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A Content-based Active-Set Method for Pressure-Dependent Models of Water Distribution Systems with Flow Controls

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Abstract

In this paper a new method is proposed that solves for the steady state of pressure dependent models (PDMs) with flow control valves. Rather than model flow devices individually, the method solves the more general problem in which a water distribution system (WDS) has some link flows constrained to lie between upper and lower, or possibly equal, set limits. No heuristics are used to determine device states. The method is shown to be fast and its effectiveness is demonstrated on PDM WDSs with up to about 20,000 links and 18,000 nodes and 60 link flow constraints, some of which prescribe a fixed flow. The method has application in network management, network design and flow control to deal with water distribution where there is insufficient supply.

INTRODUCTION

Hydraulic simulation solvers are used by water engineers in the design and management of large, complex, water distribution system (WDS) networks. Newton-type methods are frequently used to solve the non-linear model equations for the steady-state demand dependent

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16 model (DDM) link flows and nodal heads (Todini & Rossman 2013) and very good methods
17 now exist for pressure dependent model (PDM) WDSs in which there are no control devices
18 (Deuerlein et al. 2019). However, real WDSs normally utilize control devices such as throttle
19 control valves (TCVs), check valves (CHVs), flow control valves (FCVs), pressure sustaining
20 valves (PSVs), pressure reducing valves (PRVs) and pumps but early methods developed for
21 models which include some or all of these elements had considerable shortcomings. For example,
22 iterative schemes for such models sometimes failed to converge or even converged to the wrong
23 solution (Gorev et al. 2016). The status of PRVs, PSVs and FCVs was usually determined using
24 heuristics: at each iteration the control devices are assigned states based on certain assumptions
25 and if at the next iteration those assumptions no longer hold, changes of state are recorded
26 for the devices. But even for very simple networks comprising just two regulating devices (e.g.
27 one pressure regulating device and one flow regulating device) in series, hydraulic modelling
28 software failed to converge to the correct solution for particular configurations and settings
29 (see Simpson (1999) and Deuerlein et al. (2008)). More troubling is the fact that in most cases
30 that produced a false solution, it was not immediately evident that a false solution had been
31 produced. By comparison, Piller & Bremond (2001) used a least-squares global optimization
32 approach to determine the states of the PRVs in a system. Rather than the discrete control
33 problem formulation, they solve the Karush-Kuhn-Tucker (KKT) equations for a constrained
34 optimization problem.

35 FCVs restrict the flow through a valve to a certain preset maximum: a closed control loop
36 is implemented consisting of flow measurement combined with a motor valve. From a mod-
37 elling point of view, flow control devices can be classified into two categories: valves with fixed
38 status (open, closed, fixed partly-opened state) and those whose hydraulic behavior or status
39 is described by inequality conditions for the flow. Deuerlein et al. (2009) used content and
40 co-content theory to characterize the conditions that ensure the existence and uniqueness of
41 solutions in demand driven model (DDM) systems with flow control devices. They introduced
42 a sub-differential analysis to deal with the non-differentiable flow versus head relationship that
43 exists in WDSs with flow control devices and this led to a content-based, constrained optimiza-
44 tion problem. The concept of content (which has the dimensions of power) was first introduced
45 in the context of WDSs by Collins et al. (1978) and the content of a flow control device here
46 is modelled in a way that is similar to that used previously for the content of a PDM node
47 The flows range between a lower and upper bound in the same way that a pressure outflow
48 relation (POR) describes how the nodal outflow is restricted to lie between zero and the nom-
49 inal demand for a node according to the node's pressure. The head loss along a control device
50 link is modelled by a nonlinear function of the flow (the given head loss function for pipes
51 and a minor head loss function for devices). Thus, an FCV restricts the link flow to a preset

52 maximum, q_{max} , which is independent of the current difference between the heads of the link's
53 initial and final nodes. If the flow is below q_{max} , the valve is opened fully and behaves like
54 a minor loss element. If conditions are such that the unrestricted flow would be higher than
55 q_{max} , the head loss coefficient is increased (by reducing the opening of the valve until the preset
56 flow level is reached again). In steady-state modelling this control behaviour can be modelled
57 by a multivalued mapping like the one shown in Fig. 1. If the valve is in active control mode,
58 it operates on the vertical line in Fig. 1. In this case the head difference between upstream
59 and downstream nodes of the valve is composed of the head loss h_{set} of the open valve for the
60 maximum flow q_{max} and an additional minor head loss penalty which is incurred in restricting
61 the flow to q_{max} . In the mathematical model the additional minor head loss is represented by
62 the Lagrange multiplier of the active flow constraint.

63 Piller & van Zyl (2014) used external quadratic penalty function terms added to a valve's
64 head loss equation to model FCVs. CHVs were modelled, taking into account the direction
65 of flow, as FCVs with a minimum flow setting of zero. In this method the pressure control
66 valves are handled by an optimization process which is external to the hydraulic solver and
67 the method was shown to work well on DDM problems although it sometimes needed damping
68 techniques or re-starting to achieve convergence. The authors did not apply this method to
69 PDM problems although the method can be extended to these models.

70 Alvarruiz et al. (2015) modelled closed CHVs as zero flow pipes and FCVs as valves with
71 flow at a preset level. Their scheme is based on the loop method, used the same heuristics as
72 EPANET to determine device status and was applied only to DDM problems. In Alvarruiz
73 et al. (2018) the authors improved on this work by using penalty methods (high resistance
74 links).

75 In a later development, Deuerlein et al. (2019) presented a content-based active set method
76 (ASM) for PDM problems without link flow constraints which is fast and reliable for a wide
77 range of pressure outflow relations (PORs). The ASM solves an optimization problem with
78 equality and inequality constraints. If in such optimizations an inequality constraint reaches
79 equality at a point, the constraint is said to be active, binding or saturated at that point.
80 ASMs get their name from the fact that in quadratic programming, apart from the feasibility
81 requirement, the conditions for optimality involve only the set of active constraints, sometimes
82 called the working set.

83 In another recent development Gorev et al. (2018) treated FCVs, PRVs, PSVs as links
84 with adjustable resistance. Their focus was on a technique which extends EPANET 2 and as
85 a consequence the hydraulic analysis of PDMs depended on adding to each demand node an
86 artificial FCV, a fictitious node, an artificial CHV and an artificial source. The addition of
87 this number of devices to large networks can increase the number of network components by

88 percentages of thousands or hundreds of thousands. Searching the very much larger virtual
89 network for valve states at each iteration in this approach presents a challenge to the method
90 for large networks.

91 In this paper, the content function used in Deuerlein et al. (2019) forms the basis of a new
92 ASM for PDM WDSs with FCVs and pumps. It was shown there that if a solution exists the
93 flows are unique because of the strict convexity of the system content function. The range of
94 models for which such solutions exist is greater than that for DDM problems by virtue of the
95 relaxation of demand constraints in PDM modelling. There is no risk of isolated demands in this
96 case since in PDM problems the nodal outflow can reduce to zero if the pressure is insufficient.
97 In fact, for this model the non-existence of a solution can result only when the (wrong) choice
98 of constraints for the flow control devices has the consequence that the polyhedral feasible set
99 which is composed of (i) the continuity equation, (ii) the flow constraints of the control devices
100 and (iii) the outflow conditions, is empty. Whether or not the feasible set is empty can be
101 established using a linear program (LP) (see Boyd & Vandenberghe (2009, 579) for details).
102 It is shown that if 0 is included in all the constraint intervals then a solution always exists
103 although it is only flows which are then determined uniquely and the heads may not be unique.
104 The authors stress that the approach in this paper is somewhat more general than dealing with
105 particular flow devices since it deals directly with constraints. Thus, the new method functions
106 by including upper and lower flow bounds on links in the network. Assuming, without loss
107 of generality, a positive flow direction, choosing upper flow bounds which fall below the link's
108 unconstrained flow models an FCV while choosing a lower flow bound which is above the
109 link's unconstrained flow models a pump. Using equal upper and lower link flow bounds, or
110 setting link flow equality constraints (LFEC), amounts to prescribing, or fixing, a flow. The
111 new method, referred to as an active set method for flow constraint (ASMFC) handles LFECs
112 without difficulty.

113 The operation of the ASMFC is illustrated on a small example network and it's efficacy is
114 demonstrated by applying it to eight case study networks with between 934 and 19,647 links and
115 between 848 and 17,971 nodes. The case study networks each had 20, 40 or 60 cotree link flow
116 constraints which either (i) limit the maximum flow in a link to 10% of its unconstrained value
117 or (ii) prescribe a LFEC. The method determines, for various tested starting sets, the steady-
118 state solutions, even on the largest case study network, in fewer than 14 iterations and with a
119 termination test that uses the (smaller than would be used in practice) stopping tolerance of
120 10^{-10} . The small stopping tolerance allows the quadratic convergence usually associated with
121 Newton's method, which occurred in all cases, to be observed.

122 In summary, this paper presents a new method which solves for the heads, outflows and
123 link flows of a WDS which models FCVs, pumps with flow control, check valves and closed

124 valves. Pumps and FCVs are implemented as appropriate bounds on flow constraints. Fixed
 125 flows are introduced to model closed valves (zero flow equality constraints) and more com-
 126 plex controls while check valves are implemented as sign-constrained inequalities. It presents
 127 network managers with a convenient tool to study network decomposition. It establishes new
 128 conditions for the existence and uniqueness of solutions to the PDM FCV problem. The class
 129 of problems it solves is larger than the class of DDM problems which can be solved and extends
 130 the applicability of the method for DDM problems of Deuerlein et al. (2009) which used the
 131 loops method. The method does not use penalty functions which can frequently require more
 132 iterations than ASM methods.

133 The next section in the paper sets out some definitions and establishes some notation and
 134 the one following very briefly reviews the ASM PDM content model. The section following
 135 derives the new ASMFC and outlines some details that are necessary for the implementation of
 136 the practical algorithm: a set assignment algorithm, an initialization scheme and the handling
 137 of LFECs. The sections with examples are followed by some conclusions and suggestions for
 138 future work.

139

140 DEFINITIONS AND NOTATION

141 Consider a WDS whose network graph has n_p links, or arcs, and $n_j + n_f$ nodes, or vertices: n_j
 142 is the number of nodes at which the heads are unknown and $n_f \geq 1$ is the number of source nodes
 143 with fixed heads. The links of the network include control valves, pumps and pipes. Denote by
 144 $\mathbf{q} = (q_1, q_2, \dots, q_{n_p})^T \in \mathbb{R}^{n_p}$ the vector of unknown flows in the system, $\mathbf{h} = (h_1, h_2, \dots, h_{n_j})^T \in$
 145 \mathbb{R}^{n_j} the unknown heads at the nodes in the system, $\mathbf{u} = (u_1, u_2, \dots, u_{n_j})^T \in \mathbb{R}^{n_j}$ the vector of
 146 node elevations and $\mathbf{r}(\mathbf{q}) = (r_1, r_2, \dots, r_{n_p})^T$ the vector of link resistance factors. Let \mathbf{A} denote
 147 the $n_p \times n_j$, full rank, unknown-head arc-node incidence matrix, (ANIM): the ji element of \mathbf{A} is
 148 (i) -1 if node i is at the end of arc j , (ii) 0 if arc j does not connect to the node i , and (iii) 1 if arc
 149 j starts at node i . Let \mathbf{A}_f denote the ANIM, with a similar definition, for the fixed-head nodes.
 150 Let \mathbf{h}^0 denote the vector of elevations of the n_f fixed-head nodes. Denote $\mathbf{a} = \mathbf{A}_f \mathbf{h}^0$. Denote
 151 by η the exponent used in the head loss formula: $\eta = 2$ for the Darcy-Weisbach model and
 152 $\eta = 1.852$ for the Hazen-Williams model. Furthermore, denote by $\mathbf{G}(\mathbf{q}) \in \mathbb{R}^{n_p \times n_p}$ the diagonal
 153 matrix whose diagonal elements are defined as $[\mathbf{G}(\mathbf{q})]_{jj} = r_j |q_j|^{\eta-1}$. Then, $\boldsymbol{\xi}(\mathbf{q}) = \mathbf{G}(\mathbf{q})\mathbf{q}$
 154 is the vector whose elements model the head losses of the links in the system. In general,
 155 (e.g. for the Darcy-Weisbach formula) $\mathbf{r} = \mathbf{r}(\mathbf{q})$ but for the Hazen-Williams formula \mathbf{r} is
 156 independent of \mathbf{q} . Denote the vector of the nominal demands at the nodes with unknown-head
 157 by $\mathbf{d} = (d_1, d_2, \dots, d_{n_j})^T \in \mathbb{R}^{n_j}$. Denote by $\mathbf{c}(\mathbf{h}, \mathbf{d}) \in \mathbb{R}^{n_j}$ the vector whose elements are the
 158 POR function values at the n_j nodes of the system. Throughout what follows, the symbol \mathbf{O}
 159 denotes a zero matrix and \mathbf{o} denotes a zero column vector of appropriate dimension for the

particular case. The shorthand notation $\mathbf{x} + a$, where \mathbf{x} is a vector and a is a scalar, will be used to denote the case where every component of \mathbf{x} has a added to it. Furthermore, it will be assumed that any matrix inverses which are shown do exist.

Turning now to PDM problems, assume, for simplicity and without loss of generality, that every node has the same minimum pressure head, h_m , and the same service pressure head, h_s . Individualized minimum and service pressure heads can be implemented by replacing h_m by h_{mi} and h_s by h_{si} throughout but presents no further difficulty. This modification does not change the method and only complicates data management and notation.

Denote a node's elevation by u and define the pressure fraction, $z(h - u)$, by $z(h - u) = (h - u - h_m)/(h_s - h_m)$. Suppose that $\gamma(t)$ is a bounded, smooth, monotonically increasing function which maps the interval $[0, 1] \rightarrow [0, 1]$. The POR at a node is defined by

$$c(h) = \begin{cases} 0 & \text{if } z(h - u) \leq 0 \\ d\gamma(z(h - u)) & \text{if } 0 < z(h - u) < 1. \\ d & \text{if } z(h - u) \geq 1 \end{cases} \quad (1)$$

The inverse function of the POR, the head, $h_i(c)$ expressed as a function of outflow c at node i , will be required for the development of the ASMFC which is the subject of this paper. But, the function $h_i(c)$ is not in general everywhere differentiable and so in its place a multivalued, sub-differential mapping is considered:

$$h_i(c) = \begin{cases} \emptyset & \text{if } c < 0 \\ (-\infty, h_m + u_i] & \text{if } c = 0 \\ (h_s - h_m)\gamma^{-1}\left(\frac{c}{d_i}\right) + h_m + u_i & \text{if } 0 < c < d_i. \\ [h_s + u_i, +\infty) & \text{if } c = d_i \\ \emptyset & \text{if } c > d_i \end{cases} \quad (2)$$

The definitions (1) and (2) are not, as they stand, applicable to the 2-side regularized Wagner or the logistic sigmoidal POR. The new method is, nevertheless, applicable for these PORs by adapting the intervals ($[0, 1]$ and $[0, d_i]$) in the definitions of (1) and (2) (See Deuerlein et al. (2019) for details)

Note that, in what follows, we will carefully distinguish between the scalar variables, h , and the multivalued, sub-differential mapping, $h(c)$.

THE PRESSURE DEPENDENT CONTENT MODEL AND THE ASM

185 Denote the PDM content function

$$186 \quad C(\mathbf{q}) = \sum_{j=1}^{n_p} \int_0^{q_j} \xi_j(s) ds - \mathbf{a}^T \mathbf{q} + \sum_{i=1}^{n_j} \int_0^{-\mathbf{e}_i^T \mathbf{A}^T \mathbf{q}} h_i(s) ds \quad (3)$$

187 and define the set $U = \{\mathbf{q} \in \mathbb{R}^{n_p} | \mathbf{o} \leq -\mathbf{A}^T \mathbf{q} \leq \mathbf{d}\}$. For appropriate PORs the function $C(\mathbf{q})$ is
 188 strictly convex by virtue of the strict monotonicity of the head loss and consumption functions
 189 and it is also norm-coercive ($|C(\mathbf{q})| \rightarrow \infty$ if $\|\mathbf{q}\| \rightarrow \infty$). The problem of finding $\min_{\mathbf{q} \in U} C(\mathbf{q})$ is
 190 associated with the Lagrangian $L(\mathbf{q}, \mathbf{h}) = \sum_{j=1}^{n_p} \int_0^{q_j} \xi_j(s) ds - \mathbf{a}^T \mathbf{q} - \mathbf{h}^T \mathbf{A}^T \mathbf{q} - \sum_{i=1}^{n_j} \int_{h_m}^{h_i} c(s) ds$
 191 and this leads to the unconstrained, equivalent problem of finding $\min_{\mathbf{q}} \max_{\mathbf{h}} L(\mathbf{q}, \mathbf{h})$ (see Elhay
 192 et al. (2016) for details). The gradient of $L(\mathbf{q}, \mathbf{h})$ is the familiar system

$$193 \quad \mathbf{f}(\mathbf{q}, \mathbf{h}) = \begin{pmatrix} \mathbf{G}(\mathbf{q})\mathbf{q} - \mathbf{A}\mathbf{h} - \mathbf{a} \\ -\mathbf{A}^T \mathbf{q} - \mathbf{c}(\mathbf{h}) \end{pmatrix} \stackrel{\text{def}}{=} \begin{pmatrix} \boldsymbol{\rho}_e \\ \boldsymbol{\rho}_m \end{pmatrix} \quad (4)$$

194 and the PDM steady-state heads and flows are found as the solution of $\mathbf{f}(\mathbf{q}, \mathbf{h}) = \mathbf{o}$. Here $\boldsymbol{\rho}_e$
 195 is the energy residual and $\boldsymbol{\rho}_m$ is the mass balance residual. The Jacobian of \mathbf{f} is

$$196 \quad \nabla_{\mathbf{q}, \mathbf{h}} \mathbf{f}(\mathbf{q}, \mathbf{h}) = \begin{pmatrix} \mathbf{F}(\mathbf{q}) & -\mathbf{A} \\ -\mathbf{A}^T & -\mathbf{E}(\mathbf{h}) \end{pmatrix} \quad (5)$$

197 where $\mathbf{F}(\mathbf{q})$ and $\mathbf{E}(\mathbf{h})$ are diagonal matrices which are such that (i) the terms on the diagonal
 198 of $\mathbf{F}(\mathbf{q})$ are the q -derivatives of the corresponding terms in $\mathbf{G}(\mathbf{q})\mathbf{q}$ and (ii) the terms on the
 199 diagonal of \mathbf{E} are the h -derivatives of the corresponding terms in $\mathbf{c}(\mathbf{h})$.

200 From this formulation the authors developed an ASM for the equivalent box-constrained
 201 minimization problem in which the nodal outflows, \mathbf{c} are considered additional unknowns. The
 202 restriction of the content function $C(\mathbf{q}, \mathbf{c})$, where the components of \mathbf{c} are defined only on the
 203 intervals $0 \leq c_i \leq d_i$,

$$204 \quad C(\mathbf{q}, \mathbf{c}) = \sum_{j=1}^{n_p} \int_0^{q_j} \xi_j(s) ds - \mathbf{a}^T \mathbf{q} + \mathbf{c}^T (\mathbf{u} + \mathbf{h}_m) + \sum_{\substack{1 \leq i \leq n_j \\ d_i > 0}} (h_s - h_m) \int_0^{c_i} \gamma^{-1} \left(\frac{s}{d_i} \right) ds \quad (6)$$

205 is minimized subject to $-\mathbf{A}^T \mathbf{q} - \mathbf{c} = \mathbf{o}$, $-\mathbf{c} \leq \mathbf{o}$ and $\mathbf{c} \leq \mathbf{d}$. Let $\boldsymbol{\psi}(\mathbf{c})$ denote (for later use) a
 206 vector whose components are the individual terms under the summation sign in the last term
 207 in Eq. (6). In order for a solution to exist it is only necessary that the polyhedral constraint
 208 set $-\mathbf{A}^T \mathbf{q} - \mathbf{c} = \mathbf{o}$ and $\mathbf{o} \leq \mathbf{c} \leq \mathbf{d}$ be non-empty. The link flows $\mathbf{q} = \mathbf{o}$ and nodal outflows
 209 $\mathbf{c} = \mathbf{o}$ are trivially feasible solutions for the constraint set and so the PDM problem consists of
 210 the minimization of a strictly convex content function formulated in terms of unknown flows

211 \mathbf{q}, \mathbf{c} over a polyhedral set. Associated with the problem

$$212 \quad \min_{\mathbf{q}, \mathbf{c}} C(\mathbf{q}, \mathbf{c}), \text{ subject to } -\mathbf{A}^T \mathbf{q} - \mathbf{c} = \mathbf{o}, \quad \mathbf{o} \leq \mathbf{c} \leq \mathbf{d} \quad (7)$$

213 is the Lagrangian

$$214 \quad L(\mathbf{q}, \mathbf{c}, \mathbf{h}, \bar{\boldsymbol{\lambda}}, \bar{\boldsymbol{\mu}}) = \sum_{j=1}^{n_p} \int_0^{q_j} \xi_j(s) ds - \mathbf{a}^T \mathbf{q} + \mathbf{1}^T \boldsymbol{\psi}(\mathbf{c}) + \mathbf{c}^T (\mathbf{u} + h_m) - \mathbf{h}^T (\mathbf{A}^T \mathbf{q} + \mathbf{c}) \\ + \bar{\boldsymbol{\mu}}^T (\mathbf{c} - \mathbf{d}) - \bar{\boldsymbol{\lambda}}^T \mathbf{c}, \quad \bar{\boldsymbol{\lambda}} \geq \mathbf{o}, \quad \bar{\boldsymbol{\mu}} \geq \mathbf{o} \quad (8)$$

215 where $\mathbf{1} = (1, 1, \dots, 1)^T$, the heads, \mathbf{h} , represent the non-negative Lagrange multipliers for the
216 mass balance equality constraint and $\bar{\boldsymbol{\lambda}}$ and $\bar{\boldsymbol{\mu}}$ are the non-negative Lagrange multipliers for
217 the inequality constraints on the outflows, \mathbf{c} .

218
219 **THE CONTENT MODEL FOR PRESSURE DRIVEN DEMANDS WITH LINK**
220 **FLOW CONSTRAINTS**

221 If flow constraints are added to the system, the minimization problem (7) becomes

$$222 \quad \min_{\mathbf{q}, \mathbf{c}} C(\mathbf{q}, \mathbf{c}) \text{ subject to } , -\mathbf{A}^T \mathbf{q} - \mathbf{c} = \mathbf{o}, \quad -\mathbf{c} \leq \mathbf{o}, \quad \mathbf{c} \leq \mathbf{d}, \quad \mathbf{q} - \mathbf{q}_{max} \leq \mathbf{o}, \quad -\mathbf{q} + \mathbf{q}_{min} \leq \mathbf{o}. \quad (9)$$

223 As a formalism, any links which do not have finite constraints are considered to lie in the
224 interval $(-\infty, \infty)$.

225 The notation we adopt for Lagrange multipliers is as follows. The symbols $\bar{\boldsymbol{\kappa}}, \bar{\boldsymbol{\nu}} \in \mathbb{R}^{n_p}$
226 and denote generic Lagrange multiplier variables but $\hat{\boldsymbol{\kappa}}, \hat{\boldsymbol{\nu}}$ (e.g. in (11)) have generally smaller
227 dimension: $\hat{\boldsymbol{\kappa}}$ has the dimension of the number of constraints active at the lower link flow
228 constraint boundary and $\hat{\boldsymbol{\nu}}$ has the dimension of the number of constraints active at the upper
229 link flow constraint boundary, in both cases, at the solution point. The Lagrange multipliers
230 $\boldsymbol{\kappa}^{(m)}, \boldsymbol{\nu}^{(m)}$ (e.g. in (19)) also have generally smaller dimensions but these can change from one
231 iteration to the next: their dimensions match the number of (lower and upper, respectively)
232 link flow constraints which are active at the m -th iteration.

233 The associated Lagrangian is now

$$234 \quad L(\mathbf{q}, \mathbf{c}, \mathbf{h}, \bar{\boldsymbol{\lambda}}, \bar{\boldsymbol{\mu}}, \bar{\boldsymbol{\kappa}}, \bar{\boldsymbol{\nu}}) = \sum_{j=1}^{n_p} \int_0^{q_j} \xi_j(s) ds - \mathbf{a}^T \mathbf{q} + \mathbf{1}^T \boldsymbol{\psi}(\mathbf{c}) + \mathbf{c}^T (\mathbf{u} + h_m) - \mathbf{h}^T (\mathbf{A}^T \mathbf{q} + \mathbf{c}) \\ + \bar{\boldsymbol{\mu}}^T (\mathbf{c} - \mathbf{d}) - \bar{\boldsymbol{\lambda}}^T \mathbf{c} + \bar{\boldsymbol{\kappa}}^T (-\mathbf{q} + \mathbf{q}_{min}) + \bar{\boldsymbol{\nu}}^T (\mathbf{q} - \mathbf{q}_{max}) \\ \bar{\boldsymbol{\lambda}} \geq \mathbf{o}, \quad \bar{\boldsymbol{\mu}} \geq \mathbf{o}, \quad \bar{\boldsymbol{\kappa}} \geq \mathbf{o}, \quad \bar{\boldsymbol{\nu}} \geq \mathbf{o} \quad (10)$$

235 with $\bar{\boldsymbol{\lambda}}$ and $\bar{\boldsymbol{\mu}}$ the Lagrange multipliers for the outflow constraints and $\bar{\boldsymbol{\kappa}}$ and $\bar{\boldsymbol{\nu}}$, the Lagrange
236 multipliers for the link flow constraints. The necessary and sufficient KKT conditions for a

237 minimum are, considering the complementary slackness conditions for the inequality constraints
 238 (and having zero Lagrange multipliers for the inactive constraints),

$$239 \quad \boldsymbol{\xi}(\mathbf{q}) - \mathbf{A}\mathbf{h} - \mathbf{a} - \mathbf{L}_q^T \widehat{\boldsymbol{\kappa}} + \mathbf{U}_q^T \widehat{\boldsymbol{\nu}} = \mathbf{o} \quad (11)$$

$$240 \quad \mathbf{h}(\mathbf{c}) - \mathbf{h} - \mathbf{L}_c^T \widehat{\boldsymbol{\lambda}} + \mathbf{U}_c^T \widehat{\boldsymbol{\mu}} = \mathbf{o} \quad (12)$$

$$241 \quad -\mathbf{A}^T \mathbf{q} - \mathbf{c} = \mathbf{o} \quad (13)$$

$$242 \quad -\mathbf{L}_c \mathbf{c} = \mathbf{o} \quad (14)$$

$$243 \quad \mathbf{U}_c (\mathbf{c} - \mathbf{d}) = \mathbf{o} \quad (15)$$

$$244 \quad \mathbf{L}_q (-\mathbf{q} + \mathbf{q}_{min}) = \mathbf{o} \quad (16)$$

$$245 \quad \mathbf{U}_q (\mathbf{q} - \mathbf{q}_{max}) = \mathbf{o} \quad (17)$$

$$246 \quad \widehat{\boldsymbol{\lambda}} \geq \mathbf{o}, \quad \widehat{\boldsymbol{\mu}} \geq \mathbf{o}, \quad \widehat{\boldsymbol{\kappa}} \geq \mathbf{o}, \quad \widehat{\boldsymbol{\nu}} \geq \mathbf{o} \quad (18)$$

247 where (i) $\widehat{\boldsymbol{\lambda}}$, $\widehat{\boldsymbol{\mu}}$, $\widehat{\boldsymbol{\kappa}}$ and $\widehat{\boldsymbol{\nu}}$ are the Lagrange multipliers of the active PORs and link flow bounds
 248 at the solution, (ii) \mathbf{L}_c and \mathbf{U}_c are matrices made up of the rows of an identity matrix which
 249 correspond to the active set indices for the lower and upper constraints for the outflows and
 250 (iii) \mathbf{L}_q and \mathbf{U}_q are the matrices made up of the rows of identity matrices which correspond to
 251 the active set indices for the lower and upper link flow constraints. Eqs. (14) - (17) represent
 252 the binding constraints and Eqs. (13)-(17) define what is known as the linear independence
 253 constraint qualification (LICQ): the matrix of the gradient of the active inequality constraints
 254 together with the gradient of the equality constraints. If this matrix has full rank then LICQ
 255 is said to hold. Now, if the head losses and the PORs are strictly monotonic then the content
 256 function is strictly convex and there is at most one solution. An LP can be used to determine
 257 existence. Thus, the KKT conditions together with norm-coercivity of the content function,
 258 convexity and the LICQ imply uniqueness of both heads and flows. By contrast, if the LICQ is
 259 violated then the heads may not be unique because the Lagrange multipliers are not uniquely
 260 defined. However, the flows are always unique by virtue of strict convexity.

261 In computation, convergence failures for this problem are often a result of the violation of
 262 the LICQ. Even if the LP establishes that the LICQ holds at the solution point, the LICQ may
 263 be violated at an intermediate iteration on the way to the solution. This is manifest in the
 264 singularity of the Schur complement (Golub & Van Loan 1983, 58), a matrix which is key to
 265 the solution process.

266 Denote $\mathbf{M} = \text{diag} \{h'_1(c), h'_2(c), \dots, h'_{n_j}(c)\}$. The Newton method for (11) to (17) is

$$\begin{array}{c}
267 \\
268
\end{array}
\begin{array}{c}
n_p \quad n_j \quad n_j \quad n_{L_c} \quad n_{U_c} \quad n_{L_q} \quad n_{U_q} \\
\begin{pmatrix}
n_p \\
n_j \\
n_j \\
n_{L_c} \\
n_{U_c} \\
n_{L_q} \\
n_{U_q}
\end{pmatrix}
\begin{pmatrix}
\mathbf{F}^{(m)} & \mathbf{O} & -\mathbf{A} & \mathbf{O} & \mathbf{O} & -\mathbf{L}_q^{(m)T} & \mathbf{U}_q^{(m)T} \\
\mathbf{O} & \mathbf{M}^{(m)} & -\mathbf{I} & -\mathbf{L}_c^{(m)T} & \mathbf{U}_c^{(m)T} & \mathbf{O} & \mathbf{O} \\
-\mathbf{A}^T & -\mathbf{I} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
\mathbf{O} & -\mathbf{L}_c^{(m)} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
\mathbf{O} & \mathbf{U}_c^{(m)} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
-\mathbf{L}_q^{(m)} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
\mathbf{U}_q^{(m)} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O}
\end{pmatrix}
\begin{pmatrix}
\mathbf{q}^{(m+1)} - \mathbf{q}^{(m)} \\
\mathbf{c}^{(m+1)} - \mathbf{c}^{(m)} \\
\mathbf{h}^{(m+1)} - \mathbf{h}^{(m)} \\
\boldsymbol{\lambda}^{(m+1)} - \boldsymbol{\lambda}^{(m)} \\
\boldsymbol{\mu}^{(m+1)} - \boldsymbol{\mu}^{(m)} \\
\boldsymbol{\kappa}^{(m+1)} - \boldsymbol{\kappa}^{(m)} \\
\boldsymbol{\nu}^{(m+1)} - \boldsymbol{\nu}^{(m)}
\end{pmatrix}
= \\
- \begin{pmatrix}
\mathbf{G}^{(m)} \mathbf{q}^{(m)} - \mathbf{A} \mathbf{h}^{(m)} - \mathbf{a} - \mathbf{L}_q^{(m)T} \boldsymbol{\kappa} + \mathbf{U}_q^{(m)T} \boldsymbol{\nu} \\
\mathbf{h}(\mathbf{c}^{(m)}) - \mathbf{h}^{(m)} - \mathbf{L}_c^{(m)T} \boldsymbol{\lambda}^{(m)} + \mathbf{U}_c^{(m)T} \boldsymbol{\mu}^{(m)} \\
-\mathbf{A}^T \mathbf{q}^{(m)} - \mathbf{c}^{(m)} \\
-\mathbf{L}_c^{(m)} \mathbf{c}^{(m)} \\
\mathbf{U}_c^{(m)} (\mathbf{c}^{(m)} - \mathbf{d}) \\
\mathbf{L}_q^{(m)} (-\mathbf{q}^{(m)} + \mathbf{q}_{min}) \\
\mathbf{U}_q^{(m)} (\mathbf{q}^{(m)} - \mathbf{q}_{max})
\end{pmatrix}
\end{array} \tag{19}$$

269 The rows and columns of matrices $\mathbf{M}^{(m)}$, \mathbf{I} and \mathbf{A} are now partitioned into a block three-
270 by-three configuration. The matrix $\mathbf{M}^{(m)}$ has three diagonal blocks: the block $\mathbf{M}_{c_b}^{(m)}$ which
271 represents those nodes at which the head lies between the minimum and service pressure head,
272 the block $\mathbf{M}_{c_l}^{(m)}$ which represents the active sets of those nodes at which no outflow is possible
273 because the pressure is below the minimum pressure head and the block $\mathbf{M}_{c_u}^{(m)}$ which represents
274 the active sets of those nodes at which the outflow is at the nominal demand, d , because the
275 head is at least at the service pressure head level:

$$\begin{array}{c}
276
\end{array}
\mathbf{M}^{(m)} = \begin{array}{c}
n_{c_b} \quad n_{c_l} \quad n_{c_u} \\
n_{c_b} \begin{pmatrix}
\mathbf{M}_{c_b}^{(m)} & & \\
& \mathbf{M}_{c_l}^{(m)} & \\
& & \mathbf{M}_{c_u}^{(m)}
\end{pmatrix} \\
n_{c_u}
\end{array}$$

277 The ANIM, \mathbf{A} is similarly partitioned into block three-by-three form where the block's first
278 subscript refers to rows (links) sets and the second subscript refers to columns (nodes) sets: the
279 subscripts indicate (i) the set for which the constraints are not active, b , (ii) the set for which
280 the lower constraint is active, l , and (iii) the set for which the upper constraint is active, u .

$$\begin{array}{c}
281
\end{array}
\mathbf{A} = \begin{array}{c}
n_{q_b} \quad n_{q_l} \quad n_{q_u} \\
n_{q_l} \begin{pmatrix}
\mathbf{A}_{bb} & \mathbf{A}_{bl} & \mathbf{A}_{bu} \\
\mathbf{A}_{lb} & \mathbf{A}_{ll} & \mathbf{A}_{lu} \\
\mathbf{A}_{ub} & \mathbf{A}_{ul} & \mathbf{A}_{uu}
\end{pmatrix} = \begin{pmatrix}
\mathbf{A}_b \\
\mathbf{A}_l \\
\mathbf{A}_u
\end{pmatrix}
\end{array}$$

282 Thus, $\mathbf{A}_{bl} \in \mathbb{R}^{n_{qb} \times n_{cl}}$ represents those links for which the link flows are between the upper and
 283 lower constraint boundaries and the nodes for which the pressure heads are below the minimum
 284 pressure head. The various identity matrix partition blocks are designated by \mathbf{I}_q , for link flows
 285 and \mathbf{I}_c , for outflows. If the matrix $\mathbf{G}^{(m)}$, and the head loss derivatives matrix $\mathbf{F}^{(m)}$ and the
 286 identity are partitioned conformally with $\mathbf{M}^{(m)}$ and \mathbf{A} the resulting system is

$$287 \quad \mathbf{P}^{(m)}(\mathbf{x}^{(m+1)} - \mathbf{x}^{(m)}) = \mathbf{r}^{(m)} \quad (20)$$

288 where, dropping subscripts and superscripts where there is no ambiguity,

$$289 \quad \mathbf{P} = \left(\begin{array}{ccc|ccc|ccc|cccc} \mathbf{F}_{qb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & -\mathbf{A}_{bb} & -\mathbf{A}_{bl} & -\mathbf{A}_{bu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{F}_{ql} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & -\mathbf{A}_{lb} & -\mathbf{A}_{ll} & -\mathbf{A}_{lu} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{ql} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{F}_{qu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & -\mathbf{A}_{ub} & -\mathbf{A}_{ul} & -\mathbf{A}_{uu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{I}_{qu} \\ \hline \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{M}_{cb} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{M}_{cl} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{M}_{cu} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cu} & \mathbf{O} & \mathbf{I}_{cu} & \mathbf{O} & \mathbf{O} \\ \hline -\mathbf{A}_{bb}^T & -\mathbf{A}_{lb}^T & -\mathbf{A}_{ub}^T & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ -\mathbf{A}_{bl}^T & -\mathbf{A}_{ll}^T & -\mathbf{A}_{ul}^T & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ -\mathbf{A}_{bu}^T & -\mathbf{A}_{lu}^T & -\mathbf{A}_{uu}^T & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \hline \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{I}_{cu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & -\mathbf{I}_{ql} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{I}_{qu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \end{array} \right),$$

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291

$$\mathbf{x}^{(m+1)} - \mathbf{x}^{(m)} = \begin{pmatrix} \mathbf{q}_b^{(m+1)} - \mathbf{q}_b^{(m)} \\ \mathbf{q}_l^{(m+1)} - \mathbf{q}_l^{(m)} \\ \mathbf{q}_u^{(m+1)} - \mathbf{q}_u^{(m)} \\ \mathbf{c}_b^{(m+1)} - \mathbf{c}_b^{(m)} \\ \mathbf{c}_l^{(m+1)} - \mathbf{c}_l^{(m)} \\ \mathbf{c}_u^{(m+1)} - \mathbf{c}_u^{(m)} \\ \mathbf{h}_{c_b}^{(m+1)} - \mathbf{h}_{c_b}^{(m)} \\ \mathbf{h}_{c_l}^{(m+1)} - \mathbf{h}_{c_l}^{(m)} \\ \mathbf{h}_{c_u}^{(m+1)} - \mathbf{h}_{c_u}^{(m)} \\ \lambda^{(m+1)} - \lambda^{(m)} \\ \mu^{(m+1)} - \mu^{(m)} \\ \kappa^{(m+1)} - \kappa^{(m)} \\ \nu^{(m+1)} - \nu^{(m)} \end{pmatrix}$$

292

293

$$\mathbf{r}^{(m)} = - \begin{pmatrix} \mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_{bb} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{bl} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{bu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{q_b} \\ \mathbf{G}_{q_l} \mathbf{q}_l^{(m)} - \mathbf{A}_{lb} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{ll} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{lu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{q_l} - \kappa^{(m)} \\ \mathbf{G}_{q_u} \mathbf{q}_u^{(m)} - \mathbf{A}_{ub} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{ul} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{uu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{q_u} + \nu^{(m)} \\ \mathbf{h}(c_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} \\ -\mathbf{h}_{c_l}^{(m)} + h_m + \mathbf{u}_{c_l} - \lambda^{(m)} \\ -\mathbf{h}_{c_u}^{(m)} + h_s + \mathbf{u}_{c_u} + \mu^{(m)} \\ -\mathbf{A}_{bb}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lb}^T \mathbf{q}_l^{(m)} - \mathbf{A}_{ub}^T \mathbf{q}_u^{(m)} - \mathbf{c}_b^{(m)} \\ -\mathbf{A}_{bl}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{ll}^T \mathbf{q}_l^{(m)} - \mathbf{A}_{ul}^T \mathbf{q}_u^{(m)} - \mathbf{c}_l^{(m)} \\ -\mathbf{A}_{bu}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lu}^T \mathbf{q}_l^{(m)} - \mathbf{A}_{uu}^T \mathbf{q}_u^{(m)} - \mathbf{c}_u^{(m)} \\ -\mathbf{c}_l^{(m)} \\ \mathbf{c}_u^{(m)} - \mathbf{d}_u \\ -\mathbf{q}_l^{(m)} + \mathbf{q}_{l,min} \\ \mathbf{q}_u^{(m)} - \mathbf{q}_{u,max} \end{pmatrix}$$

294 In this formulation of the problem the heads are unconstrained but for convenience we
 295 denote by \mathbf{h}_{c_b} the heads which are between the minimum and service pressure heads, by \mathbf{h}_{c_l}
 296 the heads which are at or below the minimum pressure head and by \mathbf{h}_{c_u} the heads which are at
 297 or above the service pressure head. By analytically solving for some of the unknowns in terms
 298 of the others (see the Appendix for details and the notation defining $\hat{\mathbf{I}}_{cb}$ and $\hat{\mathbf{I}}_{cu}$) the system

299 (20) can be rewritten

$$\begin{pmatrix} \mathbf{F}_{q_b} & \mathbf{O} & | & -\mathbf{A}_b \\ \mathbf{O} & \mathbf{M}_{c_b} & | & -\widehat{\mathbf{I}}_{cb} \\ -\mathbf{A}_b^T & -\widehat{\mathbf{I}}_{cb}^T & | & \mathbf{O} \end{pmatrix} \begin{pmatrix} \mathbf{q}_b^{(m+1)} - \mathbf{q}_b^{(m)} \\ \mathbf{c}_b^{(m+1)} - \mathbf{c}_b^{(m)} \\ \mathbf{h}^{(m+1)} - \mathbf{h}^{(m)} \end{pmatrix} = - \begin{pmatrix} \mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_b \mathbf{h}^{(m)} - \mathbf{a}_{q_b} \\ \mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} \\ -\mathbf{A}_b^T \mathbf{q}_b^{(m)} - \mathbf{A}_l^T \mathbf{q}_{l,min} - \mathbf{A}_{u,.}^T \mathbf{q}_{u,max} - \widehat{\mathbf{I}}_{cb}^T \mathbf{c}_b^{(m)} - \widehat{\mathbf{I}}_{cu}^T \mathbf{d}_u \end{pmatrix} \quad (21)$$

300
301 Denote the Schur complement of the matrix on the left of (21) by

$$\mathbf{V}_b^{(m)} = \left(\mathbf{A}_b^T \mathbf{F}_{q_b}^{-1} \mathbf{A}_b + \widehat{\mathbf{I}}_{cb}^T \mathbf{M}_{c_b}^{-1} \widehat{\mathbf{I}}_{cb} \right) \in \mathbb{R}^{n_j \times n_j}. \quad (22)$$

302
303 The system (21) leads to three update equations

$$\begin{aligned} \mathbf{V}_b^{(m)} \left(\mathbf{h}^{(m+1)} - \mathbf{h}^{(m)} \right) &= -\mathbf{A}^T \mathbf{q}^{(m)} - \widehat{\mathbf{I}}_{cb}^T \mathbf{c}_b^{(m)} - \widehat{\mathbf{I}}_{cu}^T \mathbf{d}_u \\ &+ \mathbf{A}_b^T \mathbf{F}_{q_b}^{-1} \left(\mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_b \mathbf{h}^{(m)} - \mathbf{a}_{q_b} \right) + \widehat{\mathbf{I}}_{cb}^T \mathbf{M}_{c_b}^{-1} \left(\mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} \right) \end{aligned} \quad (23)$$

$$\mathbf{q}_b^{(m+1)} = \mathbf{q}_b^{(m)} - \mathbf{F}_{q_b}^{-1} \left(\mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_b \mathbf{h}^{(m+1)} - \mathbf{a}_{q_b} \right) \quad (24)$$

$$\mathbf{c}_b^{(m+1)} = \mathbf{c}_b^{(m)} - \mathbf{M}_{c_b}^{-1} \left(\mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m+1)} \right). \quad (25)$$

304
305
306
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308
309 The updated Lagrange multipliers are given by

$$\boldsymbol{\lambda}^{(m+1)} = h_m + \mathbf{u}_{c_l} - \mathbf{h}_{c_l}^{(m+1)}, \quad \boldsymbol{\mu}^{(m+1)} = \mathbf{h}_{c_u}^{(m+1)} - \mathbf{u}_{c_u} - h_s, \quad (26)$$

$$\boldsymbol{\kappa}^{(m+1)} = \mathbf{G}_{q_l} \mathbf{q}_l^{(m)} - \mathbf{A}_{lb} \mathbf{h}_{c_b}^{(m+1)} - \mathbf{A}_{ll} \mathbf{h}_{c_l}^{(m+1)} - \mathbf{A}_{lu} \mathbf{h}_{c_u}^{(m+1)} - \mathbf{a}_{q_l} \quad (27)$$

$$\boldsymbol{\nu}^{(m+1)} = - \left(\mathbf{G}_{q_u} \mathbf{q}_u^{(m)} - \mathbf{A}_{ub} \mathbf{h}_{c_b}^{(m+1)} - \mathbf{A}_{ul} \mathbf{h}_{c_l}^{(m+1)} - \mathbf{A}_{uu} \mathbf{h}_{c_u}^{(m+1)} - \mathbf{a}_{q_u} \right) \quad (28)$$

310
311
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316 Eqs. (23)–(28), all but the first of which are explicit, form the basis of an active set method
317 to solve this constrained optimization problem. Before presenting the algorithm for the new
318 method a few preliminaries are necessary.

319

320 The index sets

321 Let N_q be the index set of links with flow constraints and N_c be the set of all nodes with
322 unknown-head and $d_i > 0$. Six index sets are defined: three, \mathcal{I}_{q_b} , \mathcal{I}_{q_l} , and \mathcal{I}_{q_u} , for the links which
323 are flow constrained and three, \mathcal{I}_{c_b} , \mathcal{I}_{c_l} , and \mathcal{I}_{c_u} , which are defined only for the nodes at which
324 the nominal demand is positive, $d_i > 0$. All the links which have no finite flow constraints are
325 considered to satisfy $-\infty < q_i^{(m+1)} < \infty$ and so always fall into the interior of their constraint
326 intervals: their constraints are never active. Note that the elements and the number of elements

327 in these sets can change from one iteration to the next. Strictly speaking, the sets represent
 328 the states of the link flows and the outflows only at the end of each iteration (i.e. after any
 329 flows outside the constraint intervals have been projected onto the constraint boundaries).

330 The first three sets in question are the link flow index sets. Set \mathcal{I}_{q_b} has the indices of the
 331 links for which the flows are either in the interior of the constraint interval or are unconstrained.
 332 The other two sets, \mathcal{I}_{q_l} and \mathcal{I}_{q_u} , hold the indices of the links for which the constraints are active.
 333 They can, in fact, be considered together as one index set for all the inequality constraints but
 334 they are treated separately here in the interests of clarity.

335 The last three sets are the outflow index sets. The set \mathcal{I}_{c_b} holds the indices of the nodes at
 336 which the head is between the minimum head, h_m , and service head h_s , and the other two sets
 337 hold the indices of the nodes at which the head is either less than or equal to h_m or greater
 338 than or equal to h_s . The sets \mathcal{I}_{c_u} and \mathcal{I}_{c_l} can also be considered together. The sets themselves
 339 are defined by:

(a)

$$340 \quad \mathcal{I}_{q_b}^{(m+1)} = \left\{ j \in N_q \mid \left(q_j^{(m+1)} > q_{min,j} \wedge q_j^{(m+1)} < q_{max,j} \right) \vee \right. \\ \left. \left(q_j^{(m+1)} = q_{min,j} \wedge \kappa_j^{(m+1)} < 0 \right) \vee \left(q_j^{(m+1)} = q_{max,j} \wedge \nu_j^{(m+1)} < 0 \right) \right\}$$

$$341 \quad (b) \quad \mathcal{I}_{q_l}^{(m+1)} = \left\{ j \in N_q \mid \left(q_j^{(m+1)} < q_{min,j} \right) \vee \left(q_j^{(m+1)} = q_{min,j} \wedge \kappa_j^{(m+1)} \geq 0 \right) \right\}$$

$$342 \quad (c) \quad \mathcal{I}_{q_u}^{(m+1)} = \left\{ j \in N_q \mid \left(q_j^{(m+1)} > q_{max,j} \right) \vee \left(q_j^{(m+1)} = q_{max,j} \wedge \nu_j^{(m+1)} \geq 0 \right) \right\}.$$

343 and

(d)

$$344 \quad \mathcal{I}_{c_b}^{(m+1)} = \left\{ i \in N_c \mid d_i > 0 \wedge \left(\left(c_i^{(m+1)} > 0 \wedge c_i^{(m+1)} < d_i \right) \vee \right. \right. \\ \left. \left. \left(c_i^{(m+1)} = 0 \wedge \lambda_i^{(m+1)} < 0 \right) \vee \left(c_i^{(m+1)} = d_i \wedge \mu_i^{(m+1)} < 0 \right) \right) \right\}$$

$$345 \quad (e) \quad \mathcal{I}_{c_l}^{(m+1)} = \left\{ i \in N_c \mid d_i > 0 \wedge \left(c_i^{(m+1)} < 0 \vee \left(c_i^{(m+1)} = 0 \wedge \lambda_i^{(m+1)} \geq 0 \right) \right) \right\}$$

$$346 \quad (f) \quad \mathcal{I}_{c_u}^{(m+1)} = \left\{ i \in N_c \mid d_i > 0 \wedge \left(c_i^{(m+1)} > d_i \vee \left(c_i^{(m+1)} = d_i \wedge \mu_i^{(m+1)} \geq 0 \right) \right) \right\}.$$

347

348 Set assignment algorithms

349 Once the heads, link flows, outflows and Lagrange multipliers have all been updated, the
 350 links need to be classified according to their values and the values of their associated Lagrange
 351 multipliers.

- 352 Thus, for each link flow q_j
- 353 (a) If $q_{min,j} < q_j < q_{max,j}$ then $j \rightarrow \mathcal{I}_{q_b}$
- 354 (b) If $q_j < q_{min,j}$ then $j \rightarrow \mathcal{I}_{q_l}$
- 355 (c) If $q_j > q_{max,j}$ then $j \rightarrow \mathcal{I}_{q_u}$
- 356 (d) If $q_j = q_{min,j}$ then
- 357 (i) If $\kappa_j \geq 0$ then $j \rightarrow \mathcal{I}_{q_l}$
- 358 (ii) otherwise $j \rightarrow \mathcal{I}_{q_b}$.
- 359 (e) If $q_j = q_{max,j}$ then
- 360 (i) If $\nu_j \geq 0$ then $j \rightarrow \mathcal{I}_{q_u}$
- 361 (ii) otherwise $j \rightarrow \mathcal{I}_{q_b}$.

362 Similarly, the outflows are assigned to their index sets by the following algorithm. For each
 363 node with $d_i > 0$

- 364 (a) If $0 < c_i < d_i$ then $i \rightarrow \mathcal{I}_{c_b}$
- 365 (b) If $c_i < 0$ then $i \rightarrow \mathcal{I}_{c_l}$
- 366 (c) If $c_i > d_i$ then $i \rightarrow \mathcal{I}_{c_u}$
- 367 (d) If $c_i = 0$ then
- 368 (i) If $\lambda_i \geq 0$ then $i \rightarrow \mathcal{I}_{c_l}$
- 369 (ii) otherwise $i \rightarrow \mathcal{I}_{c_b}$.
- 370 (e) If $c_i = d_i$ then
- 371 (i) If $\mu_i \geq 0$ then $i \rightarrow \mathcal{I}_{c_u}$
- 372 (ii) otherwise $i \rightarrow \mathcal{I}_{c_b}$.

373

374 **Initialization**

375 Initial heads $\mathbf{h}^{(0)}$, link flows $\mathbf{q}^{(0)}$, nodal outflows $\mathbf{c}^{(0)}$, Lagrange multipliers $\boldsymbol{\lambda}^{(0)}$, $\boldsymbol{\mu}^{(0)}$, $\boldsymbol{\kappa}^{(0)}$,
 376 $\boldsymbol{\mu}^{(0)}$, and the corresponding index sets $\mathcal{I}_{q_b}, \mathcal{I}_{q_l}, \mathcal{I}_{q_u}, \mathcal{I}_{c_b}, \mathcal{I}_{c_l}, \mathcal{I}_{c_u}$ are required. The initial outflows

377 for nodes with positive nominal demand, $d > 0$ are set to mid-interval values, $c_i = d_i/2$. The
378 corresponding initial heads are given by the general formula $h_i^{(0)} = (h_s - h_m)\gamma^{-1}(1/2) + h_m + u_i$.
379 This translates, for particular PORs, to $h_i^{(0)} = u_i + (h_s + a_2 h_m)/a_1$ with (i) $a_1 = 2$, $a_2 = 1$
380 for the linear, cubic and logistic PORs; (ii) $a_1 = 3$, $a_2 = 2$ for the quadratic POR; and (iii)
381 $a_1 = 4$, $a_2 = 3$ for the unregularized, 1-side regularized and 2-side regularized Wagner PORs

382 The initial flows for links which have no flow constraints are set (in SI units) to $q_i^{(0)} =$
383 $D_i^2\pi/12$, (equivalent to a fluid velocity of 1/3 m/s) and the initial flows for links which have
384 flow constraints are set to $\mathbf{q}^{(0)} = (\alpha\mathbf{q}_{min} + \beta\mathbf{q}_{max})/(\alpha + \beta)$ with $\alpha = \beta = 1$ for mid-interval
385 initial link flows. Other choices of α , and β were also investigated and the results are reported
386 below.

387 The initial Lagrange multipliers are set to $\lambda_i^{(0)} = \mu_i^{(0)} = \kappa_i^{(0)} = \nu_i^{(0)} = 0$, $\forall i$ and all Lagrange
388 multipliers are zeroed at the beginning of each iteration.

389 With $c_i/d_i = 1/2$ and $\alpha = \beta = 1$ the corresponding initial index sets are $\mathcal{I}_{q_b} = \{1, 2, \dots, n_p\}$,
390 $\mathcal{I}_{c_b} = \{1, 2, \dots, n_j\}$, $\mathcal{I}_{c_u} = \mathcal{I}_{c_l} = \mathcal{I}_{q_u} = \mathcal{I}_{q_l} = \emptyset$. Note that where there are LFECs the initial
391 set assignments of the corresponding link indices will be to either \mathcal{I}_{q_l} or \mathcal{I}_{q_u} according to the
392 random choice made. These starting values may not be in the feasible set but provided the LP
393 confirms the existence of a solution this is not a problem because mass balance will be satisfied
394 at the solution.

395

396 **Regularizing the Schur complement**

397 It is possible that the Schur complement in (22) becomes singular. When this happens
398 at a point which is away from the solution point, failure of the method can be avoided by
399 regularizing the Schur complement. This does not affect the generally quadratic convergence
400 of the procedure unless there is degeneracy at the solution point. Regularization would usually
401 only be necessary if there are constraints applied to links in the network's spanning tree since
402 this can lead to a violation of the LICQ: a phenomenon which cannot occur if constraints are
403 only applied to co-tree links.

404 One simple heuristic regularization that has succeeded in the experience of the authors,
405 and represents a variation on the Levenberg-Marquardt method (LMM), is to replace any of
406 those zeros on the diagonal of the Schur complement by non-zeros. The choice of regularization
407 parameter value can be varied adaptively, as is done in the LMM, if convergence remains slow
408 but regularization will usually only be necessary until the iterates move away from the region
409 where the Schur complement is singular or has large condition number. In many cases a value
410 of 1 is sufficient but larger regularization parameters may be necessary and indeed were used
411 in a few of the tests reported later which used the unregularized Wagner POR. The technique
412 works well in the experience of the authors. A full Levenberg-Marquardt regularization scheme

413 may address more difficult cases where matrix conditioning arrests or delays convergence but
 414 the investigation of this is beyond the scope of this paper.

415

416 **The iteration loop**

417 The iteration loop which implements the ASMFC is now described.

418 Start loop: For $m = 0, 1, 2, \dots$ repeat steps (a) to (l) until the stopping test is satisfied

419 (a) Zero all the Lagrange multipliers.

420 (b) Compute $\mathbf{M}_{c_b}^{(m)} = \text{diag} \{h'(c_{i_1}), h'(c_{i_2}), \dots, h'(c_{i_{n_b}})\}$, $i_k \in \mathcal{I}_{c_b}^{(m)}$, $1 \leq k \leq n_{c_b}^{(m)}$, $\mathbf{V}_b^{(m)}$ of
 421 (22) and the right-hand-side of (23).

422 (c) Solve (23) for the corrections $\mathbf{h}^{(m+1)} - \mathbf{h}^{(m)}$ and use the corrections to update $\mathbf{h}^{(m+1)}$.

423 (d) Use (24) to update the link flows $q_i^{(m+1)}$ for $i \in \mathcal{I}_{q_b}$

424 (e) Use (25) to update the nodal outflows $c_i^{(m+1)}$ for which $i \in \mathcal{I}_{c_b}$.

425 (f) Use (26) to update the lower bound nodal outflow constraint Lagrange multipliers $\boldsymbol{\lambda}^{(m)}$
 426 for the nodes with index $i \in \mathcal{I}_{c_l}$.

427 (g) Use (26) to update the upper bound nodal outflow constraint Lagrange multipliers, $\boldsymbol{\mu}^{(m)}$
 428 for the nodes with index $i \in \mathcal{I}_{c_u}$.

429 (h) Use (27) to update the lower bound link flow constraint Lagrange multipliers $\boldsymbol{\kappa}^{(m)}$ for the
 430 links with index $i \in \mathcal{I}_{q_l}$.

431 (i) Use (28) to update the upper bound link flow constraint Lagrange multipliers $\boldsymbol{\nu}^{(m)}$ for
 432 the links with index $i \in \mathcal{I}_{q_u}$.

433 (j) Assign those links and nodes with unequal upper and lower bound constraints to the
 434 index sets $\mathcal{I}_{q_b}, \mathcal{I}_{q_l}, \mathcal{I}_{q_u}, \mathcal{I}_{c_b}, \mathcal{I}_{c_l}$, and \mathcal{I}_{c_u} . Then assign, if there are any, the LFEC links to
 435 the appropriate sets using the scheme described earlier.

436 (k) Project the exterior link flows onto the constraint boundaries $\mathbf{q}^{(m+1)} \leftarrow \max(\mathbf{q}^{(m+1)}, \mathbf{q}_{min})$
 437 and then $\mathbf{q}^{(m+1)} \leftarrow \min(\mathbf{q}^{(m+1)}, \mathbf{q}_{max})$

438 (l) Project the exterior outflows onto the constraint boundaries $\mathbf{c}^{(m+1)} \leftarrow \max(\mathbf{c}^{(m+1)}, 0)$,
 439 $\mathbf{c}^{(m+1)} \leftarrow \min(\mathbf{c}^{(m+1)}, \mathbf{d})$

441 **ILLUSTRATIVE EXAMPLES**

442 In this section the ASMFC is demonstrated on the illustrative network shown in Fig. 2.
 443 The constrained links are not confined to the cotree and this leaves open the possibility that
 444 zero flows or active constraints in some links could isolate parts of the network and thereby
 445 violate the LICQ.

446 The basic parameters of the network are given in Table 1. The steady-state solution shown
 447 is for the (unregularized) Wagner POR, a source head of 250 m, minimum pressure head,
 448 $h_m = 0$ m, and a service pressure head, $h_s = 20$ m. All nodes have an elevation of 100 m. Also
 449 shown in Fig. 2 are the nominal demands, d , the solution heads, h , flows q , delivery fractions
 450 as percentages of the nominal demands and the constraint upper and lower limits (shown in
 451 parentheses). Thus, links 2-10 have flow constraints and of these links 5, 7 and 8 have LFECs.
 452 All initial values were shown to be inside the feasible set.

453 The iterations were run until the relative differences between successive iterates

$$\delta_h^{(m+1)} = \frac{\|\mathbf{h}^{(m+1)} - \mathbf{h}^{(m)}\|_\infty}{1 + \|\mathbf{h}^{(m+1)}\|_\infty}, \quad \delta_q^{(m+1)} = \frac{\|\mathbf{q}^{(m+1)} - \mathbf{q}^{(m)}\|_\infty}{1 + \|\mathbf{q}^{(m+1)}\|_\infty}, \quad \delta_c^{(m+1)} = \frac{\|\mathbf{c}_b^{(m+1)} - \mathbf{c}_b^{(m)}\|_\infty}{1 + \|\mathbf{c}_b^{(m+1)}\|_\infty} \quad (29)$$

454
 455 were smaller than the prescribed stopping tolerance, 10^{-10} . The choice $\alpha = \beta = 1$ took 6
 456 iterations to satisfy the stopping test, the choice $\alpha = 0, \beta = 1$ took 7 iterations and the choice
 457 $\alpha = 1, \beta = 0$ took 11 iterations. Extensive tests were conducted with different values of α and
 458 β on this and other networks with link flow constraints but in the experience of the authors the
 459 values $\alpha = \beta = 1$ most often took the fewest iterations. The convergence data show the typical
 460 quadratic convergence associated with Newton's method. It is worth noting that the derivative
 461 assignment technique described in Deuerlein et al. (2019) was necessary in the solution of this
 462 network (because the derivative of the Wagner POR is undefined at $h = h_m$). It was also
 463 necessary to invoke the Schur complement regularization scheme described above to counteract
 464 the singularity of the Schur complement during one of the early iterations.

465 At steady-state (i) the set memberships are: $\mathcal{I}_{q_b} = \{1, 9, 10\}$, $\mathcal{I}_{q_u} = \{2, 3, 4, 5, 8\}$, $\mathcal{I}_{q_l} =$
 466 $\{6, 7\}$, $\mathcal{I}_{c_b} = \{3, 4, 5, 6, 7, 8\}$ and $\mathcal{I}_{c_u} = \{1\}$, $\mathcal{I}_{c_l} = \{2\}$ (ii) the KKT conditions were satisfied
 467 and (iii) the LICQ condition was not violated. The steady-state energy, mass and outflow
 468 residuals all had norm smaller than 10^{-13} , a value consistent with the fact that all calculations
 469 (including those for other examples in this paper) were performed using Matlab (Mathworks
 470 2016) which uses a floating point number system that conforms with IEEE standard double
 471 precision arithmetic (IEEE 2008) for which machine epsilon is about 2.2×10^{-16} .

472 It is seen that the flow constraints on links 9 and 10 are inactive and the sum of their flows

473 into node 2 exactly cancels the fixed flow in link 8 thereby delivering zero outflow to node 2.
474 The flow in link 6 is at the lower link flow constraint boundary and, since the corresponding
475 multiplier in this case can be interpreted as a negative head loss, this constraint can be seen as
476 acting as a pump. Similarly, the flow in link 8 has direction opposite to that of the unconstrained
477 flow and so that too can be seen as acting as a pump.

478 The ASMFC was also applied to eight case study networks N_1-N_8 (four of which are available
479 online in the ASCE Library (www.ascelibrary.org) which have between 934 and 19,647 links
480 and between 848 and 17,971 nodes, to demonstrate the effectiveness of the method on realistic
481 problems. Each of the eight networks had 60 cotree link flow constraints: 57 links were flow-
482 constrained to 10% of that link's unconstrained steady-state PDM flow and another 3 had
483 LFEC. This has the effect of simulating 60 flow control valves in each network.

484 In all cases (i) the nominal demands were magnified, in repeated tests, by factors of 5, 20
485 and 40 to assess the behaviour of the method in solving increasingly difficult PDM problems (ii)
486 the 1-side regularized Wagner POR was used (iii) the mid-interval starting schemes described
487 above were used and (iv) the values $\alpha = \beta = 1$ were used in the starting values formula and
488 (v) the stopping tolerance for the infinity norms of the relative differences between successive
489 iterates was set at 10^{-10} . This stopping tolerance (even though it is smaller than would normally
490 be used in practice) was chosen to ensure that the quadratic convergence normally associated
491 with Newton's method was evident.

492 Columns 2, 3 and 4 of Table 2 show the number of links, nodes and sources for the eight case
493 study networks. The other columns of Table 2 show the convergence data for the application
494 of the method to the case study network N_1-N_8 with a demand magnification factor $f = 5$:
495 column 5 shows the number, m , of iterations to satisfy the stopping test, column 6 shows the
496 delivery fraction, ζ , as a percentage of the nominal demand, columns 7–9 show the quantities
497 $\tau_{q,h,c} = -\log_{10}(\delta_{q,h,c}^{(m)})$ which represent the numbers of decimal digits of agreement between the
498 two last iterates for the link flows, heads and outflows, respectively, and columns 10–12 show
499 the accuracy of the final energy, mass and outflow residuals shown as the negative base-10
500 logarithms of the residual norms themselves. All these results are consistent with a stopping
501 test based on a relative norm difference no greater than 10^{-10} . The corresponding convergence
502 results for the other networks, other PORs and the other demand magnification factors are
503 remarkably similar to those in Table 2.

504 In runs on all the case study networks and with all 3 demand magnification factors, the
505 method took at best 9 and at most 13 iterations to satisfy the stopping test based on the
506 measures in (29). The mean of the number of iterations was 11.6 with a standard deviation of
507 1.2. With the starting values $\alpha = 0, \beta = 1$ and $\alpha = 1, \beta = 0$ all cases converged in no more
508 than 14 iterations and the quadratic convergence was evident in all cases. The behaviour of the

509 method for these problems with, for example, the linear or the unregularized Wagner PORs
510 was almost identical with the behaviour described so far although the delivery fractions were,
511 naturally, different for the other PORs.

512 The derivative assignment technique described in Deuerlein et al. (2019), which is part
513 of the implementation code for these tests was automatically invoked for the unregularized
514 Wagner POR to overcome the difficulties created by the fact that the derivative of that POR
515 is undefined when $h = h_m = 0$. Where the (unreasonable) demand magnification factor of
516 40 was used to engineer a more difficult problem, a larger Schur complement regularization
517 parameter was, in 2 cases, necessary to ensure convergence.

518

519 CONCLUSIONS

520 A new content-based active set method, ASMFC, for the determination of link flows, nodal
521 heads and outflows in a PDM WDS which has link flow constraints is presented. The method
522 extends the authors' previous work which was an active set method for the determination
523 of link flows, nodal heads and outflows in a PDM WDS with unconstrained link flows. The
524 necessary and sufficient KKT conditions for a minimum of the content function optimization
525 problem are given and the Newton method based on this formulation leads, after some algebraic
526 simplifications, to the ASMFC. For this model the non-existence of a solution can result only
527 when the (wrong) choice of constraints has the consequence that the polyhedral feasible set
528 which is composed of (i) the continuity equation, (ii) the flow constraints and (iii) the outflow
529 conditions, is empty. Whether or not the feasible set is empty can be easily tested using a
530 linear program. The uniqueness of the solution to the problem is assured provided the LICQ
531 is not violated at the solution.

532 FCVs and pumps can be modelled and heuristics are not needed to determine the status of
533 control devices in the system: their states are found as part of the solution. Choosing equal
534 upper and lower bound constraints (LFEC) is equivalent to specifying a fixed link flow rate
535 and is easily handled by the method. The range of models for which such solutions exist is
536 greater than that for DDM problems by virtue of the relaxation of demand constraints in PDM
537 modeling. There is no risk of isolated demands in this case since in PDM problems the nodal
538 outflow can reduce to zero if the pressure is insufficient.

539 The operation of the ASMFC is illustrated on a small example network and it's efficacy is
540 demonstrated by applying it to eight case study networks with between 934 and 19,647 links
541 and between 848 and 17,971 nodes. The case study networks each had 60 cotree link flow
542 constraints which either (i) limit the maximum flow in a link to 10% of its unconstrained value
543 or (ii) prescribe a LFEC. The method found, for various tested starting sets, the steady-state
544 solutions, even on the largest case study network, in fewer than 14 iterations. The quadratic

545 convergence usually associated with Newton's method was evident in all cases. A regularization
546 of the Schur complement may be necessary in some cases. The new method is applicable to
547 all the PORs for which the ASM of Deuerlein et al. (2019) is applicable provided the special
548 methods introduced there to account for irregularities in the inverse POR are invoked.

549 The ASMFC method has application in real-time operations. The operation of drinking
550 water distribution systems is becoming more and more complex for a variety of reasons. For
551 instance, as events in recent years have shown, even in Europe the availability of the water
552 as a resource is not guaranteed in every region during the increasingly hot and dry summer
553 periods. As a consequence water suppliers are forced to develop alternative resources that may
554 be shared by different supply utilities. This means that there is a rapidly growing need for
555 enhanced system operations such as control of the flow from different sources. In a worst-case
556 scenario where the available resources are not sufficient to cover the demand, flow control is
557 also an indispensable tool for efficient distribution of the available water.

558 Improved simulation techniques are also required that are able to deal with new develop-
559 ments in the management of WDSs. An invaluable tool for operation of such systems is a near
560 real-time hydraulic solver that solves the control equations and may be integrated within newly
561 developed IOT platforms in the future. The ASMFC solver is such a tool.

562 In addition to real-time simulations ASMFC also has application in the optimal design
563 of future new supply systems and their control strategies. The ASMFC has, for example,
564 application in pump system design: for a given positive lower flow bound the solver calculates
565 the required pumping head that is necessary to maintain that desired flow. This technique can
566 be used in system design as well as in control optimization.

567 Last, but not least, stable solution methods for systems under control conditions form the
568 basis of all optimization applications or Monte Carlo simulations that require a huge number
569 of simulation runs with a great variety of boundary conditions (that may have a strong impact
570 on the operation of flow control devices). Future research will be focussed on the integration
571 of pressure control devices and pumps.

572

573

574

575 ANALYTICAL SEPARATION

576 Certain unknowns in the system (20) can, by exploiting the structure of the system, be
 577 expressed analytically in terms of other parts and this analytical separation helps to clarify
 578 the exposition and to simplify the algorithmic implementation of the ASMFC. This separation
 579 process is now described.

580 The 12-th block row of (20) is $-\mathbf{I}_{ql}(\mathbf{q}_l^{(m+1)} - \mathbf{q}_l^{(m)}) = \mathbf{q}_l^{(m)} - \mathbf{q}_{l,min}$ from which it is evident
 581 that $\mathbf{q}_l^{(m+1)} = \mathbf{q}_{l,min}$, where $\mathbf{q}_{l,min}$ is the vector of constraint lower bounds for the links in \mathcal{I}_{ql} .
 582 By similar reasoning the 13-th block row of (20) gives $\mathbf{q}_u^{(m+1)} = \mathbf{q}_{u,max}$. Substituting these into
 583 (20) gives the reduced, 11×11 equivalent system (with block columns 2 and 3 removed and
 584 block rows 12 and 13 of (20) removed) where

$$\begin{pmatrix}
 \mathbf{F}_{qb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & -\mathbf{A}_{bb} & -\mathbf{A}_{bl} & -\mathbf{A}_{bu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
 \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & -\mathbf{A}_{lb} & -\mathbf{A}_{ll} & -\mathbf{A}_{lu} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{ql} & \mathbf{O} \\
 \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & -\mathbf{A}_{ub} & -\mathbf{A}_{ul} & -\mathbf{A}_{uu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{I}_{qu} \\
 \mathbf{O} & \mathbf{M}_{cb} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
 \mathbf{O} & \mathbf{O} & \mathbf{M}_{cl} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
 \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{M}_{cu} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cu} & \mathbf{O} & \mathbf{I}_{cu} & \mathbf{O} & \mathbf{O} \\
 -\mathbf{A}_{bb}^T & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
 -\mathbf{A}_{bl}^T & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
 -\mathbf{A}_{bu}^T & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
 \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
 \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{I}_{cu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O}
 \end{pmatrix} \times$$

$$\begin{pmatrix}
 \mathbf{q}_b^{(m+1)} - \mathbf{q}_b^{(m)} \\
 \mathbf{c}_b^{(m+1)} - \mathbf{c}_b^{(m)} \\
 \mathbf{c}_l^{(m+1)} - \mathbf{c}_l^{(m)} \\
 \mathbf{c}_u^{(m+1)} - \mathbf{c}_u^{(m)} \\
 \mathbf{h}_{c_b}^{(m+1)} - \mathbf{h}_{c_b}^{(m)} \\
 \mathbf{h}_{c_l}^{(m+1)} - \mathbf{h}_{c_l}^{(m)} \\
 \mathbf{h}_{c_u}^{(m+1)} - \mathbf{h}_{c_u}^{(m)} \\
 \boldsymbol{\lambda}^{(m+1)} - \boldsymbol{\lambda}^{(m)} \\
 \boldsymbol{\mu}^{(m+1)} - \boldsymbol{\mu}^{(m)} \\
 \boldsymbol{\kappa}^{(m+1)} - \boldsymbol{\kappa}^{(m)} \\
 \boldsymbol{\nu}^{(m+1)} - \boldsymbol{\nu}^{(m)}
 \end{pmatrix} = - \begin{pmatrix}
 \mathbf{G}_{qb} \mathbf{q}_b^{(m)} - \mathbf{A}_{bb} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{bl} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{bu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{qb} \\
 \mathbf{G}_{ql} \mathbf{q}_l^{(m)} - \mathbf{A}_{lb} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{ll} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{lu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{ql} - \boldsymbol{\kappa}^{(m)} + \mathbf{F}_{ql} (\mathbf{q}_{l,min} - \mathbf{q}_l^{(m)}) \\
 \mathbf{G}_{qu} \mathbf{q}_u^{(m)} - \mathbf{A}_{ub} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{ul} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{uu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{qu} + \boldsymbol{\nu}^{(m)} + \mathbf{F}_{qu} (\mathbf{q}_{u,max} - \mathbf{q}_u^{(m)}) \\
 \mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} \\
 -\mathbf{h}_{c_l}^{(m)} + h_m + \mathbf{u}_{c_l} - \boldsymbol{\lambda}^{(m)} \\
 -\mathbf{h}_{c_u}^{(m)} + h_s + \mathbf{u}_{c_u} + \boldsymbol{\mu}^{(m)} \\
 -\mathbf{A}_{bb}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lb}^T \mathbf{q}_{l,min} - \mathbf{A}_{ub}^T \mathbf{q}_{u,max} - \mathbf{c}_b^{(m)} \\
 -\mathbf{A}_{bl}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{ll}^T \mathbf{q}_{l,min} - \mathbf{A}_{ul}^T \mathbf{q}_{u,max} - \mathbf{c}_l^{(m)} \\
 -\mathbf{A}_{bu}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lu}^T \mathbf{q}_{l,min} - \mathbf{A}_{uu}^T \mathbf{q}_{u,max} - \mathbf{c}_u^{(m)} \\
 -\mathbf{c}_l^{(m)} \\
 \mathbf{c}_u^{(m)} - \mathbf{d}_u
 \end{pmatrix}$$

585

586

587 The 10-th block equation in this system leads to $\mathbf{c}_l^{(m+1)} = 0$ and the 11-th leads to $\mathbf{c}_u^{(m+1)} = \mathbf{d}_u$
588 from which it follows that the reduced system (with block columns 3 and 4 and block rows 10
589 and 11 removed) can be written

$$\begin{aligned}
& \begin{pmatrix} \mathbf{F}_{q_b} & \mathbf{O} & -\mathbf{A}_{bb} & -\mathbf{A}_{bl} & -\mathbf{A}_{bu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & -\mathbf{A}_{lb} & -\mathbf{A}_{ll} & -\mathbf{A}_{lu} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{ql} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & -\mathbf{A}_{ub} & -\mathbf{A}_{ul} & -\mathbf{A}_{uu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{I}_{qu} \\ \hline \mathbf{O} & \mathbf{M}_{c_b} & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & -\mathbf{I}_{cl} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & -\mathbf{I}_{cu} & \mathbf{O} & \mathbf{I}_{cu} & \mathbf{O} & \mathbf{O} \\ \hline -\mathbf{A}_{bb}^T & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ -\mathbf{A}_{bl}^T & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ -\mathbf{A}_{bu}^T & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \end{pmatrix} \times \tag{30} \\
& \begin{pmatrix} \mathbf{q}_b^{(m+1)} - \mathbf{q}_b^{(m)} \\ \mathbf{c}_b^{(m+1)} - \mathbf{c}_b^{(m)} \\ \mathbf{h}_{c_b}^{(m+1)} - \mathbf{h}_{c_b}^{(m)} \\ \mathbf{h}_{c_l}^{(m+1)} - \mathbf{h}_{c_l}^{(m)} \\ \mathbf{h}_{c_u}^{(m+1)} - \mathbf{h}_{c_u}^{(m)} \\ \lambda^{(m+1)} - \lambda^{(m)} \\ \mu^{(m+1)} - \mu^{(m)} \\ \kappa^{(m+1)} - \kappa^{(m)} \\ \nu^{(m+1)} - \nu^{(m)} \end{pmatrix} = - \begin{pmatrix} \mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_{bb} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{bl} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{bu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{q_b} \\ \mathbf{G}_{q_l} \mathbf{q}_l^{(m)} - \mathbf{A}_{lb} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{ll} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{lu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{q_l} - \kappa^{(m)} + \mathbf{F}_{q_l} (\mathbf{q}_{l,min} - \mathbf{q}_l^{(m)}) \\ \mathbf{G}_{q_u} \mathbf{q}_u^{(m)} - \mathbf{A}_{ub} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{ul} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{uu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{q_u} + \nu^{(m)} + \mathbf{F}_{q_u} (\mathbf{q}_{u,max} - \mathbf{q}_u^{(m)}) \\ \hline \mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} \\ -\mathbf{h}_{c_l}^{(m)} + h_m + \mathbf{u}_{c_l} - \lambda^{(m)} - \mathbf{M}_{c_l} \mathbf{c}_l^{(m)} \\ -\mathbf{h}_{c_u}^{(m)} + h_s + \mathbf{u}_{c_u} + \mu^{(m)} - \mathbf{M}_{c_u} (\mathbf{c}_u^{(m)} - \mathbf{d}_u) \\ \hline -\mathbf{A}_{bb}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lb}^T \mathbf{q}_{l,min} - \mathbf{A}_{ub}^T \mathbf{q}_{u,max} - \mathbf{c}_b^{(m)} \\ -\mathbf{A}_{bl}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{ll}^T \mathbf{q}_{l,min} - \mathbf{A}_{ul}^T \mathbf{q}_{u,max} \\ -\mathbf{A}_{bu}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lu}^T \mathbf{q}_{l,min} - \mathbf{A}_{uu}^T \mathbf{q}_{u,max} - \mathbf{d}_u \end{pmatrix}
\end{aligned}$$

592 Consider the submatrix of (30) made up of block rows 1,4,7,8,9. This subsystem is independent
593 of the last four unknowns and so can be written

$$\begin{pmatrix} \mathbf{F}_{q_b} & \mathbf{O} & -\mathbf{A}_{bb} & -\mathbf{A}_{bl} & -\mathbf{A}_{bu} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{M}_{c_b} & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \hline -\mathbf{A}_{bb}^T & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ -\mathbf{A}_{bl}^T & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ -\mathbf{A}_{bu}^T & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \end{pmatrix} \times$$

$$\begin{pmatrix} \mathbf{q}_b^{(m+1)} - \mathbf{q}_b^{(m)} \\ \mathbf{c}_b^{(m+1)} - \mathbf{c}_b^{(m)} \\ \mathbf{h}_{c_b}^{(m+1)} - \mathbf{h}_{c_b}^{(m)} \\ \mathbf{h}_{c_l}^{(m+1)} - \mathbf{h}_{c_l}^{(m)} \\ \mathbf{h}_{c_u}^{(m+1)} - \mathbf{h}_{c_u}^{(m)} \\ \boldsymbol{\lambda}^{(m+1)} - \boldsymbol{\lambda}^{(m)} \\ \boldsymbol{\mu}^{(m+1)} - \boldsymbol{\mu}^{(m)} \\ \boldsymbol{\kappa}^{(m+1)} - \boldsymbol{\kappa}^{(m)} \\ \boldsymbol{\nu}^{(m+1)} - \boldsymbol{\nu}^{(m)} \end{pmatrix} = - \begin{pmatrix} \mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_{bb} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{bl} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{bu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{q_b} \\ \mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} \\ -\mathbf{A}_{bb}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lb}^T \mathbf{q}_{l,min} - \mathbf{A}_{ub}^T \mathbf{q}_{u,max} - \mathbf{c}_b^{(m)} \\ -\mathbf{A}_{bl}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{ll}^T \mathbf{q}_{l,min} - \mathbf{A}_{ul}^T \mathbf{q}_{u,max} \\ -\mathbf{A}_{bu}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lu}^T \mathbf{q}_{l,min} - \mathbf{A}_{uu}^T \mathbf{q}_{u,max} - \mathbf{d}_u \end{pmatrix}$$

or more simply as

$$\begin{pmatrix} \mathbf{F}_{q_b} & \mathbf{O} & -\mathbf{A}_{bb} & -\mathbf{A}_{bl} & -\mathbf{A}_{bu} \\ \mathbf{O} & \mathbf{M}_{c_b} & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} \\ -\mathbf{A}_{bb}^T & -\mathbf{I}_{cb} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ -\mathbf{A}_{bl}^T & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ -\mathbf{A}_{bu}^T & \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{O} \end{pmatrix} \begin{pmatrix} \mathbf{q}_b^{(m+1)} - \mathbf{q}_b^{(m)} \\ \mathbf{c}_b^{(m+1)} - \mathbf{c}_b^{(m)} \\ \mathbf{h}_{c_b}^{(m+1)} - \mathbf{h}_{c_b}^{(m)} \\ \mathbf{h}_{c_l}^{(m+1)} - \mathbf{h}_{c_l}^{(m)} \\ \mathbf{h}_{c_u}^{(m+1)} - \mathbf{h}_{c_u}^{(m)} \end{pmatrix} = \tag{31}$$

$$- \begin{pmatrix} \mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_{bb} \mathbf{h}_{c_b}^{(m)} - \mathbf{A}_{bl} \mathbf{h}_{c_l}^{(m)} - \mathbf{A}_{bu} \mathbf{h}_{c_u}^{(m)} - \mathbf{a}_{q_b} \\ \mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} \\ -\mathbf{A}_{bb}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lb}^T \mathbf{q}_{l,min} - \mathbf{A}_{ub}^T \mathbf{q}_{u,max} - \mathbf{c}_b^{(m)} \\ -\mathbf{A}_{bl}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{ll}^T \mathbf{q}_{l,min} - \mathbf{A}_{ul}^T \mathbf{q}_{u,max} \\ -\mathbf{A}_{bu}^T \mathbf{q}_b^{(m)} - \mathbf{A}_{lu}^T \mathbf{q}_{l,min} - \mathbf{A}_{uu}^T \mathbf{q}_{u,max} - \mathbf{d}_u \end{pmatrix}. \tag{32}$$

Once the unknowns in (31) have been found, the Lagrange multipliers can be found from block equations 2,3,5, and 6 of (31) which can be rewritten, after some manipulations as

$$\boldsymbol{\lambda}^{(m+1)} = h_m + \mathbf{u}_{c_l} - \mathbf{h}_{c_l}^{(m+1)} - \mathbf{M}_{c_l} \mathbf{c}_l^{(m)}$$

$$\boldsymbol{\mu}^{(m+1)} = \mathbf{h}_{c_u}^{(m+1)} - h_s - \mathbf{u}_{c_u} + \mathbf{M}_{c_u} (\mathbf{c}_u^{(m)} - \mathbf{d}_u)$$

$$\boldsymbol{\kappa}^{(m+1)} = \mathbf{G}_{q_l} \mathbf{q}_l^{(m)} - \mathbf{A}_{lb} \mathbf{h}_{c_b}^{(m+1)} - \mathbf{A}_{ll} \mathbf{h}_{c_l}^{(m+1)} - \mathbf{A}_{lu} \mathbf{h}_{c_u}^{(m+1)} - \mathbf{a}_{q_l} + \mathbf{F}_{q_l} (\mathbf{q}_{l,min} - \mathbf{q}_l^{(m)})$$

$$\boldsymbol{\nu}^{(m+1)} = - \left(\mathbf{G}_{q_u} \mathbf{q}_u^{(m)} - \mathbf{A}_{ub} \mathbf{h}_{c_b}^{(m+1)} - \mathbf{A}_{ul} \mathbf{h}_{c_l}^{(m+1)} - \mathbf{A}_{uu} \mathbf{h}_{c_u}^{(m+1)} - \mathbf{a}_{q_u} + \mathbf{F}_{q_u} (\mathbf{q}_{u,max} - \mathbf{q}_u^{(m)}) \right)$$

Omitting the last terms in parentheses, which vanish by definition, gives

$$\boldsymbol{\lambda}^{(m+1)} = h_m + \mathbf{u}_{c_l} - \mathbf{h}_{c_l}^{(m+1)}$$

$$\boldsymbol{\mu}^{(m+1)} = \mathbf{h}_{c_u}^{(m+1)} - h_s - \mathbf{u}_{c_u}$$

$$\boldsymbol{\kappa}^{(m+1)} = \mathbf{G}_{ql} \mathbf{q}_l^{(m)} - \mathbf{A}_{lb} \mathbf{h}_{c_b}^{(m+1)} - \mathbf{A}_{ll} \mathbf{h}_{c_l}^{(m+1)} - \mathbf{A}_{lu} \mathbf{h}_{c_u}^{(m+1)} - \mathbf{a}_{ql}$$

$$\boldsymbol{\nu}^{(m+1)} = - \left(\mathbf{G}_{qu} \mathbf{q}_u^{(m)} - \mathbf{A}_{ub} \mathbf{h}_{c_b}^{(m+1)} - \mathbf{A}_{ul} \mathbf{h}_{c_l}^{(m+1)} - \mathbf{A}_{uu} \mathbf{h}_{c_u}^{(m+1)} - \mathbf{a}_{qu} \right)$$

if we denote, $\widehat{\mathbf{I}}_{cb} = (\mathbf{I}_{cb} \quad \mathbf{O} \quad \mathbf{O})$ and $\widehat{\mathbf{I}}_{cu} = (\mathbf{O} \quad \mathbf{O} \quad \mathbf{I}_{cu})$ the first block row of

$$\begin{pmatrix} \mathbf{q}_b^{(m+1)} - \mathbf{q}_b^{(m)} \\ \mathbf{c}_b^{(m+1)} - \mathbf{c}_b^{(m)} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_{q_b}^{-1} & \mathbf{O} \\ \mathbf{O} & \mathbf{M}_{c_b}^{-1} \end{pmatrix} \left[- \begin{pmatrix} \mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_b \mathbf{h}^{(m)} - \mathbf{a}_{q_b} \\ \mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} \end{pmatrix} + \begin{pmatrix} \mathbf{A}_b \cdot \\ \widehat{\mathbf{I}}_{cb} \end{pmatrix} (\mathbf{h}^{(m+1)} - \mathbf{h}^{(m)}) \right]$$

is

$$\begin{pmatrix} \mathbf{q}_b^{(m+1)} - \mathbf{q}_b^{(m)} \\ \mathbf{c}_b^{(m+1)} - \mathbf{c}_b^{(m)} \end{pmatrix} = -\mathbf{F}_{q_b}^{-1} \left(\mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_b \mathbf{h}^{(m)} - \mathbf{a}_{q_b} - \mathbf{A}_b \cdot (\mathbf{h}^{(m+1)} - \mathbf{h}^{(m)}) \right) \quad (33)$$

$$= -\mathbf{F}_{q_b}^{-1} \left(\mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_b \mathbf{h}^{(m+1)} - \mathbf{a}_{q_b} \right) \quad (34)$$

or

$$\mathbf{q}_b^{(m+1)} = \mathbf{q}_b^{(m)} - \mathbf{F}_{q_b}^{-1} \left(\mathbf{G}_{q_b} \mathbf{q}_b^{(m)} - \mathbf{A}_b \mathbf{h}^{(m+1)} - \mathbf{a}_{q_b} \right) \quad (35)$$

and the second block row is

$$\begin{aligned} \mathbf{c}_b^{(m+1)} &= \mathbf{c}_b^{(m)} - \mathbf{M}_{c_b}^{-1} \left(\mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} - \widehat{\mathbf{I}}_{cb} (\mathbf{h}^{(m+1)} - \mathbf{h}^{(m)}) \right) \\ &= \mathbf{c}_b^{(m)} - \mathbf{M}_{c_b}^{-1} \left(\mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m)} - (\mathbf{h}_{c_b}^{(m+1)} - \mathbf{h}_{c_b}^{(m)}) \right) \\ &= \mathbf{c}_b^{(m)} - \mathbf{M}_{c_b}^{-1} \left(\mathbf{h}(\mathbf{c}_b^{(m)}) - \mathbf{h}_{c_b}^{(m+1)} \right). \end{aligned} \quad (36)$$

LINEAR INDEPENDENCE CONSTRAINT QUALIFICATION

The inequality constraints in the system are $-c_i \leq 0$, $c_i \leq d_i$, $i = 1, 2, \dots, n_j$ $q_j \leq q_{max,j}$, $-q_j \leq -q_{min,j}$, $j = 1, 2, \dots, n_p$. Suppose that certain of these inequality constraints are, at some point during the optimization process active, or binding: $c_{i_1} = 0$, $c_{i_2} = d_{i_2}$, $i_1, i_2 \in S$ and $q_{j_1} = q_{max,j_1}$, $q_{j_2} = q_{min,j_2}$, $j_1, j_2 \in T$, S and T , subsets of the index sets $\{1, 2, \dots, n_j\}$ and $\{1, 2, \dots, n_p\}$, respectively. In order for the Lagrange multipliers to be uniquely defined during the optimization process these binding constraints, together with the conservation of mass equations (another set of equality constraints) must form a set of linearly independent equations. More precisely, let \mathbf{U}_{q_l} be a matrix made up of the rows of an n_{q_l} identity which correspond to an active link flow lower constraint, \mathbf{U}_{q_u} a matrix made up of the rows of an n_{q_u} identity which correspond to an active link flow upper constraint, and let \mathbf{U}_{c_l} be a matrix made up of the rows of an n_{c_l} identity which correspond to an active outflow lower constraint, \mathbf{U}_{c_u} a matrix made up of the rows of an n_{c_u} identity which correspond to an active outflow upper constraint. Let $\mathbf{q}_{l,min} \in \mathbb{R}^{n_{q_l}}$ be a vector of the link flow lower constraint values of those

642 links for which the lower constraint is active and let $\mathbf{q}_{u,max} \in \mathbb{R}^{n_{qu}}$ be a vector of the link flow
 643 upper constraint values of those links for which the upper constraints are active. Let $\mathbf{d}_u \in \mathbb{R}^{n_{cu}}$
 644 be a vector of the demands for nodes at which the upper outflow constraints are active. The
 645 general full equality constraint system is

$$646 \quad \mathbf{C} \begin{pmatrix} \mathbf{q} \\ \mathbf{c} \end{pmatrix} \stackrel{\text{def}}{=} \begin{matrix} & n_p & n_j \\ n_j & \begin{pmatrix} \mathbf{A}^T & \mathbf{I} \\ -\mathbf{U}_{q_l} & \\ \mathbf{U}_{q_u} & \\ & -\mathbf{U}_{c_l} \\ & \mathbf{U}_{c_u} \end{pmatrix} & \\ n_{q_l} & & \\ n_{q_u} & & \\ n_{c_l} & & \\ n_{c_u} & & \end{matrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{c} \end{pmatrix} = \begin{pmatrix} \mathbf{o} \\ -\mathbf{q}_{l,min} \\ \mathbf{q}_{u,max} \\ \mathbf{o} \\ \mathbf{d}_u \end{pmatrix}.$$

647 The top block represents the equality constraints that make up the conservation of mass e-
 648 quations and are constant and the bottom four blocks represent the link flow and outflow
 649 constraints which are active and can change from one iteration to the next. Some, or all, of
 650 the lower four blocks may be empty at any given iteration. The LICQ is said to hold when
 651 the matrix \mathbf{C} has full rank. The LICQ is necessary for the KKT conditions hold at a local
 652 minimizer.

653
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 658 BMBF-13N13690).

659
 660 **DATA AVAILABILITY**

661 The network shown in Fig. 2 and the networks N_1 , N_3 , N_4 and N_7 , which are listed in Table
 662 2, and their EPANET .inp files were previously published in Deuerlein et al. (2019). The other
 663 four networks N_2 , N_5 , N_6 and N_8 are not freely available either because they are proprietary
 664 or because of security concerns.

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Pipe or node i	L_i (m)	D_i (m)	ϵ_i (mm)	$q_{min,i}$ (lps)	q_i (lps)	$q_{max,i}$ (lps)	h_i (m)	δ_i (%)
1	1000	0.30	0.250	$-\infty$	295.00	∞	193.3	100
2	1000	0.20	0.250	0.00	110.00	110.00	99.5	0
3	1500	0.15	0.250	1.00	10.00	10.00	108.9	67
4	1200	0.20	0.250	2.00	50.00	50.00	100.0	4
5	800	0.20	0.250	85.00	85.00	85.00	100.9	21
6	800	0.15	0.250	12.00	12.00	89.00	101.2	24
7	800	0.15	0.250	8.00	8.00	8.00	100.0	1
8	1200	0.10	0.250	-3.00	-3.00	-3.00	100.0	2
9	1000	0.10	0.250	0.00	1.43	2.00	—	—
10	800	0.10	0.250	0.00	1.57	5.00	—	—

Table 1: The network parameters and the steady-state solution values for the illustrative network shown in Fig. 2. Also shown are the link flow constraints and the delivery fractions as percentages.

ID	n_p	n_j	n_f	m	ζ (%)	τ_q	τ_h	τ_c	ρ_e	ρ_m	ρ_o
N_1	934	848	8	11	82.4	14	16	17	17	6	11
N_2	1118	1039	2	11	54.2	11	13	15	17	7	12
N_3	1976	1770	4	12	93.3	11	16	17	17	8	9
N_4	2465	1890	3	13	23.3	11	12	15	16	12	15
N_5	2508	2443	2	12	28.4	12	16	18	17	5	9
N_6	8584	8392	2	10	60.8	11	16	18	17	8	12
N_7	14830	12523	7	13	47.5	12	14	15	16	10	14
N_8	19647	17971	15	10	97.6	10	14	18	16	8	11

Table 2: Convergence results for the ASMFC applied to the N_1 – N_8 case study networks with 60 cotree links flow-constrained, 3 of which have LFEC, and demand magnification factor $f = 5$.

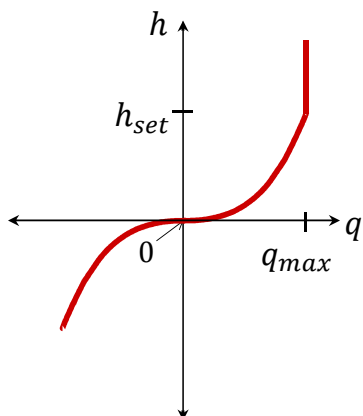


Figure 1: The multivalued subdifferential mapping modelling an FCV.

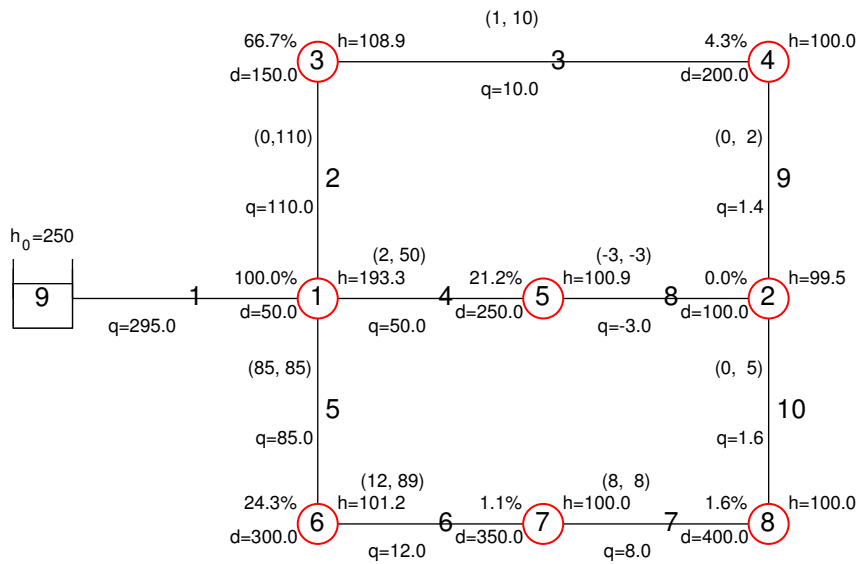


Figure 2: The illustrative network discussed in the text showing the steady-state solution and the link flow constraints.

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719 2 Convergence results for the ASMFC applied to the N_1-N_8 case study network-
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