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Modeling the behavior of flow regulating devices in water distribution systems using constrained non-linear programming

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Abstract

Currently the modeling of check valves and flow control valves in water distribution systems is based on heuristics intermixed with solving the set of non-linear equations governing flow in the network. At the beginning of a simulation, the operating status of these valves is not known and must be assumed. The system is then solved. The status of the check valves and flow control valves are then changed to try to determine their correct operating status, at times leading to incorrect solutions even for simple systems. This paper proposes an entirely different approach. Content and Co-Content theory is used to define conditions that guarantee the existence and uniqueness of the solution. The work here focuses solely on flow control devices with a defined head discharge versus head loss relationship. A new modeling approach for water distribution systems based on subdifferential analysis that deals with the non-differentiable flow versus head relationships is proposed in this paper. The water distribution equations are solved as a constrained non-linear programming problem based on the Content model where the Lagrangian multipliers have important physical meanings. This new method gives correct solutions by dealing appropriately with inequality and equality constraints imposed by the presence of the flow regulating devices (check valves, flow control valves and temporarily closed isolating valves). An example network is used to illustrate the concepts.

Keywords: water distribution system modeling, flow control valves, check valves, nonlinear programming, variational inequalities, Content, Co-Content, subdifferential, convex analysis

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Introduction

The presence of flow regulating devices and pressure regulating devices in water distribution systems (WDSs) complicates the computer analysis of water distribution systems. This paper presents details of the theory and solution techniques required related to the presence of flow regulating devices in WDSs. The main type of devices considered in this paper are the check valve that prevents reverse flow (a lower limit on the flow) and the flow control valve (FCV) that limits the flow to be equal to or less than a set flow value (an upper limit on the flow). A "Content" approach to understanding the physics of these devices in water distribution systems is presented. A discussion of the Content and Co-Content functions for normal pipes and nodes is firstly given. Then details of the Content and Co-Content functions for check valves and flow control valves are given and their difference in behavior compared to pipes is noted. Currently heuristics dominate the modeling of these devices in state-ofthe-art computer hydraulic simulation packages. In particular, the proof of existence and uniqueness of the hydraulic steady-state of networks with feedback devices is lacking. Difficulties arise due to the fact that control devices with inequality conditions (associated with check valves and flow control valves) have multi-valued mappings for the hydraulic functions and are not differentiable in the classical sense. In this paper the mathematical modeling of check valves and flow control valves is proposed by the use of subdifferential hydraulic laws. Then, the conditions for existence and uniqueness of the hydraulic steady-state as well as appropriate algorithms for the numerical calculation are discussed.

A formulation of the equations in terms of unknowns of loop flow corrections is developed based on the Content model. Details of a constrained convex non-linear programming formulation that is required to properly solve the governing equations are presented. Lagrangian multipliers in the nonlinear programming formulation coming from the Content analysis are physically linked to either the head drop across a closed check valve or the actual head loss across the flow control valve that is required to produce the set flow. Case study examples are provided to demonstrate the concepts presented in the paper.

Background

For the operation of water supply networks control devices are very important. These devices possess different functional characteristics and various control modes with specific hydraulic characteristics. Only flow regulating devices in terms of check valves, flow control valves and temporarily closed isolating valves are considered in detail in this paper, although the principles presented also apply to pressure breaker valves, pressure dependent demands and leakages.

Two groups of different flow regulating devices are now defined as

1. *Flow regulating devices* whose operational state depends on the actual flow conditions. Examples include check valves (CHV, also referred to as non-return valves or back flow preventers) and also flow control valves (FCVs) for which a set flow is selected for the valve. The difficulty in modeling this group of valves is that the operating status of the valve is not known a priori. For example, for a check valve, it is not known whether it is open or closed. For a flow control valve it is not known whether it is active (partly open) or inactive (fully open). The analytic description of the hydraulic behavior of those devices in terms of system Content and sub-differential analysis is given in this paper. These flow regulating devices can be modeled as multi-valued mappings resulting from lower or upper inequality conditions for the hydraulic equations.

2. *Isolating valves* (CIV) may have time varying operational states in a WDS. The operational states are assumed to be constant during certain time intervals and are altered by the system operator at particular times during the day. For instance some valves may be temporarily closed at a certain time. These are easier to model as the operating status of the device (usually an opened or closed valve) is known ahead of time unlike for check valves and flow regulating valves in Group 1 above. Closed valves invoke an equality constraint.

In contrast to the flow regulating devices, another form of regulating device is also present in water distribution systems. These are referred to as distributed feedback devices or pressure regulating devices. Examples are pressure reducing valves (PRVs), pressure sustaining valves (PSVs) and remote pressure controlled variable speed pumps. The hydraulic state of these valves is operated in order to reach a given set pressure at the control node. The location of the control node for the pressure can

either be immediately downstream of the PRV or at a location that is distant from the valve – for example at a node that is at the extremity of the system. The hydraulic behavior of these pressure regulating devices cannot be modeled with a specified relationship between flow and head loss. The operational state of those devices depends on the actual pressure of the assigned control node which is controlled by the conditions in the water distribution system both upstream and downstream of the valve. These devices require a different approach to modeling using the Nash Equilibrium in a competitive non-linear programming formulation (Deuerlein 2002, Deuerlein et. al. 2005) and the result of the significantly more complex requirements are not considered in this paper. The stark difference in the fundamental behavior of flow control devices and pressure regulating devices is an important observation of the research. This is the reason that flow controlling devices are considered separately in this paper.

A number of publications deal with modeling of flow regulating control devices. Shamir and Howard (1968) took into account valves and pumps for the development of hydraulic simulation models while Kesavan and Chandrashekar (1972) presented a graph theoretical method for the consideration of flow control valves (FCVs) and pressure breaker valves (PBVs). Chandrashekar (1980) modeled booster stations and check valves (CHVs). Convergence problems for networks that include several check valves and pressure reducing valves (PRVs) are mentioned and the question of existence and uniqueness of a solution arises. Collins et al. (1979) show examples for multiple operating points of a system, if the network includes pumps with non-monotone pump curves.

A comprehensive discussion of the uniqueness of solutions for networks with distributed feedback devices can be found in Berghout and Kuczera (1997). The authors stated that multiple solutions had not been found so far, as long as the control devices were controlled locally. In other words the control node must be directly connected to the device. The authors claim as an 'intuitive proof' for the uniqueness of the solution that PRVs have balancing impacts and the downstream pressure is kept constant.

Steady-State Calculation of the Network Hydraulics

There are a number of ways to choose the unknowns to be solved for in a water distribution system. The Q-H Formulation where the combined unknown head and flow equations are used (made up of continuity equations for each node and a head loss equation for each link in terms of the unknown nodal heads at each end of the link related to the discharge through the link) is the basis of the Todini and Pilati (1988) algorithm. This algorithm is the basis for many government (EPANET, Rossman 2000) and commercially available computer hydraulic solvers.

Consider a water distribution network of links and nodes in which the system has m links (for example pipe, pumps and valves), n variable-head nodes, r fixed-head nodes (for example, reservoirs or tanks) and a total of l loops and independent paths and also assume the network is completely connected. For simplicity pumps will not be included in the analysis although they can be easily incorporated. The relevant vectors are:

- $\mathbf{q} = (q_1, q_2, \dots, q_m)^{\mathrm{T}}$, where q_j is the unknown flow for the *j*-th link,
- $\mathbf{h} = (h_1, h_2, \dots, h_m)^{\mathrm{T}}$, where h_j is the head loss for the *j*-th link,
- $\mathbf{r} = (r_1, r_2, ..., r_m)^T$, where r_j is the resistance factor for the *j*-th link (for example based on Darcy-Weisbach or Hazen-Williams).
- $\mathbf{H} = (H_1, H_2, \dots, H_n)^{\mathrm{T}}$, where H_i is the unknown head for the *i*-th node.
- $\mathbf{Q} = (Q_1, Q_2, \dots, Q_n)^T$, where Q_i is the known demand at the *i*-th node.

Three topology matrices for the network need to be defined. First, each link in the network needs to have a direction assigned to it (see Figure 1). The first topology matrix is the unknown head node incidence matrix **A** of dimension *m* x *n* that defines the node identifiers at the ends of links such that: A(j, i) = -1 if link *j* leaves node *i*; A(j, i) = 0 if link *j* does not connect to node *i*; and A(j, i) = +1 if link *j* enters node *i*.

The second topology matrix that is required is the fixed head node incidence matrix A_R of dimension $m \ge r$ that defines the fixed head node identifiers at the end of links such that: $A_R(j, m) = -1$ if link j

leaves fixed head node *m*; $\mathbf{A}_{\mathbf{R}}(j, m) = 0$ if link *j* does not connect to fixed head node *m*; and $\mathbf{A}_{\mathbf{R}}(j,m) = +1$ if link *j* enters fixed head node *m*.

The third topology matrix is the loop and independent path incidence matrix **C** that is of dimension *m* x *l* that defines which links are in each loop in the network such that: C(j, k) = -1 if the link *j* is in loop *k* where the defined direction of the link is opposite to the assumed loop direction (see Figure 1); C(j, k) = 0 if link *j* is not part of loop *k*; and C(j, k) = +1 if the link *j* is in loop *k* where the defined direction of the assumed loop direction.

The continuity equations in matrix form in terms of the unknown flows **q** can be expressed as (Nielsen 1989):

$$\mathbf{A}^{\mathrm{T}}\mathbf{q} = \mathbf{Q} \tag{1}$$

The energy equations are:

$$\mathbf{h} + \mathbf{A}\mathbf{H} = -\mathbf{A}_{\mathrm{R}}\mathbf{H}_{\mathrm{R}}$$
(2)

Finally the head loss-flow relationships for the links in the network are

$$\mathbf{h} = f(\mathbf{q}) \tag{3}$$

Eq. (2) and Eq. (3) are formulated in terms of the link head losses. These head losses could have easily been eliminated. However they are presented in this form to explain the nonlinear relationship between the head loss and the discharge and are important for the later development of the Content and Co-Content for the system.

The Loop Flow Correction Formulation of the Pipe Network Equations

Based on the definition of topology matrices **A** and **C** (Todini and Pilati 1988, Deuerlein 2002) it holds that $\mathbf{A}^{\mathrm{T}} \mathbf{C} = \mathbf{0}$ and therefore $\mathbf{C}^{\mathrm{T}} \mathbf{A} = \mathbf{0}$ (Nielsen 1989). Multiplication of Eq. (2) by \mathbf{C}^{T} yields the equations for zero head loss around the loops or the head difference between fixed head nodes for the independent paths:

$$\mathbf{C}^{T}\mathbf{D}\mathbf{q} + \mathbf{C}^{T}\mathbf{A}\mathbf{D}\mathbf{q} + \mathbf{C}^{T}\mathbf{A}_{R}\mathbf{H}_{R} = \mathbf{0} \Leftrightarrow \mathbf{C}^{T}(\mathbf{D}\mathbf{q} + \mathbf{A}_{R}\mathbf{H}_{R}) = \mathbf{0}$$
(4)

with **D** being a diagonal matrix with non-zero elements defined as $D_{jj} = r_j |q_j|^{\alpha-1}$, j = 1,..., m, where α is the head loss exponent that depends on the type of head loss equation being used ($\alpha = 2$ for the Darcy-Weisbach equation, $\alpha = 1.852$ for Hazen-Williams). This formulation is a flow formulation in terms of the unknown flows **q** only and does not contain the nodal heads **H**. For the calculation of the *m* unknown flows in vector **q** the total number of loops and independent paths is given by l=m-n equations. Thus the system of equations in Eq. (4) is underdetermined.

The flow vector \mathbf{q} can be written as sum of the flows of an arbitrary flow vector \mathbf{q}_0 that solves the continuity equation (Eq. (1)) and a loop flow correction vector \mathbf{u} :

$$\mathbf{q} = \mathbf{q}_0 + \mathbf{C}\mathbf{u} \tag{5}$$

For the example network in Figure 1 there are two loops and one independent path between the reservoirs and thus three loop flow corrections u_1 , u_2 and u_3 . One way of calculating the flow vector \mathbf{q}_0 is to select one of the fixed grade nodes as a reference node and to compute the vector \mathbf{q}_0 by solving the linear system of continuity equations for a spanning tree of the network (spanning tree matrix \mathbf{A}_t):

$$\mathbf{q}_0 = [\mathbf{A}_1^{\mathrm{T}}]^{-1} \mathbf{Q} \tag{6}$$

The flows \mathbf{q} of Eq. (5) satisfy the continuity equations (Eq. (1)) independently of the choice of \mathbf{u} . The stationary point calculation is reduced to the solution of the nonlinear equation system in the loop correction vector variables \mathbf{u} :

$$\mathbf{C}^{\mathrm{T}}\mathbf{D}\mathbf{q}_{0} + \mathbf{C}^{\mathrm{T}}\mathbf{D}\mathbf{C}\mathbf{u} + \mathbf{C}^{\mathrm{T}}\mathbf{A}_{\mathrm{R}}\mathbf{H}_{\mathrm{R}} = \mathbf{0}$$
(7)

Eq. (7) represents the formulation of the unknown loop flow correction (\mathbf{u}) equations based on the head loss equations around loops and along independent paths between fixed head nodes. Thus the sum of head losses around each loop must be zero.

Nodal equations

Alternatively, the hydraulic equation can be obtained by the elimination of the vector of unknown flows **q** in Eq. (1) with use of Eq. (3). If the condition $D_{jj} \neq 0$ holds for all network links then the equality $\mathbf{A}\mathbf{H} = -\mathbf{D}\mathbf{q} - \mathbf{A}_{R}\mathbf{H}_{R}$ of Eq. (2) can be solved for **q** and applied to the continuity equation (Eq. (1)). As result the equation of the hydraulic steady-state calculation of pipe networks follows formulated in the variables of the unknown heads **H**:

$$\mathbf{A}^{\mathrm{T}}\mathbf{D}^{-1}\mathbf{A}\mathbf{H} + \mathbf{A}^{\mathrm{T}}\mathbf{D}^{-1}\mathbf{A}_{\mathrm{R}}\mathbf{H}_{\mathrm{R}} = -\mathbf{Q}$$
(8)

Analytical Approach for Problem Formulation Based on Variational Calculus

Formulation of a Nonlinear Optimization Problem without Constraints

An alternative solution approach for the various formulations above is based on nonlinear minimization methods (NLP). Birkhoff and Diaz (1956) and Birkhoff (1963) have shown that the calculation of the looped electrical circuit systems with consideration of the first and second laws of Kirchhoff is equivalent to the minimization of a convex function. These principles can be applied to solving the pipe network equations. Based on the work of Cherry (1951) and Millar (1951) for the calculation of electrical networks, Collins et al. (1978) applied the minimization of the so called Content and Co-Content functions to the calculation of the steady-state for hydraulic networks. The minimization of the Co-Content refers to the variational principle of Birkhoff (1963) who proved conditions for the existence and uniqueness of a solution to the problem. Two assumptions are introduced in this paper. The first is:

Assumption A: For each link of the hydraulic model there exists a (i) continuous and (ii) a (strictly) monotonically increasing relation of the vector form $\mathbf{h} = f(\mathbf{q})$ which represents a functional relation between the flow \mathbf{q} and the head loss \mathbf{h} .

The hydraulic equations that represent the bilateral relation between head loss and flow within a link have to be continuous (Assumption $A^{(i)}$) which guarantees the differentiability of the above mentioned Content and Co-Content functions (being the sum of the integrals of the headloss function) and strictly monotonically increasing (Assumption $A^{(i)}$) which guarantees the strict convexity of the Content and Co-Content functions.

Minimization of the Co-Content Function for Pipes and Unknown Head Nodes

Co-Content for water distribution systems may be specified in an analogous way to which Millar (1951) proposed definitions for electrical networks. First, define the function Π as the Co-Content for both the pipes and unknown head nodes in the network as (Birkhoff 1963):

$$\Pi = \sum_{j=1}^{m} W_j + \sum_{i=1}^{n} V_i \tag{9}$$

The quantity W_j for pipe j (j=1,2,...,m) is defined as the integral of the curve $q_j = g(h_j)$ in Eq. (3) and is shown in Figure 2 (a) (Cherry 1951, Millar 1951):

$$W_{j} = \int_{0}^{h_{j}} g(\mathbf{h}) d\mathbf{h} = \int_{0}^{h_{j}} (\mathbf{r}_{j}^{-1} |\mathbf{h}|)^{\frac{1}{\alpha}} \operatorname{sign}(\mathbf{h}) d\mathbf{h} = \frac{\alpha \mathbf{r}_{j}}{\alpha + 1} (\mathbf{r}_{j}^{-1} |\mathbf{h}_{j}|)^{\frac{\alpha + 1}{\alpha}}$$
(10)

where h_j is the head loss in pipe j, r_j is the pipe resistance factor. The Co-Content value V_i is for node i(i=1,...,n) with an unknown nodal head and is defined as the integral of the non increasing function F_{H_i} that describes the demand – head relationship at node i (Birkhoff (1963)):

$$V_{i} = -\int_{0}^{H_{i}} F_{H,i}(x) dx$$
 (11)

Figure 2 (b) shows the characteristics for a unknown head node with a given demand ($F_{H,i}$ = constant). There is a one to one correspondence for a pipe between flow and head loss and between nodal demand and head in Figure 2 (a) and Figure 2 (b), respectively. Later, we will see that this is not the case for check valves and flow control valves and as a result subdifferential calculus will need to be used.

Birkhoff (1963) has shown, in his Theorem 1, that the condition $\delta \Pi = 0$ is equivalent to the nodal equations (according to Eq. (1)). If the hydraulic equations $\mathbf{q} = g(\mathbf{h})$ are monotonically increasing functions and $F_{H,i}$, i=1,2,...,n monotone decreasing, then Π is convex (Theorem 2 in Birkhoff, 1963). If, for both, the condition of strict monotonicity holds then Π is even strictly convex (Theorem 3, Birkhoff 1963). In this case there exists at the most only one solution to the problem, that is, the

solution is unique. This outcome of existence and uniqueness of solutions is especially important to the development of this paper.

The Co-Content $\Pi : \mathbf{R}^n \to R$ can be formulated in terms of the unknown heads:

$$\min_{\mathbf{H}\in\mathbf{R}^{n}}\Pi(\mathbf{H}) \quad \text{with } \Pi(\mathbf{H}) = \sum_{j=1}^{m} W_{j} + \sum_{i=1}^{n} V_{i} = \frac{\alpha}{\alpha+1} \left[\left(\mathbf{A}\mathbf{H} + \mathbf{A}_{R}\mathbf{H}_{R} \right)^{T} \mathbf{D}^{-1} \left(\mathbf{A}\mathbf{H} + \mathbf{A}_{R}\mathbf{H}_{R} \right) \right] + \mathbf{H}^{T} \mathbf{Q}$$
(12)

Since $\Pi(\mathbf{H})$ is a continuously differentiable function that is defined on the whole \mathbf{R}^n the gradient $\nabla \Pi(\mathbf{H})$ can be calculated. It is necessary for a minimum \mathbf{H}^* of Π that it solves the variational equation

$$\delta \Pi = \nabla \Pi \left(\mathbf{H}^* \right)^T \left(\mathbf{H} - \mathbf{H}^* \right) = 0$$
(13)

where $\mathbf{H} - \mathbf{H}^*$ is an arbitrary variation $\delta \mathbf{H}$. The condition of Eq. (13) is valid for arbitrary variations $\delta \mathbf{H}$, if

$$\nabla \Pi = \mathbf{A}^T \mathbf{D}^{-1} \mathbf{A} \mathbf{H} + \mathbf{A}^T \mathbf{D}^{-1} \mathbf{A}_R \mathbf{H}_R + \mathbf{Q} = \mathbf{0}$$
(14)

Eq. (14) corresponds to the formulation of the nodal equations (Eq. (8)). Therefore the minimization of the Co-Content function is equivalent to the steady-state calculation (based on Proposition 2, Collins et al. 1978). Assumption $A^{(i)}$ guarantees the differentiability of the objective function $\Pi(\mathbf{H})$. Assumption $A^{(ii)}$ is sufficient for the (strict) convexity of $\Pi(\mathbf{H})$ (Collins et al. 1978). For h = 0, in Figure 2 (a), the slope of the curve is infinite, which causes problems in the iterative solution of the set of nonlinear nodal H-equations (Todini 2006).

Minimization of the Content Function for Pipes and Fixed Head Nodes

Now define the function Π^{c} as the Content for the pipes and fixed head nodes in the network as

$$\Pi^{c} = \sum_{j=1}^{m} W_{j}^{c} + \sum_{k=1}^{r} Z_{k}^{c}$$
(15)

For the calculation of the Content-function $\Pi^c : \mathbf{R}^1 \mapsto \mathbf{R}$ the integrals W_j^c for each of the pipes are required. The value W_j^c for pipe j (j=1,2,...,m) is defined as the area under the curve of head loss

versus flow $h_j = f(q_j)$ and is shown in Figure 3 (a) (Cherry (1951), Millar (1951)):

$$W_{j}^{c} = \int_{0}^{q_{j}} f(\mathbf{q}) d\mathbf{q} = \int_{0}^{q_{j}} r_{j} |\mathbf{q}|^{\alpha - 1} q \, d\mathbf{q} = \frac{1}{\alpha + 1} r_{j} |\mathbf{q}_{j}|^{\alpha - 1} q_{j}^{2}$$
(16)

where h_j is the head loss in pipe *j*, r_j is the pipe resistance factor. The value Z_k^c for a fixed head node *k* (*k*=1,...,*r*) is defined as the integral of the constant known head difference along the independent paths:

$$Z_{k}^{c} = -\int_{0}^{u_{k}} (H_{k,b} - H_{k,e}) dx$$
(17)

where $H_{k,b}$ is the beginning (fixed grade) node of the independent path k and $H_{k,e}$ is the end (fixed grade) node of the independent path k.

In the Content model the nodes with fixed given demands do not contribute to the Content function Here, in addition to the nodes with functional relation between demand and head (pumps, pressure dependent demands) the Content of the fixed grade nodes (Figure 3 (b)) has been included within the total system content. In contrast to Collins et al. (1978) in this paper the continuity equation Eq. (1) is not considered as a constraint of the minimization problem. Here, it is assumed that a flow distribution vector has already been found that solves the continuity equation (Eq. (1)) (for example - the flow vector of a spanning tree \mathbf{q}_0 as defined previously is determined by Eq. (6)) and based on this assumption the minimization problem is now formulated in terms of the unknown loop flow corrections **u** to minimize the system's Content:

$$\min_{\mathbf{u}\in\mathbf{R}^{1}}\Pi^{c}(\mathbf{u}) \text{ with } \Pi^{c}(\mathbf{u}) = \sum_{j=1}^{m} W_{j}^{c} + \sum_{k=1}^{r} Z_{k}^{c} = \frac{1}{\alpha+1} (\mathbf{q}_{0} + \mathbf{C}\mathbf{u})^{T} \mathbf{D}(\mathbf{q}_{0} + \mathbf{C}\mathbf{u}) + \mathbf{u}^{T} \mathbf{C}^{T} \mathbf{A}_{R} \mathbf{H}_{R}$$
(18)

A solution for the loop flow corrections \mathbf{u}^* must necessarily solve the variational equation

$$\delta \Pi^{c} = \nabla \Pi^{c} \left(\mathbf{u}^{*} \right)^{T} \left(\mathbf{u} - \mathbf{u}^{*} \right) = 0 \quad \forall \mathbf{u} \in \mathbf{R}^{1}$$
⁽¹⁹⁾

Implying that for arbitrary variations $\delta \mathbf{u} = \mathbf{u} - \mathbf{u}^*$ the vector \mathbf{u}^* is a solution of the following equation system:

$$\nabla \Pi^{c}(\mathbf{u}) = \mathbf{C}^{\mathrm{T}} \left[\mathbf{D}(\mathbf{q}_{0} + \mathbf{C}\mathbf{u}) + \mathbf{A}_{\mathrm{R}} \mathbf{H}_{\mathrm{R}} \right] = \mathbf{0}$$
(20)

Eq. (20) refers to the loop flow correction equations of Eq. (7). Thus the minimization of the system Content is equivalent to the calculation of the hydraulic steady-state (see Proposition 1, Collins et al. 1978). From Assumption A⁽ⁱ⁾ it follows that the integrals of the headloss functions can be calculated. Consequently the Content function as the sum of the resulting integrals is differentiable. Assumption A⁽ⁱⁱ⁾ of this paper guarantees the (strict) convexity of the Content function Π^c (Collins et al. 1979 and Collins et. al. 1978). Thus, there exists a unique solution for the minimization of the system Content. If according to Assumption A⁽ⁱⁱ⁾ strict monotonicity of all the hydraulic equations of the system features holds then it follows that there is strict convexity of the Content function Π^c . Therefore there exists at the most one *unique* solution to the problem. Due to the continuity and coercivity of Π^c ($\lim_{\|u\to\infty\|}\Pi^c(\mathbf{u})=+\infty$) it is guaranteed that there exists at least one solution to the hydraulic equations for the network system.

Systems including Flow Regulating Devices

In the following section, flow regulating control devices within water supply systems that have hydraulic laws complying with the subdifferential of a convex function are considered. The results are used for the development of an extended mathematical model of the hydraulic simulation of water supply networks. Eventually, the Content of control devices with subdifferential hydraulic laws in combination with the Content of conventional (not subdifferential) hydraulic equations for pipes and contributions of inflows and outflows of the system yields the Content Π^c of the system.

It will be shown that the minimization of Π^{c} is equivalent to the solution of the hydraulic equations with consideration of equality and inequality constraints for the flows. The system Content Π^{c} as a sum of convex functions is always convex (Rockafellar1970, Theorem 5.2). The problem can then be solved by using methods of constrained convex programming. For detailed information on the theoretical background of subdifferential calculus and convex analysis the reader is referred to Rockafellar (1970), Rockafellar and Wets (1998) and Hiriart-Urruty and Lemaréchal (1993). In order to distinguish network features (for example nodes and links of the network graph) that have a certain property from the other features, the indicator matrix I_p of features with property P with respect to the set M is introduced (see Definition 5, Appendix A)

An Extended Mathematical Model for Systems with Flow Regulating Devices

Preliminary requirements

The application of subdifferential calculus allows the extension of the mathematical model of hydraulic simulation of water supply networks by using hydraulic relations that can be assigned to a subdifferential according to Definition 3, Appendix A. Those relationships appear if flow regulating devices have to be considered. The hydraulic equations h = f(q) and q = g(h) are replaced by the subdifferential formulations $q \in \partial W$ and $h \in \partial W^c$. Assumption A is replaced by the following:

Assumption B: There exists for each link *j* of the model a hydraulic law in the form of a subdifferential mapping $\partial W_j^c: q_j \rightarrow h_j$ ($\partial W_j: h_j \rightarrow q_j$), which satisfies the specifications of a strictly monotone mapping according to Definition 4, Appendix A.

With Assumption B it follows (Theorem 12.17 of Rockafellar and Wets 1998) that the related system Content function is convex. The hydraulic equations of the previous section (normal pipes) are included in the subdifferential formulation as a special case $\partial W_j^c(q_j) = \{\nabla W_j^c(q)\}$ and $\partial W_i(h_i) = \{\nabla W_i(h)\}$.

Control Devices Having Subdifferential Hydraulic Laws

Overview

In the following section, various control devices and their subdifferential formulations of the hydraulic equations are presented together with the related Co-Content and Content functions. The variational equations presented in Eq. (13) and Eq. (19) being necessary conditions of a minimum of the Co-Content function Π and Content function Π^c in this case are replaced by inequalities. The definition of the subdifferential of a general non-differentiable function can be found in the Appendix A (Definition 3).

Check valves

Check Valves (CHV) are a one-way valve primarily used in combination with pumps to prevent reverse flow from draining the upper tank. Such valves appear as non-return flaps, non-return valves, check valves and membrane valves. In steady-state calculations the hydraulic operational state of the check valve, either opened or closed, is not known a priori. In fact the state depends on the water distribution systems' conditions both upstream and downstream of the check valve. The flow through the check valve is subject to inequality constraints and must satisfy the inequality for the flow through the check valve $q_{CHV} \ge 0$. If $q_{CHV} > 0$ then the check valve head loss will be the minor loss associated with the check valve in a fully open position.

$$h_{\rm CHV} = \zeta \frac{v^2}{2g} = \zeta \frac{q_{\rm CHV}^2}{2A_{\rm CHV}^2 g} = k_{\rm CHV} q_{\rm CHV}^2$$
(21)

where ζ is the minor head loss coefficient, A_{CHV} is the cross section area and k_{CHV} is the coefficient for the head loss equation of the check valve. For example the link 8 in the example network of Figure 1 can be considered to be a check valve that prevents a flow from node "d" to node "e". If the head H_e at the exit or end node increases and finally exceeds the head of the entrance or initial node H_d, the flow direction would change, which is then prohibited by the closure of the check valve. In this case an arbitrary head difference h_{CHV} = H_e -H_d < 0 across the closed valve can be observed that is not related to the hydraulic relation of check valve. There is a lack of a functional relation between flow and head drop across a closed check valve that complies with the described behavior. In that case the mapping $q \mapsto h$ is multivalued in contrast to the one to one correspondence of a normal pipe. In the following, the subdifferential hydraulic laws and the calculation of the convex Co-Content and Content functions of a check valve are described.

The Co-Content for a Check Valve

The subdifferential mapping of the hydraulic function of a check valve $q_{CHV}(h): R \mapsto R$ and the related Co-Content W_{CHV} are (Theorem 12.17, Rockafellar and Wets 1998) (see also Figure 4):

$$q_{CHV}(h) = \partial W_{CHV}(h) = \begin{cases} 0, & h \le 0 \\ \sqrt{h / k_{CHV}}, & h > 0 \end{cases}$$
(22)
$$W_{CHV}(h) = \begin{cases} 0, & h \le 0 \\ \int_{0}^{h} [h / k_{CHV}]^{\frac{1}{2}} dh = \frac{2k_{CHV}}{3} \left[\frac{h}{k_{CHV}}\right]^{\frac{3}{2}}, & h > 0 \end{cases}$$
(23)

In Eq. (22) and Figure 4 (a) there are two regions of interest for the check valve when the Co-Content of the function is considered including:

- 1. Where the check valve is closed ($q_{CHV} = 0$) the head drop across the valve is equal to or less than zero (in the region of $h_{CHV} \le 0$). Note that the term "head drop" is used here rather than "head loss" as there is no flow occurring. For this case the discharge is zero along the negative x-axis. The amount of head drop across the closed check valve depends on the difference in head on the upstream side of the valve (H_d in Figure 1) and the head on the downstream of the valve (H_e).
- 2. Once the head loss across the check value is positive ($h_{CHV} > 0$) corresponding to a positive flow, the relationship between flow and head loss for the check value becomes like a normal minor loss caused by the fully opened value. This behavior is represented by the upper right hand quadrant of Figure 4 (a).

Note in Figure 4 (a) the discontinuity in slope of the function at h=0, while in Figure 4 (b), integration to obtain the Co-Content function has led to a function with continuous slope at h=0.

The Content for a Check Valve

The dual formulation of the Content W_{CHV}^c follows from the inversion of the hydraulic relationship q = g(h) with consideration of $q_{CHV} \ge 0$. The head across the check value in terms of the subdifferential of the Content function and the Content function itself are defined as:

$$h_{CHV}(q) = \partial W_{CHV}^{c}(h) = \begin{cases} \emptyset, & q < 0\\ (-\infty, 0], & q = 0\\ k_{CHV}q^{2} = dq, & q > 0 \end{cases}$$
(24)
$$W_{CHV}^{c}(q) = \begin{cases} \infty, & q < 0\\ \int_{0}^{q} k_{CHV}q^{2}dq = \frac{1}{3}k_{CHV}q^{3}, & q \ge 0 \end{cases}$$
(25)

In Eq. (24) and Figure 5 (a) there are also two regions of interest when the Content of the function is considered. These include:

- 1. When the flow is positive ($q_{CHV} > 0$) through the check valve the head loss varies as normal for the case of the minor loss through a fully opened check valve. This zone is the upper right hand quadrant Figure 5 (a).
- 2. When the flow is zero the head difference across the check valve can vary anywhere in the range from (-∞,0] along the negative-y axis depending on heads on either side of the check valve being the upstream head (H_d Figure 1) and the downstream head (H_e). The mapping is multi-valued along the negative y-axis.

In Figure 5 (a) the slope of the Content function is discontinuous at q=0. In fact, the flow versus head loss relationship is not a one to one function anymore but is rather a multivalued mapping. In Figure 5 (b) integration of the subdifferential to obtain the Content function also leads to a function that has a discontinuity in both value and slope at q=0 (unlike the Co-Content function in Figure 4 (b)). In the terminology of convex analysis the Content function is lower semi-continuous. It is important to note that it is also convex.

Constraints of a Non-Linear Optimization Problem for a Check Valve

In contrast to the Co-Content function W_{CHV} whose subdifferential is defined on the entire domain of $(-\infty, +\infty)$, the Content function W_{CHV}^c is defined as $W_{CHV}^c = \infty$ for negative flows q < 0 where $\partial W_{CHV}^c = \emptyset$. For that reason in convex analysis the effective domain (see Definition 1, Appendix A) dom (W_{CHV}^c) of the Content function is introduced with dom $(W_{CHV}^c) = \left\{ q_{CHV} \in \mathbb{R} | W_{CHV}^c(q_{CHV}) < +\infty \right\}$ (see for example Rockafellar 1970, Theorem 3.4). If the indicator matrix as defined by Eq. (52) of the set \mathbf{M}_{CHV} of links that include check valves is denoted by \mathbf{I}_{CHV} , the constraints of the nonlinear optimization model in terms of the link flows, the loop incidence matrix \mathbf{C} and the unknown loop flow corrections \mathbf{u} are:

$$\mathbf{I}_{\mathrm{CHV}}^{\mathrm{T}} \left[\mathbf{q}_{0} + \mathbf{C} \mathbf{u} \right] \ge \mathbf{0}$$
(26)

It is assumed that the positive direction of the independent path coincides with the direction of flow. In the last part of the paper an example of the formulation of the non-linear programming problem for a check valve is given.

Flow Control Valves

Flow Control Valves (FCV) are used to limit the flow to be a maximum value q_{max} (called the set flow). The flow through the valve is monitored. If the flow exceeds q_{max} then the valve closes to create an additional head loss to reduce the flow to be equal to q_{max} and the FCV is in an active state. If the flow is less than the set flow q_{max} then the valve opens to try to achieve the set flow. For flows of $q < q_{max}$ the FCV will be totally opened and the behavior will be like a minor loss element corresponding to the fully opened FCV. Assume the minor loss coefficient for the fully open valve k_{OPEN} (see Figure 6) is the same for flow in either direction through the valve.

The Co-Content Function for Flow Control Valves

For the Co-Content function, Figure 6 shows the subdifferential for an FCV expressed in terms of discharge through the FCV as:

$$q_{FCV}(h) = \partial W_{FCV}(h) = \begin{cases} \left[\frac{|h|}{k_{FCV}}\right]^{\frac{1}{2}} \operatorname{sign}(h), & h \le h_{0} \\ q_{max}, & h > h_{0} \end{cases}$$
(27)

$$W_{FCV}(h) = \begin{cases} \int_{0}^{h} \left[\frac{|h|}{k_{FCV}}\right]^{\frac{1}{2}} \operatorname{sign}(h) dh = \frac{2k_{FCV}}{3} \left[\frac{|h|}{k_{FCV}}\right]^{\frac{3}{2}}, & h \le h_{0} \\ \int_{0}^{h_{0}} \left[\frac{|h|}{k_{FCV}}\right]^{\frac{1}{2}} \operatorname{sign}(h) dh + \int_{h_{0}}^{h} q_{max} dh = q_{max}(h - h_{0}) + \frac{2k_{FCV}}{3} \left[\frac{|h_{0}|}{k_{FCV}}\right]^{\frac{3}{2}}, & h > h_{0} \end{cases}$$
(28)

In Eq. (27) and Figure 6 (a) there are three regions of interest for the operation of a FCV including:

- 1. When the head loss (h as a minor loss) across the FCV is negative ($h_{FCV} < 0$) then the valve will be fully open and the reverse discharge will only be determined by the flow through the FCV (the lower left quadrant of Figure 6 (a)).
- 2. To the right of the vertical line $h_{FCV} = h_0$ on the x-axis where the discharge is constant given by the $q_{FCV} = q_{max}$ line, the FCV (active mode) is causing a head loss due to its partly closed position such that the minor head loss factor k is greater than the k value when the FCV is fully opened. The flow is constant and is maintained at the set value of q_{max} .
- 3. In the region where the head loss across the valve is in the range $(0 \le h_{FCV} \le h_0)$ where q is positive but less than q_{max} the FCV is full opened (inactive mode) and the flow through the valve is like a normal minor loss due to the FCV being fully open.

In each of these regions in Figure 6 (a) where the valve is fully opened it is assumed that a minor loss occurs across the FCV itself. In Figure 6 (a) the slope of the function is discontinuous at $h = h_0$. In Figure 6 integration of the subdifferential to obtain the Content function leads (Figure 6 (b)) to a function that has no discontinuity in value and slope at $h = h_0$ (unlike the Content function in Figure 7 (b)).

The Content Function for Flow Control Valves

For the Content function, Figure 7 shows the subdifferential for an FCV expressed in terms of head loss across the valve as:

$$h_{FCV}(q) = \partial W^{c}_{FCV}(q) = \begin{cases} k_{FCV} |q|q, & q \le q_{max} \\ [h_{0,\infty}), & q = q_{max} \\ \emptyset, & q > q_{max} \end{cases}$$
(29)

$$W_{FCV}^{c}(q) = \begin{cases} \int_{0}^{q} k_{FCV} |q| q dq = \frac{1}{3} k_{FCV} |q| q^{2}, & q \le q_{max} \\ \infty, & q > q_{max} \end{cases}$$
(30)

In Eq. (29) and Figure 7 (a) there are three zones of interest including:

- 1. For $(q_{FCV} \le 0)$, there is reverse flow through the FCV, the FCV is fully opened and the flow is governed by the minor head loss coefficient for reverse flow.
- 2. For $q_{FCV} = q_{max}$, the head loss (h_{FCV}) through the FCV can vary anywhere in the range $(h_0, +\infty)$ along the $q_{FCV} = q_{max}$ vertical line above the horizontal line $h_{FCV} = h_0$. This mapping is multi-valued. The head loss is created by the amount by which the FCV is closed to ensure it delivers only the set value of q_{max} .
- 3. For the region between $q_{FCV} = 0$ and $q_{FCV} = q_{max}$ the FCV is fully opened. The set flow cannot be achieved. The head loss across the FCV is the minor loss for the fully opened FCV.

Constraints of a Non-Linear Optimization Problem for a Flow Control Valve

For the minimization of the system-Content (see Figure 7) within the effective domain the following constraints have to be considered for FCV (I_{FCV} : Indicator matrix of the set M_{FCV} of links that include FCVs):

$$\mathbf{I}_{\text{FCV}}^{\text{T}} \left[\mathbf{q}_{0} + \mathbf{C} \mathbf{u} \right] \leq \mathbf{q}_{\text{max}}$$
(31)

Temporarily Closed Isolating Valves

In addition to control devices considered earlier in the paper, water supply networks often include a number of valves that may be used for total closure of particular links. The valves are closed for instance during rehabilitation or control of the system. Temporary closure of isolating valves can also be useful for calibration in order to provide different flow distributions. The information that is gained from pressure measurements is thus increased.

For modeling of temporarily closed isolating valves (CIV) the related links can be removed from the graph. For the minimization of the system Co-Content Π this can be realized easily by removing the columns of those links from the incidence matrix of the network graph. With regard to the minimization of the system Content function Π^c the effort would be much more complex because the loop matrix also has to be modified. For this case it is more efficient to model the temporarily closed valves with equality constraints that are added to the mathematical model:

$$\mathbf{I}_{\text{CIV}}^{\text{T}}[\mathbf{q}_{0} + \mathbf{C}\mathbf{u}] = \mathbf{0}$$
(32)

Matrix I_{CIV} is again the indicator matrix of the set of isolating valves that are temporarily closed.

Variational Inequalities and the Nonlinear Optimization Formulation

In this section the general formulations for the minimization of the system Content and system Co-Content for networks that include features with subdifferential hydraulic laws shall be derived. It is assumed that the hydraulic equations of subdifferential type for pipe or control device *j* are known. Let $s(h_j) \in \partial W_j(h_j), h_j \in \mathbb{R}$ and M_{h_j} be the feasible range for the head loss of link *j*. Then, the Co-Content is given by (see Remark 4.2.5, Hiriart-Urruty and Lemarechal 1993)

$$W_{j}(h_{j}) = \begin{cases} W_{j}(a) + \int_{a}^{h_{j}} s(x) dx, & h_{j} \in M_{h_{j}} \\ \infty, & h_{j} \notin M_{h_{j}} \end{cases}$$
(33)

for all $x \in [a,b]$. Correspondingly the function for the Content of link *j* can also be stated. Let $t(q_j) \in \partial W_j^c(q_j), q_j \in R$ and Q_j be the set of admissible flows of link *j*. It follows that the Content function is as follows:

$$W_{j}^{c}(q_{j}) = \begin{cases} W_{j}^{c}(a) + \int_{a}^{q_{j}} t(x) dx, & q_{j} \in Q_{j} \\ \infty, & q_{j} \notin Q_{j} \end{cases}$$
(34)

for all $x \in [a, b]$. It is further assumed that the possibly multivalued hydraulic relation satisfies the requirements of a strictly monotone subdifferential mapping (see Assumption B and Definition 4, Appendix A). Since the Content (and the Co-Content) functions are proper and lower semicontinuous

(see Definition 2, Appendix A), it follows that they are convex (Theorem 12.17, Rockafellar and Wets 1998). With Assumption B, the equations (33) and (34) are due to the definition of the subdifferential (see Definition 3 of the Appendix A) equivalent to the variational inequalities for both the Co-Content and Content

$$\delta W_{j} = W_{j} (\mathbf{h}_{j} + \delta \mathbf{h}_{j}) - W_{j} (\mathbf{h}_{j}) \ge q_{j} \delta \mathbf{h}_{j} \quad \forall q_{j} \in \partial W_{j} (\mathbf{h}_{j})$$
(35)

and

$$\delta W_{j}^{c} = W_{j}^{c} \left(\mathbf{q}_{j} + \delta \mathbf{q}_{j} \right) - W_{j}^{c} \left(\mathbf{q}_{j} \right) \ge \mathbf{h}_{j} \delta \mathbf{q}_{j} \qquad \forall \mathbf{h}_{j} \in \partial W_{j}^{c} \left(\mathbf{q}_{j} \right)$$
(36)

The hydraulic equations of the *j*-th link $q_j = g_j(h_j)$ with a continuous and strictly monotone increasing function $g_j : \mathbb{R} \to \mathbb{R}$ are replaced by the more general subdifferential conditions $q_j \in \partial W_j(h_j)$ and $h_j \in \partial W_j^c(q_j)$, respectively, which is equivalent to the inequalities of Eq. (35) and Eq. (36) where $\partial W_j(h_j)$ ($\partial W_j^c(q_j)$) is the subdifferential of the proper, convex and lower semi continuous (see Definition 2 of Appendix A) Co-Content function $W_j(h_j)$ (Content function $W_j^c(q_j)$). Following the same ideas as in the previous section as to systems without control devices the total systems Co-Content function can be calculated as the sum of the Co-Content functions of the particular network features.

According to Eq. (12) the minimization problem of the Co-Content function of systems including features with non-differentiable but *sub-differentiable* hydraulic laws can be stated as

$$\min_{\mathbf{H}\in\mathbf{R}^{n}}\widetilde{\Pi}(\mathbf{H}) \tag{37}$$

In contrast to Eq. (12) the objective function in Eq. (37) is not twice continuous differentiable which is indicated by the tilde. A necessary condition for a minimum \mathbf{H}^* is that it solves the variational inequality:

$$\nabla \widetilde{\Pi} (\mathbf{H}^*)^{\mathrm{T}} (\mathbf{H} - \mathbf{H}^*) \ge 0 \quad \forall \mathbf{H} \in \mathbf{R}^{\mathrm{n}}$$
(38)

In an analogous way, the minimization problem of the Content function is derived. As shown previously, the check valve and FCV control devices have subdifferentiable, possibly multivalued hydraulic laws that include the indicator functions of the convex sets that represent the unilateral behavior of the control devices. If the contributions of the indicator functions (see Appendix A, Definition 6) are removed from the objective function and replaced by inequality conditions then the problem can be formulated as a nonlinear minimization problem of a twice continuously differentiable objective function over a polyhedral set instead of a minimization problem of the unconstrained subdifferentiable convex function $\widetilde{\Pi}^c(\mathbf{u}): \mathbf{R}^1 \mapsto \mathbf{R}$. Note that due to the monotonicity properties of the hydraulic laws of the different network features (pipes, check valves, FCVs) both the function $\widetilde{\Pi}^c$ and Π^c are convex. In addition since the flow is subject to friction everywhere in the system both functions are even strictly convex. For example the content of the check valve (Eq. (25)) can be written as the sum

$$W_{\rm CHV}^{\rm c} = I_{\rm C} + \frac{1}{3} k_{\rm CHV} |q| q$$
(39)

 $C_{CHV} = \{q | q \ge 0\}$ represents the convex feasible set for the flow through a check valve and $I_{C_{CHV}}$ is the indicator function (Definition 6, Appendix A) of the set C_{CHV} . For the minimization of the total system Content function the unconstrained minimization problem of Eq. (18) is replaced by:

$$\min_{\mathbf{u}\in\mathbf{U}}\Pi^{c}(\mathbf{u}) \tag{40}$$

The feasible set U consists of a convex polyhedral subspace of \mathbf{R}^1 and is defined by:

$$\mathbf{U} = \left\{ \mathbf{u} \in \mathbf{R}^1 | \mathbf{g}(\mathbf{u}) \le \mathbf{0}, \mathbf{h}(\mathbf{u}) = \mathbf{0} \right\} \subseteq \mathbf{R}^1$$
(41)

The function $g(\mathbf{u})$ refers to the flow inequality constraints due to check valves (Eq. (26)) and FCVs (Eq. (31)):

$$g(\mathbf{u}) = \begin{bmatrix} -\mathbf{I}_{CHV} & \mathbf{I}_{FCV} \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \mathbf{q}_{0} + \mathbf{C}\mathbf{u} \end{bmatrix} - \begin{bmatrix} \mathbf{I}_{FCV} \end{bmatrix}^{\mathrm{T}} \mathbf{q}_{\max} \le \mathbf{0}$$
(42)

Temporarily closed valves are modeled with the equality constraints of Eq. (32):

$$\mathbf{h}(\mathbf{u}) = [\mathbf{I}_{CIV}]^{\mathrm{T}}[\mathbf{q}_{0} + \mathbf{C}\mathbf{u}] = \mathbf{0}$$
(43)

The Content function Π^{c} is the sum of the single Content-functions of control devices, pipes and linear contributions of inflows and outflows at the fixed grade nodes. In contrast to the Co-Content function Π , the Content function without the terms belonging to the indicator functions of the flow constraints is twice continuous differentiable. The necessary condition for a solution of the problem in Eq. (40) can be stated as a variational inequality (see Harker and Pang, 1990, page 165):

$$\nabla \Pi^{c} \left(\mathbf{u}^{*} \right)^{T} \left(\mathbf{u} - \mathbf{u}^{*} \right) \geq 0 \quad \forall \mathbf{u} \in \mathbf{U}$$

$$\tag{44}$$

Application of Nonlinear Optimization

Overview

For the calculation of the hydraulic steady-state with consideration of control devices using subdifferential hydraulic laws, the methods of constrained nonlinear optimization are applied. The minimization of the system Co-Content Π as well as the minimization of the system Content Π^c is presented. For both of these, a nonlinear convex objective function has to be minimized over a polyhedral set that is defined by linear constraints. The objective function for the Co-Content formulation Π (Eq. (37)) is defined in a piecewise way and is only one times continuous differentiable (see hydraulic laws of check valves and FCVs) whereas the objective function for the Co-Content to the content formulation Π^c of the second problem (Eq. (40)) is twice continuous differentiable over the total feasible range U. This will be seen to be clearly advantageous.

Minimization of the Co-Content Function

The total Co-Content of the system is composed of the sum of the Co-Content of the individual links and nodes. One significant discrepancy in the formulation of the system Co-Content according to Eq. (12) consists of the lack of twice differentiability (e.g. check valves and FCVs) of the Co-Content contributions. With consideration of the control devices of subdifferential hydraulic type, the hydraulic steady-state is completely described by the following Convex Optimization problem with the convex nonlinear objective function Π over the feasible set \mathbf{R}^n (Abbreviation: CO(\mathbf{R}^n, Π)):

$$\operatorname{CO}(\mathbf{R}^{n}, \widetilde{\Pi}): \min_{\mathbf{H} \in \mathbf{R}^{n}} \widetilde{\Pi}(\mathbf{H})$$

$$with: \quad \widetilde{\Pi} = \frac{\alpha}{\alpha + 1} (\mathbf{A}\mathbf{H} + \mathbf{A}_{R}\mathbf{H}_{R})^{T} \widetilde{\mathbf{D}}^{-1} (\mathbf{A}\mathbf{H} + \mathbf{A}_{R}\mathbf{H}_{R}) + \mathbf{H}^{T}\mathbf{Q}$$

$$(45)$$

Thus the outcome here is an unconstrained optimization problem in terms of unknown nodal heads. The difficulty is that the matrix $\tilde{\mathbf{D}}$ is made up of pipes, check valves and flow control valves. In contrast to the formulation of the hydraulic steady-state that contains no control devices with subdifferential hydraulic laws (see matrix \mathbf{D} in Eq. (12)), $\tilde{\mathbf{D}}^{-1}$ contains piecewise defined functions $d_i : R \mapsto R$ that are not continuous for the whole range R (see for instance relation $q_{CHV}(h_{CHV})$ or $q_{FCV}(h_{FCV})$).

Minimization of the Content Function

In contrast to the Co-Content function Π , the objective function for the Content Π^{c} of systems including control devices as described above is twice continuously differentiable. The minimization of the system Content according to Eq. (18) extended by the linear constraints of the control devices complies with the dual formulation of the minimization of the Co-Content (see Eq. (45)):

with:
$$\Pi^{c} = \frac{1}{\alpha + 1} (\mathbf{q}_{0} + \mathbf{C}\mathbf{u})^{\mathrm{T}} \mathbf{D}(\mathbf{q}_{0} + \mathbf{C}\mathbf{u}) + \mathbf{u}^{\mathrm{T}} \mathbf{C}^{\mathrm{T}} \mathbf{A}_{\mathrm{R}} \mathbf{H}_{\mathrm{R}}$$
(46)

Thus the outcome here is a constrained optimization problem in terms of loop flow corrections, but the objective function Π^{c} is twice continuously differentiable (thus the **D** matrix is in terms of functions that are continuous). In addition, the check valves, FCVs are dealt with as inequality constraints. The Lagrangian multipliers turn out to be the local head losses (FCVs) or head drops (check valves) of the control devices. As a result the Content model is selected for implementation.

The Lagrangian function of the convex optimization problem $CO(U,\Pi^c)$ is:

$$L_{\text{CO}(\mathbf{U},\Pi^{c})} = (\mathbf{C}\mathbf{u})^{\mathrm{T}} \frac{1}{\alpha+1} \left[\mathbf{D}(\mathbf{q}_{0} + \mathbf{C}\mathbf{u}) + \mathbf{A}_{\mathrm{R}}\mathbf{H}_{\mathrm{R}} \right] + \sum_{i=1}^{s} \mu_{i} g_{i}(\mathbf{u}) + \sum_{j=1}^{d} \lambda_{j} h_{j}(\mathbf{u})$$
(47)

where $\mu_i :=$ Lagrangian multipliers of the inequality constraints for the check values and FCVs (i = 1,..., s), $\lambda_j :=$ Lagrangian multipliers of the equality constraints for the temporarily closed isolating values (j=1,...,d), *s* is the number of control devices with inequality constraints and *d* is the number of temporarily closed links with equality constraints. The twice continuous differentiability of Π^e with respect to the variables **u** allows the calculation of the gradient $\nabla_{\mathbf{u}} L_{CO(\mathbf{U},\Pi^e)}$ and Hessian matrix $\nabla_{\mathbf{u}}^2 L_{CO(\mathbf{U},\Pi^e)}$ of the Lagrangian $L_{CO(\mathbf{U},\Pi^e)}$. Using the gradients of the linear constraints $\nabla_{\mathbf{u}} g(\mathbf{u}) = \mathbf{G}_1$ and $\nabla_{\mathbf{u}} h(\mathbf{u}) = \mathbf{H}$, the derivatives of the Lagrangian can be written as:

$$\nabla_{\mathbf{u}} L_{\mathrm{CO}(\mathbf{U},\Pi^{c})} = \mathbf{C}^{\mathrm{T}} \left[\mathbf{D} (\mathbf{q}_{0} + \mathbf{C}\mathbf{u}) + \mathbf{A}_{\mathrm{R}} \mathbf{H}_{\mathrm{R}} \right] + \mathbf{G}_{1}^{\mathrm{T}} \boldsymbol{\mu} + \mathbf{H}^{\mathrm{T}} \boldsymbol{\lambda}$$
(48)

$$\nabla_{\mathbf{u}}^{2} L_{\mathrm{CO}(\mathbf{U},\Pi^{c})} = \mathbf{C}^{\mathrm{T}} \mathbf{D} \mathbf{C}$$
(49)

A necessary condition for a solution of the problem $CO(U,\Pi^c)$ are the Kuhn-Tucker conditions of nonlinear programming, which can be written as:

$$\nabla_{\mathbf{u}} L_{\text{CO}(\mathbf{U},\Pi^{c})} = \mathbf{C}^{\mathrm{T}} \left[\mathbf{D} (\mathbf{q}_{0} + \mathbf{C}\mathbf{u}) + \mathbf{A}_{\mathrm{R}} \mathbf{H}_{\mathrm{R}} \right] + \mathbf{G}_{1}^{\mathrm{T}} \boldsymbol{\mu} + \mathbf{H}^{\mathrm{T}} \boldsymbol{\lambda} = \mathbf{0}$$

$$g(\mathbf{u}) \leq \mathbf{0}; \quad h(\mathbf{u}) = \mathbf{0}; \quad \mu_{i} g(\mathbf{u})_{i} = 0, i = 1, \dots, s; \quad \boldsymbol{\mu} \geq 0$$
 (50)

Assumption B guarantees the positive definiteness of the Hessian matrix (Eq. (49)).

The assumed strict monotonicity of the mappings ∂W_j^c and ∂W_j (compared with Assumption B) implies strict convexity of the functions Π^c and Π , which by theorems in nonlinear programming guarantees that the problem CO(U, Π^c) has at most one unique local (and hence global) optimal solution. If in addition $\mathbf{U} \neq \emptyset$ the existence of a unique solution is proven. Sufficient for the uniqueness of the Lagrangian multipliers is the Linear Independence Constraint Qualification (LICQ) of Nonlinear Programming that requires that the gradients of the active inequality constraints together with the gradients of the equality constraints are linearly independent at the solution point. As a result of the development of this constrained nonlinear optimization formulation, the correct operating status of check valves and flow control valves can be determined and guaranteed by the solution process. Use of the Content function approach ensures that the solution to the nonlinear optimization problem gives a unique solution that has been shown to exist. This represents a significant improvement over the current use of heuristics in combination with solving the non-linear equations for simulation of water distribution systems. Examples of problems with the heuristic approaches have been described by Simpson (1999) and Deuerlein et al. (2008).

Example Systems

For illustration of the solution of the constrained minimization problem $CO(U, \Pi^c)$ for the Content of a system, the network presented in Figure 1 serves as an example. It consists of two supply areas that are each supplied by one storage tank. The zones are connected by a pipe including a FCV between nodes a and c, which restricts the possible flow from S1 to S2 up to a certain maximum set flow (q_{max}) and a check valve in link 8 between nodes d and e that only allows flow from supply area 1 (S1) to supply area 2 (S2). Two different scenarios are considered. In the first case the demand Q_c at node c is less than the set value of the FCV and a feasible solution exists. In the second case the demand at node c is increased such that it exceeds the set value of the FCV. Since the CHV prohibits a flow from S2 to node c, a feasible solution does not exist in this case.

The necessary conditions for a minimum of the Content function for the system without flow control devices according to Eq. (20) are:

$$\mathbf{C}^{\mathrm{T}}\mathbf{D}(\mathbf{q}_{0} + \mathbf{C}\mathbf{u}) = -\mathbf{C}^{\mathrm{T}}\mathbf{A}_{\mathrm{R}}\mathbf{H}_{\mathrm{R}}$$
 with $\mathbf{q}_{0} = [\mathbf{A}_{\mathrm{t}}^{\mathrm{T}}]^{-1}\mathbf{Q}$

where \mathbf{q}_0 denotes the flow distribution of the spanning tree. The iterative calculation can be carried out by application of the Newton-Raphson-method for the solution of the nonlinear system:

$$\left[\mathbf{C}^{\mathrm{T}}\mathbf{D}\mathbf{C}\right]_{k}\mathbf{u}_{k+1} = -\mathbf{C}^{\mathrm{T}}\left(\mathbf{D}_{k}\mathbf{q}_{k} + \mathbf{A}_{\mathrm{R}}\mathbf{H}_{\mathrm{R}}\right), \qquad \mathbf{q}_{k+1} = \mathbf{q}_{k} + \frac{1}{\alpha}\mathbf{C}\mathbf{u}_{k+1}$$

Case 1: Demand at Node c is less than FCV flow setting $(q_{max} > Q_c)$

Two additional inequalities have to be considered, which in this example is equivalent to $q_8 \ge 0$ and $q_4 \le q_{max}$. The necessary conditions for the solution of the problem are expressed by the Kuhn-Tucker conditions of nonlinear optimization including the derivative of the Lagrangian function, the constraints and the complementary slackness condition:

$$\mathbf{C}^{\mathsf{T}} \mathbf{D} (\mathbf{q}_{0} + \mathbf{C} \mathbf{u}) + \mathbf{C}^{\mathsf{T}} \mathbf{I}_{\mathsf{FCV}} \boldsymbol{\mu}_{\mathsf{FCV}} - \mathbf{C}^{\mathsf{T}} \mathbf{I}_{\mathsf{CHV}} \boldsymbol{\mu}_{\mathsf{CHV}} = -\mathbf{C}^{\mathsf{T}} \mathbf{A}_{\mathsf{R}} \mathbf{H}_{\mathsf{R}}$$

$$q_{0,4} + u_{2} - q_{\max} \le 0; \quad \boldsymbol{\mu}_{\mathsf{FCV}} \ge 0; \quad \boldsymbol{\mu}_{\mathsf{FCV}} (q_{0,4} + u_{2} - q_{\max}) = 0;$$

$$-(q_{0,8} + u_{2}) \le 0; \quad \boldsymbol{\mu}_{\mathsf{CHV}} \ge 0; \quad (q_{0,8} + u_{2}) \boldsymbol{\mu}_{\mathsf{CHV}} = 0$$
(51)

where **u** is the vector of loop flow corrections and the Lagrangian multiplier μ_{FCV} and μ_{CHV} are the local headloss of theactive flow control valve and head drop across the check valve, respectively. Assuming that in iteration k the FCV is inactive (open) and the check valve is closed (active) the following system of equations for the system in Figure 1 has to be solved:

$$\begin{pmatrix} d_3 + d_4 + d_{10} & -d_3 & 0 & 0 \\ -d_3 & d_1 + d_2 + d_3 + d_5 + d_6 + d_8 + d_{11} & -d_5 & -1 \\ 0 & -d_5 & d_1 + d_3 + d_4 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}_k \begin{pmatrix} \Delta u_1 \\ \Delta u_2 \\ \Delta u_3 \\ \mu_{\text{CHV}} \end{pmatrix}_{k+1} = - \begin{pmatrix} -\sum h_{LI} \\ -\sum h_{LII} \\ -\sum h_{LII} \\ 0 \end{pmatrix}_k$$

where for pipes $d_j = r_j |q_j|^{\alpha-1}$ and for check values $d_j = \frac{2}{\alpha} k_{CHV} q$. If in the solution the check value is closed that means that the inequality condition for the flow through link 8 is fulfilled with equality $q_8 = 0$. In that case the Lagrangian multiplier of the constraint is positive and represents the head drop across the check value in Figure 1 of $H_d - H_e = \mu$.

Case 2: Demand at Node c exceeds the FCV flow setting $(q_{max} < Q_c)$

Now the FCV link 4 is considered to be active. The necessary conditions for the solution of the problem expressed by the Kuhn-Tucker are the same as in Eq. (51). In this case the system of linear inequalities $q_{0,4} + u_2 - q_{max} \le 0$ and $-q_{0,8} - u_2 \le 0$ has no solution (from the continuity equation it follows that $q_{0,4} - q_{0,8} - Q_c = 0$). Consequently there is no feasible solution to the nonlinear optimization problem. Existing hydraulic solvers that are based on heuristics fail to calculate proper results for this

system. For example, EPANET finds an incorrect solution, in which both set flows are exceeded (which is incorrect) and 50% of the excess flow is allocated to both the FCV and the CHV. Thus the fact that a solution to the problem did not exist was not detected by the heuristic approach. The new computational procedure for FCVs based on NLP described in this paper is able to compute the correct answer. At the beginning of the iterative procedure, a point in the interior of the feasible set U (Eq. (41)) is calculated by use of a modified Simplex Algorithm guaranteeing that all of the inequality constraints are in an inactive state and that the multiplier vector is zero. In case 2, the non-existence of a feasible flow vector is detected before the iterative calculation takes place. In case 1 (with this initial flow distribution) the system of equations, resulting from the Kuhn-Tucker-conditions is solved for the new flows by using a modified Newton-Raphson-algorithm. After each iteration it is checked as to whether the new calculated iteration point is within the feasible set U or outside its boundary. If the new point is outside of U, it is reset to the intersection of the line that connects x_{n+1} and x_n with the constraint that is violated first. Consequently at the most, one constraint can become active within each iteration step. In contrast, the heuristic procedure in the EPANET-algorithm checks after each second iteration all constraints simultaneously and modifies the system at places where the constraints are violated, which may lead to non-convergence or the incorrect solution.

The new NLP solution method as proposed in this paper has been implemented for a number of networks ranging from theoretical systems to real networks with more than 20,000 nodes and pipes. Compared with EPANET, in most of the tested cases the calculation requires more time depending on the number of flow control devices. However, the new algorithm in this paper always provides the correct solution to the flow distribution in contrast to EPANET which on some of these networks gave the wrong solution.

Conclusions

This paper presents a theoretical framework for the correct simulation of water distribution system networks that contain flow controlling devices comprising check valves, flow control valves and/or temporarily closed isolation valves. The new method presented in this paper replaces the existing approach where heuristics are used to determine the operating state of check valves and flow control

valves during the iterative process in which the nonlinear pipe network equations are solved. An important observation about flow regulating valves is that the flow versus head relationship is clearly defined for these devices, which is in stark contrast to pressure regulating devices.

In this paper, a Content and Co-Content approach has been considered. Subdifferential analysis has been introduced due to the head versus flow relationships for check valves and flow control valves not being twice continuously differentiable. This leads to the definition of a convex problem that is proven to have a solution that both exists and is unique. The uniqueness proof is an important advantage in framing the solution as a constrained nonlinear optimization problem with inequality constraints (check valves, FCVs) and equality constraints (temporarily closed isolating valves) rather than just the solution of a set of non-linear equations. The new method based on an optimization approach based on the Content function appropriately deals with the equality and inequality constraints associated with flow regulating devices thereby enabling the correct solutions for the operating status of valves to be found for the hydraulic flows and heads in networks containing these devices. The Lagrangian multipliers arising in the approach have been shown to have a unique physical interpretation. For a check valve and a temporarily closed isolation valve the Lagrangian multiplier is the head drop across the closed valve. For a flow control valve, the Lagrangian multiplier is the head loss created by the valve maintaining the flow through the valve at the set flow. The non-linear constrained optimization formulation based on the Content model has been implemented. Two cases for an example network configuration containing a check valve and a flow control valve have been investigated. The methodology presented here represents a significant improvement over the current methods used in hydraulic modeling that are based on heuristics for dealing with flow control valves.

Appendix A: Definitions

For the following definitions the function $f : \mathbb{R}^n \mapsto \overline{\mathbb{R}} := \mathbb{R} \cup \{-\infty, \infty\}$ is considered. For reference see Rockafellar and Wets (1998).

Definition 1 (Domain): The domain of the function is defined as dom $f := \{x : f(x) < \infty\}$.

Definition 2 (Properties of the function *f* (proper, convex, lower semi-continuous)):

(a) A function is called proper if it is never equal to $-\infty$ and dom $f :\neq \emptyset$.

(b) A function $f: \mathbf{R}^n \mapsto \overline{\mathbf{R}}$ is convex if for all $x, y \in \mathbf{R}$ and for all $\lambda \in (0,1)$ it holds that $f(\lambda x + (1 - \lambda)y) \le \lambda f(x) + (1 - \lambda)f(y).$

(c) A function $f: \mathbf{R}^n \mapsto \overline{\mathbf{R}}$ is called lower semi-continuous at a point $\overline{\mathbf{x}}$, if $\liminf f(\mathbf{x}) \ge f(\overline{\mathbf{x}})$.

Definition 3 (Subgradients, Subdifferential): The set of regular subgradients $\hat{\partial} f(\bar{\mathbf{x}})$ of a function

 $f: \mathbb{R} \mapsto \overline{\mathbb{R}}$ is the set of all points χ such that $\liminf_{x \to \overline{x}, x = \overline{x}} \frac{f(x) - f(\overline{x}) - \chi^{T}(x - \overline{x})}{\|x - \overline{x}\|} \ge 0$. The subdifferential

 $\partial f(\overline{x})$ of $f: \mathbb{R}^n \to \mathbb{R}$ is the set of all cluster points of elements of $\hat{\partial} f(\overline{x})$ for $x \to \overline{x}$. (see Figure 8) For convex functions it coincides with $\hat{\partial} f(\overline{x})$.

Definition 4 (Monotonicity): The subdifferential mapping $\mathbf{x} \rightarrow \partial f(\mathbf{x})$ is monotone if

 $(\mathbf{u} - \mathbf{v})^{\mathrm{T}}(\mathbf{x} - \mathbf{y}) \ge 0$ for all $\mathbf{x}, \mathbf{y} \in \mathbf{R}^{\mathrm{n}}$ and all $\mathbf{u} \in \partial f(\mathbf{x}), \mathbf{v} \in \partial f(\mathbf{y})$ and strictly monotone if

 $(\mathbf{u} - \mathbf{v})^{\mathrm{T}}(\mathbf{x} - \mathbf{y}) > 0$ for all $\mathbf{x}, \mathbf{y} \in \mathbf{R}^{\mathrm{n}}$ and all $\mathbf{u} \in \partial f(\mathbf{x}), \mathbf{v} \in \partial f(\mathbf{y})$.

Definition 5 (Indicator matrix): Consider the index set **M** of the total set of elements $|\mathbf{M}| = m$ and the index set $\mathbf{P} \subseteq \mathbf{M}$ of elements having property \mathbb{P} with $|\mathbf{P}| = k$. The $(m \times k)$ matrix \mathbf{I}_p is denoted as indicator matrix of the set **P** with respect to **M** and is defined by:

$$\mathbf{I}_{\mathbf{P}_{(i,j)}} = \begin{cases} 1, & \text{if } i \in \mathbf{M} \text{ and } j \in \mathbf{P} \\ 0, & \text{else} \end{cases}$$
(52)

Definition 6 (Indicator function of the convex set C): A convex set C can be analytically represented by its convex indicator function:

$$I_{\rm C}(\mathbf{x}) = \begin{cases} 0 & \text{for } \mathbf{x} \in \mathbf{C} \subset \mathbf{R} \\ \infty & \text{for } \mathbf{x} \notin \mathbf{C} \end{cases}, \quad \mathbf{x} \in \mathbf{R}^n$$

Appendix B: Notation

Α	$(m \ge n)$ incidence matrix of unknown head nodes
A _{CHV}	cross section area of a check valve
\mathbf{A}_{R}	$(m \ge r)$ incidence matrix of fixed grade nodes
С	$(m \ge l)$ loop incidence matrix
D	(<i>m</i> x <i>m</i>) diagonal matrix of derivatives of head loss functions
d	number of links with equality flow constraints
Н	<i>n</i> vector of heads at unknown head nodes
\mathbf{H}_{R}	r vector of heads at fixed grade nodes
\mathbf{H}^{*}	heads at minimum point
h	<i>m</i> vector of head losses of the links
\mathbf{I}_P	indicator matrix of subset of links having property P (P = CHV, FCV or CIV)
$\mathbf{k}_{\mathbf{v}}$	valve head loss coefficient
l	number of loops plus independent paths
$M_{h_{j}}$	feasible range for the head loss of pipe j
т	number of links
n	number of nodes with unknown head
q _{max}	set flow of flow control valve
q	<i>m</i> vector of link flows of the network
q ₀	<i>n</i> vector of flows of a spanning tree
Q	n vector of nodal demands
r	number of nodes with fixed head
r	<i>m</i> vector of resistances of the links
S	number of links with inequality flow constraints
u	<i>l</i> vector of loop flow corrections,
u [*]	loop flow corrections at minimum point
U	polyhedral set of feasible loop flows

 V_{i} Co-Content of unknown head node *i* Co-Content of pipe *j* W_{i} W_{i}^{c} Content of pipe *j* Z_{k}^{c} Content of fixed grade node k exponent in head loss equation α λ d vector of Lagrange multipliers of equality constraints d vector of Lagrange multipliers of equality constraints μ system Co-Content П Π^{c} system Content W_{i}^{c} Content of pipe j loss coefficient ζ ∂ subdifferential operator $\sum h_{\rm LI}$ sum of headloss in loop I CIV temporarily closed isolating valve $CO(U, \Pi^{c})$ convex optimization problem of the function Π^{c} over the feasible set U FCV flow control valve KKT Karush-Kuhn-Tucker conditions PRV pressure reducing valve PSV pressure sustaining valve

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Todini, E. (2006). On the Convergence Properties of the Different Pipe Network Algorithms. Proceedings of the 8th Annual Water Distribution Systems Analysis Symposium, Water Distribution Systems Analysis Symposium 2006, Cincinnati, Ohio, USA. Figure 1: A 7-pipe and 2-reservoir example network with a valve (R = reservoir, S1, S2 are supply areas, the roman numerals indicate the loops and independent path)

Figure 2: Hydraulic head loss equations, Co-Content functions of (a) pipe j and (b) demand node i

Figure 3: Hydraulic head loss equation, Content functions of (a) pipe j and (b) fixed head node i

Figure 4: (a) Hydraulic mapping $h_{CHV} \mapsto q_{FCV}$ and (b) Co-Content W_{CHV} for a check value

Figure 5: Hydraulic mapping (a) $q_{CHV} \mapsto h_{CHV}$ and (b) Content W_{CHV}^c for a check value

Figure 6: Hydraulic mapping (a) $h_{FCV} \mapsto q_{FCV}$ and (b) Co-Content W_{FCV} for an FCV

Figure 7: Hydraulic mapping $q_{FCV} \mapsto h_{FCV}$ and Content W_{FCV}^c for an FCV

Figure 8: Subdifferential of a non differentiable but subdifferentiable function $f : \mathbb{R} \mapsto \mathbb{R}$



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