is modelled by nonlinear constraints (1a) and linear constraints (1c), (1d). In comparison, in Eck and Mevissen (2012); Dai and Li (2014); Pecci et al. (2016a), this is expressed by two nonlinear inequalities, one of them being a polynomial expression of degree 3 involving both flow and hydraulic head variables. In conclusion, the introduction of the vectors η^t together with linear constraints (1c) and (1d) results in a simplification of the problem formulation.

3. OUTER APPROXIMATION

In the present section we outline the application of an outer-approximation (OA) method for the solution of (P). Such approach is based on the solution of an alternating sequence of nonlinear programs (NLP) subproblems (obtained fixing the integer variables to particular values) and linear relaxations of the original mixed integer nonlinear program (MINLP). For a more general description of the OA algorithm and its properties we refer the reader to (Floudas, 1995, Sections 6.4-6.7).

Since the formulation of Problem (P) includes nonlinear equality constraints, we consider an Equality-Relaxation (OA/ER) variant to the standard outer approximation algorithm, as presented in Kocis and Grossmann (1987) and (Floudas, 1995, Section 6.5), where a detailed discussion of its theoretical properties can be found. In particular, outer approximation approaches are expected to perform well for the considered problem formulation, where many of the constraints and variables are linear (Grossmann, 2002). On the other hand, we have already observed that (P) is nonconvex, as it involves nonconvex nonlinear constraints. Consequently, OA/ER will not provide any global optimality guarantee and it is expected to generate local optimal solutions (Grossmann, 2002). Nonetheless, as reported also in Section 4, the application of the OA/ER method to nonconvex problems often produces solutions close to the global optimum (Grossmann, 2002). Moreover, we also consider a practical heuristic modification of the OA/ER which tries to minimise, the effects of nonconvex constraints as proposed in Viswanathan and Grossmann (1990).

Let a sequence $\{\hat{v}^+_{(k)}, \hat{v}^-_{(k)}\}_{k \in \mathscr{F} \cup \mathscr{N}} \subset V$ be defined as follows: if $k \in \mathscr{F}$, then (NLP($\hat{v}^+_{(k)}, \hat{v}^-_{(k)}$)) is feasible and we indicate with $\hat{x}_{(k)}$ a solution of such problem; on the contrary, if $k \in \mathscr{N}$, we have that (NLP($\hat{v}^+_{(k)}, \hat{v}^-_{(k)}$)) is not feasible. Let $k \in \mathscr{F}$ and $\hat{x}_{(k)}$ be the solution of (NLP($\hat{v}^+_{(k)}, \hat{v}^-_{(k)}$)). The associated vector of optimal Lagrange multipliers corresponding to the nonlinear constraints $c^t(\cdot)$ is denoted by $\lambda^t_{(k)} \in \mathbb{R}^{n_p}$, for all $t = 1, \ldots, n_l$. We define a diagonal matrix $S^t \in \mathbb{R}^{n_p \times n_p}$ given by:

$$S^t_{(k)}(j,j) := \begin{cases} -1 & \text{if } {\lambda_{(k)}}^t_j < 0 \\ \ \ 0 & \text{if } {\lambda_{(k)}}^t_j = 0 \\ +1 & \text{if } {\lambda_{(k)}}^t_j > 0 \end{cases} \tag{2}$$

for every $t = 1, \ldots, n_l$.

Following the formulation in Kocis and Grossmann (1987), we define the following MILP master problem:

$$\begin{aligned} &\min \mu \\ &\quad \text{s.t. } \mu \geq \widehat{f} + \widehat{\nabla f}^T \begin{bmatrix} x - \hat{x}_{(k)} \\ v^+ - \hat{v}^+_{(k)} \\ v^- - \hat{v}^-_{(k)} \end{bmatrix}, \quad \forall k \in \mathscr{F}, \\ &\qquad S^t_{(k)} \widehat{J}^t (x - \hat{x}_{(k)}) \leq 0, \ t = 1, .., n_l, \forall k \in \mathscr{F}, \\ &\qquad x \in X(v^+, v^-), \\ &\qquad (\hat{v}^+_{(k)})^T v^+ + (\hat{v}^-_{(k)})^T v^- \leq n_v - 1, \quad \forall k \in \mathscr{F} \cup \mathscr{N}, \\ &\qquad (v^+, v^-) \in V. \end{aligned} \tag{M($\mathscr{F}, \mathscr{N}$)}$$

where $J^t(\cdot)$ is the Jacobian matrix of the function $c^t(\cdot)$ for all $t \in \{1, \ldots, n_l\}$. Moreover, for all $k \in \mathscr{F}$, we have set $\widehat{f} := f(\hat{x}_{(k)}, \hat{v}^+_{(k)}, \hat{v}^-_{(k)})$, $\widehat{\nabla f} := \nabla f(\hat{x}_{(k)}, \hat{v}^+_{(k)}, \hat{v}^-_{(k)})$, and $\widehat{J}^t := J^t(\hat{x}_{(k)})$.

The OA/ER method implemented in the present work is described in Algorithm 1. Viswanathan and Grossmann (1990) proposed a strategy for the computation of an initial integer vector; in the case considered here, the initialisation procedure is simplified since the algorithm can start from the vector corresponding to a configuration where no valve is installed. Analogously, the initial guess of each nonlinear program corresponds to a solution of the hydraulic equations where no valve is considered. The study of tailored initialisation strategies that promote convergence towards global optima is subject of future research. The algorithm terminates with a feasible solution $(x_{\text{best}}, v^+_{\text{best}}, v^-_{\text{best}})$ and corresponding objective function value f_{best}, which represents an upper bound to the the optimal objective function value of (P). Since the considered nonlinear constraints are nonconvex, the solution of $(\mathrm{M}(\mathscr{F},\mathscr{N}))$ does not provide a valid lower bound to (P), unlike the convex case. Therefore, in our case, we do not use the termination criterion $\mu_{(k)} \geq f_{\text{best}}$ as in Kocis and Grossmann (1987). Algorithm 1 stops when the objective function evaluated at successive feasible solutions is no more decreasing, as suggested in Viswanathan and Grossmann (1990).

Algorithm 1 OA/ER Algorithm from Kocis and Grossmann (1987) where binary cuts are used to discard infeasible integer solutions

Initialization:
  Set $\mathscr{F} = \emptyset$, $\mathscr{N} = \emptyset$, $f_{\text{best}} = +\infty$,
  $\hat{v}^+_{(0)} = \hat{v}^-_{(0)} = 0$.
while $(\mathrm{M}(\mathscr{F},\mathscr{N}))$ is feasible **do**
  if $(\mathrm{NLP}(\hat{v}^+_{(k)}, \hat{v}^-_{(k)}))$ is infeasible **then**
    $\mathscr{N} := \mathscr{N} \cup \{k\}$.
  else
    Let $\hat{x}_{(k)}$ be a solution for $(\mathrm{NLP}(\hat{v}^+_{(k)}, \hat{v}^-_{(k)}))$
    Set $\mathscr{F} := \mathscr{F} \cup \{k\}$
    if $f(\hat{x}_{(k)}, \hat{v}^+_{(k)}, \hat{v}^-_{(k)}) < f_{\text{best}}$ **then**
      $f_{\text{best}} := f(\hat{x}_{(k)}, \hat{v}^+_{(k)}, \hat{v}^-_{(k)})$;
      $v^+{}_{\text{best}} := \hat{v}^+_{(k)}$; $v^-{}_{\text{best}} := \hat{v}^-_{(k)}$; $x_{\text{best}} := \hat{x}_{(k)}$;
    else
      Stop
    end if
  end if
  Solve $(\mathrm{M}(\mathscr{F},\mathscr{N}))$ obtaining $\hat{v}^+_{(k+1)}, \hat{v}^-_{(k+1)}$.
  Set $k = k+1$.
end while

Finally, note that constraints

$$(\hat{v}^+_{(k)})^T v^+ + (\hat{v}^-_{(k)})^T v^- \leq n_v - 1, \quad \forall k \in \mathscr{F} \cup \mathscr{N}, \tag{3}$$

are introduced to prevent a binary solution from repeating itself. In particular, it ensures that if a binary choice corresponds to an infeasible NLP this is discarded from the optimisation process. These binary cuts are weak when the number of binary unknowns is large, as observed in Grossmann (2002). However, they avoid the solution of an additional feasibility NLP problem when an infeasible binary choice is generated - see the discussion in Fletcher and Leyffer (1994) where general integer constraints are considered.

In the practical experience of the authors, once the locations of the valves are chosen, the optimisation of their operation using standard NLP solvers always generates a near-optimal solution, even though such a Problem is nonconvex - see also Wright et al. (2015). The main effect of the nonconvexity of the constraints is observed in the solution of $(\mathrm{M}(\mathscr{F},\mathscr{N}))$. In fact, the linear constraints in $(\mathrm{M}(\mathscr{F},\mathscr{N}))$ do not represent a valid outer approximation of the nonconvex feasibility region and can exclude feasible solutions preventing Algorithm 1 from converging to the global optimum of (P). In order to contrast such phenomenon, the work in Viswanathan and Grossmann (1990) suggests the introduction of slack variables to allow controlled violations of the linear constraints in $(\mathrm{M}(\mathscr{F},\mathscr{N}))$. Recall that we denote with $\lambda^t_{(k)}$ the Lagrange multipliers associated to the constraints $c^t(\cdot)$ and corresponding to a local optimal solution of $(\mathrm{NLP}(\hat{v}^+_{(k)}, \hat{v}^-_{(k)}))$, for all $t = 1, \ldots, n_l$ and $k \in \mathscr{F}$. We can define an augmented penalty (AP) objective function and formulate the following MILP master problem:

$$\begin{aligned}
&\min \ \mu + \sum_{k\in\mathscr{F}} \sum_{t=1}^{n_l} \alpha^t_{(k)} \rho^t_k \\
&\text{s.t. } \mu \geq \widehat{f} + \widehat{\nabla f}^T \begin{bmatrix} x - \hat{x}_{(k)} \\ v^+ - \hat{v}^+_{(k)} \\ v^- - \hat{v}^-_{(k)} \end{bmatrix}, \quad \forall k \in \mathscr{F}, \\
&\quad S^t_{(k)} \widehat{J}^t (x - \hat{x}_{(k)}) \leq \rho^t_k, \ t = 1,..,n_l, \forall k \in \mathscr{F}, \\
&\quad x \in X(v^+, v^-), \\
&\quad (\hat{v}^+_{(k)})^T v^+ + (\hat{v}^-_{(k)})^T v^- \leq n_v - 1, \quad \forall k \in \mathscr{F} \cup \mathscr{N}, \\
&\quad (v^+, v^-) \in V, \\
&\quad \rho^t_k \geq 0, \quad t = 1,..,n_l, \quad \forall k \in \mathscr{F}.
\end{aligned} \tag{$\mathrm{R}(\mathscr{F},\mathscr{N})$}$$

where $\alpha^t_{(k)} := 10^3 |\lambda^t_{(k)}|$, as suggested in Viswanathan and Grossmann (1990). The AP/OA/ER method is described in detail in Viswanathan and Grossmann (1990); in this work, the considered AP/OA/ER algorithm is analogous to Algorithm 1, where $(\mathrm{M}(\mathscr{F},\mathscr{N}))$ is substituted by $(\mathrm{R}(\mathscr{F},\mathscr{N}))$.

3.1 Global optimality bounds

Since the problem considered here is nonconvex, both OA/ER and AP/OA/ER can not provide theoretical guarantee of global optimality. The application of global optimisation approaches (e.g. the method proposed in D'Ambrosio et al. (2012)) can be computationally impractical for large scale instances. Alternatively, it is possible to compute tight global optimality bounds using some "convexification" of (P). Future research will consider this strategy.

4. NUMERICAL EXPERIENCE

The optimisation methods presented in Section 3 are applicable provided the objective is a smooth convex function. As an example application, here we consider the minimisation of pressure driven leakage. The average zone pressure (AZP), which is an indicator for the level of leakage in the zone of the network being controlled Lambert (2001), is used as the objective function to be minimised. The AZP is defined as:

$$f(x, v^+, v^-) := \frac{1}{n_l W} \sum_{t=1}^{n_l} \sum_{i=1}^{n_n} w_i (h^t_i - e_i) \tag{4}$$

where $w_i = \sum_{j \in I(i)} L_j / 2$ and $I(i)$ is the set of indices for links incident at node i, counted only once. Moreover, we have a normalization factor $W = \sum_{i=1}^{n_n} w_i$.

In this study, the commercial solver `Gurobi` (Gurobi Optimization, 2016) is applied for the solution of all the MILPs considered by OA/ER and AP/OA/ER methods. In addition, the solution of each (NLP($\hat{v}^+, \hat{v}^-$)), corresponding to a specific choice of valve locations, is performed by the solver Ipopt (Waechter and Biegler, 2006) .

4.1 Case study 1

In order to provide a preliminary numerical experiments on the proposed OA/ER and AP/OA/ER methods, we consider the same benchmarking water network studied in Eck and Mevissen (2012); Dai and Li (2014); Pecci et al. (2016a). Such network as 22 nodes, 3 water sources and 37 pipes; in our optimisation framework we consider a control over a typical diurnal operation with 24 different demand conditions - see Figure 1. The minimum hydraulic head is set to $e_i + 30m$ for all nodes $i \in \{1, \ldots, n_n\}$, while we set the maximum velocity allowed to $1\,\frac{m}{s}$ in every pipe. The quadratic approximation for friction head losses is chosen so that it minimises absolute errors, as shown in Pecci et al. (2016b).

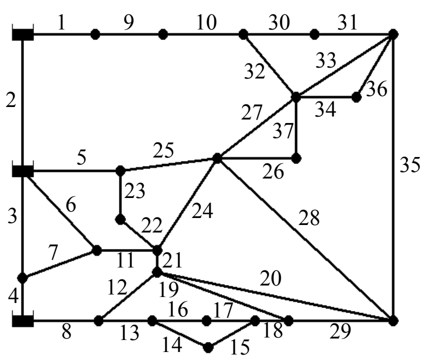

Fig. 1. Benchmarking network layout

Table 1 reports the number of continuous and binary variables together with the number of nonlinear and linear constraints.

Table 1. Problem size characteristics

No. cont. var.	No. bin. var.	No. lin. const.	No. nonlin. const.
2304	74	5174	888

In the present study we consider the number of valves to be installed in the network ranging from 1 to 5 - so we have $n_v \in \{1, \ldots, 5\}$. For each value of n_v we have applied the OA/ER and OP/OA/ER methods to determine local optimal solutions to Problem (P). Furthermore, we have applied the mixed-integer nonlinear programming solver Bonmin (Bonami et al., 2008) with branch-and-bound algorithm (B-BB) to determine a local optimal solution for Problem (P).

In Table 2 we report the optimisation results obtained from the solver Bonmin. In comparison with previous literature, the application of Bonmin resulted in the best known local solutions for the case study.- this was observed also in Pecci et al. (2016a) where a different problem formulation was used to solve optimal valve placement and operation for the same benchmarking network. Tables 3 and 4 show the results obtained from the application of OA/ER and AP/OA/ER, respectively. In particular, in Tables 2-4, the 'Link' column includes the indices of the computed valve locations, with reference to Figure 1, while the 'AZP' column lists the corresponding values of the objective function.

Table 2. Local solutions obtained by the solver Bonmin, together with computational performances.

n_v	Link	AZP	CPU time	B-BB iter
1	11	33.63 m	9 s	69
2	11, 1	32.67 m	396 s	3114
3	11, 1, 21	32.16 m	606 s	13667
4	11, 1, 21, 8	31.75 m	878 s	21381
5	11, 1, 21, 8, 20	31.47 m	3306 s	116243

Table 3. Local solutions obtained by the OA/ER algorithm and computational performances.

n_v	Link	AZP	CPU time	OA/ER iter
1	11	33.63 m	0.87 s	2
2	11, 1	32.67 m	1.18 s	2
3	11, 1, 5	32.46 m	1.5 s	2
4	11, 1, 5, 21	31.95 m	1.27 s	2
5	11, 1, 5, 21, 8	31.75 m	1.27 s	2

Table 4. Local solutions obtained by the AP/OA/ER algorithm and computational performances.

n_v	Link	AZP	CPU time	AP/OA/ER iter
1	11	33.63 m	2.05 s	3
2	11, 1	32.67 m	2.60 s	3
3	11, 1, 5	32.46 m	6.00 s	3
4	11, 1, 5, 21	31.95 m	5.80 s	3
5	11, 1, 5, 21, 20	31.56 m	14.00 s	4

The two proposed algorithms converged to the same local solutions in most cases. The only exception is encountered for $n_v = 5$, when AP/OA/ER has converged to solution with a slightly lower AZP than OA/ER. Nonetheless, in all cases, the outer approximation based methods have converged to solutions with AZP values very close to the best known solutions obtained from Bonmin.

Furthermore, from Table 3 we observe that the OA/ER method has converged after only two iterations in all the scenarios considered here. Such good computational performance was expected; in fact, as discussed in Section 2, only a minority of optimisation constraints and variables are nonlinear -see also Table 1. The OA/ER algorithm is known to be computationally efficient on mostly linear problems Grossmann (2002). With reference to the computational time reported in Table 3, we observe a reduction of up to three orders with respect to what reported for Bonmin - see Table 2. The solution of the optimal valve placement and operation problem for the considered case study was also studied in Eck and Mevissen (2012); Dai and Li (2014); Pecci et al. (2016a). A different, highly nonlinear problem formulation was presented and the binary constraints were reformulated through the use of penalization and relaxation schemes showing a reduction in computational time with respect to the application of Bonmin. Nonetheless, the computational time required by the OA/ER algorithm to converge is at least one order smaller that what reported in Eck and Mevissen (2012); Dai and Li (2014); Pecci et al. (2016a), while maintaining good quality of the solutions.

4.2 Case study 2

We now consider the Smart Water Network Demonstrator operated by Bristol Water, InfraSense Labs at Imperial College London and Cla-Val presented in Wright et al. (2015) - in the following we refer to the case study model as BWFLnet. This water supply network consists of 2374 nodes, 2434 pipes and 2 inlets (with fixed known hydraulic heads); its graph and elevation map is presented in Figure 2. BWFLnet is composed of two interconnected District Metered Areas (DMAs) and it is currently operated with a dynamic topology Wright et al. (2015). Two originally closed boundary valves (BVs) between the DMAs have been replaced by two dynamic boundary valves (DBVs) that are closed at night hours and open during diurnal network operation. Three pressure reducing valves (PRVs) are optimally operated in order to minimise AZP. The network model and control options have been expanded from the model presented in Wright et al. (2015). The quadratic approximation proposed in Eck and Mevissen (2015) is used to model friction losses within the BWFLnet, where the maximum velocity in each pipe is set to $8\,\frac{m}{s}$.

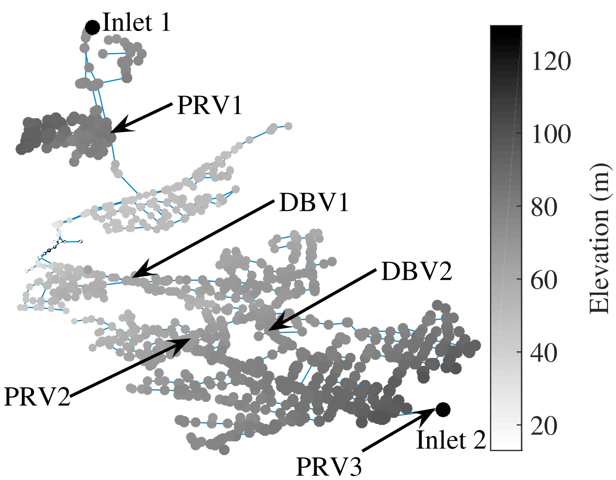

Fig. 2. BWFLnet network model

In the present formulation we consider 24 different demand conditions, one for each hour of the day. We model the existing PRVs as open smooth pipes. Moreover, the operation of the two DBVs is embedded within the optimisation constraints by varying in time the coefficients of the quadratic head loss approximation to model the valves opening and closing. Details on the operation of the DBVs have been provided by the valves' manufacturer. The links corresponding to the DBVs are excluded from the set of possible valve locations. In addition, for all the nodes $i \in \{1,\ldots,n_n\}$, we set a minimum hydraulic head requirement of $e_i + 18\,m$.

We formulate Problem (1) for the optimal placement and operation of 3 control valves, addressing the minimisation of AZP. The number of continuous variables, binary variables and constraints is reported in Table 5.

Table 5. Problem size characteristics for the second case study

No. cont. var.	No. bin. var.	No. lin. const.	No. nonlin. const.
221808	4864	407027	58412

The OA/ER method outlined in Algorithm 1 was applied to the considered case study. Convergence was achieved after two iterations requiring a CPU time of $8198\,s$. The optimal locations on V_1^*, V_2^*, V_3^* are presented in Figure 3 and corresponds to an AZP of $36.72\,m$. In comparison, the AZP corresponding to the optimal operation of PRV1, PRV2 and PRV3 is $37.02\,m$. Therefore, new valve locations result in a reduction of the objective function compared to the actual valve configuration. To the best of authors' knowledge, the presented case study is the only example of solution of the optimal valve placement and operation problem for a large network as BWFLnet when considering multiple demand conditions. The reported computational results show that the OA algorithm represents a scalable approach for the large scale mixed integer nonlinear programs arising in the framework of water distribution networks. Finally, both the MINLP solver `Bonmin` and the reformulation approaches considered in Pecci et al. (2016a) were applied to the same problem formulation but failed to converge.

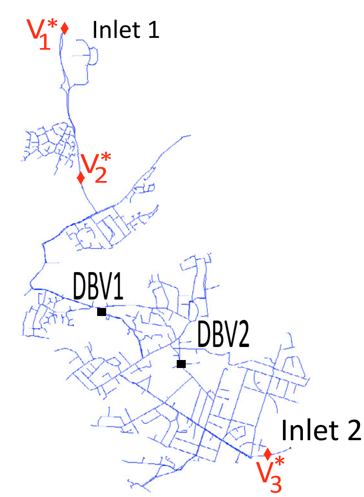

Fig. 3. Optimal valve placement found by the OA/ER method

5. CONCLUSIONS

We have proposed a new problem formulation of the optimal valve placement and operation problem, where different objectives can be considered. The newly reformulated optimisation constraints have a lower degree of nonlinearity with respect to those commonly presented in literature. The resulting optimisation problem is a nonconvex mixed integer nonlinear program with mostly linear constraints. We have investigated the application of outer approximation approaches for the solution of the problem in study. We have presented two outer approximation algorithms and implemented them for the solution of the optimal valve placement and operation problem where the minimization of average zone pressure is the objective. We have considered two case studies, a published benchmarking network and the hydraulic model of a large operational water distribution network from the UK. The computational results are promising and show that the considered methods are scalable approaches for the solution of the large scale mixed integer nonlinear programs arising in the framework of water distribution networks. In particular, the proposed approach has enabled the convergence to a (local) solution in a large problem instance. In comparison with previous literature, the presented case study is the only example of solution of the optimal valve placement and operation problem for a large network as the one considered here, where the valves' operation is optimized under multiple demand conditions. In addition, although the presence of nonconvex constraints prevents theoretical global optimality guarantees, the outer approximation methods have resulted in good quality solutions, in practice. Future work will investigate the generation of rigorous global optimality bounds for the problem in study.

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