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

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The optimisation problem for optimal valve placement and operation is formulated as:

$$
\begin{aligned}
\text{minimise} \quad & \frac{1}{n_l W}\sum_{t=1}^{n_l} \mathbf{w}^T(\mathbf{h}^t - \boldsymbol{\xi}) \\
\text{subject to} \quad & \boldsymbol{\Phi}(\mathbf{q}^t) + \mathbf{A_{12}}\mathbf{h}^t + \boldsymbol{\eta}^t + \mathbf{A_{10}}\mathbf{h_0}^t = 0, \quad t = 1,\dots,n_l, && \text{(1a)}\\
& \mathbf{A_{12}}^T\mathbf{q}^t - \mathbf{d}^t = 0, \quad t = 1,\dots,n_l, && \text{(1b)}\\
& \boldsymbol{\eta}^t - \mathbf{M}^+\mathbf{z}^+ \le 0, \quad t = 1,\dots,n_l, && \text{(1c)}\\
& -\boldsymbol{\eta}^t - \mathbf{M}^-\mathbf{z}^- \le 0, \quad t = 1,\dots,n_l, && \text{(1d)}\\
& \mathbf{q}^t + \mathbf{Q}^{\max}\mathbf{z}^- \le \mathbf{q}^{\max}, \quad t = 1,\dots,n_l, && \text{(1e)}\\
& -\mathbf{q}^t + \mathbf{Q}^{\max}\mathbf{z}^+ \le \mathbf{q}^{\max}, \quad t = 1,\dots,n_l, && \text{(1f)}\\
& \mathbf{h}^t \le \mathbf{h}^t_{\max}, \quad t = 1,\dots,n_l, && \text{(1g)}\\
& -\mathbf{h}^t \le -\mathbf{h}^t_{\min}, \quad t = 1,\dots,n_l, && \text{(1h)}\\
& \mathbf{z}^+ + \mathbf{z}^- \le \mathbf{e}, && \text{(1i)}\\
& \sum_{j=1}^{n_p}(z_j^+ + z_j^-) = n_v, && \text{(1j)}\\
& \mathbf{z}^+, \mathbf{z}^- \in \{0,1\}^{n_p}, && \text{(1k)}
\end{aligned}
$$

where all mathematical symbols are defined as in the main manuscript.

Appendix I : Model Reduction

In this appendix, we described the implemented model reduction algorithm in details. Let P and V be initialised to the index sets of all network links and nodes, respectively. We also define empty index lists F, G, Y, and S. Sets G and F contain the indices of forest nodes and links, respectively. On the other hand, the indices of nodes and links discarded by contraction are assigned to sets Y and S, respectively. The present discussion adopts the following notation: 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. Since each time step can be considered separately, we omit the temporal index t in the description of the algorithmic development. We define $\mathbf{A} := \mathbf{A_{12}}(P,V)$.

Forest-Core decomposition

Let $V(j)$ be the index of a leaf node, i.e. such that the column $\mathbf{A}(:,j)$ has only one non-zero entry. Let $P(m)$ be the unique link connected to node $V(j)$ and let $V(k)$ be an unknown node connected to link $P(m)$ - see also Figure 1. Furthermore, we assume that $|\xi_{V(i)} - \xi_{V(k)}| \leq \varepsilon_{\text{tres}}$. Flow across link $P(m)$ is determined by the demand at $V(j)$:

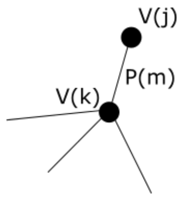

Fig. 1. Example of forest node and link.

$$q_{P(m)} = A(m, j)d_{V(j)} \tag{2}$$

Therefore, the value of $q_{P(m)}$ is known a priori and in order to ensure the satisfaction of mass balance at $V(j)$, we update the demand at $V(k)$:

$$d_{V(k)} \leftarrow d_{V(k)} + d_{V(j)} \tag{3}$$

and its minimum and maximum hydraulic head:

$$h_{\min}(V(k)) \leftarrow \max\left\{h_{\min}(V(j)) + A(m, j)d_{V(j)} \cdot (a_{P(m)}d_{V(j)} + b_{P(m)}),\, h_{\min}(V(k))\right\} \tag{4}$$

$$h_{\max}(V(k)) \leftarrow \min\left\{h_{\max}(V(j)) + A(m, j)d_{V(j)} \cdot (a_{P(m)}d_{V(j)} + b_{P(m)}),\, h_{\max}(V(k))\right\} \tag{5}$$

Provided that $\varepsilon_{\text{tres}}$ is sufficiently small, the assumption that no valve is placed on $P(m)$ will not result in a significantly sub-optimal solution. Finally, we move $V(j)$ from V to G and $P(m)$ from P to F and eliminate the $j-$th column and $m-$th row from matrix $\mathbf{A}$. The case of link $P(m)$ connecting to a fixed-head node follows similarly.

Trivial **loops**

Assume that $N+1$ nodes $V(k), V(j_1), \ldots, V(j_N)$ and links $P(m_1), \ldots, P(m_{N+1})$ form a *trivial loop* according to Definition 3.4 of the main manuscript - see Figure 2. Each link involved in such a loop is not to be considered a candidate for valve placement. The following holds:

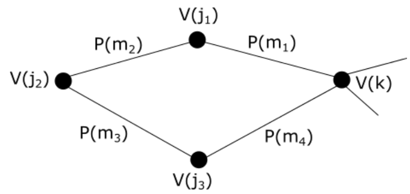

Fig. 2. A loop composed by zero-demand nodes. In this example, N=3.

$$q_{P(m_i)} = 0, \quad \forall i = 1, \ldots, N+1 \tag{6}$$

$$h_{V(j_i)} = h_{V(k)}, \quad \forall j = i = 1, \ldots, N \tag{7}$$

and we update the the minimum and maximum hydraulic head at $V(k)$:

$$h_{\min}(V(k)) \leftarrow \max\left\{h_{\min}(V(j_1)), \ldots, h_{\min}(V(j_N)), h_{\min}(V(k))\right\} \tag{8}$$

$$h_{\max}(V(k)) \leftarrow \min\left\{h_{\max}(V(j_1)), \ldots, h_{\max}(V(j_N)), h_{\max}(V(k))\right\}. \tag{9}$$

The considered nodes and links can be handled as member of the forest, moving them to G and F, respectively.

Pipe contraction

Consider a sequence of candidate links for contraction into a pseudo-link as depicted in Figure 3, where $(V(i_j))_{j=0,\dots,N+1}$ are a sequence of nodes defined as follows. Given $j \in \{1,\dots,N\}$, assume that node $V(i_j)$ has zero demand and is connected only to $V(i_{j-1})$ and $V(i_{j+1})$ by links $P(l_{j-1})$ and $P(l_j)$, respectively. Assume that nodes $V(i_0)$ and $V(i_{N+1})$ either have non-zero demand or they are connected to more than two links. In addition, since we want to preserve links with high elevation variation between their start and end nodes, we consider the case where

$$|\xi_{V(i_{k-1})} - \xi_{V(i_k)}| \leq \varepsilon_{tres}, \quad \forall k = 1,\dots,N+1 \tag{10}$$

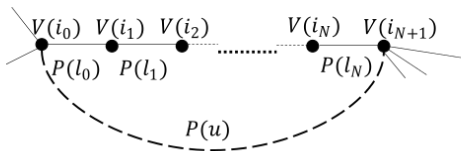

Fig. 3. Example of node sequence considered for contraction into the pseudo-link $P(u)$

Mass conservation constraints (1b) at nodes $V(i_0),\dots,V(i_1)$ are written as:

$$A(l_{j-1},i_j)q_{P(l_{j-1})} + A(l_j,i_j)q_{P(l_j)} = 0, \quad j = 1,\dots,N \tag{11}$$

The above equation implies that $q_{P(l_j)} = q_{P(l_0)}$, for all $j = 1,\dots N$ and hence $q^{max}_{P(l_j)} = q^{max}_{P(l_0)}$, for all $j = 1,\dots,N$. Energy conservation equations (1a), restricted on links $P(l_0),\dots,P(l_N)$, are:

$$A(l_k,i_k)h_{V(i_k)} + A(l_k,i_{k+1})h_{V(i_{k+1})} + q_{P(l_k)}(a_{P(l_k)}|q_{P(l_k)}| + b_{P(l_k)}) + \eta_{P(l_k)} = 0, \tag{12}$$

for $k = 0,\dots,N$. Similarly to the example ToyNet, we define a pseudo-link $P(u)$ between nodes $V(i_0)$ and $V(i_{N+1})$, with the following properties:

$$\begin{aligned} &A(u,i_0) := A(l_0,i_0), \quad A(u,i_{N+1}) := A(l_0,i_1), \quad q^{max}_{P(u)} := q^{max}_{P(l_0)} \\ &a_{P(u)} := \sum_{k=0}^{N} a_{P(l_k)}, \quad b_{P(u)} := \sum_{k=0}^{N} b_{P(l_k)} \end{aligned} \tag{13}$$

Furthermore, it is convenient to introduce additional variables $q_{P(u)}$, $\eta_{P(u)}$, $z^+_{P(u)}$ and $z^-_{P(u)}$. The conservation of energy for the pseudo-link is written as

$$A(u,i_0)h_{V(i_0)} + A(u,i_{N+1})h_{V(i_{N+1})} + q_{P(u)}(a_{P(u)}|q_{P(u)}| + b_{P(u)}) + \eta_{P(u)} \tag{14}$$

Nodes $\{V(i_j)\}_{j=1,\dots,N}$ are moved to Y while links $\{P(l_k)\}_{k=0,\dots,N}$ to S. The case of a sequence of nodes involving a fixed-head node can be dealt with analogously.

The outlined process terminates when all pipe sequences involving zero demand nodes have been considered. We observe that omitting the minimum operational pressure constraints at nodes discarded by pipe-contraction can result in infeasible solutions. Hence, we consider the following two-stage approach. Firstly, Problem (1) is solved for the reduced network model identified by (P,V); the resulting optimal valve locations are used to determine a restricted set of candidates among the links of the full scale network. There is the possibility that the resulting solution is sub-optimal, since the proposed scheme is ignoring operational pressure constraints at some discarded nodes. Nonetheless, if ε_{tres} is small enough, the sub-optimality will be limited - see the numerical results reported in the main manuscript. We re-introduce the time index $t \in \{1,\dots,n_l\}$ and define

$\mathbf{\Phi}_P(\mathbf{q}^t(P)) := \text{diag}(\phi_{P(1)}(q^t_{P(1)}), \ldots, \phi_{P(|P|)}(q^t_{P(|P|)}))$. The restriction of Problem (1) to the network defined by (P,V) can be formulated as follows:

$$
\begin{aligned}
\text{minimise} \quad & \frac{1}{n_l \hat{W}} \sum_{t=1}^{n_l} \hat{\mathbf{w}}^T (\hat{\mathbf{h}}^t - \xi(\mathbf{V})) \\
\text{subject to} \quad & \mathbf{\Phi}_P(\hat{\mathbf{q}}^t) + \mathbf{A}\hat{\mathbf{h}}^t + \mathbf{A_{10}}(P,:)\mathbf{h_0}^t + \hat{\boldsymbol{\eta}}^t = 0, \quad t = 1, \ldots, n_l, && \text{(15a)} \\
& \mathbf{A}^T \hat{\mathbf{q}}^t - \mathbf{d}(\mathbf{V})^t = 0, \quad t = 1, \ldots, n_l, && \text{(15b)} \\
& \hat{\boldsymbol{\eta}}^t - \mathbf{M}^+(P,P)^t \hat{\mathbf{z}}^+ \leq 0, \quad t = 1, \ldots, n_l, && \text{(15c)} \\
& -\hat{\boldsymbol{\eta}}^t - \mathbf{M}^-(P,P)^t \hat{\mathbf{z}}^- \leq 0, \quad t = 1, \ldots, n_l, && \text{(15d)} \\
& \hat{\mathbf{q}}^t + \mathbf{Q}^{\max}(P,P)\hat{\mathbf{z}}^- \leq \mathbf{q}^{\max}(P), \quad t = 1, \ldots, n_l, && \text{(15e)} \\
& -\hat{\mathbf{q}}^t + \mathbf{Q}^{\max}(P,P)\hat{\mathbf{z}}^+ \leq \mathbf{q}^{\max}(P), \quad t = 1, \ldots, n_l, && \text{(15f)} \\
& \hat{\mathbf{h}}^t \leq \mathbf{h}(V)^t_{\max}, \quad t = 1, \ldots, n_l, && \text{(15g)} \\
& -\hat{\mathbf{h}}^t \leq -\mathbf{h}(V)^t_{\min}, \quad t = 1, \ldots, n_l, && \text{(15h)} \\
& \hat{\mathbf{z}}^+ + \hat{\mathbf{z}}^- \leq \mathbf{e}(P), && \text{(15i)} \\
& \sum_{k=1}^{|P|} (\hat{z}_k^+ + \hat{z}_k^-) = n_v, && \text{(15j)} \\
& \hat{\mathbf{q}}^t \in \mathbb{R}^{|P|}, \quad \forall t = 1, \ldots, n_l, && \text{(15k)} \\
& \hat{\mathbf{h}}^t \in \mathbb{R}^{|V|}, \quad \forall t = 1, \ldots, n_l, && \text{(15l)} \\
& \hat{\boldsymbol{\eta}}^t \in \mathbb{R}^{|P|}, \quad \forall t = 1, \ldots, n_l, && \text{(15m)} \\
& \hat{\mathbf{z}}^+, \hat{\mathbf{z}}^- \in \{0,1\}^{|P|}. && \text{(15n)}
\end{aligned}
$$

Appendix II : Outer Approximation

In this Appendix, we described a detailed formulation of the OA/ER algorithm. We start this section by defining a more compact form for Problem (1). We can define the following vector of continuous unknowns:

$$\mathbf{x} := [\mathbf{q}^{1^T}\,\mathbf{h}^{1^T}\,\boldsymbol{\eta}^{1^T}\cdots\mathbf{q}^{n_l T}\,\mathbf{h}^{n_l T}\,\boldsymbol{\eta}^{n_l T}]^T \tag{16}$$

Let $\mathbf{c}^t(\cdot)$ be the function whose components correspond to the rows of constraints in (1a), for every t. Let $f(\mathbf{x}) := \frac{1}{n_l W}\sum_{t=1}^{n_l}\mathbf{w}^T(\mathbf{h}^t - \boldsymbol{\xi})$ and define the following set:

$$Z := \left\{(\mathbf{z}^+,\mathbf{z}^-) \in \{0,1\}^{n_p}\times\{0,1\}^{n_p} \,|\, (\mathbf{z}^+,\mathbf{z}^-) \text{ satisfies (1i)-(1j) } \right\}. \tag{17}$$

In addition, given $(\mathbf{z}^+,\mathbf{z}^-)\in Z$, we consider the compact polyhedral set :

$$X(\mathbf{z}^+,\mathbf{z}^-) := \left\{\mathbf{x}\in\mathbb{R}^{n_l(n_n+2n_p)} \,|\, \mathbf{x} \text{ satisfies (1b)-(1h)}\right\}. \tag{18}$$

Problem (1) can be rewritten as:

$$\begin{aligned} \text{minimise} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{c}^t(\mathbf{x}) = 0, \quad t = 1,\ldots,n_l \\ & \mathbf{x}\in X(\mathbf{z}^+,\mathbf{z}^-) \\ & (\mathbf{z}^+,\mathbf{z}^-)\in Z. \end{aligned} \tag{19}$$

The solution approaches considered in this manuscript are based on the Outer Approximation with Equality-Relaxation (OA/ER) introduced by [2]. For a sequence of valve placement choices $\{\mathbf{z}^+_{(k)},\mathbf{z}^-_{(k)}\}_{k\in\{1,2,\ldots,k_{maxIter}\}}\subset Z$, consider the nonlinear program:

$$\begin{aligned} \text{minimise} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{c}^t(\mathbf{x}) = 0, \quad t = 1,\ldots,n_l, \\ & \mathbf{x}\in X(\mathbf{z}^+_{(k)},\mathbf{z}^-_{(k)}), \end{aligned} \tag{NLP($\mathbf{z}^+_{(k)},\mathbf{z}^-_{(k)}$)}$$

and the index sets $\mathscr{F}$ and $\mathscr{N}$. We say $k\in\mathscr{F}$ if NLP($\mathbf{z}^+_{(k)},\mathbf{z}^-_{(k)}$) is feasible and indicate with $\mathbf{x}_{(k)}$ the corresponding solution. On the other hand, if NLP($\mathbf{z}^+_{(k)},\mathbf{z}^-_{(k)}$) is not feasible, then $k\in\mathscr{N}$.

Let $k\in\mathscr{F}$ and $\mathbf{x}_{(k)}$ be the solution of NLP($\mathbf{z}^+_{(k)},\mathbf{z}^-_{(k)}$). The associated vector of optimal Lagrange multipliers corresponding to the nonlinear constraints $\mathbf{c}^t(\cdot)$ is denoted by $\boldsymbol{\lambda}^t_{(k)}\in\mathbb{R}^{n_p}$, for all $t = 1,\ldots,n_l$. We define a diagonal matrix $\boldsymbol{\Lambda}^t_{(k)} := \text{diag}(\text{sign}(\boldsymbol{\lambda}^t_{(k)}))$, for every $t = 1,\ldots,n_l$. Following the definitions given in [1, Section 6.5], we consider Problem (19) and define its *master* MILP $\mathscr{M}(\mathscr{F},\mathscr{N})$ as:

$$\begin{aligned} \text{minimise} \quad & \mu \\ \text{subject to} \quad & \mu \geq f_{(k)} + \nabla\mathbf{f}^T_{(k)}(\mathbf{x}-\mathbf{x}_{(k)}), \quad \forall k\in\mathscr{F} && \text{(20a)} \\ & \boldsymbol{\Lambda}^t_{(k)}\mathbf{J}^t_{(k)}(\mathbf{x}-\mathbf{x}_{(k)}) \leq 0,\ t = 1,..,n_l, \forall k\in\mathscr{F} && \text{(20b)} \\ & \mathbf{x}\in X(\mathbf{z}^+,\mathbf{z}^-) && \text{(20c)} \\ & (\mathbf{z}^+_{(k)})^T\mathbf{z}^+ + (\mathbf{z}^-_{(k)})^T\mathbf{z}^- \leq n_v - 1, \quad \forall k\in\mathscr{F}\cup\mathscr{N}\setminus\{0\} && \text{(20d)} \\ & (\mathbf{z}^+,\mathbf{z}^-)\in Z, && \text{(20e)} \end{aligned}$$

where $\mathbf{J}^t(\cdot)$ is the Jacobian matrix of the function $\mathbf{c}^t(\cdot)$ for all $t\in\{1,\ldots,n_l\}$. Moreover, for all $k\in\mathscr{F}$, we have set $f_{(k)} := f(\mathbf{x}_{(k)})$, $\nabla f_{(k)} := \nabla\mathbf{f}(\mathbf{x}_{(k)})$, and $\mathbf{J}^t_{(k)} := \mathbf{J}^t(\mathbf{x}_{(k)})$. The linear constraints (20d) prevents the repetition of any of the binary vectors corresponding to indices in $\mathscr{F}\cup\mathscr{N}$. The OA/ER algorithm implemented in the present manuscript is described in Algorithm 1.

Algorithm 1 OA/ER algorithm

Select $\mathbf{x}_{(0)} \in \mathbb{R}^{n_l(n_n+2n_p)}$ satisfying (1a) and corresponding multipliers $\boldsymbol{\lambda}^t_{(0)}$;
Set $\mathscr{F} = \{0\}$, $\mathscr{N} = \emptyset$, $f_{\text{best}} = +\infty$, $k = 1$; $k_{maxIter} = 30$;
while $\mathscr{M}(\mathscr{F},\mathscr{N})$ is feasible **and** $k \leq k_{maxIter}$ **do**
    Solve $\mathscr{M}(\mathscr{F},\mathscr{N})$ obtaining $\mathbf{z}^+_{(k)}, \mathbf{z}^-_{(k)}$.
    if NLP($\mathbf{z}^+_{(k)}, \mathbf{z}^-_{(k)}$) is infeasible **then**
        $\mathscr{N} := \mathscr{N} \cup \{k\}$.
    else
        Let $\mathbf{x}_{(k)}$ be a solution of NLP($\mathbf{z}^+_{(k)}, \mathbf{z}^-_{(k)}$) with Lagrangian multipliers $\boldsymbol{\lambda}^t_{(k)}$;
        Set $\mathscr{F} := \mathscr{F} \cup \{k\}$;
        if $f(\mathbf{x}_{(k)}) < f_{\text{best}}$ **then**
            $f_{\text{best}} := f(\mathbf{x}_{(k)})$;
            $\mathbf{z}^+_{\text{best}} := \mathbf{z}^+_{(k)}$; $\mathbf{z}^-_{\text{best}} := \mathbf{z}^-_{(k)}$; $\mathbf{x}_{\text{best}} := \mathbf{x}_{(k)}$;
        else
            Stop
        end if
    end if
    Set $k = k + 1$.
end while

References

[1] Christodoulos A Floudas. *Nonlinear and mixed-integer optimization: fundamentals and applications*. Oxford University Press, 1995.

[2] Gary R Kocis and I. E. Grossmann. Relaxation Strategy for the Structural Optimization of Process Flow Sheets. *Industrial & Engineering Chemistry Research*, 26(205):1869–1880, 1987.