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1 **PRESSURE-LEAK DUALITY FOR LEAK DETECTION AND**
2 **LOCALIZATION IN WATER DISTRIBUTION SYSTEMS**

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12 **ABSTRACT**

13 Water utilities are challenged to reduce their water losses through detecting, localizing, and
14 repairing leaks as fast as possible in their aging distribution systems. In this work, we solve this
15 challenging problem by detecting multiple leaks simultaneously in a water distribution network for
16 the *Battle of the Leak Detection and Isolation Methods*. The performance of leak detection and
17 localization depends on how well the system roughness and demand are calibrated. In addition,
18 existing leaks affect the diagnosis performance unless they are identified and explicitly represented
19 in the model. To circumvent this "chicken-and-egg" dilemma, we decompose the problem into
20 multiple levels of decision making (a hierarchical approach) where we iteratively improve the water
21 distribution network model and so are able to solve the multi-leak diagnosis problem.

22 First, a combination of time series and cluster analysis is used on smart meter data to build
23 patterns for demand models. Second, point and interval estimates of pipe roughnesses are retrieved

24 using least squares to calibrate the hydraulic model, utilizing the demand models from the first
25 step. Finally, the calibrated primal model is transformed into a dual model that intrinsically
26 combines sensor data and network hydraulics. This dual model automatically converts small
27 pressure deviations caused by leaks into sharp and localized signals in the form of virtual leak
28 flows. Analytical derivations of sensitivities with respect to these virtual leak flows are calculated
29 and used to estimate the leakage impulse responses at candidate nodes. Subsequently, we use the
30 dual network to (i) detect the start time of the leaks and (ii) compute the Pearson correlation of
31 pressure residuals, which allows further localization of leaks. This novel dual modeling approach
32 resulted in the highest true-positive rates for leak isolation among all participating teams in the
33 competition.

34 INTRODUCTION

35 The detection, localization and control of leakage from aging water distribution networks
36 (WDNs) remains one of the main challenges for water utilities (WUs), because the direct financial
37 cost of water loss can be high. By detecting and dealing with leaks and bursts fast, utilities can also
38 mitigate deterioration of pipes and surrounding infrastructure in addition to lost revenues (Gupta
39 and Kulat 2018). The aim to reduce leakage is further motivated by stringent regulations and
40 financial incentives (OECD 2016).

41 Conventional techniques for detecting leakage include random and regular sounding surveys
42 using listening sticks and acoustic loggers (Adedeji et al. 2017), and step-testing of metered
43 subsystems as district metered areas (DMAs) through gradual valve closures (Farley and Trow
44 2003; Wu 2008). More advanced leakage pin-pointing methods like *leak noise correlators*, *pig-*
45 *mounted acoustic sensing* and *gas-injection techniques* (Puust et al. 2010) are the most precise at
46 locating leaks. However, all these techniques come with expensive equipment cost and are man-
47 hour intensive, and so are not scalable. In addition, the suppression of leakage sound signatures by
48 reduced pressures in active pressure management or increasing use of plastic pipes in the network
49 has also made these methods less effective (Wu 2008; Puust et al. 2010).

50 More recent advanced approaches use model-based analysis of near real-time telemetry data

51 from pressure sensors and flow meters distributed over the network. Starting with the work of
52 [Pudar and Liggett 1992](#), model-based leak localization was intensively studied with diverse set of
53 methods ranging from sensitivity matrix-based approaches ([Pérez et al. 2011](#); [Perez et al. 2014](#)),
54 meta-heuristic optimization ([Wu 2008](#); [Steffelbauer and Fuchs-Hanusch 2016b](#)), error-domain
55 model falsification ([Goulet et al. 2013](#); [Moser et al. 2017](#)), to combinations of model-based and
56 data-driven approaches ([Soldevila et al. 2016](#); [Soldevila et al. 2017](#)). An extensive review of leak
57 localization techniques including their limitations can be found in [Hu et al. 2021](#). This manuscript
58 deals with a novel model-based approach that leverages time-series analysis of demand models and
59 new hydraulic modeling approaches for both detecting and localizing potential leaks. One of the
60 main challenges for model-based leak detection approaches is the sparse number of pressure sensors
61 compared to the number of candidate leak location nodes. For methods that solve for multiple leaks
62 by posing inverse problems to determine leak parameters in the network model ([Pudar and Liggett
63 1992](#)) (*i.e.* leak levels and locations), this creates an under-determined and ill-posed problem.
64 Additionally, the performance of model-based approaches can also be very sensitive to errors in
65 two important model parameters: the demand at nodes and pipe roughness coefficients ([Hutton et al.
66 2014](#)). [Sanz et al. 2016](#) reduce this error by including existing leaks in the calibration process. This
67 is done by co-optimizing the calibration and detection, and updating the calibrated model through
68 iteration as new data becomes available and leaks are discovered and fixed. This is achieved
69 through an iterative calibration process, where demands at nodes are composed of geographically
70 distributed demand components. Due to the fact that a leak occurs as a less geographically spread
71 component in this approach, they become easier to find. The method of [Sanz et al. 2016](#) belongs to
72 a class of methods that rely on first-order pressure sensitivities to changes in demand at nodes, and
73 the projection of pressure residuals (differences of measured pressures from leak free case, usually
74 retrieved from time series or well calibrated hydraulic models) onto the sensitivities ([Sanz et al.
75 2016](#)). However, this class of methods have the limitations that they assume a single leak in the
76 system at one time, and are known to be less reliable for small leak sizes, since the leak induced
77 pressure deviations and, hence, the pressure residuals are very small in that case.

78 In this manuscript, we address these limitations of pressure residual projection approaches (i.e.,
79 the applicability on single as well as small leaks) by combining multiple methods. As in [Sanz
80 et al. 2016](#), we utilize an iterative calibration of the system roughness and demand parameters
81 using multiple measurements, including automatic meter readings (AMRs). To deal with multiple
82 leaks, we separate the detection and localization process; time series analysis (TSA) is used to
83 automatically find deviations in demand and flow measurements, thus, estimating the start and end
84 time of multiple growing and non-growing leaks that can coincide. The detected leaks are then
85 localized by using a residual projection approach ([Steffelbauer et al. 2020](#)), where the model is
86 updated when leaks are discovered or fixed. A new duality-based approach is then proposed to
87 improve the sensitivity of the localization process to smaller leaks. We formulate a dual network
88 model, where thanks to a mathematical trick — by transforming the network model with pressure
89 measurements to an equivalent model with additional virtual reservoirs and valves — we are able
90 to translate pressure heads directly to virtual leakage outflows at the measurement locations, which
91 provide a first estimate for the leak’s size and location in the network.

92 Subsequently, we use the virtual leak flows of the dual model for leak detection with anomaly
93 detection algorithms (i.e., the cumulative sum control chart (CUSUM) algorithm and the likelihood
94 ratio test ([Peach et al. 1995](#))) to obtain information on the leak start-time; and the residual-based
95 localization to retrieve the location of the leak. Finally, the information from the detection and
96 localization methods are combined to get accurate estimates for the actual size and location of the
97 leaks.

98 In the next section, an exposition of the different methods will be presented. We will then
99 discuss the results using the L-Town network model of the *Battle of the Leak Detection and Isolation*
100 *Methods* (BattLeDIM) competition ([Vrachimis et al. 2020](#)), which the authors of this manuscript
101 won under the team name *Under Pressure*. The final section will present the conclusions, limitations
102 and future directions to improve the proposed method.

103 METHODS

104 **Overview**

105 We solve the leak detection and isolation problem through utilizing a hierarchical approach. An
106 overview of the two stages where different methods are combined as well as the order in which they
107 are applied is illustrated in Figure 1, depicting how we attempted to find *leaks* in the measurement
108 *data* via model *calibration* and then *simulation* with the dual model. In the first stage, the hydraulic
109 model is calibrated, since a well-calibrated model is essential to reliably localize leaks (Savic et al.
110 2009). The model is itself calibrated in two-stages; starting with demand calibration and followed
111 by pipe roughness parameter estimation. The demand calibration method makes use of TSA on
112 AMR data d , and infers estimated demands \hat{d} to unmeasured nodes with respect to their average
113 demand \bar{d} stored in the EPANET file. The pipe roughnesses \hat{C} are estimated through solving
114 a differentiable, constrained, weighted least squares (WLS) problem, which uses the estimated
115 demands \hat{d} , measured pressure heads h , and the initial roughness values C as found in the original
116 EPANET file. In the second, a dual model is built based on the calibrated values (\hat{d} and \hat{C}) and
117 used for leak detection and localization, where pressure measurements are replaced with virtual
118 reservoirs. The dual model magnifies leak signals by transforming pressures in virtual leakage
119 outflows q_v . Moreover, dual model leak sensitivities S are computed. Finally, the sensitivities S
120 and virtual flows q_v are used to locate the leaks with a correlation-based method similar to Sanz
121 et al. 2016. In cases with multiple leaks that appear simultaneously, the leaks are localized one by
122 one, eliminated from the dual model, and the remaining leaks are detected and located subsequently
123 through an iterative approach.

124 **Calibration**

125 *Nodal demand calibration*

126 The AMRs data is used to develop a demand model through TSA for the unmeasured customers
127 within the network. Various time series models (Shumway and Stoffer 2010) are tested on the
128 AMRs aiming to extract weekly seasonalities and yearly trends for different customer types (e.g.,
129 residential, commercial). The best performance is achieved with a rather simple model, consisting
130 of a multiplicative superposition of weekly seasonalities ($S(t)$), a time varying trend ($T(t)$) and a

131 random component ($R(t)$) accounting for stochastic variations and measurement noise

$$d(t) = \bar{d} \cdot T(t) \cdot S(t) \cdot R(t), \quad (1)$$

132 with \bar{d} being the customer's base demand. For each AMR time series, the trend component $T(t)$
 133 is estimated using a convolution filter and subsequently removed by dividing the original time
 134 series through $T(t)$, followed by estimation of $S(t)$ through periodical averages over the trend-free
 135 series (Seabold and Perktold 2010). After removing the seasonal component by dividing the trend-
 136 free series by $S(t)$, only the random component $R(t)$ remains. Subsequently, similarities in the
 137 individual seasonal patterns are identified through time series clustering (Steffelbauer et al. 2021).
 138 Furthermore, cluster analysis is used to identify the number of distinct patterns n_d and outliers.
 139 For each demand node i of the network model, a time-varying demand time series \hat{d}_i is built as a
 140 superposition of the distinct patterns weighted by their individual averages \bar{d}_{ij} associated with the
 141 patterns

$$\hat{d}_i(t) = \sum_{j=1}^{n_d} \bar{d}_{ij} \cdot T_j(t) \cdot S_j(t). \quad (2)$$

142 Note that the random time series components are neglected when building the estimates \hat{d}_i .

143 *Pipe roughness calibration*

144 Pipes with the same material, age, diameter, hydraulic conditions and locations are grouped in
 145 clusters with the same roughness value (in this case a Hazen-Williams (HW) coefficient)

$$\mathbf{C}_{HW} = \mathbf{M}_{HW} \mathbf{x}, \quad (3)$$

146 where \mathbf{M}_{HW} is the membership matrix of the n_p pipes to n_c clusters of HW coefficients, $\mathbf{x} \in \mathbb{R}^{n_c}$ is
 147 the vector of roughness cluster values to calibrate, and $\mathbf{C}_{HW} \in \mathbb{R}^{n_p}$ is the vector of HW coefficients
 148 of pipes. Roughness calibration aims to fit the measurements by adjusting the roughness coefficients

149 of the hydraulic model. Following nonlinear regression equations have to be considered

$$[\mathbf{z}^j]_i = [\mathbf{S}\mathbf{y}(t_j, \mathbf{x})]_i + \varepsilon_{ij}, \quad (4)$$

150 where $\mathbf{y}(t_j, \mathbf{x})$ is the hydraulic state that is implicitly defined by the extended period simulations at
 151 time t_j , $\mathbf{z}^j \in \mathbb{R}^{n_m}$ is the vector of measurements at time t_j , \mathbf{S} is the selection matrix to select state
 152 vectors that correspond to the measurements, and $\varepsilon_{ij} \sim \mathcal{N}(0, \sigma_{ij}^2)$ are independent and identically
 153 distributed Gaussian error terms with zero expectation and standard deviation σ_{ij} .

154 The box-constrained WLS problem for parameter calibration consists of seeking to minimize
 155 the differentiable criterion

$$\min_{\mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U} f(\mathbf{x}) \triangleq \frac{1}{2} \sum_{j=1}^{n_t} \sum_{i=1}^{n_m} H_\kappa \left(\frac{[\mathbf{S}\mathbf{y}(t_j, \mathbf{x})]_i - [\mathbf{z}^j]_i}{\sigma_{ij}} \right) + \frac{\alpha}{2} \|\mathbf{x} - \mathbf{x}^0\|_2^2, \quad (5)$$

156 where in place of the traditional least-squares criterion the weighted Huber function H_κ with
 157 parameter κ is used, as in [Preis et al. \(2011\)](#), to increase the robustness of parameter estimates
 158 against outliers, n_t is the number of observation times, n_m the number of measurements, \mathbf{x}^L and \mathbf{x}^U
 159 are the lower and upper bounds, \mathbf{x}^0 is prior information about \mathbf{x} (e.g. initial value in the EPANET
 160 file) and α is a Tikhonov regularization coefficient, which penalizes large departures from \mathbf{x}^0 for
 161 sufficiently large α and increases the robustness of parameter estimates against outliers. The state
 162 of the art algorithm for solving a differentiable WLS problem is the iterative Levenberg-Marquardt
 163 algorithm. At each iteration step, the gradient of f is calculated to estimate the Hessian at the last
 164 estimate \mathbf{x}^k . The gradient of f at \mathbf{x}^k is:

$$\nabla f^k = \sum_{j=1}^{n_t} \mathbf{J}(t_j, \mathbf{x}^k)^T \mathbf{W}_j \tilde{\mathbf{R}}(t_j, \mathbf{x}^k) + \alpha (\mathbf{x}^k - \mathbf{x}^0), \quad (6)$$

165 where \mathbf{W}_j is the diagonal weight matrix at time t_j , $\mathbf{J}(t_j, \mathbf{x}^k) = \mathbf{S} \partial_x \mathbf{y}(t_j, \mathbf{x}^k)$ is the Jacobian matrix of
 166 the prediction function at \mathbf{x}^k , with $\partial_x \mathbf{y}$ using the postmultiplication by $\mathbf{P} = \mathbf{M}_{HW}$ as in [Piller et al.](#)

167 (2017), and $\tilde{\mathbf{R}}(t_j, \mathbf{x}^k)$ is the $(n_m, 1)$ -vector of truncated unreduced residuals

$$[\tilde{\mathbf{R}}(t_j, \mathbf{x}^k)]_i = \begin{cases} [\mathbf{S}\mathbf{y}(t_j, \mathbf{x}^k) - \mathbf{z}]_i & \dots \text{ if } |[\mathbf{S}\mathbf{y}(t_j, \mathbf{x}^k) - \mathbf{z}]_i| \leq \kappa\sigma_{ij} \\ \kappa\sigma_{ij}\text{sign}([\mathbf{S}\mathbf{y}(t_j, \mathbf{x}^k) - \mathbf{z}]_i) & \dots \text{ else} \end{cases} . \quad (7)$$

168 The estimate of the Hessian is following symmetric, positive definite matrix:

$$\mathbf{H}_k = \sum_{j=1}^{n_t} \mathbf{J}(t_j, \mathbf{x}^k)^T \mathbf{W}_j \tilde{\mathbf{J}}(t_j, \mathbf{x}^k) + \alpha \mathbf{I}_{nc} = \sum_{j=1}^{n_t} \tilde{\mathbf{J}}(t_j, \mathbf{x}^k)^T \mathbf{W}_j \tilde{\mathbf{J}}(t_j, \mathbf{x}^k) + \alpha \mathbf{I}_{nc} , \quad (8)$$

169 where $\tilde{\mathbf{J}}$ is given by

$$[\tilde{\mathbf{J}}(t_j, \mathbf{x}^k)]_{mn} = \begin{cases} [\mathbf{J}(t_j, \mathbf{x}^k)]_{mn} & \dots \text{ if } |[\mathbf{S}\mathbf{y}(t_j, \mathbf{x}^k) - \mathbf{z}]_m| \leq \kappa\sigma_{mj} \\ 0 & \dots \text{ else} \end{cases} . \quad (9)$$

170 The constraints are taken into account through a saturation/desaturation process by checking the
171 Karush-Kuhn-Tucker optimality conditions to identify the optimal Lagrange multipliers.

172 The projected Levenberg-Marquardt algorithm consists of solving following linear system

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \mathbf{C}_k^T \left(\mathbf{C}_k \mathbf{H}_k \mathbf{C}_k^T \right)^{-1} \mathbf{C}_k \nabla f_k , \quad (10)$$

173 where \mathbf{C}_k is the selection matrix for the unsaturated components \mathbf{x}^k . To cope with ill conditioned
174 Hessians, a damping factor with a regularization parameter is introduced to scale the gradient
175 according to the curvature

$$\mathbf{H}_k(\lambda) = \mathbf{H}_k + \lambda [\mathbf{diag}(\mathbf{H}_k) + \phi \mathbf{I}_{nc}] , \quad (11)$$

176 where ϕ is a positive parameter and λ is the damping parameter. Furthermore, we make use of

177 following relation to calculate confidence intervals for the roughness estimates (Piller 2019)

$$-[\Delta_x]_i \leq \delta \mathbf{x}_i \leq [\Delta_x]_i, \text{ with } \mathbf{M} = \left(\mathbf{W}^{0.5} \mathbf{J} \right)^+, [\Delta_x]_i = 3 \sum_{k=1}^{n_m} |\mathbf{M}_{ik}|, i = 1, \dots, n_c \quad (12)$$

178 with \mathbf{J} is the block matrix $\mathbf{J} = \left(\mathbf{J}(t_1, \mathbf{x})^T \quad \dots \quad \mathbf{J}(t_{n_t}, \mathbf{x})^T \right)^T$ and $\mathbf{W}^{0.5}$ is the diagonal matrix
 179 $\mathbf{W}^{0.5} = \left(\mathbf{W}_j^{0.5} \right) = (\sigma_{ij})$.

180 The Dual Model

181 We introduce a so-called ‘‘Dual Approach (DA)’’ for detecting and localizing leaks, that is
 182 depicted in Figure 2 (b). In the DA, the model is *augmented* with n_s *virtual reservoirs* that are
 183 connected with pressure measurement nodes by valves. The origin of the name ‘‘dual’’ stems from
 184 the fact that, instead of using the fixed demand boundary condition at the sensor nodes (*i.e.* the
 185 original or ‘‘primal’’ hydraulic model), the measured pressure heads are used as fixed head boundary
 186 conditions at the corresponding virtual reservoirs. Consequently, the heads at the measurement
 187 nodes become free variables and imbalances in the system compared to a leak-free model lead to
 188 flows to the virtual reservoirs. If there are no leaks, and if we set the minor loss of each virtual
 189 reservoir’s valve to zero, the two networks are equivalent. In the hydraulic model, we normally
 190 set these valves’ minor loss to a sufficiently low but non-zero value, and so the primal and dual
 191 networks are ‘numerically equivalent’ but not mathematically equivalent.

192 If a new leak appears in the primal model, the residuals between measured and calculated
 193 pressures change. The pressure drops caused by higher flow velocities towards the leak in the
 194 real system are not observed in the model that is still based on the leak free system. In the dual
 195 approach, the measured pressure drop is applied to the fixed head reservoirs and, as a consequence,
 196 an additional outflow is generated. This outflow can be understood as an outflow residual or *virtual*
 197 *leak flow*. The advantage of the DA is that the calculated outflows act as amplifiers that deliver
 198 significant and localized signals even for small pressure drops. In addition, the outflows at the
 199 virtual reservoirs serve a good first estimate for the leak’s size and location.

200 *Dual Model Sensitivities*

201 We consider the dual WDN with n_p pipes, n_s virtual links and n_j junction nodes at which the
 202 heads are unknown. We also denote the vector of unknown flows in the pipes and virtual links
 203 by $\mathbf{q} \in \mathbb{R}^{n_p+n_s}$, the unknown heads and demands at the (free) nodes by $\mathbf{h} \in \mathbb{R}^{n_j}$ and $\mathbf{d} \in \mathbb{R}^{n_j}$,
 204 respectively. The sensitivities of heads and pipe flow rates with respect to nodal outflows are
 205 derived among other sensitivities in Piller et al. (2017). The local sensitivities $\nabla_{\mathbf{d}}\mathbf{h}$ and $\nabla_{\mathbf{d}}\mathbf{q}$ can be
 206 calculated in demand driven analysis as follows

$$\begin{aligned}\nabla_{\mathbf{d}}\mathbf{h} &= -\left(\mathbf{A}^T\mathbf{F}^{-1}\mathbf{A}\right)^{-1} \\ \nabla_{\mathbf{d}}\mathbf{q} &= -\mathbf{F}^{-1}\mathbf{A}\left(\mathbf{A}^T\mathbf{F}^{-1}\mathbf{A}\right)^{-1},\end{aligned}\quad (13)$$

207 where \mathbf{A} is the link-node-incidence matrix of the dual network graph reduced to junction nodes
 208 (all links, including pipes and virtual links, are taken), and \mathbf{F} is the diagonal matrix of head loss
 209 derivatives with respect to \mathbf{q} .

210 Let $\mathbf{A}_f \in \mathbb{R}^{(n_p+n_s) \times (n_f+n_s)}$ be the link-node-incidence matrix of the dual network graph reduced
 211 to fixed-head nodes (the n_f initial tanks and reservoirs, and the n_s virtual reservoirs), and let
 212 $\mathbf{q}_{in} = \mathbf{A}_f\mathbf{q}$ represent the unknown flow rate entering in the system (leaving the fixed-head nodes if
 213 positive). Then the sensitivity of the \mathbf{q}_{in} can be written as using Eq. (13)

$$\nabla_{\mathbf{d}}\mathbf{q}_{in} = -\mathbf{A}_f^T\mathbf{F}^{-1}\mathbf{A}\left(\mathbf{A}^T\mathbf{F}^{-1}\mathbf{A}\right)^{-1}.\quad (14)$$

214 The Jacobian in Eq. (14) is the matrix of first order derivatives of the inflows calculated at virtual
 215 pressure nodes at measurement locations and real pressure boundary conditions such as reservoirs.
 216 The (i, j) element of $\nabla_{\mathbf{d}}\mathbf{q}_{in}$ represents the first order change rate of the calculated in- or outflow at
 217 a fixed-head node i as a consequence of a change in demand at node j .

218 In the dual model the in- and outflows at virtual reservoir are an indicator for a real existing leak
 219 or model errors. In a perfect model, where all the parameters are known, the calculated pressures
 220 of the dual model would be exactly the same as the measurements from a primal model. In the

221 corresponding dual model, the calculated in- and outflows at junctions would be zero and the primal
 222 and the dual models would give approximately the same results (*i.e.* except for small numerical
 223 differences due to the minor losses across the virtual reservoir valves).

224 In presence of an unknown leak, the measured pressure heads and the values calculated by the
 225 leak-free primal model diverge. In the dual model, the pressures at the measurement nodes become
 226 free and the measurements are set as virtual fixed heads (Figure 2 (b)). The imbalance caused by
 227 the unknown leak is then expressed as in- and outflows calculated at pressure measurement nodes.
 228 However, as we have shown in the BattLeDIM (Steffelbauer et al. 2020), the sensitivity is much
 229 higher in the dual model. Inverting the problem acts as an amplifier of leaks. Another advantage
 230 is that the imbalances and the value in question (leaks) have the same unit of flow. The sum of all
 231 the imbalances normally gives a good first estimate of the size of the leak. For explanation of the
 232 amplifying effect, a deeper investigation of the equation (14) may be useful: from the balance of
 233 inflows and outflows, it is possible to deduce each column of $\nabla_{\mathbf{d}}\mathbf{q}_{in}$ including the fraction of in-
 234 and outflows as a response to the change in outflow at the corresponding demand node equation

$$\mathbf{1}_{n_f+n_s}^T \mathbf{q}_{in} = \mathbf{1}_{n_j}^T \mathbf{d} \Rightarrow \mathbf{1}_{n_f+n_s}^T \nabla_{\mathbf{d}} \mathbf{q}_{in} = \mathbf{1}_{n_j}^T . \quad (15)$$

235 The sum of the column vector must be one. Naturally, the response should be an inflow for all
 236 fixed-head nodes.

237 **Leak detection and localization**

238 *Leak detection with the dual model*

239 Whereas in the past, human operators were in charge of small single supply areas, modern WU
 240 employees are responsible for multiple DMAs simultaneously (Bakker et al. 2014). That is why
 241 automatic anomaly detection algorithms are of particular interest for providing a rapid response to
 242 leaks and pipe burst (Romano et al. 2013). However, a correct estimation of the total leakage outflow
 243 over their time of existence (from the start t_S until the end t_E when they are repaired) is of utmost
 244 importance to assess water losses (Hamilton and McKenzie 2014). The correct identification of

245 t_S is also one of the objectives in the BattLeDIM (Vrachimis et al. 2020). We developed a two-
 246 stage approach to tackle both tasks: (i) using anomaly detection algorithms to detect leaks as fast
 247 as possible, and (ii) using regression analysis to retrieve good leak start time t_S estimates. For
 248 both approaches the virtual leak flows $[\mathbf{q}_v]_i = -[\mathbf{q}_{in}]_{i+n_f}$ (the dual model's outflows to the virtual
 249 reservoirs) are used (see Figure 4, for example).

250 Two algorithms were used to detect leaks in the \mathbf{q}_v : (i) the CUSUM algorithm, where a leak
 251 is detected when the cumulative sum of positive and negative differences in the signal exceeds a
 252 certain threshold τ_1 , (ii) and the likelihood ratio test (Peach et al. 1995), where a leak is detected if
 253 the ratio between the likelihood of the leak versus the leak-free case exceeds a certain threshold τ_2 .
 254 The ideal thresholds for both methods are obtained through calibration on leak free data.

255 Visual inspection of the virtual leakage outflows \mathbf{q}_v of detected leaks revealed two different
 256 types of leaks. The first leak type T_I is a sudden pipe burst that happen instantaneously at t_S

$$q_L(t) = \begin{cases} 0 & \text{for } t < t_S \\ q_S & \text{for } t \geq t_S \end{cases}, \quad (16)$$

257 where $q_L(t)$ is the leakage outflow over time and q_S is the saturated (maximum) leak flow (e.g.,
 258 Leak 3 in Figure 4). Note that leaks are not modeled as pressure dependent demands in contrast to
 259 the leaks generated in the BattLeDIM. The second leak type T_{II} is a slowly growing leak starting
 260 at t_S and saturating at a certain time t_{SA} , modeled as a piecewise function with a quadratic growth
 261 rate before the saturation ((e.g., Leak 1, 2 and 4 in Figure 4).)

$$q_L(t) = \begin{cases} 0 & \text{for } t < t_S \\ a \cdot t^2 + b \cdot t + c & \text{for } t_S \leq t \leq t_{SA} \\ q_S & \text{for } t > t_{SA} \end{cases}. \quad (17)$$

262 The coefficients of the quadratic outflow model connect the curves through following relationships
 263 $a = (q_S - b(t_{SA} - t_S))/(t_{SA}^2 - t_S^2)$ and $c = -at_S^2 - bt_S$. Additionally, it was found that leaks are

264 evolving simultaneously in the system, which makes the detection more difficult. If a single leak
 265 evolves over time, a Bayesian inference approach based on Hamilton Monte Carlo (Hoffman and
 266 Gelman 2014) is used (e.g. in Area C) to identify the parameters $t_S, t_{SA}, q_S, a, b,$ and c plus the
 267 confidence intervals of the leak model parameters. In the case of multiple evolving leaks (Area
 268 A&B), differential evolution is used to identify the best combination of leak outflows over time
 269 plus the leak parameters of each single leak (Storn and Price 1997). The identified leak outflows
 270 were compared against the outcomes of the DA and subsequently used for the leak localization.

271 *Leak localization with the dual model*

272 The Pearson correlation for flow and pressure residuals and the first-order estimates using
 273 sensitivities are calculated for the localization (Perez et al. 2014). It is more convenient for
 274 implementation purposes to work with the pressure residuals and sensitivities of the original
 275 measurement nodes instead of using the inflow sensitivities in Eq. (14) (e.g. no need for calculating
 276 \mathbf{A}_f and changing the set of variable pressure nodes). This does not affect the main idea, because
 277 the sensitivity of the head is equivalent to the headloss of the virtual valve and, hence, proportional
 278 to the flow sensitivity in the linearized system.

279 The vector of the sensitivities of measured head is determined by

$$\nabla_{\mathbf{d}} \mathbf{h}_{\mathbf{m}} = -\mathbf{S} \left(\mathbf{A}^T \mathbf{F}^{-1} \mathbf{A} \right)^{-1}. \quad (18)$$

280 The term \mathbf{S} is the same selection matrix for the measurement nodes as in Eq. (4).

281 The difference between Eq. (18) and Eq. (14) consists in the multiplication by the derivative of
 282 the valve headloss: $([\mathbf{Sh}]_i - h_{n_f+i}^f = K_i |[\mathbf{q}_v]_i| [\mathbf{q}_v]_i \Rightarrow \partial_{d_j} ([\mathbf{Sh}]_i) = -2K_i |[\mathbf{q}_v]_i| \partial_{d_j} ([\mathbf{q}_{in}]_{n_f+i}))$. If
 283 the sensitivities following Eq. (18) are used, the pressure residuals are used for the calculation of
 284 the correlation, whereas the simulated external flows at the virtual reservoirs are considered in the
 285 case of Eq. (14).

286 It proved to be beneficial to calculate the correlations only for measurement nodes where the
 287 leak flow (calculated by the dual model) exceeds a certain threshold (e.g. 0.5 L/s). This adjustment

288 eliminates the noise from the pressure measurements and stabilizes the calculated set of candidates
289 for the unknown leak. The Pearson correlation $\rho_{\mathbf{r}, \mathbf{S}_{(:,i)}}$ is calculated as

$$\rho_{\mathbf{r}, \mathbf{S}_{(:,i)}} = \frac{cov(\mathbf{r}, \mathbf{S}_{(:,i)})}{\sigma_{\mathbf{r}} \cdot \sigma_{\mathbf{S}_{(:,i)}}}, \quad (19)$$

290 where \mathbf{r} is the vector of residuals, $\mathbf{S}_{(:,i)}$ is the sensitivity vector of node i , $cov(\cdot)$ is the co-variance
291 and $\sigma_{\mathbf{r}}$ and $\sigma_{\mathbf{S}_{(:,i)}}$ are the standard deviations of the residual vector and the sensitivity vector,
292 respectively. The residuals and the sensitivity coefficients are very small. However, this did not
293 show any negative impact in the allocation in our tests. In contrast, the system is stabilized by the
294 additional pressure boundary conditions, which makes the correlation more stable compared to the
295 conventional primal model approach. One important limitation of the correlation method is that it
296 does not work for two or more leaks appearing at the same time. Therefore, a single leak must first
297 be isolated in time from other leaks in order to be localized. The leakage curves that have been
298 calculated for detection serve as a basis for choosing the best time for allocation, and we use a step
299 by step procedure for localizing simultaneously growing leaks.

- 300 1. Identification of time interval that starts briefly before the new unknown leak starts and ends
301 before the next leak starts. The time intervals from t_S to t_{SA} are found by a combination
302 of CUSUM or likelihood ratio tests with Hamilton Monte Carlo or differential evolution
303 (depending on the single or multiple leak case) as described in the leak detection paragraph
304 in the methods section.
- 305 2. Initialize calculation for the selected time interval (load all measurements as well as the
306 estimated demands)
- 307 3. Run Extended Period Simulations for selected time interval; for each time step do:
 - 308 (a) Update boundary conditions via toolkit functions including demand patterns, heads at
309 virtual reservoirs, pump flow.
 - 310 (b) Update all known leaks with their calculated leak flows as fixed demands and define the

- 311 start time of the unknown leak based on the results of the detection.
- 312 (c) Simulation of the time step (here the EPANET toolkit is used) and after each time step
313 with active new unknown leak, calculate correlation in Eq. (19) for all nodes based on
314 the sensitivities.
- 315 (d) Consider only the nodes with a correlation score higher than a given minimum threshold
316 (*e.g.* 0.95) and add those eligible correlations to the sum of correlation taken over all
317 calculated time steps.
- 318 4. The node with the highest correlation sum is identified as the candidate for the new leak
319 within this time interval.
- 320 5. The new leak is added to the list of known leaks and the leakage flow is considered as known
321 demand for the localization of the next leak and the procedure is repeated from point 1 until
322 all leaks have been identified in the given period.

323 **L-Town case study and measurement data**

324 The case study network *L-Town* was provided by the organizers of the BattLeDIM ([Vrachimis](#)
325 [et al. 2020](#)). *L-Town* is a small hypothetical town based on a real WDN in Cyprus with approximately
326 10,000 inhabitants, which receive water from two reservoirs. The WDN consists of pipes with
327 diameters ranging from 63 mm to 225 mm and a total pipe length of 43 km. *L-Town* consists of
328 three distinct hydraulic areas: (i) Area A is the main part of the network, (ii) Area B is a low lying
329 part that is supplied through a pressure reduction valve, and (iii) Area C is an area with higher
330 elevation that is supplied by an elevated tank fed from Area A through a pumping station. An
331 overview of the network and the location of the three measurement zones can be found in Figure 2.

332 To enhance the water loss monitoring capabilities, the WU of *L-Town* installed three flow meters
333 (two at the reservoirs and one at the pumping station), a tank level sensor and 33 pressure sensors
334 (depicted as circles in Figure 2). All sensors measure and transmit data every 5 minutes to the
335 utility's supervisory control and data acquisition (SCADA) system. Additionally, the WU installed
336 82 smart water meters or AMRs in Area C, measuring three different customer types: residential,

337 commercial and industrial. There is no flow meter installed at the tank that feeds Area C. Therefore,
338 a virtual inflow measurement to Area C has to be reconstructed from the tank level measurements
339 and the inflow measurement measured at the pump that supplies the tank.

340 The dataset of the BattLeDIM contains two years of sensor data for years 2018 (historical
341 dataset) and 2019 (validation dataset), an EPANET model of the water distribution network, plus
342 the time and repair location of ten pipe bursts that have been fixed in 2018. Three types of leaks
343 exist: (i) small background leaks with 1 % - 5% of the average inflow, (ii) medium pipe breaks with
344 5 % - 10%, and (iii) large pipe bursts with leakage flows of more than 10 % of the average system
345 inflow ($\approx 180 \text{ m}^3/h$). Large leakages with outflows over $15 \text{ m}^3/h$ are fixed by the water utility after
346 a reasonable amount of time within two months. The leakages have two different time profiles, (i)
347 either abrupt pipe bursts with constant leak flow rates, (ii) or background leakages with growing
348 leak rates which evolve over time until large outflow rates at which they remain constant. In total,
349 14 leakages occurred in 2018 with outflow rates between 5 to $35 \text{ m}^3/h$, of which 10 leaks have
350 been repaired. The remaining 4 leaks are not repaired and continue into the 2019 validation dataset.
351 The BattLeDIM challenge is to find the 19 leaks that happened in 2019 plus the 4 remaining leaks.
352 The outflows and locations of the 33 leaks can be found in Figures 7 to 10 (dashed lines in the
353 outflow time series plots and circles in the location overview plots). More details on the dataset
354 can be found in (Vrachimis et al. 2020).

355 **RESULTS AND DISCUSSION**

356 **Demand calibration**

357 Each AMR time series is decomposed into its trend, seasonal (with a period length of a
358 week), and random components using the multiplicative time series model described in Eq. (1).
359 Subsequently, cluster analysis is used to identify similarities in the trend and seasonal patterns. Two
360 distinct demand patterns emerge in the trend $T(t)$ and in the seasonal components $S(t)$, a residential
361 ($T_R(t), S_R(t)$) and a commercial ($T_C(t), S_C(t)$) one. The seasonal and the trend components are
362 shown in Figure 3 for each AMR measurement. Furthermore, some patterns are found to be a
363 superposition of both pattern types. These patterns belong to houses with mixed user groups (e.g.

364 commercial space in the ground floor and apartments in the floors above). Subsequently, these
365 patterns are called *mixed* patterns. Generally, all demand patterns can be described through the
366 superposition (see Eq.(2)) of the residential and the commercial pattern. During workdays (Monday
367 to Friday), water consumption follows a similar behavior, whereas during the weekend (Saturday
368 and Sunday) higher consumption during late hours occur as the result of night life (see Figure 3
369 (a)). Furthermore, cluster analysis revealed four outlier pattern in the AMR measurements. After
370 closer examination, these outlier patterns were explained as industrial users with a periodicity
371 differing from a week (*i.e.* 9, 11 or 13 days). Hence, those industrial users do not follow the same
372 pattern of consumption as described in Eq. (2) and are not further used in the demand modeling.
373 The trend components in Figure 3 (b) show higher water usage during July/August, and lower in
374 December/January.

375 The demand model is used to model the unmeasured customers within the L-town network.
376 Additionally, a virtual inflow measurement of Area C has been constructed from the pump flow
377 measurements and the tank's water level. This virtual inflow is used to (i) validate the demand
378 model and to (ii) estimate the leak outflow in Area C. Figure 4 (a) shows the estimated leakage
379 outflow, which is constructed as the difference between the virtual inflow measurement and the
380 total estimated demand for Area C. Three different strategies for the demand estimation are used
381 in Area C. First, only the measured demand at the AMRs is subtracted (*just AMR* in Figure 4 (a)),
382 which leads to an overestimation or an offset of the leak flow, because of the unmeasured customers.
383 Second, the demand for the whole zone is estimated based on the model as described in Eq. 2 using
384 the base demands from the BattLeDIM EPANET model (*Inferred*), which leads to a high noise in
385 the leak outflow estimates. Third, the AMR measurements are combined with demand estimates for
386 the unmeasured customers (*Combined*). The last approach leads to the best leak outflow estimates
387 with low levels of noise as well as no offset. Clearly, four different leaks can be seen in the data,
388 three are growing over time until they are saturated (Leak 1, 2, and 4), and a sudden pipe burst
389 (Leak 3). This information proved to be useful for the leakage modeling (see Eq. (16) and (17)).

Roughness calibration

The internal diameters of pipes are nominal diameters defined by a discrete number of values that depend on the manufacturer and the material. In the L-Town INP file, it is assumed that the outside diameters of plastic pipes are entered instead of the inside diameters, which is first corrected with the most usual inside diameter for PVC and PE pipes (see Table 1).

After inspection and several tests, the pipes are divided in six different roughness clusters according to their diameter, material, initial roughness values and managing zones in which they are located : Because of the small number of observations and pipes, one cluster with $C_{HW} = x_5$ is assigned for Zone B and one to Zone C (x_6). Cluster with same x_1 roughness value consists of the plastic pipes in Zone A; pipes in cluster 2 are in Zone A with diameters 100 mm or 150 mm, and original INP roughness $x_2 = 120$. Similarly, pipes in zone A with diameters 100 mm or 150 mm and original $C_{HW} = 140$ define the cluster 3: $x_3 = 140$. Finally, cluster 4 is made of pipes with internal diameter 200 mm in Zone A. Figure 2 shows an overview of the roughness groups. Through visual inspection of the measurements from the first week of 2018, it is assumed that no leaks are present in the dataset during that time. Consequently, measurements for this week are used for the roughness calibration. The roughness calibration is performed for the six clusters, $n_c = 6$, and by solving the WLS problem in Eq. (5) with $\kappa = 3$, $\alpha = 0$ and box constraints $x^L = 60$ and $x^U = 160$ with the Levenberg-Marquardt method (10). The $n_s = 33$ pressure measurements in Figure 2 are used ($n_m = 33$). They repeat every five minutes for 7 days ($n_t = 2016$). All measurements are chosen to be of the same accuracy $\sigma_{ij} = 1$.

The algorithm converges after 11 iterations. The results are given in terms of estimates in Table 2. For the first cluster, plastic pipes in Zone A, the initial estimate $x_1^0 = 146$ belongs to the 99% confidence interval [141.9, 163.7]. Consequently, the final estimate 152.8 is not significantly different from the initial value. However, the initial estimates for the other five clusters differ significantly from the point estimates at iteration $k = 11$ (they do not belong to the five 99% confidence intervals). Based on the confidence intervals and the initial estimates, the bold values are selected. The pressure residuals are represented in Figure 2. It can be seen that the mean

417 squared error (MSE) is about 6 cm H₂O.

418 **Virtual leak flows with the dual model**

419 A dual model is constructed from the EPANET model containing the calibrated pipe roughnesses
420 and demand patterns from the demand calibration. The heads of the virtual reservoirs are set to
421 the corresponding pressure measurements. If leaks appear in the network, the dual model reacts
422 with virtual leak outflows caused by the pressure differences of the hydraulic model and the lower
423 reservoir heads. The virtual leak flows for each sensor location within Area C are depicted in
424 Figure 4 (b). Furthermore, the total sum of all virtual leak flows is shown. This sum gives a good
425 first approximation of the leak size. The second leak in Area C was repaired and, hence, its end
426 time and its location (pipe p31) are known. The leak is closest to sensor node n31, which shows
427 the strongest reaction to the leak by producing the biggest virtual outflow. Same reasoning leads
428 to the conclusion that Leak 1 is close to sensor n1, Leak 3 is in proximity of n31, and Leak 4 is
429 somewhere in the middle of all three sensors.

430 Comparison of Figure 4 (a) with the total virtual leak outflow in (b) shows that the real leakage
431 outflows have similar magnitudes as the virtual outflows. However, the dual model seems to
432 underestimate the real outflows in Area C slightly.

433 Figure 5 shows an comparison of the effect of leakages on the measured pressure signals versus
434 the virtual leak flows in the dual model for the first two leakages in 2019 that appear in Area A
435 (pipe p523 and p810). In this Figure, solid lines are four hour moving averages, whereas the shaded
436 lines are the original five minutes signal. The dual model amplifies the leak signal compared to
437 the pressures (compare Figure 5 (a) and (b)). Furthermore, the leaks have a more local effect on
438 the virtual leak flows than in the pressures, which allows already a rough estimation of the leak's
439 location. The sum of all virtual leak outflows in Figure 5 (c) gives already a good estimate of the
440 leak sizes, which are approximately $27 \text{ m}^3/h$ for each leak.

441 **Leak Detection**

442 Two different signals are used for leak detection; (i) the flow residual between the measured
443 inflow and total demand plus already known leaks in an area, (ii) the dual model's outflows to the

444 virtual reservoirs (see Figure 4 or Figure 5). Two different types of leaks are found in the data –
445 instant bursts and leaks that are growing over time. Growing leakage flows are modeled with the
446 quadratic function in Eq. (17). Data from the dual model is used to identify the leak start times
447 and their shapes (*i.e.* instant or growing). For that reason, thresholds are extracted from the DA
448 flows at each sensor using the leak free case in the first week of 2018. If the DA signal exceeds the
449 threshold, a leak is detected in the system. The detection time is used as the start time of the leak
450 for our BattLeDIM solution. To estimate the leakage outflow, the start times and the shapes of the
451 leaks are used to fit the leak shape on the flow residuals. If a single leak evolves over time, Bayesian
452 inference is used, for multiple simultaneously appearing leaks, a faster differential evolution is used
453 to identify the best combination of leak outflows over time. The detected leaks are double checked
454 against the DA and subsequently used for the leak localization.

455 The results for leak detection and localization for 2019 are summarized in Table 3. Additionally,
456 the leak detection and localization results are broken down by the different areas are shown in
457 Figures 7 to 10, where shaded lines are daily moving averages of the real leakages, solid dashed
458 lines are the estimated leakages. Circles in the network maps are the real leak locations, while
459 crosses show our estimates. The leak detection results for Area C are shown in Figure 7 (a). The
460 shapes of the leaks are resembled very well by our method for all three leaks, and the differences in
461 the final leak outflows are negligible for Area C. The sudden pipe burst (Leak C3 at pipe p280) is
462 detected instantaneously, while the detection of the growing leaks takes a bit longer. Nevertheless,
463 leakages are detected on average within less than 9 days. A less conservative detection threshold
464 potentially decreases the detection time.

465 The leak detection results for Area B are shown in Figure 8 (a), where the instant pipe burst is
466 perfectly detected, although the leakage outflow is slightly overestimated.

467 The leak detection results for Area A are shown in Figure 9. For a better visibility of the
468 simultaneously appearing leaks, the Figure is split into the two half-years of 2019, with (a) for the
469 first half until July, and (b) showing the second half of the year. Additionally, the leaks from the first
470 half are depicted as gray shaded lines in Figure 9 (b) as they are still present in the network. Sudden

471 pipe bursts are again detected instantaneously, while the thresholds for growing leaks seemed a bit
472 too conservative. However, the shapes of all leaks are very well described through the coefficients
473 that our model found. One leak that started in February 2018 at pipe p427 with a magnitude of
474 $5m^3/h$ is not detected at all. All leak shapes are identified correctly until August, when Leak A17
475 at pipe p721 appears (see Figure 9 (b)). However, this leak is detected very late and its size is
476 underestimated by almost $5 m^3/h$. This influences the detection of subsequent leaks, which results
477 in a decrease in the detection as well as the localization performance. Nevertheless, leakages in
478 Zone A were detected within 10 days on average.

479 **Leak Localization**

480 For the localization of the leaks the network is divided into two separate parts (A+B and C) and
481 the pump is replaced by the flow measurement for Zone A and B. All calculations are executed by
482 use of EPANET 2.00.12 (Rossman 2000) and the EPANET toolkit integrated in an application for
483 data management and visualization that is exclusively developed for the performance of the project.

484 Figure 6 visualizes the GUI-output at a certain time step. The circles indicate the locations of the
485 pressure measurement nodes and the numbers show the calculated in- and outflows calculated by the
486 dual model. The two biggest virtual reservoirs outflows are marked by a bigger circle as expected
487 in the neighborhood of these two nodes. The diamonds show the nodes with highest correlation
488 scores at the current time and the bigger diamonds show the nodes with highest correlation sum.
489 Their size is scaled by the sum value which means that they are growing over time.

490 Figure 7 (b) shows the localization results for Area C. Leak C1 is perfectly isolated at the real
491 location (p257). Leak C3 is found within 50 m of the real leak. However, if the closed valve in Area
492 C is added to the hydraulic model, the isolation of this leak might improve further. Leak C4 is not
493 localized correctly, since the distance exceeds 300 m as stated in the BattLeDIM rules. Reasons for
494 that might be that the closed valve is not taken into account, or the fact that we are using demand
495 driven models, while the BattLeDIM organizers used a pressure-driven model. The more leakages
496 occur in the network, the greater the difference between a demand-driven and a pressure-driven
497 demand model become, and the more inexact our localization gets, since the localization errors

498 accumulate. On average, all leaks are found within 130 m of the real leak in Area C. For Area B,
499 the leak is perfectly isolated in time as well as in space (see Figure 8).

500 The results for Area A can be found in Figure 10, and are split again into half-years. Figure 10
501 (a) also contains the leak that was not detected by our method (white cross). Early leaks are
502 isolated almost perfectly, while the localization gets worse during later simulations. This might be
503 a consequence of the demand-driven model that is used. For the leaks in Figure 10 (a), the average
504 distance of the real leaks to the estimated leak position is around 150 m. During later simulations,
505 this distance increases to 250 m (see Figure 10 (b) and Table 3). It has to be noted that a typo
506 occurred while submitting the results for the BattLeDIM. Leak p654 was inserted as p645. Taken
507 this into account, the final score of the Team *Under Pressure* would even further increase from
508 already the highest rate of true positives of 65% of all participating teams.

509 **CONCLUSION**

510 In this work, we present a novel solution to detect and isolate multiple-leaks in WDN that we
511 developed while participating in the BattLeDIM competition. Our method consists of calibrating
512 the nodal demand and pipe roughness, and introducing a dual model for the calibrated primal
513 problem to detect and locate leaks.

514 The calibration uses time series analysis and cluster analysis to build a multiplicative predictive
515 model for ultimately two network-wide demand models, a residential and a commercial model.
516 This is used for both, (i) modeling unknown demands over time in the hydraulic model, as well
517 as distinguishing leakages and consumption in the measurements. Subsequently, six roughness
518 clusters were calibrated using 33 pressure loggers for the first week of 2018. Confidence intervals
519 are given for the least-squares estimates. The pressure residuals are very well reproduced for the
520 entire week with a small root mean square error of 6 cm.

521 The core of our method is a dual model that transforms a pressure measurement node into a
522 free junction node plus a link to a virtual reservoir, whose head is equal to the measured values.
523 Significant inflows or outflows, either sudden or gradual, to these virtual reservoirs are indications
524 of leaks. In the dual model, the pressure signal is transformed into a virtual leakage outflow

525 signal that is easier to analyze since it amplifies and localizes the effects of leaks in the network.
526 Sensitivities of nodal pressures to virtual outflows are also derived. They are essential to understand
527 the behavior of the model at first order.

528 For leak detection, the CUSUM algorithm and likelihood-ratio tests are used jointly on the
529 virtual leak flows, where the parameters are tuned to limit the global false positive rate under
530 normal operation conditions. When multiple leaks are present, differential evolution is used to
531 identify the best combination of leak modeling parameters over time (*i.e.* start times and shapes
532 of leaks over time). These detection methods were employed for both, the primal and the dual
533 data. The localization is achieved by analyzing the correlation between the calibrated pressure (or
534 virtual inlet-outlet model predictions) and the corresponding first-order leakage impulse response
535 predictions at the candidate nodes. This solution recovered 65% of true leaks with only four false
536 positives in all of 2019, which is a notable result (shared #1 ranking).

537 Using a pressure-driven model instead of a demand-driven one, improving the calibration by
538 reliably detecting closed valves, as well as using less conservative threshold parameters for the
539 detection of the growing leaks might increase the already notable result further. Certainly, a lot
540 of potential lies in a deeper understanding of the dual model to further improve the detection and
541 isolation of multiple simultaneously occurring leaks.

542 With 33 pressure sensors, the BattLeDIM dataset contains an unrealistic high number of
543 sensors in a WDN of that size. Indeed, the leak detection and localization performance will
544 decrease with a lower number of sensors. However, optimal sensor placement algorithms might
545 recover similar leak detection and localization performances with fewer sensors. Furthermore,
546 the BattLeDIM organizers constructed the nodal demand patterns through a superposition of
547 residential and commercial demands multiplied with noise. That is why we were able to almost
548 precisely reconstruct the demands on the unmeasured locations through the information contained
549 in the AMR data with our demand calibration approach. In reality, demand patterns are more
550 variable (Steffelbauer et al. 2021). Consequently, the dual model might perform worse in systems
551 with limited demand information and, hence, less accurate demand models.

552 That is why for future work, we want to focus on optimal sensor placement (Steffelbauer and
553 Fuchs-Hanusch 2016a) with the dual model and on applying the dual model on challenging real
554 data sets, with model errors, outliers, uncertainty, and more variable and realistic water demands.
555 Furthermore, we are planning to investigate the importance of each step for the final classification,
556 enhancing the method to reduce the false positive rate, and study the effect of the dual model on
557 fitness landscapes of WDN optimization problems (Steffelbauer and Fuchs-Hanusch 2016b).

558 **DATA AVAILABILITY STATEMENT**

559 All data, models, or code that support the findings of this study are available from the corre-
560 sponding author upon reasonable request.

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568 **APPENDIX**

569 **AMR** automatic meter reading

570 **BattLeDIM** *Battle of the Leak Detection and Isolation Methods*

571 **CUSUM** cumulative sum control chart

572 **DA** Dual Approach

573 **DMA** district metered area

574 **HW** Hazen-Williams

575 **MSE** mean squared error

576 **SCADA** supervisory control and data acquisition

577 **TSA** time series analysis

578 **WLS** weighted least squares

579 **WDN** water distribution network

580 **WU** water utility

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678
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680
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List of Tables

- 1 Original pipe characteristics in the INP file and corresponding cluster membership;
in red the original external parameters that were corrected for PVC and PE pipes. 30
- 2 Calibration of HW coefficients; the first three columns are the lower bound, initial
estimate, and upper bound values for the six clusters; the last three columns are the
99% confidence intervals centered on the value at convergence; in bold the final
point estimate. 31
- 3 Results of leak detection and localization: The true location, the start time and the
maximum leakage outflow $\max(Q_L)$ are taken from the BattLeDIM solutions. The
estimated location is found with the leak localization algorithm. t_D is the detection
time measured in hours since the true start time of the leak. The distance between
the true and the estimated leak location is the shortest topological distance over
the pipes in meter. Zone shows in which area of the network the leak is located.
Perfectly located leaks are shown in boldface (plus minus 10 m), while leaks with
a distance greater than 300 m (missed leaks according to the BattLeDIM rules) are
highlighted with an asterisk. 32

TABLE 1. Original pipe characteristics in the INP file and corresponding cluster membership; in red the original external parameters that were corrected for PVC and PE pipes.

Diameter in mm	C_{HW}	Zone	Cluster # in Eq. (3)	# pipes	Length in m
53.6 (63)	146	A	1	3	71.40
53.6 (63)	146	B	5	1	9.21
64 (75)	146	A	1	1	60.08
100	120	A	2	76	3639.10
100	120	B	5	25	1190.11
100	140	A	3	500	24069.65
100	140	C	6	104	5201.60
150	120	A	2	7	313.62
150	140	A	3	90	4102.87
150	120	B	5	6	226.56
141 (160)	146	A	1	16	713.73
200	90	A	4	59	2749.71
200	90	C	6	5	195.90
198.2 (225)	146	A	1	12	558.58

TABLE 2. Calibration of HW coefficients; the first three columns are the lower bound, initial estimate, and upper bound values for the six clusters; the last three columns are the 99% confidence intervals centered on the value at convergence; in bold the final point estimate.

Cluster #	\mathbf{x}^L	\mathbf{x}^0	\mathbf{x}^U	$\mathbf{x}^{11} - \Delta_x$	\mathbf{x}^{11}	$\mathbf{x}^{11} + \Delta_x$
1	60	146	160	141.9	152.8	163.7
2	60	120	160	108.1	109.7	111.3
3	60	140	160	141.1	141.6	142.1
4	60	90	160	126.5	126.8	127.1
5	60	136	160	100.4	111.2	122.0
6	60	133	160	133.1	134.0	134.9

TABLE 3. Results of leak detection and localization: The true location, the start time and the maximum leakage outflow $\max(Q_L)$ are taken from the BattLeDIM solutions. The estimated location is found with the leak localization algorithm. t_D is the detection time measured in hours since the true start time of the leak. The distance between the true and the estimated leak location is the shortest topological distance over the pipes in meter. Zone shows in which area of the network the leak is located. Perfectly located leaks are shown in boldface (plus minus 10 m), while leaks with a distance greater than 300 m (missed leaks according to the BattLeDIM rules) are highlighted with an asterisk.

True Loc.	start time	$\max(Q_L)$ (m^3/h)	Est. Loc.	t_D (h)	Distance (m)	Zone
-	-	-	-	-	-	-
p427	2018-02-13 08:25	5.11	-	-	-	A
p654	2018-07-05 03:40	5.49	p654	956.33	0	A
p810	2018-07-28 03:05	6.91	p810	668.92	0	A
p523	2019-01-15 23:00	28.39	p500	0.00	205	A
p827	2019-01-24 18:30	26.46	p827	-0.08	0	A
p653	2019-03-03 13:10	18.28	p655	273.42	106	A
p710	2019-03-24 14:15	5.58	p702	0.00	222	A
p514	2019-04-02 20:40	15.58	p226	0.00	90	A
p331 ^(*)	2019-04-20 10:10	10.93	p905	0.00	355	A
p193 ^(*)	2019-05-19 10:40	10.36	p185	417.33	398	A
p142	2019-06-12 19:55	27.04	p623	0.00	2	A
p586	2019-07-26 14:40	20.52	p586	215.50	0	A
p721 ^(*)	2019-08-02 03:00	13.18	p703	222.92	354	A
p800	2019-08-16 14:00	21.95	p820	110.50	196	A
p123	2019-09-13 20:05	9.19	p201	588.33	133	A
p455	2019-10-03 14:00	11.05	p109	584.92	142	A
p762	2019-10-09 10:15	15.71	p745	301.00	179	A
p426 ^(*)	2019-10-25 13:25	13.56	p42	0.00	779	A
p879	2019-11-20 11:55	10.93	p884	342.50	256	A
p680	2019-07-10 08:45	5.37	p680	0.00	0	B
p257	2018-01-08 13:30	6.87	p257	104.50	0	C
p280	2019-02-10 13:05	5.26	p251	0.00	49	C
p277 ^(*)	2019-05-30 21:55	7.36	p8	541.83	358	C

682 **List of Figures**

683 1 Overview of the hierarchical leak detection and isolation approach from left to
684 right: Starting with the *data* analysis (measurements and EPANET model), then
685 model *calibration* (nodal demand and pipe roughness), followed by *simulations*
686 with the dual model approach, to finally detect and localize *leaks*. 35

687 2 Network colored by calibration clusters of Hazen-Williams roughness coefficients.
688 Pressure measurements are shown as circles. In a) the roughness iterations are
689 plotted ; in b), the inset shows the principle of the dual model, where the pressure
690 measurements are replaced by the combination of a valve and a virtual reservoir
691 whose head is equal to the measured head h_i ; the dual model transforms h_i into
692 virtual leakage flows q_{v_i} ; in (c) the pressure residuals are shown for the first week
693 of 2018; and finally, in (d) the minimum, maximum, and root mean square errors
694 (RMSE) are shown in increasing RMSE order. 36

695 3 Weekly seasonality (a) and yearly trend (b) extracted from the AMR measurements
696 for the different customer types (Residential and Commercial) and nodes consisting
697 of a mix of them (Mixed). 37

698 4 Leakage outflow in Area C (a) estimated by comparing the “virtual” inflow mea-
699 surement and the demand model and (b) as provided by the dual model. 38

700 5 Dual model signals for first two leaks in Area A in 2019 (location at pipes p827 and
701 p523 with magnitudes of approximately $27 \text{ m}^3/h$ each). (a) Pressure measurements
702 p over time, (b) sharp and localized signal of the virtual leak outflows q_v over time
703 calculated by the dual model at the same measurement locations, (c) the sum over
704 all virtual leak flows in the dual model serves as good estimates for leak size. . . . 39

705 6 Snapshot of the leakage isolation tool: calculated outflows at virtual reservoirs of
706 sensor nodes and correlation results: small diamonds for current time step and large
707 diamonds for sum of all time steps (the size represents the score). 40

708	7	Results of leak detection and localization for the unknown leaks in Area C in 2019:	
709		(a) Identified leakage outflows over time and (b) estimated locations of the leaks.	
710		Crosses are the estimated leak locations, circles indicate the real locations.	41
711	8	Results of leak detection and localization for the unknown leaks in Area B in 2019:	
712		(a) Identified leakage outflows over time; and (b) estimated locations of the leaks.	
713		The Cross is the estimated leak location, the circle indicates the real location.	42
714	9	Results of leak detection for the unknown leaks in Area A in 2019: (a) Leakage	
715		outflows for the first half of the year / leaks, and (b) for the second half of the year	
716		/ leaks. The second half also includes the ongoing leaks from (a) as shaded lines.	
717		Additionally, the missed detected leak at pipe p427 is shown in (a).	43
718	10	Results of leak localization for the unknown leaks in Area A in 2019: (a) First half	
719		of the year from January to June, and (b) for the second half of the year from July	
720		to December. The not detected leak at pipe 427 is shown as a white cross in (a).	
721		Crosses are the estimated leak locations, circles indicate the real locations.	44

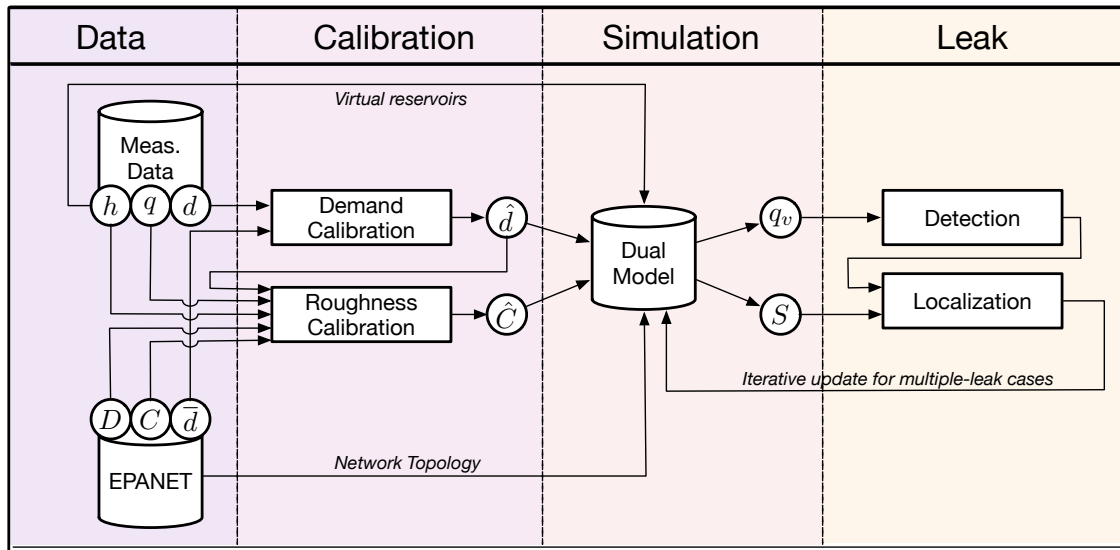


Fig. 1. Overview of the hierarchical leak detection and isolation approach from left to right: Starting with the *data* analysis (measurements and EPANET model), then model *calibration* (nodal demand and pipe roughness), followed by *simulations* with the dual model approach, to finally detect and localize *leaks*.

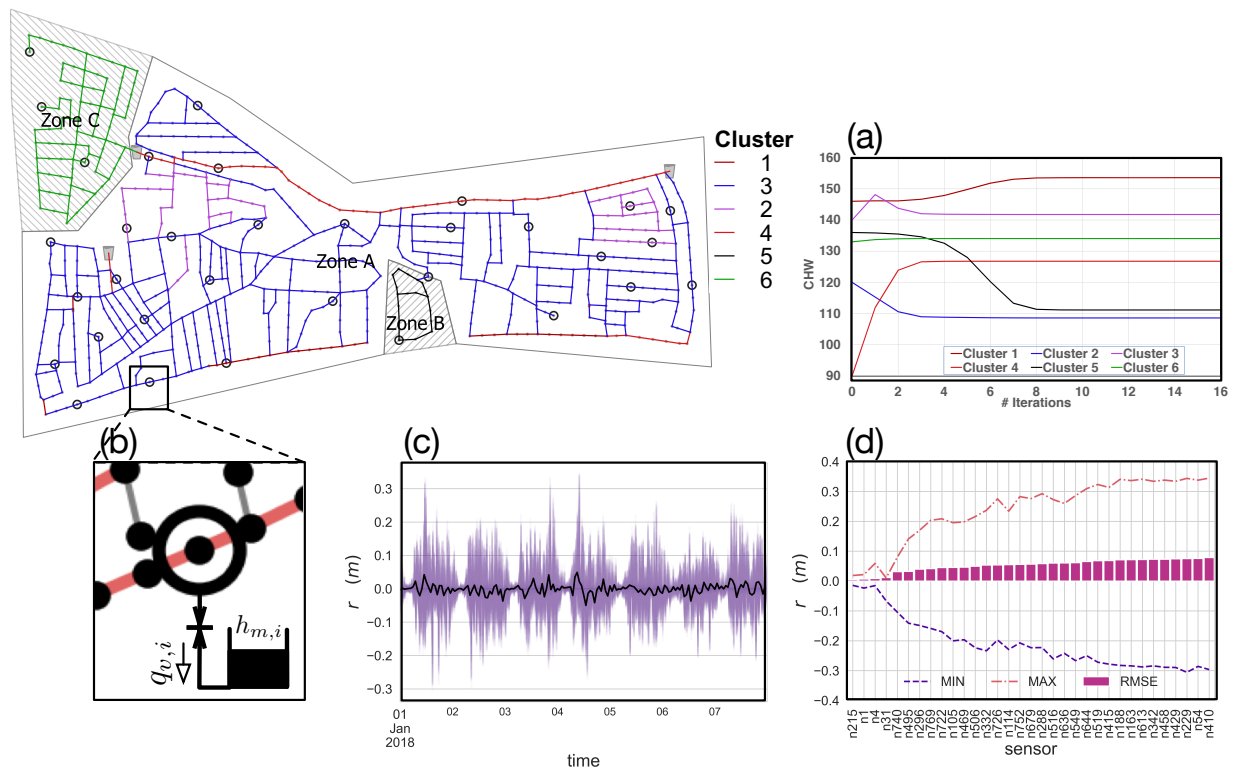


Fig. 2. Network colored by calibration clusters of Hazen-Williams roughness coefficients. Pressure measurements are shown as circles. In a) the roughness iterations are plotted ; in b), the inset shows the principle of the dual model, where the pressure measurements are replaced by the combination of a valve and a virtual reservoir whose head is equal to the measured head h_i ; the dual model transforms h_i into virtual leakage flows $q_{v,i}$; in (c) the pressure residuals are shown for the first week of 2018; and finally, in (d) the minimum, maximum, and root mean square errors (RMSE) are shown in increasing RMSE order.

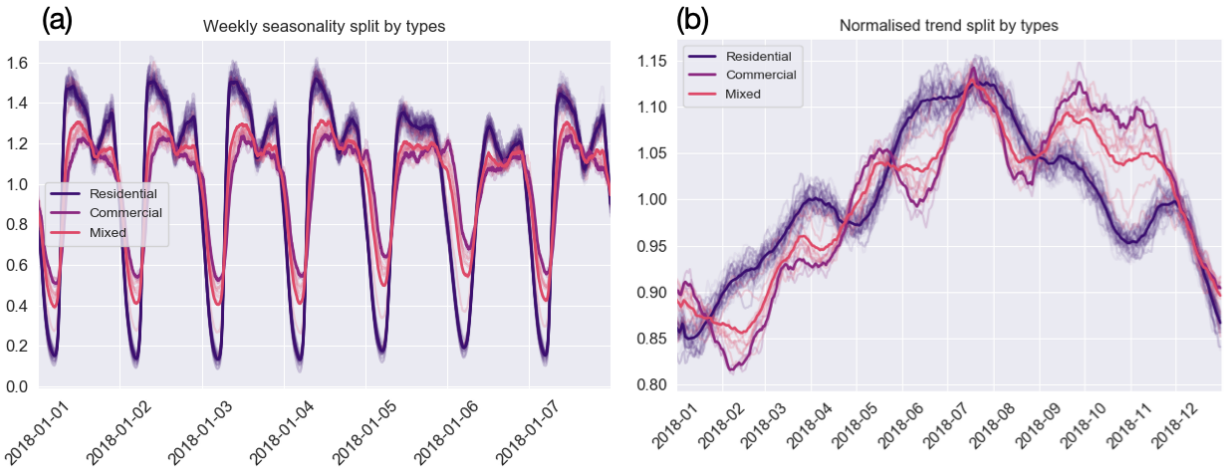


Fig. 3. Weekly seasonality (a) and yearly trend (b) extracted from the AMR measurements for the different customer types (Residential and Commercial) and nodes consisting of a mix of them (Mixed).

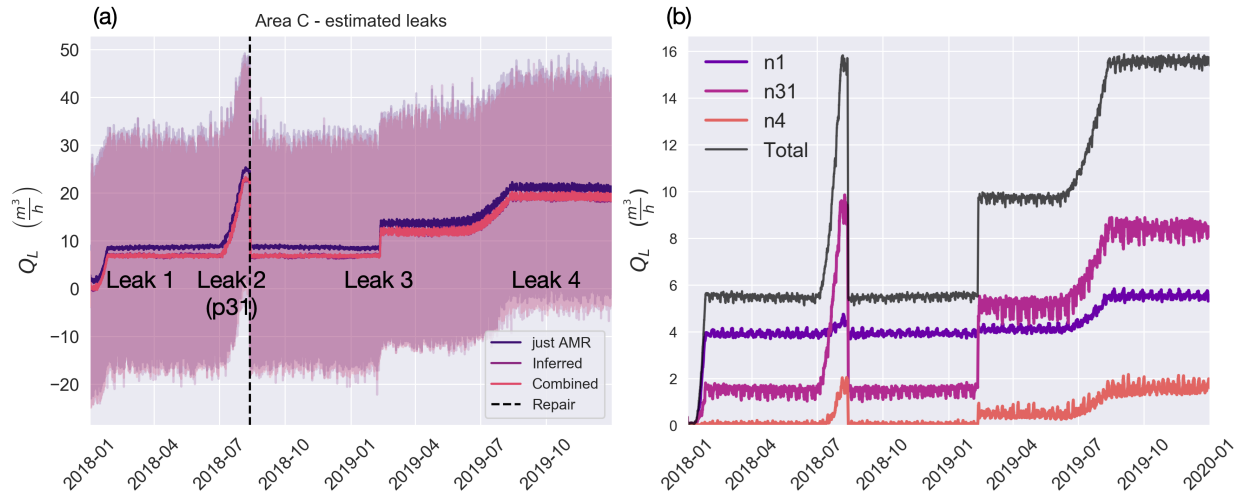


Fig. 4. Leakage outflow in Area C (a) estimated by comparing the “virtual” inflow measurement and the demand model and (b) as provided by the dual model.

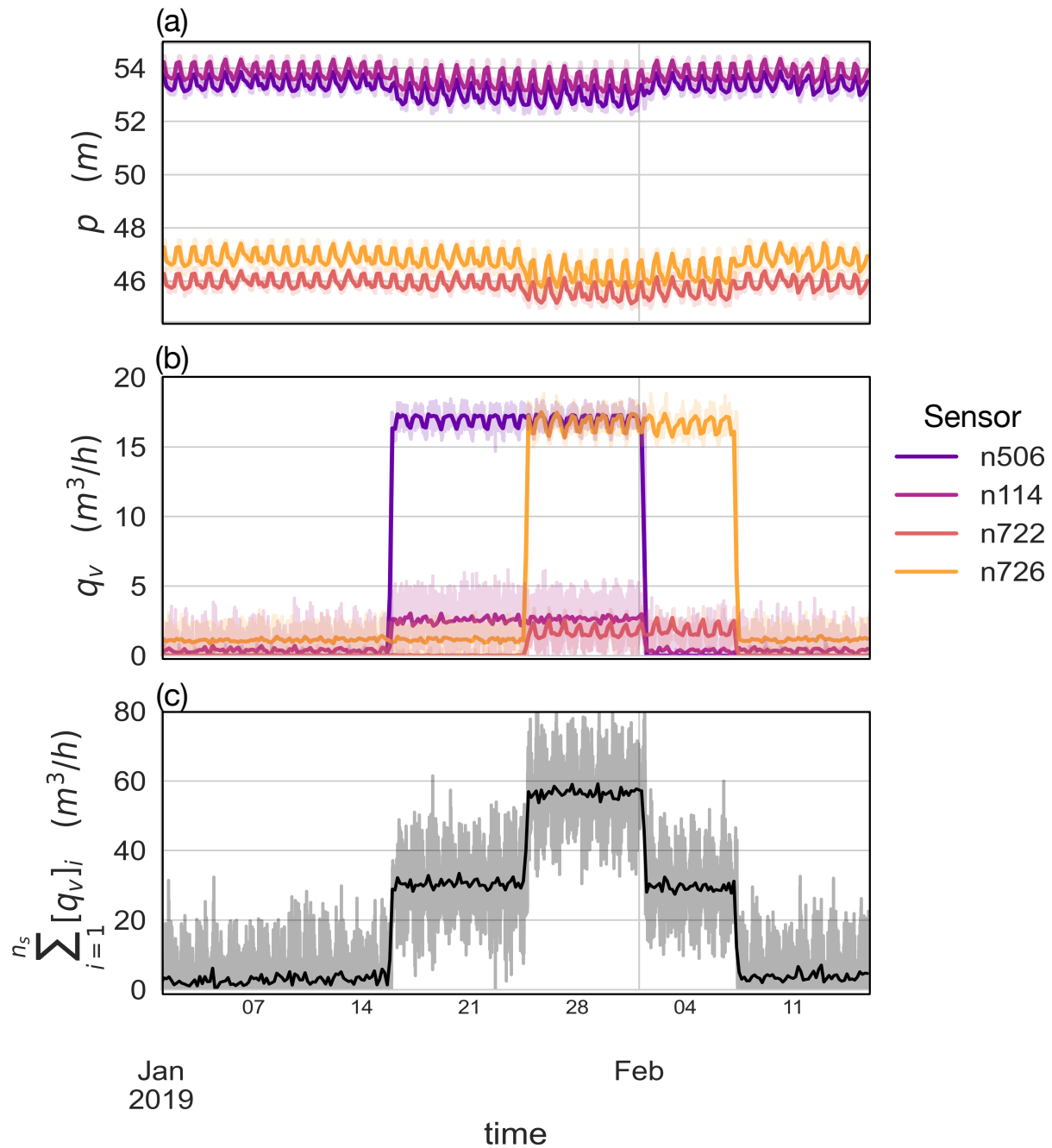


Fig. 5. Dual model signals for first two leaks in Area A in 2019 (location at pipes p827 and p523 with magnitudes of approximately $27 m^3/h$ each). (a) Pressure measurements p over time, (b) sharp and localized signal of the virtual leak outflows q_v over time calculated by the dual model at the same measurement locations, (c) the sum over all virtual leak flows in the dual model serves as good estimates for leak size.

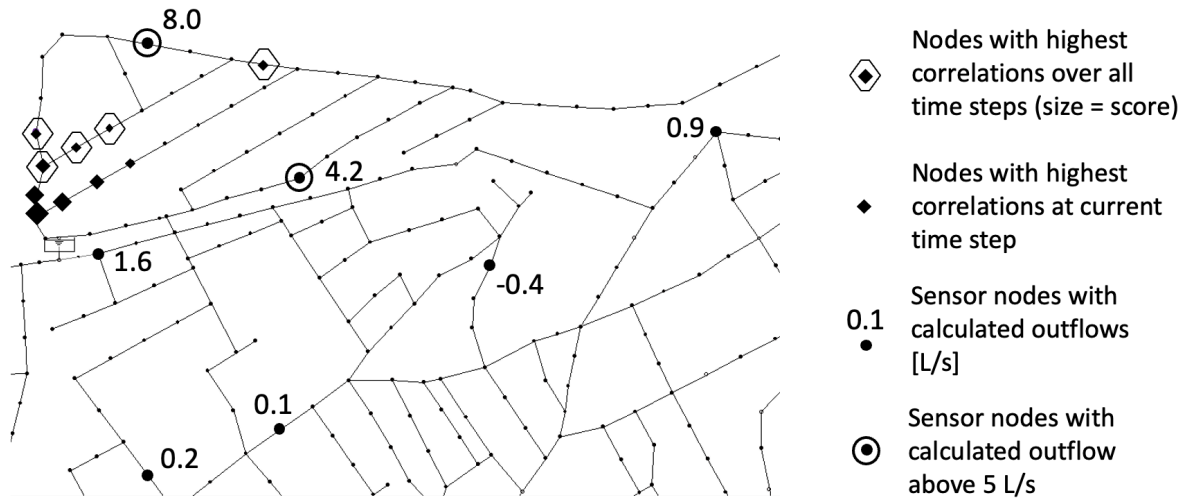


Fig. 6. Snapshot of the leakage isolation tool: calculated outflows at virtual reservoirs of sensor nodes and correlation results: small diamonds for current time step and large diamonds for sum of all time steps (the size represents the score).

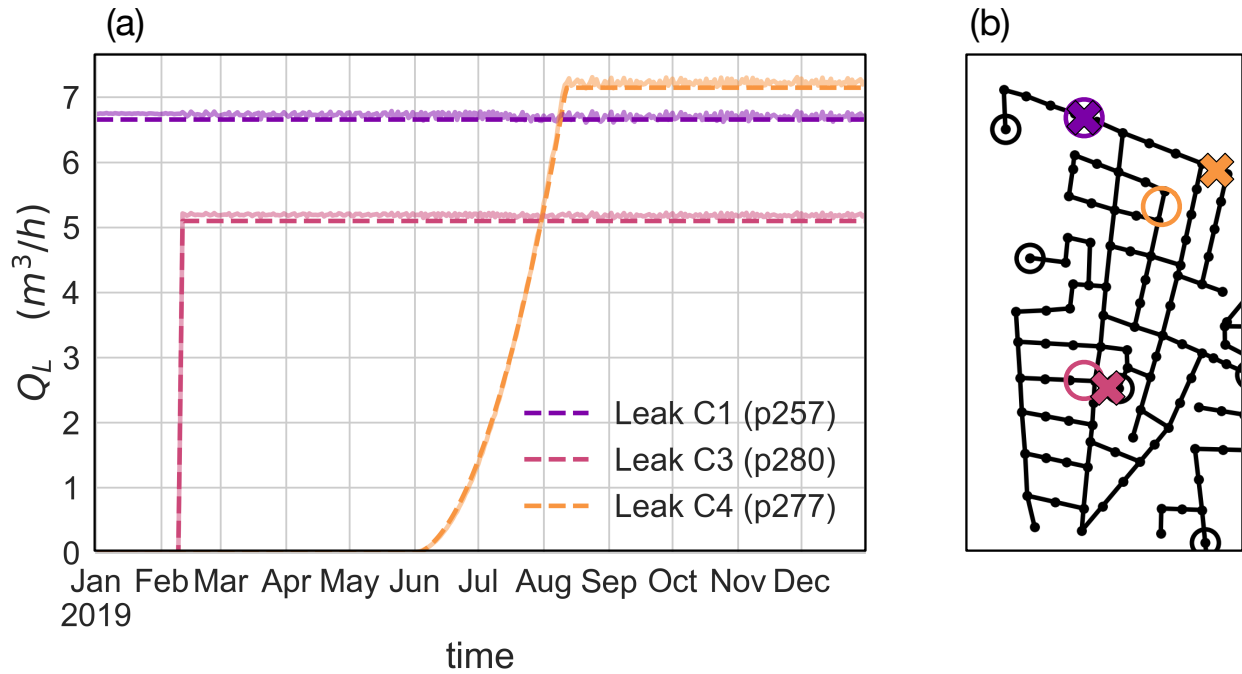


Fig. 7. Results of leak detection and localization for the unknown leaks in Area C in 2019: (a) Identified leakage outflows over time and (b) estimated locations of the leaks. Crosses are the estimated leak locations, circles indicate the real locations.

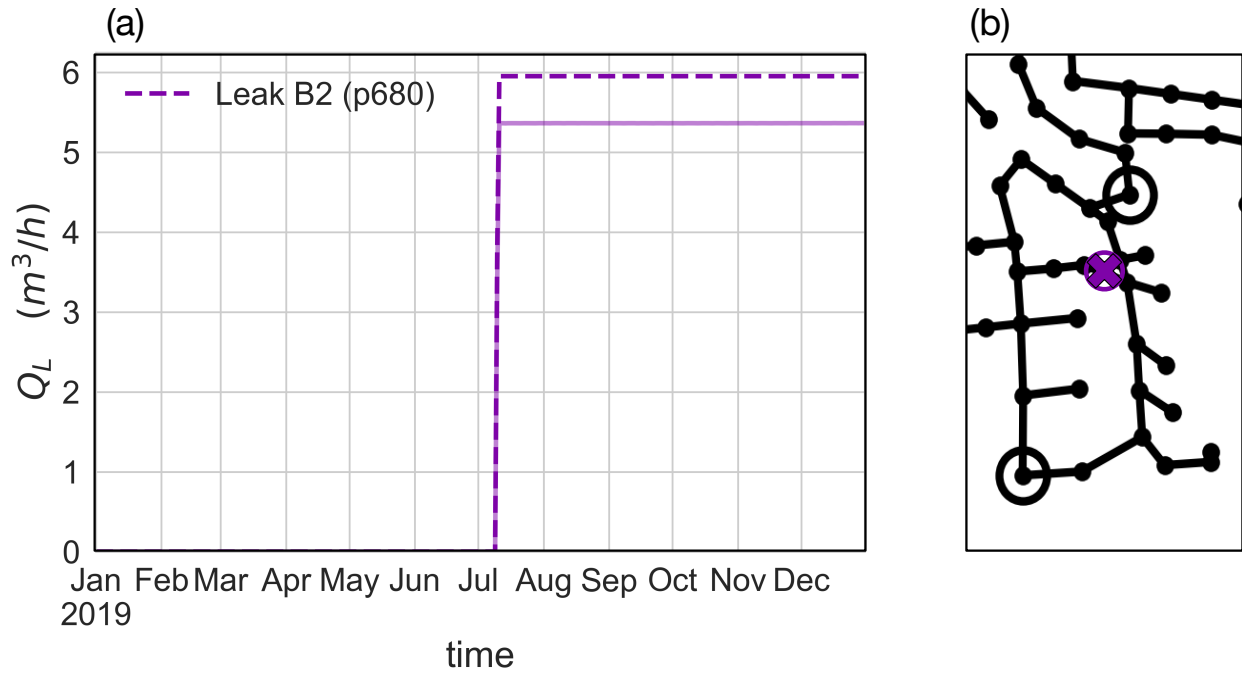


Fig. 8. Results of leak detection and localization for the unknown leaks in Area B in 2019: (a) Identified leakage outflows over time; and (b) estimated locations of the leaks. The Cross is the estimated leak location, the circle indicates the real location.

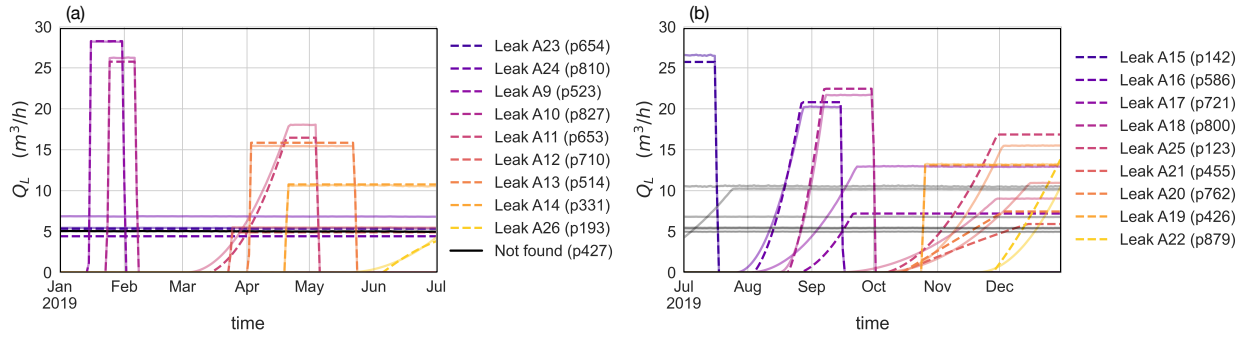


Fig. 9. Results of leak detection for the unknown leaks in Area A in 2019: (a) Leakage outflows for the first half of the year / leaks, and (b) for the second half of the year / leaks. The second half also includes the ongoing leaks from (a) as shaded lines. Additionally, the missed detected leak at pipe p427 is shown in (a).

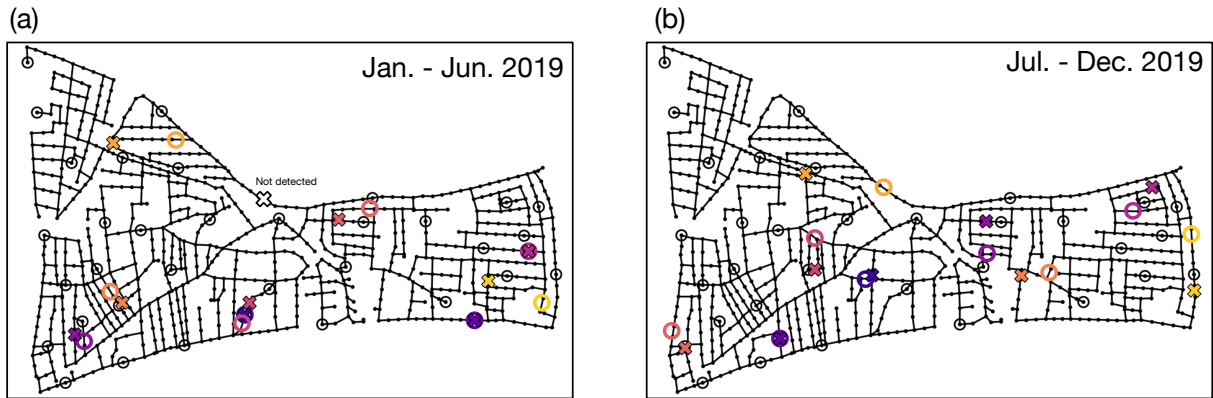


Fig. 10. Results of leak localization for the unknown leaks in Area A in 2019: (a) First half of the year from January to June, and (b) for the second half of the year from July to December. The not detected leak at pipe 427 is shown as a white cross in (a). Crosses are the estimated leak locations, circles indicate the real locations.

1 **PRESSURE-LEAK DUALITY FOR LEAK DETECTION AND**
2 **LOCALIZATION IN WATER DISTRIBUTION SYSTEMS**

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12 **ABSTRACT**

13 Water utilities are challenged to reduce their water losses through detecting, localizing, and
14 repairing leaks as fast as possible in their aging distribution systems. In this work, we solve this
15 challenging problem by detecting multiple leaks simultaneously in a water distribution network for
16 the *Battle of the Leak Detection and Isolation Methods*. The performance of leak detection and
17 localization depends on how well the system roughness and demand are calibrated. In addition,
18 existing leaks affect the diagnosis performance unless they are identified and explicitly represented
19 in the model. To circumvent this "chicken-and-egg" dilemma, we decompose the problem into
20 multiple levels of decision making (a hierarchical approach) where we iteratively improve the water
21 distribution network model and so are able to solve the multi-leak diagnosis problem.

22 First, a combination of time series and cluster analysis is used on smart meter data to build
23 patterns for demand models. Second, point and interval estimates of pipe roughnesses are retrieved

24 using least squares to calibrate the hydraulic model, utilizing the demand models from the first
25 step. Finally, the calibrated primal model is transformed into a dual model that intrinsically
26 combines sensor data and network hydraulics. This dual model automatically converts small
27 pressure deviations caused by leaks into sharp and localized signals in the form of virtual leak
28 flows. Analytical derivations of sensitivities with respect to these virtual leak flows are calculated
29 and used to estimate the leakage impulse responses at candidate nodes. Subsequently, we use the
30 dual network to (i) detect the start time of the leaks and (ii) compute the Pearson correlation of
31 pressure residuals, which allows further localization of leaks. This novel dual modeling approach
32 resulted in the highest true-positive rates for leak isolation among all participating teams in the
33 competition.

34 INTRODUCTION

35 The detection, localization and control of leakage from aging water distribution networks
36 (WDNs) remains one of the main challenges for water utilities (WUs), because the direct financial
37 cost of water loss can be high. By detecting and dealing with leaks and bursts fast, utilities can also
38 mitigate deterioration of pipes and surrounding infrastructure in addition to lost revenues (Gupta
39 and Kulat 2018). The aim to reduce leakage is further motivated by stringent regulations and
40 financial incentives (OECD 2016).

41 Conventional techniques for detecting leakage include random and regular sounding surveys
42 using listening sticks and acoustic loggers (Adedeji et al. 2017), and step-testing of metered
43 subsystems as district metered areas (DMAs) through gradual valve closures (Farley and Trow
44 2003; Wu 2008). More advanced leakage pin-pointing methods like *leak noise correlators*, *pig-*
45 *mounted acoustic sensing* and *gas-injection techniques* (Puust et al. 2010) are the most precise at
46 locating leaks. However, all these techniques come with expensive equipment cost and are man-
47 hour intensive, and so are not scalable. In addition, the suppression of leakage sound signatures by
48 reduced pressures in active pressure management or increasing use of plastic pipes in the network
49 has also made these methods less effective (Wu 2008; Puust et al. 2010).

50 More recent advanced approaches use model-based analysis of near real-time telemetry data

51 from pressure sensors and flow meters distributed over the network. Starting with the work of
52 [Pudar and Liggett 1992](#), model-based leak localization was intensively studied with diverse set of
53 methods ranging from sensitivity matrix-based approaches ([Pérez et al. 2011](#); [Perez et al. 2014](#)),
54 meta-heuristic optimization ([Wu 2008](#); [Steffelbauer and Fuchs-Hanusch 2016b](#)), error-domain
55 model falsification ([Goulet et al. 2013](#); [Moser et al. 2017](#)), to combinations of model-based and
56 data-driven approaches ([Soldevila et al. 2016](#); [Soldevila et al. 2017](#)). An extensive review of leak
57 localization techniques including their limitations can be found in [Hu et al. 2021](#). This manuscript
58 deals with a novel model-based approach that leverages time-series analysis of demand models and
59 new hydraulic modeling approaches for both detecting and localizing potential leaks. One of the
60 main challenges for model-based leak detection approaches is the sparse number of pressure sensors
61 compared to the number of candidate leak location nodes. For methods that solve for multiple leaks
62 by posing inverse problems to determine leak parameters in the network model ([Pudar and Liggett
63 1992](#)) (*i.e.* leak levels and locations), this creates an under-determined and ill-posed problem.
64 Additionally, the performance of model-based approaches can also be very sensitive to errors in
65 two important model parameters: the demand at nodes and pipe roughness coefficients ([Hutton et al.
66 2014](#)). [Sanz et al. 2016](#) reduce this error by including existing leaks in the calibration process. This
67 is done by co-optimizing the calibration and detection, and updating the calibrated model through
68 iteration as new data becomes available and leaks are discovered and fixed. This is achieved
69 through an iterative calibration process, where demands at nodes are composed of geographically
70 distributed demand components. Due to the fact that a leak occurs as a less geographically spread
71 component in this approach, they become easier to find. The method of [Sanz et al. 2016](#) belongs to
72 a class of methods that rely on first-order pressure sensitivities to changes in demand at nodes, and
73 the projection of pressure residuals (differences of measured pressures from leak free case, usually
74 retrieved from time series or well calibrated hydraulic models) onto the sensitivities ([Sanz et al.
75 2016](#)). However, this class of methods have the limitations that they assume a single leak in the
76 system at one time, and are known to be less reliable for small leak sizes, since the leak induced
77 pressure deviations and, hence, the pressure residuals are very small in that case.

78 In this manuscript, we address these limitations of pressure residual projection approaches (i.e.,
79 the applicability on single as well as small leaks) by combining multiple methods. As in [Sanz
80 et al. 2016](#), we utilize an iterative calibration of the system roughness and demand parameters
81 using multiple measurements, including automatic meter readings (AMRs). To deal with multiple
82 leaks, we separate the detection and localization process; time series analysis (TSA) is used to
83 automatically find deviations in demand and flow measurements, thus, estimating the start and end
84 time of multiple growing and non-growing leaks that can coincide. The detected leaks are then
85 localized by using a residual projection approach ([Steffelbauer et al. 2020](#)), where the model is
86 updated when leaks are discovered or fixed. A new duality-based approach is then proposed to
87 improve the sensitivity of the localization process to smaller leaks. We formulate a dual network
88 model, where thanks to a mathematical trick — by transforming the network model with pressure
89 measurements to an equivalent model with additional virtual reservoirs and valves — we are able
90 to translate pressure heads directly to virtual leakage outflows at the measurement locations, which
91 provide a first estimate for the leak’s size and location in the network.

92 Subsequently, we use the virtual leak flows of the dual model for leak detection with anomaly
93 detection algorithms (i.e., the cumulative sum control chart (CUSUM) algorithm and the likelihood
94 ratio test ([Peach et al. 1995](#))) to obtain information on the leak start-time; and the residual-based
95 localization to retrieve the location of the leak. Finally, the information from the detection and
96 localization methods are combined to get accurate estimates for the actual size and location of the
97 leaks.

98 In the next section, an exposition of the different methods will be presented. We will then
99 discuss the results using the L-Town network model of the *Battle of the Leak Detection and Isolation*
100 *Methods* (BattLeDIM) competition ([Vrachimis et al. 2020](#)), which the authors of this manuscript
101 won under the team name *Under Pressure*. The final section will present the conclusions, limitations
102 and future directions to improve the proposed method.

103 METHODS

104 **Overview**

105 We solve the leak detection and isolation problem through utilizing a hierarchical approach. An
106 overview of the two stages where different methods are combined as well as the order in which they
107 are applied is illustrated in Figure 1, depicting how we attempted to find *leaks* in the measurement
108 *data* via model *calibration* and then *simulation* with the dual model. In the first stage, the hydraulic
109 model is calibrated, since a well-calibrated model is essential to reliably localize leaks (Savic et al.
110 2009). The model is itself calibrated in two-stages; starting with demand calibration and followed
111 by pipe roughness parameter estimation. The demand calibration method makes use of TSA on
112 AMR data d , and infers estimated demands \hat{d} to unmeasured nodes with respect to their average
113 demand \bar{d} stored in the EPANET file. The pipe roughnesses \hat{C} are estimated through solving
114 a differentiable, constrained, weighted least squares (WLS) problem, which uses the estimated
115 demands \hat{d} , measured pressure heads h , and the initial roughness values C as found in the original
116 EPANET file. In the second, a dual model is built based on the calibrated values (\hat{d} and \hat{C}) and
117 used for leak detection and localization, where pressure measurements are replaced with virtual
118 reservoirs. The dual model magnifies leak signals by transforming pressures in virtual leakage
119 outflows q_v . Moreover, dual model leak sensitivities S are computed. Finally, the sensitivities S
120 and virtual flows q_v are used to locate the leaks with a correlation-based method similar to Sanz
121 et al. 2016. In cases with multiple leaks that appear simultaneously, the leaks are localized one by
122 one, eliminated from the dual model, and the remaining leaks are detected and located subsequently
123 through an iterative approach.

124 **Calibration**

125 *Nodal demand calibration*

126 The AMRs data is used to develop a demand model through TSA for the unmeasured customers
127 within the network. Various time series models (Shumway and Stoffer 2010) are tested on the
128 AMRs aiming to extract weekly seasonalities and yearly trends for different customer types (e.g.,
129 residential, commercial). The best performance is achieved with a rather simple model, consisting
130 of a multiplicative superposition of weekly seasonalities ($S(t)$), a time varying trend ($T(t)$) and a

131 random component ($R(t)$) accounting for stochastic variations and measurement noise

$$d(t) = \bar{d} \cdot T(t) \cdot S(t) \cdot R(t), \quad (1)$$

132 with \bar{d} being the customer's base demand. For each AMR time series, the trend component $T(t)$
 133 is estimated using a convolution filter and subsequently removed by dividing the original time
 134 series through $T(t)$, followed by estimation of $S(t)$ through periodical averages over the trend-free
 135 series (Seabold and Perktold 2010). After removing the seasonal component by dividing the trend-
 136 free series by $S(t)$, only the random component $R(t)$ remains. Subsequently, similarities in the
 137 individual seasonal patterns are identified through time series clustering (Steffelbauer et al. 2021).
 138 Furthermore, cluster analysis is used to identify the number of distinct patterns n_d and outliers.
 139 For each demand node i of the network model, a time-varying demand time series \hat{d}_i is built as a
 140 superposition of the distinct patterns weighted by their individual averages \bar{d}_{ij} associated with the
 141 patterns

$$\hat{d}_i(t) = \sum_{j=1}^{n_d} \bar{d}_{ij} \cdot T_j(t) \cdot S_j(t). \quad (2)$$

142 Note that the random time series components are neglected when building the estimates \hat{d}_i .

143 *Pipe roughness calibration*

144 Pipes with the same material, age, diameter, hydraulic conditions and locations are grouped in
 145 clusters with the same roughness value (in this case a Hazen-Williams (HW) coefficient)

$$\mathbf{C}_{HW} = \mathbf{M}_{HW} \mathbf{x}, \quad (3)$$

146 where \mathbf{M}_{HW} is the membership matrix of the n_p pipes to n_c clusters of HW coefficients, $\mathbf{x} \in \mathbb{R}^{n_c}$ is
 147 the vector of roughness cluster values to calibrate, and $\mathbf{C}_{HW} \in \mathbb{R}^{n_p}$ is the vector of HW coefficients
 148 of pipes. Roughness calibration aims to fit the measurements by adjusting the roughness coefficients

149 of the hydraulic model. Following nonlinear regression equations have to be considered

$$[\mathbf{z}^j]_i = [\mathbf{S}\mathbf{y}(t_j, \mathbf{x})]_i + \varepsilon_{ij}, \quad (4)$$

150 where $\mathbf{y}(t_j, \mathbf{x})$ is the hydraulic state that is implicitly defined by the extended period simulations at
 151 time t_j , $\mathbf{z}^j \in \mathbb{R}^{n_m}$ is the vector of measurements at time t_j , \mathbf{S} is the selection matrix to select state
 152 vectors that correspond to the measurements, and $\varepsilon_{ij} \sim \mathcal{N}(0, \sigma_{ij}^2)$ are independent and identically
 153 distributed Gaussian error terms with zero expectation and standard deviation σ_{ij} .

154 The box-constrained WLS problem for parameter calibration consists of seeking to minimize
 155 the differentiable criterion

$$\min_{\mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U} f(\mathbf{x}) \triangleq \frac{1}{2} \sum_{j=1}^{n_t} \sum_{i=1}^{n_m} H_\kappa \left(\frac{[\mathbf{S}\mathbf{y}(t_j, \mathbf{x})]_i - [\mathbf{z}^j]_i}{\sigma_{ij}} \right) + \frac{\alpha}{2} \|\mathbf{x} - \mathbf{x}^0\|_2^2, \quad (5)$$

156 where in place of the traditional least-squares criterion the weighted Huber function H_κ with
 157 parameter κ is used, as in [Preis et al. \(2011\)](#), to increase the robustness of parameter estimates
 158 against outliers, n_t is the number of observation times, n_m the number of measurements, \mathbf{x}^L and \mathbf{x}^U
 159 are the lower and upper bounds, \mathbf{x}^0 is prior information about \mathbf{x} (e.g. initial value in the EPANET
 160 file) and α is a Tikhonov regularization coefficient, which penalizes large departures from \mathbf{x}^0 for
 161 sufficiently large α and increases the robustness of parameter estimates against outliers. The state
 162 of the art algorithm for solving a differentiable WLS problem is the iterative Levenberg-Marquardt
 163 algorithm. At each iteration step, the gradient of f is calculated to estimate the Hessian at the last
 164 estimate \mathbf{x}^k . The gradient of f at \mathbf{x}^k is:

$$\nabla f^k = \sum_{j=1}^{n_t} \mathbf{J}(t_j, \mathbf{x}^k)^T \mathbf{W}_j \tilde{\mathbf{R}}(t_j, \mathbf{x}^k) + \alpha (\mathbf{x}^k - \mathbf{x}^0), \quad (6)$$

165 where \mathbf{W}_j is the diagonal weight matrix at time t_j , $\mathbf{J}(t_j, \mathbf{x}^k) = \mathbf{S} \partial_x \mathbf{y}(t_j, \mathbf{x}^k)$ is the Jacobian matrix of
 166 the prediction function at \mathbf{x}^k , with $\partial_x \mathbf{y}$ using the postmultiplication by $\mathbf{P} = \mathbf{M}_{HW}$ as in [Piller et al.](#)

167 (2017), and $\tilde{\mathbf{R}}(t_j, \mathbf{x}^k)$ is the $(n_m, 1)$ -vector of truncated unreduced residuals

$$[\tilde{\mathbf{R}}(t_j, \mathbf{x}^k)]_i = \begin{cases} [\mathbf{S}\mathbf{y}(t_j, \mathbf{x}^k) - \mathbf{z}]_i & \dots \text{ if } |[\mathbf{S}\mathbf{y}(t_j, \mathbf{x}^k) - \mathbf{z}]_i| \leq \kappa\sigma_{ij} \\ \kappa\sigma_{ij}\text{sign}([\mathbf{S}\mathbf{y}(t_j, \mathbf{x}^k) - \mathbf{z}]_i) & \dots \text{ else} \end{cases} . \quad (7)$$

168 The estimate of the Hessian is following symmetric, positive definite matrix:

$$\mathbf{H}_k = \sum_{j=1}^{n_t} \mathbf{J}(t_j, \mathbf{x}^k)^T \mathbf{W}_j \tilde{\mathbf{J}}(t_j, \mathbf{x}^k) + \alpha \mathbf{I}_{nc} = \sum_{j=1}^{n_t} \tilde{\mathbf{J}}(t_j, \mathbf{x}^k)^T \mathbf{W}_j \tilde{\mathbf{J}}(t_j, \mathbf{x}^k) + \alpha \mathbf{I}_{nc} , \quad (8)$$

169 where $\tilde{\mathbf{J}}$ is given by

$$[\tilde{\mathbf{J}}(t_j, \mathbf{x}^k)]_{mn} = \begin{cases} [\mathbf{J}(t_j, \mathbf{x}^k)]_{mn} & \dots \text{ if } |[\mathbf{S}\mathbf{y}(t_j, \mathbf{x}^k) - \mathbf{z}]_m| \leq \kappa\sigma_{mj} \\ 0 & \dots \text{ else} \end{cases} . \quad (9)$$

170 The constraints are taken into account through a saturation/desaturation process by checking the
171 Karush-Kuhn-Tucker optimality conditions to identify the optimal Lagrange multipliers.

172 The projected Levenberg-Marquardt algorithm consists of solving following linear system

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \mathbf{C}_k^T \left(\mathbf{C}_k \mathbf{H}_k \mathbf{C}_k^T \right)^{-1} \mathbf{C}_k \nabla f_k , \quad (10)$$

173 where \mathbf{C}_k is the selection matrix for the unsaturated components \mathbf{x}^k . To cope with ill conditioned
174 Hessians, a damping factor with a regularization parameter is introduced to scale the gradient
175 according to the curvature

$$\mathbf{H}_k(\lambda) = \mathbf{H}_k + \lambda [\mathbf{diag}(\mathbf{H}_k) + \phi \mathbf{I}_{nc}] , \quad (11)$$

176 where ϕ is a positive parameter and λ is the damping parameter. Furthermore, we make use of

177 following relation to calculate confidence intervals for the roughness estimates (Piller 2019)

$$-[\Delta_x]_i \leq \delta \mathbf{x}_i \leq [\Delta_x]_i, \text{ with } \mathbf{M} = \left(\mathbf{W}^{0.5} \mathbf{J} \right)^+, [\Delta_x]_i = 3 \sum_{k=1}^{n_m} |\mathbf{M}_{ik}|, i = 1, \dots, n_c \quad (12)$$

178 with \mathbf{J} is the block matrix $\mathbf{J} = \left(\mathbf{J}(t_1, \mathbf{x})^T \quad \dots \quad \mathbf{J}(t_{n_t}, \mathbf{x})^T \right)^T$ and $\mathbf{W}^{0.5}$ is the diagonal matrix
 179 $\mathbf{W}^{0.5} = \left(\mathbf{W}_j^{0.5} \right) = (\sigma_{ij})$.

180 The Dual Model

181 We introduce a so-called ‘‘Dual Approach (DA)’’ for detecting and localizing leaks, that is
 182 depicted in Figure 2 (b). In the DA, the model is *augmented* with n_s *virtual reservoirs* that are
 183 connected with pressure measurement nodes by valves. The origin of the name ‘‘dual’’ stems from
 184 the fact that, instead of using the fixed demand boundary condition at the sensor nodes (*i.e.* the
 185 original or ‘‘primal’’ hydraulic model), the measured pressure heads are used as fixed head boundary
 186 conditions at the corresponding virtual reservoirs. Consequently, the heads at the measurement
 187 nodes become free variables and imbalances in the system compared to a leak-free model lead to
 188 flows to the virtual reservoirs. If there are no leaks, and if we set the minor loss of each virtual
 189 reservoir’s valve to zero, the two networks are equivalent. In the hydraulic model, we normally
 190 set these valves’ minor loss to a sufficiently low but non-zero value, and so the primal and dual
 191 networks are ‘numerically equivalent’ but not mathematically equivalent.

192 If a new leak appears in the primal model, the residuals between measured and calculated
 193 pressures change. The pressure drops caused by higher flow velocities towards the leak in the
 194 real system are not observed in the model that is still based on the leak free system. In the dual
 195 approach, the measured pressure drop is applied to the fixed head reservoirs and, as a consequence,
 196 an additional outflow is generated. This outflow can be understood as an outflow residual or *virtual*
 197 *leak flow*. The advantage of the DA is that the calculated outflows act as amplifiers that deliver
 198 significant and localized signals even for small pressure drops. In addition, the outflows at the
 199 virtual reservoirs serve a good first estimate for the leak’s size and location.

200 *Dual Model Sensitivities*

201 We consider the dual WDN with n_p pipes, n_s virtual links and n_j junction nodes at which the
 202 heads are unknown. We also denote the vector of unknown flows in the pipes and virtual links
 203 by $\mathbf{q} \in \mathbb{R}^{n_p+n_s}$, the unknown heads and demands at the (free) nodes by $\mathbf{h} \in \mathbb{R}^{n_j}$ and $\mathbf{d} \in \mathbb{R}^{n_j}$,
 204 respectively. The sensitivities of heads and pipe flow rates with respect to nodal outflows are
 205 derived among other sensitivities in Piller et al. (2017). The local sensitivities $\nabla_{\mathbf{d}}\mathbf{h}$ and $\nabla_{\mathbf{d}}\mathbf{q}$ can be
 206 calculated in demand driven analysis as follows

$$\begin{aligned} \nabla_{\mathbf{d}}\mathbf{h} &= -\left(\mathbf{A}^T\mathbf{F}^{-1}\mathbf{A}\right)^{-1} \\ \nabla_{\mathbf{d}}\mathbf{q} &= -\mathbf{F}^{-1}\mathbf{A}\left(\mathbf{A}^T\mathbf{F}^{-1}\mathbf{A}\right)^{-1}, \end{aligned} \quad (13)$$

207 where \mathbf{A} is the link-node-incidence matrix of the dual network graph reduced to junction nodes
 208 (all links, including pipes and virtual links, are taken), and \mathbf{F} is the diagonal matrix of head loss
 209 derivatives with respect to \mathbf{q} .

210 Let $\mathbf{A}_f \in \mathbb{R}^{(n_p+n_s) \times (n_f+n_s)}$ be the link-node-incidence matrix of the dual network graph reduced
 211 to fixed-head nodes (the n_f initial tanks and reservoirs, and the n_s virtual reservoirs), and let
 212 $\mathbf{q}_{in} = \mathbf{A}_f\mathbf{q}$ represent the unknown flow rate entering in the system (leaving the fixed-head nodes if
 213 positive). Then the sensitivity of the \mathbf{q}_{in} can be written as using Eq. (13)

$$\nabla_{\mathbf{d}}\mathbf{q}_{in} = -\mathbf{A}_f^T\mathbf{F}^{-1}\mathbf{A}\left(\mathbf{A}^T\mathbf{F}^{-1}\mathbf{A}\right)^{-1}. \quad (14)$$

214 The Jacobian in Eq. (14) is the matrix of first order derivatives of the inflows calculated at virtual
 215 pressure nodes at measurement locations and real pressure boundary conditions such as reservoirs.
 216 The (i, j) element of $\nabla_{\mathbf{d}}\mathbf{q}_{in}$ represents the first order change rate of the calculated in- or outflow at
 217 a fixed-head node i as a consequence of a change in demand at node j .

218 In the dual model the in- and outflows at virtual reservoir are an indicator for a real existing leak
 219 or model errors. In a perfect model, where all the parameters are known, the calculated pressures
 220 of the dual model would be exactly the same as the measurements from a primal model. In the

221 corresponding dual model, the calculated in- and outflows at junctions would be zero and the primal
 222 and the dual models would give approximately the same results (*i.e.* except for small numerical
 223 differences due to the minor losses across the virtual reservoir valves).

224 In presence of an unknown leak, the measured pressure heads and the values calculated by the
 225 leak-free primal model diverge. In the dual model, the pressures at the measurement nodes become
 226 free and the measurements are set as virtual fixed heads (Figure 2 (b)). The imbalance caused by
 227 the unknown leak is then expressed as in- and outflows calculated at pressure measurement nodes.
 228 However, as we have shown in the BattLeDIM (Steffelbauer et al. 2020), the sensitivity is much
 229 higher in the dual model. Inverting the problem acts as an amplifier of leaks. Another advantage
 230 is that the imbalances and the value in question (leaks) have the same unit of flow. The sum of all
 231 the imbalances normally gives a good first estimate of the size of the leak. For explanation of the
 232 amplifying effect, a deeper investigation of the equation (14) may be useful: from the balance of
 233 inflows and outflows, it is possible to deduce each column of $\nabla_{\mathbf{d}}\mathbf{q}_{in}$ including the fraction of in-
 234 and outflows as a response to the change in outflow at the corresponding demand node equation

$$\mathbf{1}_{n_f+n_s}^T \mathbf{q}_{in} = \mathbf{1}_{n_j}^T \mathbf{d} \Rightarrow \mathbf{1}_{n_f+n_s}^T \nabla_{\mathbf{d}} \mathbf{q}_{in} = \mathbf{1}_{n_j}^T . \quad (15)$$

235 The sum of the column vector must be one. Naturally, the response should be an inflow for all
 236 fixed-head nodes.

237 **Leak detection and localization**

238 *Leak detection with the dual model*

239 Whereas in the past, human operators were in charge of small single supply areas, modern WU
 240 employees are responsible for multiple DMAs simultaneously (Bakker et al. 2014). That is why
 241 automatic anomaly detection algorithms are of particular interest for providing a rapid response to
 242 leaks and pipe burst (Romano et al. 2013). However, a correct estimation of the total leakage outflow
 243 over their time of existence (from the start t_S until the end t_E when they are repaired) is of utmost
 244 importance to assess water losses (Hamilton and McKenzie 2014). The correct identification of

245 t_S is also one of the objectives in the BattLeDIM (Vrachimis et al. 2020). We developed a two-
 246 stage approach to tackle both tasks: (i) using anomaly detection algorithms to detect leaks as fast
 247 as possible, and (ii) using regression analysis to retrieve good leak start time t_S estimates. For
 248 both approaches the virtual leak flows $[\mathbf{q}_v]_i = -[\mathbf{q}_{in}]_{i+n_f}$ (the dual model's outflows to the virtual
 249 reservoirs) are used (see Figure 4, for example).

250 Two algorithms were used to detect leaks in the \mathbf{q}_v : (i) the CUSUM algorithm, where a leak
 251 is detected when the cumulative sum of positive and negative differences in the signal exceeds a
 252 certain threshold τ_1 , (ii) and the likelihood ratio test (Peach et al. 1995), where a leak is detected if
 253 the ratio between the likelihood of the leak versus the leak-free case exceeds a certain threshold τ_2 .
 254 The ideal thresholds for both methods are obtained through calibration on leak free data.

255 Visual inspection of the virtual leakage outflows \mathbf{q}_v of detected leaks revealed two different
 256 types of leaks. The first leak type T_I is a sudden pipe burst that happen instantaneously at t_S

$$q_L(t) = \begin{cases} 0 & \text{for } t < t_S \\ q_S & \text{for } t \geq t_S \end{cases}, \quad (16)$$

257 where $q_L(t)$ is the leakage outflow over time and q_S is the saturated (maximum) leak flow (e.g.,
 258 Leak 3 in Figure 4). Note that leaks are not modeled as pressure dependent demands in contrast to
 259 the leaks generated in the BattLeDIM. The second leak type T_{II} is a slowly growing leak starting
 260 at t_S and saturating at a certain time t_{SA} , modeled as a piecewise function with a quadratic growth
 261 rate before the saturation ((e.g., Leak 1, 2 and 4 in Figure 4).)

$$q_L(t) = \begin{cases} 0 & \text{for } t < t_S \\ a \cdot t^2 + b \cdot t + c & \text{for } t_S \leq t \leq t_{SA} \\ q_S & \text{for } t > t_{SA} \end{cases}. \quad (17)$$

262 The coefficients of the quadratic outflow model connect the curves through following relationships
 263 $a = (q_S - b(t_{SA} - t_S))/(t_{SA}^2 - t_S^2)$ and $c = -at_S^2 - bt_S$. Additionally, it was found that leaks are

264 evolving simultaneously in the system, which makes the detection more difficult. If a single leak
 265 evolves over time, a Bayesian inference approach based on Hamilton Monte Carlo (Hoffman and
 266 Gelman 2014) is used (e.g. in Area C) to identify the parameters $t_S, t_{SA}, q_S, a, b,$ and c plus the
 267 confidence intervals of the leak model parameters. In the case of multiple evolving leaks (Area
 268 A&B), differential evolution is used to identify the best combination of leak outflows over time
 269 plus the leak parameters of each single leak (Storn and Price 1997). The identified leak outflows
 270 were compared against the outcomes of the DA and subsequently used for the leak localization.

271 *Leak localization with the dual model*

272 The Pearson correlation for flow and pressure residuals and the first-order estimates using
 273 sensitivities are calculated for the localization (Perez et al. 2014). It is more convenient for
 274 implementation purposes to work with the pressure residuals and sensitivities of the original
 275 measurement nodes instead of using the inflow sensitivities in Eq. (14) (e.g. no need for calculating
 276 \mathbf{A}_f and changing the set of variable pressure nodes). This does not affect the main idea, because
 277 the sensitivity of the head is equivalent to the headloss of the virtual valve and, hence, proportional
 278 to the flow sensitivity in the linearized system.

279 The vector of the sensitivities of measured head is determined by

$$\nabla_{\mathbf{d}} \mathbf{h}_{\mathbf{m}} = -\mathbf{S} \left(\mathbf{A}^T \mathbf{F}^{-1} \mathbf{A} \right)^{-1}. \quad (18)$$

280 The term \mathbf{S} is the same selection matrix for the measurement nodes as in Eq. (4).

281 The difference between Eq. (18) and Eq. (14) consists in the multiplication by the derivative of
 282 the valve headloss: $([\mathbf{Sh}]_i - h_{n_f+i}^f = K_i |[\mathbf{q}_v]_i| [\mathbf{q}_v]_i \Rightarrow \partial_{d_j} ([\mathbf{Sh}]_i) = -2K_i |[\mathbf{q}_v]_i| \partial_{d_j} ([\mathbf{q}_{in}]_{n_f+i}))$. If
 283 the sensitivities following Eq. (18) are used, the pressure residuals are used for the calculation of
 284 the correlation, whereas the simulated external flows at the virtual reservoirs are considered in the
 285 case of Eq. (14).

286 It proved to be beneficial to calculate the correlations only for measurement nodes where the
 287 leak flow (calculated by the dual model) exceeds a certain threshold (e.g. 0.5 L/s). This adjustment

288 eliminates the noise from the pressure measurements and stabilizes the calculated set of candidates
289 for the unknown leak. The Pearson correlation $\rho_{\mathbf{r}, \mathbf{S}_{(:,i)}}$ is calculated as

$$\rho_{\mathbf{r}, \mathbf{S}_{(:,i)}} = \frac{cov(\mathbf{r}, \mathbf{S}_{(:,i)})}{\sigma_{\mathbf{r}} \cdot \sigma_{\mathbf{S}_{(:,i)}}}, \quad (19)$$

290 where \mathbf{r} is the vector of residuals, $\mathbf{S}_{(:,i)}$ is the sensitivity vector of node i , $cov(\cdot)$ is the co-variance
291 and $\sigma_{\mathbf{r}}$ and $\sigma_{\mathbf{S}_{(:,i)}}$ are the standard deviations of the residual vector and the sensitivity vector,
292 respectively. The residuals and the sensitivity coefficients are very small. However, this did not
293 show any negative impact in the allocation in our tests. In contrast, the system is stabilized by the
294 additional pressure boundary conditions, which makes the correlation more stable compared to the
295 conventional primal model approach. One important limitation of the correlation method is that it
296 does not work for two or more leaks appearing at the same time. Therefore, a single leak must first
297 be isolated in time from other leaks in order to be localized. The leakage curves that have been
298 calculated for detection serve as a basis for choosing the best time for allocation, and we use a step
299 by step procedure for localizing simultaneously growing leaks.

- 300 1. Identification of time interval that starts briefly before the new unknown leak starts and ends
301 before the next leak starts. The time intervals from t_S to t_{SA} are found by a combination
302 of CUSUM or likelihood ratio tests with Hamilton Monte Carlo or differential evolution
303 (depending on the single or multiple leak case) as described in the leak detection paragraph
304 in the methods section.
- 305 2. Initialize calculation for the selected time interval (load all measurements as well as the
306 estimated demands)
- 307 3. Run Extended Period Simulations for selected time interval; for each time step do:
 - 308 (a) Update boundary conditions via toolkit functions including demand patterns, heads at
309 virtual reservoirs, pump flow.
 - 310 (b) Update all known leaks with their calculated leak flows as fixed demands and define the

- 311 start time of the unknown leak based on the results of the detection.
- 312 (c) Simulation of the time step (here the EPANET toolkit is used) and after each time step
313 with active new unknown leak, calculate correlation in Eq. (19) for all nodes based on
314 the sensitivities.
- 315 (d) Consider only the nodes with a correlation score higher than a given minimum threshold
316 (*e.g.* 0.95) and add those eligible correlations to the sum of correlation taken over all
317 calculated time steps.
- 318 4. The node with the highest correlation sum is identified as the candidate for the new leak
319 within this time interval.
- 320 5. The new leak is added to the list of known leaks and the leakage flow is considered as known
321 demand for the localization of the next leak and the procedure is repeated from point 1 until
322 all leaks have been identified in the given period.

323 **L-Town case study and measurement data**

324 The case study network *L-Town* was provided by the organizers of the BattLeDIM ([Vrachimis](#)
325 [et al. 2020](#)). *L-Town* is a small hypothetical town based on a real WDN in Cyprus with approximately
326 10,000 inhabitants, which receive water from two reservoirs. The WDN consists of pipes with
327 diameters ranging from 63 mm to 225 mm and a total pipe length of 43 km. *L-Town* consists of
328 three distinct hydraulic areas: (i) Area A is the main part of the network, (ii) Area B is a low lying
329 part that is supplied through a pressure reduction valve, and (iii) Area C is an area with higher
330 elevation that is supplied by an elevated tank fed from Area A through a pumping station. An
331 overview of the network and the location of the three measurement zones can be found in Figure 2.

332 To enhance the water loss monitoring capabilities, the WU of *L-Town* installed three flow meters
333 (two at the reservoirs and one at the pumping station), a tank level sensor and 33 pressure sensors
334 (depicted as circles in Figure 2). All sensors measure and transmit data every 5 minutes to the
335 utility's supervisory control and data acquisition (SCADA) system. Additionally, the WU installed
336 82 smart water meters or AMRs in Area C, measuring three different customer types: residential,

337 commercial and industrial. There is no flow meter installed at the tank that feeds Area C. Therefore,
338 a virtual inflow measurement to Area C has to be reconstructed from the tank level measurements
339 and the inflow measurement measured at the pump that supplies the tank.

340 The dataset of the BattLeDIM contains two years of sensor data for years 2018 (historical
341 dataset) and 2019 (validation dataset), an EPANET model of the water distribution network, plus
342 the time and repair location of ten pipe bursts that have been fixed in 2018. Three types of leaks
343 exist: (i) small background leaks with 1 % - 5% of the average inflow, (ii) medium pipe breaks with
344 5 % - 10%, and (iii) large pipe bursts with leakage flows of more than 10 % of the average system
345 inflow ($\approx 180 \text{ m}^3/h$). Large leakages with outflows over $15 \text{ m}^3/h$ are fixed by the water utility after
346 a reasonable amount of time within two months. The leakages have two different time profiles, (i)
347 either abrupt pipe bursts with constant leak flow rates, (ii) or background leakages with growing
348 leak rates which evolve over time until large outflow rates at which they remain constant. In total,
349 14 leakages occurred in 2018 with outflow rates between 5 to $35 \text{ m}^3/h$, of which 10 leaks have
350 been repaired. The remaining 4 leaks are not repaired and continue into the 2019 validation dataset.
351 The BattLeDIM challenge is to find the 19 leaks that happened in 2019 plus the 4 remaining leaks.
352 The outflows and locations of the 33 leaks can be found in Figures 7 to 10 (dashed lines in the
353 outflow time series plots and circles in the location overview plots). More details on the dataset
354 can be found in (Vrachimis et al. 2020).

355 **RESULTS AND DISCUSSION**

356 **Demand calibration**

357 Each AMR time series is decomposed into its trend, seasonal (with a period length of a
358 week), and random components using the multiplicative time series model described in Eq. (1).
359 Subsequently, cluster analysis is used to identify similarities in the trend and seasonal patterns. Two
360 distinct demand patterns emerge in the trend $T(t)$ and in the seasonal components $S(t)$, a residential
361 ($T_R(t), S_R(t)$) and a commercial ($T_C(t), S_C(t)$) one. The seasonal and the trend components are
362 shown in Figure 3 for each AMR measurement. Furthermore, some patterns are found to be a
363 superposition of both pattern types. These patterns belong to houses with mixed user groups (e.g.

364 commercial space in the ground floor and apartments in the floors above). Subsequently, these
365 patterns are called *mixed* patterns. Generally, all demand patterns can be described through the
366 superposition (see Eq.(2)) of the residential and the commercial pattern. During workdays (Monday
367 to Friday), water consumption follows a similar behavior, whereas during the weekend (Saturday
368 and Sunday) higher consumption during late hours occur as the result of night life (see Figure 3
369 (a)). Furthermore, cluster analysis revealed four outlier pattern in the AMR measurements. After
370 closer examination, these outlier patterns were explained as industrial users with a periodicity
371 differing from a week (*i.e.* 9, 11 or 13 days). Hence, those industrial users do not follow the same
372 pattern of consumption as described in Eq. (2) and are not further used in the demand modeling.
373 The trend components in Figure 3 (b) show higher water usage during July/August, and lower in
374 December/January.

375 The demand model is used to model the unmeasured customers within the L-town network.
376 Additionally, a virtual inflow measurement of Area C has been constructed from the pump flow
377 measurements and the tank's water level. This virtual inflow is used to (i) validate the demand
378 model and to (ii) estimate the leak outflow in Area C. Figure 4 (a) shows the estimated leakage
379 outflow, which is constructed as the difference between the virtual inflow measurement and the
380 total estimated demand for Area C. Three different strategies for the demand estimation are used
381 in Area C. First, only the measured demand at the AMRs is subtracted (*just AMR* in Figure 4 (a)),
382 which leads to an overestimation or an offset of the leak flow, because of the unmeasured customers.
383 Second, the demand for the whole zone is estimated based on the model as described in Eq. 2 using
384 the base demands from the BattLeDIM EPANET model (*Inferred*), which leads to a high noise in
385 the leak outflow estimates. Third, the AMR measurements are combined with demand estimates for
386 the unmeasured customers (*Combined*). The last approach leads to the best leak outflow estimates
387 with low levels of noise as well as no offset. Clearly, four different leaks can be seen in the data,
388 three are growing over time until they are saturated (Leak 1, 2, and 4), and a sudden pipe burst
389 (Leak 3). This information proved to be useful for the leakage modeling (see Eq. (16) and (17)).

Roughness calibration

The internal diameters of pipes are nominal diameters defined by a discrete number of values that depend on the manufacturer and the material. In the L-Town INP file, it is assumed that the outside diameters of plastic pipes are entered instead of the inside diameters, which is first corrected with the most usual inside diameter for PVC and PE pipes (see Table 1).

After inspection and several tests, the pipes are divided in six different roughness clusters according to their diameter, material, initial roughness values and managing zones in which they are located : Because of the small number of observations and pipes, one cluster with $C_{HW} = x_5$ is assigned for Zone B and one to Zone C (x_6). Cluster with same x_1 roughness value consists of the plastic pipes in Zone A; pipes in cluster 2 are in Zone A with diameters 100 mm or 150 mm, and original INP roughness $x_2 = 120$. Similarly, pipes in zone A with diameters 100 mm or 150 mm and original $C_{HW} = 140$ define the cluster 3: $x_3 = 140$. Finally, cluster 4 is made of pipes with internal diameter 200 mm in Zone A. Figure 2 shows an overview of the roughness groups. Through visual inspection of the measurements from the first week of 2018, it is assumed that no leaks are present in the dataset during that time. Consequently, measurements for this week are used for the roughness calibration. The roughness calibration is performed for the six clusters, $n_c = 6$, and by solving the WLS problem in Eq. (5) with $\kappa = 3$, $\alpha = 0$ and box constraints $x^L = 60$ and $x^U = 160$ with the Levenberg-Marquardt method (10). The $n_s = 33$ pressure measurements in Figure 2 are used ($n_m = 33$). They repeat every five minutes for 7 days ($n_t = 2016$). All measurements are chosen to be of the same accuracy $\sigma_{ij} = 1$.

The algorithm converges after 11 iterations. The results are given in terms of estimates in Table 2. For the first cluster, plastic pipes in Zone A, the initial estimate $x_1^0 = 146$ belongs to the 99% confidence interval [141.9, 163.7]. Consequently, the final estimate 152.8 is not significantly different from the initial value. However, the initial estimates for the other five clusters differ significantly from the point estimates at iteration $k = 11$ (they do not belong to the five 99% confidence intervals). Based on the confidence intervals and the initial estimates, the bold values are selected. The pressure residuals are represented in Figure 2. It can be seen that the mean

417 squared error (MSE) is about 6 cm H₂O.

418 **Virtual leak flows with the dual model**

419 A dual model is constructed from the EPANET model containing the calibrated pipe roughnesses
420 and demand patterns from the demand calibration. The heads of the virtual reservoirs are set to
421 the corresponding pressure measurements. If leaks appear in the network, the dual model reacts
422 with virtual leak outflows caused by the pressure differences of the hydraulic model and the lower
423 reservoir heads. The virtual leak flows for each sensor location within Area C are depicted in
424 Figure 4 (b). Furthermore, the total sum of all virtual leak flows is shown. This sum gives a good
425 first approximation of the leak size. The second leak in Area C was repaired and, hence, its end
426 time and its location (pipe p31) are known. The leak is closest to sensor node n31, which shows
427 the strongest reaction to the leak by producing the biggest virtual outflow. Same reasoning leads
428 to the conclusion that Leak 1 is close to sensor n1, Leak 3 is in proximity of n31, and Leak 4 is
429 somewhere in the middle of all three sensors.

430 Comparison of Figure 4 (a) with the total virtual leak outflow in (b) shows that the real leakage
431 outflows have similar magnitudes as the virtual outflows. However, the dual model seems to
432 underestimate the real outflows in Area C slightly.

433 Figure 5 shows an comparison of the effect of leakages on the measured pressure signals versus
434 the virtual leak flows in the dual model for the first two leakages in 2019 that appear in Area A
435 (pipe p523 and p810). In this Figure, solid lines are four hour moving averages, whereas the shaded
436 lines are the original five minutes signal. The dual model amplifies the leak signal compared to
437 the pressures (compare Figure 5 (a) and (b)). Furthermore, the leaks have a more local effect on
438 the virtual leak flows than in the pressures, which allows already a rough estimation of the leak's
439 location. The sum of all virtual leak outflows in Figure 5 (c) gives already a good estimate of the
440 leak sizes, which are approximately $27 \text{ m}^3/h$ for each leak.

441 **Leak Detection**

442 Two different signals are used for leak detection; (i) the flow residual between the measured
443 inflow and total demand plus already known leaks in an area, (ii) the dual model's outflows to the

444 virtual reservoirs (see Figure 4 or Figure 5). Two different types of leaks are found in the data –
445 instant bursts and leaks that are growing over time. Growing leakage flows are modeled with the
446 quadratic function in Eq. (17). Data from the dual model is used to identify the leak start times
447 and their shapes (*i.e.* instant or growing). For that reason, thresholds are extracted from the DA
448 flows at each sensor using the leak free case in the first week of 2018. If the DA signal exceeds the
449 threshold, a leak is detected in the system. The detection time is used as the start time of the leak
450 for our BattLeDIM solution. To estimate the leakage outflow, the start times and the shapes of the
451 leaks are used to fit the leak shape on the flow residuals. If a single leak evolves over time, Bayesian
452 inference is used, for multiple simultaneously appearing leaks, a faster differential evolution is used
453 to identify the best combination of leak outflows over time. The detected leaks are double checked
454 against the DA and subsequently used for the leak localization.

455 The results for leak detection and localization for 2019 are summarized in Table 3. Additionally,
456 the leak detection and localization results are broken down by the different areas are shown in
457 Figures 7 to 10, where shaded lines are daily moving averages of the real leakages, solid dashed
458 lines are the estimated leakages. Circles in the network maps are the real leak locations, while
459 crosses show our estimates. The leak detection results for Area C are shown in Figure 7 (a). The
460 shapes of the leaks are resembled very well by our method for all three leaks, and the differences in
461 the final leak outflows are negligible for Area C. The sudden pipe burst (Leak C3 at pipe p280) is
462 detected instantaneously, while the detection of the growing leaks takes a bit longer. Nevertheless,
463 leakages are detected on average within less than 9 days. A less conservative detection threshold
464 potentially decreases the detection time.

465 The leak detection results for Area B are shown in Figure 8 (a), where the instant pipe burst is
466 perfectly detected, although the leakage outflow is slightly overestimated.

467 The leak detection results for Area A are shown in Figure 9. For a better visibility of the
468 simultaneously appearing leaks, the Figure is split into the two half-years of 2019, with (a) for the
469 first half until July, and (b) showing the second half of the year. Additionally, the leaks from the first
470 half are depicted as gray shaded lines in Figure 9 (b) as they are still present in the network. Sudden

471 pipe bursts are again detected instantaneously, while the thresholds for growing leaks seemed a bit
472 too conservative. However, the shapes of all leaks are very well described through the coefficients
473 that our model found. One leak that started in February 2018 at pipe p427 with a magnitude of
474 $5m^3/h$ is not detected at all. All leak shapes are identified correctly until August, when Leak A17
475 at pipe p721 appears (see Figure 9 (b)). However, this leak is detected very late and its size is
476 underestimated by almost $5 m^3/h$. This influences the detection of subsequent leaks, which results
477 in a decrease in the detection as well as the localization performance. Nevertheless, leakages in
478 Zone A were detected within 10 days on average.

479 **Leak Localization**

480 For the localization of the leaks the network is divided into two separate parts (A+B and C) and
481 the pump is replaced by the flow measurement for Zone A and B. All calculations are executed by
482 use of EPANET 2.00.12 (Rossman 2000) and the EPANET toolkit integrated in an application for
483 data management and visualization that is exclusively developed for the performance of the project.

484 Figure 6 visualizes the GUI-output at a certain time step. The circles indicate the locations of the
485 pressure measurement nodes and the numbers show the calculated in- and outflows calculated by the
486 dual model. The two biggest virtual reservoirs outflows are marked by a bigger circle as expected
487 in the neighborhood of these two nodes. The diamonds show the nodes with highest correlation
488 scores at the current time and the bigger diamonds show the nodes with highest correlation sum.
489 Their size is scaled by the sum value which means that they are growing over time.

490 Figure 7 (b) shows the localization results for Area C. Leak C1 is perfectly isolated at the real
491 location (p257). Leak C3 is found within 50 m of the real leak. However, if the closed valve in Area
492 C is added to the hydraulic model, the isolation of this leak might improve further. Leak C4 is not
493 localized correctly, since the distance exceeds 300 m as stated in the BattLeDIM rules. Reasons for
494 that might be that the closed valve is not taken into account, or the fact that we are using demand
495 driven models, while the BattLeDIM organizers used a pressure-driven model. The more leakages
496 occur in the network, the greater the difference between a demand-driven and a pressure-driven
497 demand model become, and the more inexact our localization gets, since the localization errors

498 accumulate. On average, all leaks are found within 130 m of the real leak in Area C. For Area B,
499 the leak is perfectly isolated in time as well as in space (see Figure 8).

500 The results for Area A can be found in Figure 10, and are split again into half-years. Figure 10
501 (a) also contains the leak that was not detected by our method (white cross). Early leaks are
502 isolated almost perfectly, while the localization gets worse during later simulations. This might be
503 a consequence of the demand-driven model that is used. For the leaks in Figure 10 (a), the average
504 distance of the real leaks to the estimated leak position is around 150 m. During later simulations,
505 this distance increases to 250 m (see Figure 10 (b) and Table 3). It has to be noted that a typo
506 occurred while submitting the results for the BattLeDIM. Leak p654 was inserted as p645. Taken
507 this into account, the final score of the Team *Under Pressure* would even further increase from
508 already the highest rate of true positives of 65% of all participating teams.

509 **CONCLUSION**

510 In this work, we present a novel solution to detect and isolate multiple-leaks in WDN that we
511 developed while participating in the BattLeDIM competition. Our method consists of calibrating
512 the nodal demand and pipe roughness, and introducing a dual model for the calibrated primal
513 problem to detect and locate leaks.

514 The calibration uses time series analysis and cluster analysis to build a multiplicative predictive
515 model for ultimately two network-wide demand models, a residential and a commercial model.
516 This is used for both, (i) modeling unknown demands over time in the hydraulic model, as well
517 as distinguishing leakages and consumption in the measurements. Subsequently, six roughness
518 clusters were calibrated using 33 pressure loggers for the first week of 2018. Confidence intervals
519 are given for the least-squares estimates. The pressure residuals are very well reproduced for the
520 entire week with a small root mean square error of 6 cm.

521 The core of our method is a dual model that transforms a pressure measurement node into a
522 free junction node plus a link to a virtual reservoir, whose head is equal to the measured values.
523 Significant inflows or outflows, either sudden or gradual, to these virtual reservoirs are indications
524 of leaks. In the dual model, the pressure signal is transformed into a virtual leakage outflow

525 signal that is easier to analyze since it amplifies and localizes the effects of leaks in the network.
526 Sensitivities of nodal pressures to virtual outflows are also derived. They are essential to understand
527 the behavior of the model at first order.

528 For leak detection, the CUSUM algorithm and likelihood-ratio tests are used jointly on the
529 virtual leak flows, where the parameters are tuned to limit the global false positive rate under
530 normal operation conditions. When multiple leaks are present, differential evolution is used to
531 identify the best combination of leak modeling parameters over time (*i.e.* start times and shapes
532 of leaks over time). These detection methods were employed for both, the primal and the dual
533 data. The localization is achieved by analyzing the correlation between the calibrated pressure (or
534 virtual inlet-outlet model predictions) and the corresponding first-order leakage impulse response
535 predictions at the candidate nodes. This solution recovered 65% of true leaks with only four false
536 positives in all of 2019, which is a notable result (shared #1 ranking).

537 Using a pressure-driven model instead of a demand-driven one, improving the calibration by
538 reliably detecting closed valves, as well as using less conservative threshold parameters for the
539 detection of the growing leaks might increase the already notable result further. Certainly, a lot
540 of potential lies in a deeper understanding of the dual model to further improve the detection and
541 isolation of multiple simultaneously occurring leaks.

542 With 33 pressure sensors, the BattLeDIM dataset contains an unrealistic high number of
543 sensors in a WDN of that size. Indeed, the leak detection and localization performance will
544 decrease with a lower number of sensors. However, optimal sensor placement algorithms might
545 recover similar leak detection and localization performances with fewer sensors. Furthermore,
546 the BattLeDIM organizers constructed the nodal demand patterns through a superposition of
547 residential and commercial demands multiplied with noise. That is why we were able to almost
548 precisely reconstruct the demands on the unmeasured locations through the information contained
549 in the AMR data with our demand calibration approach. In reality, demand patterns are more
550 variable (Steffelbauer et al. 2021). Consequently, the dual model might perform worse in systems
551 with limited demand information and, hence, less accurate demand models.

552 That is why for future work, we want to focus on optimal sensor placement (Steffelbauer and
553 Fuchs-Hanusch 2016a) with the dual model and on applying the dual model on challenging real
554 data sets, with model errors, outliers, uncertainty, and more variable and realistic water demands.
555 Furthermore, we are planning to investigate the importance of each step for the final classification,
556 enhancing the method to reduce the false positive rate, and study the effect of the dual model on
557 fitness landscapes of WDN optimization problems (Steffelbauer and Fuchs-Hanusch 2016b).

558 **DATA AVAILABILITY STATEMENT**

559 All data, models, or code that support the findings of this study are available from the corre-
560 sponding author upon reasonable request.

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568 **APPENDIX**

569 **AMR** automatic meter reading

570 **BattLeDIM** *Battle of the Leak Detection and Isolation Methods*

571 **CUSUM** cumulative sum control chart

572 **DA** Dual Approach

573 **DMA** district metered area

574 **HW** Hazen-Williams

575 **MSE** mean squared error

576 **SCADA** supervisory control and data acquisition

577 **TSA** time series analysis

578 **WLS** weighted least squares

579 **WDN** water distribution network

580 **WU** water utility

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List of Tables

- 1 Original pipe characteristics in the INP file and corresponding cluster membership; in red the original external parameters that were corrected for PVC and PE pipes. 30
- 2 Calibration of HW coefficients; the first three columns are the lower bound, initial estimate, and upper bound values for the six clusters; the last three columns are the 99% confidence intervals centered on the value at convergence; in bold the final point estimate. 31
- 3 Results of leak detection and localization: The true location, the start time and the maximum leakage outflow $\max(Q_L)$ are taken from the BattLeDIM solutions. The estimated location is found with the leak localization algorithm. t_D is the detection time measured in hours since the true start time of the leak. The distance between the true and the estimated leak location is the shortest topological distance over the pipes in meter. Zone shows in which area of the network the leak is located. Perfectly located leaks are shown in boldface (plus minus 10 m), while leaks with a distance greater than 300 m (missed leaks according to the BattLeDIM rules) are highlighted with an asterisk. 32

TABLE 1. Original pipe characteristics in the INP file and corresponding cluster membership; in red the original external parameters that were corrected for PVC and PE pipes.

Diameter in mm	C_{HW}	Zone	Cluster # in Eq. (3)	# pipes	Length in m
53.6 (63)	146	A	1	3	71.40
53.6 (63)	146	B	5	1	9.21
64 (75)	146	A	1	1	60.08
100	120	A	2	76	3639.10
100	120	B	5	25	1190.11
100	140	A	3	500	24069.65
100	140	C	6	104	5201.60
150	120	A	2	7	313.62
150	140	A	3	90	4102.87
150	120	B	5	6	226.56
141 (160)	146	A	1	16	713.73
200	90	A	4	59	2749.71
200	90	C	6	5	195.90
198.2 (225)	146	A	1	12	558.58

TABLE 2. Calibration of HW coefficients; the first three columns are the lower bound, initial estimate, and upper bound values for the six clusters; the last three columns are the 99% confidence intervals centered on the value at convergence; in bold the final point estimate.

Cluster #	\mathbf{x}^L	\mathbf{x}^0	\mathbf{x}^U	$\mathbf{x}^{11} - \Delta_x$	\mathbf{x}^{11}	$\mathbf{x}^{11} + \Delta_x$
1	60	146	160	141.9	152.8	163.7
2	60	120	160	108.1	109.7	111.3
3	60	140	160	141.1	141.6	142.1
4	60	90	160	126.5	126.8	127.1
5	60	136	160	100.4	111.2	122.0
6	60	133	160	133.1	134.0	134.9

TABLE 3. Results of leak detection and localization: The true location, the start time and the maximum leakage outflow $\max(Q_L)$ are taken from the BattLeDIM solutions. The estimated location is found with the leak localization algorithm. t_D is the detection time measured in hours since the true start time of the leak. The distance between the true and the estimated leak location is the shortest topological distance over the pipes in meter. Zone shows in which area of the network the leak is located. Perfectly located leaks are shown in boldface (plus minus 10 m), while leaks with a distance greater than 300 m (missed leaks according to the BattLeDIM rules) are highlighted with an asterisk.

True Loc.	start time	$\max(Q_L)$ (m^3/h)	Est. Loc.	t_D (h)	Distance (m)	Zone
-	-		-			-
p427	2018-02-13 08:25	5.11	-	-	-	A
p654	2018-07-05 03:40	5.49	p654	956.33	0	A
p810	2018-07-28 03:05	6.91	p810	668.92	0	A
p523	2019-01-15 23:00	28.39	p500	0.00	205	A
p827	2019-01-24 18:30	26.46	p827	-0.08	0	A
p653	2019-03-03 13:10	18.28	p655	273.42	106	A
p710	2019-03-24 14:15	5.58	p702	0.00	222	A
p514	2019-04-02 20:40	15.58	p226	0.00	90	A
p331 ^(*)	2019-04-20 10:10	10.93	p905	0.00	355	A
p193 ^(*)	2019-05-19 10:40	10.36	p185	417.33	398	A
p142	2019-06-12 19:55	27.04	p623	0.00	2	A
p586	2019-07-26 14:40	20.52	p586	215.50	0	A
p721 ^(*)	2019-08-02 03:00	13.18	p703	222.92	354	A
p800	2019-08-16 14:00	21.95	p820	110.50	196	A
p123	2019-09-13 20:05	9.19	p201	588.33	133	A
p455	2019-10-03 14:00	11.05	p109	584.92	142	A
p762	2019-10-09 10:15	15.71	p745	301.00	179	A
p426 ^(*)	2019-10-25 13:25	13.56	p42	0.00	779	A
p879	2019-11-20 11:55	10.93	p884	342.50	256	A
p680	2019-07-10 08:45	5.37	p680	0.00	0	B
p257	2018-01-08 13:30	6.87	p257	104.50	0	C
p280	2019-02-10 13:05	5.26	p251	0.00	49	C
p277 ^(*)	2019-05-30 21:55	7.36	p8	541.83	358	C

682 **List of Figures**

683 1 Overview of the hierarchical leak detection and isolation approach from left to
684 right: Starting with the *data* analysis (measurements and EPANET model), then
685 model *calibration* (nodal demand and pipe roughness), followed by *simulations*
686 with the dual model approach, to finally detect and localize *leaks*. 35

687 2 Network colored by calibration clusters of Hazen-Williams roughness coefficients.
688 Pressure measurements are shown as circles. In a) the roughness iterations are
689 plotted ; in b), the inset shows the principle of the dual model, where the pressure
690 measurements are replaced by the combination of a valve and a virtual reservoir
691 whose head is equal to the measured head h_i ; the dual model transforms h_i into
692 virtual leakage flows q_{v_i} ; in (c) the pressure residuals are shown for the first week
693 of 2018; and finally, in (d) the minimum, maximum, and root mean square errors
694 (RMSE) are shown in increasing RMSE order. 36

695 3 Weekly seasonality (a) and yearly trend (b) extracted from the AMR measurements
696 for the different customer types (Residential and Commercial) and nodes consisting
697 of a mix of them (Mixed). 37

698 4 Leakage outflow in Area C (a) estimated by comparing the “virtual” inflow mea-
699 surement and the demand model and (b) as provided by the dual model. 38

700 5 Dual model signals for first two leaks in Area A in 2019 (location at pipes p827 and
701 p523 with magnitudes of approximately $27 \text{ m}^3/h$ each). (a) Pressure measurements
702 p over time, (b) sharp and localized signal of the virtual leak outflows q_v over time
703 calculated by the dual model at the same measurement locations, (c) the sum over
704 all virtual leak flows in the dual model serves as good estimates for leak size. . . . 39

705 6 Snapshot of the leakage isolation tool: calculated outflows at virtual reservoirs of
706 sensor nodes and correlation results: small diamonds for current time step and large
707 diamonds for sum of all time steps (the size represents the score). 40

708	7	Results of leak detection and localization for the unknown leaks in Area C in 2019:	
709		(a) Identified leakage outflows over time and (b) estimated locations of the leaks.	
710		Crosses are the estimated leak locations, circles indicate the real locations.	41
711	8	Results of leak detection and localization for the unknown leaks in Area B in 2019:	
712		(a) Identified leakage outflows over time; and (b) estimated locations of the leaks.	
713		The Cross is the estimated leak location, the circle indicates the real location.	42
714	9	Results of leak detection for the unknown leaks in Area A in 2019: (a) Leakage	
715		outflows for the first half of the year / leaks, and (b) for the second half of the year	
716		/ leaks. The second half also includes the ongoing leaks from (a) as shaded lines.	
717		Additionally, the missed detected leak at pipe p427 is shown in (a).	43
718	10	Results of leak localization for the unknown leaks in Area A in 2019: (a) First half	
719		of the year from January to June, and (b) for the second half of the year from July	
720		to December. The not detected leak at pipe 427 is shown as a white cross in (a).	
721		Crosses are the estimated leak locations, circles indicate the real locations.	44

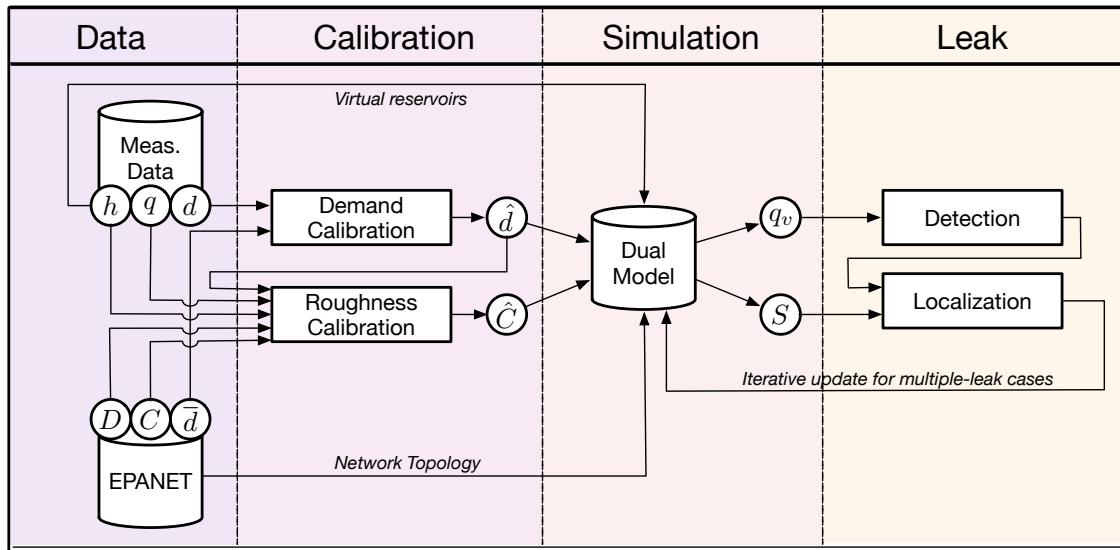


Fig. 1. Overview of the hierarchical leak detection and isolation approach from left to right: Starting with the *data* analysis (measurements and EPANET model), then model *calibration* (nodal demand and pipe roughness), followed by *simulations* with the dual model approach, to finally detect and localize *leaks*.

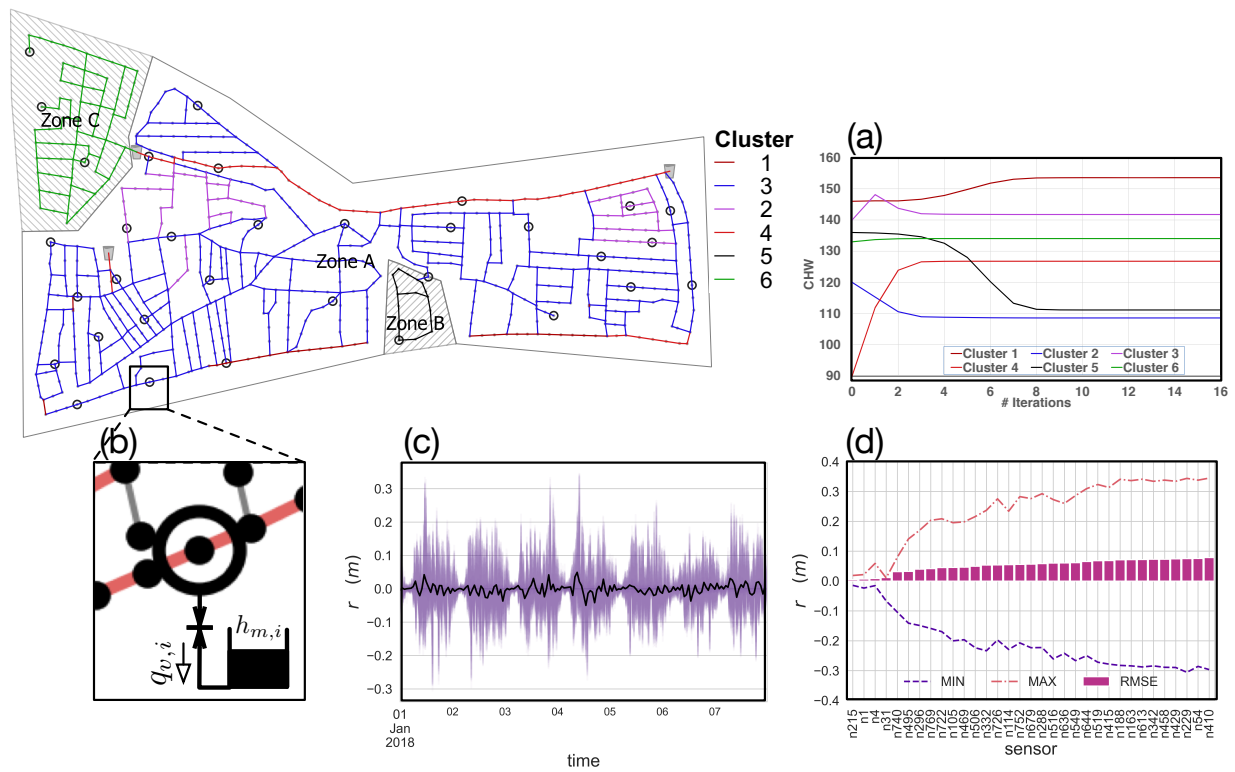


Fig. 2. Network colored by calibration clusters of Hazen-Williams roughness coefficients. Pressure measurements are shown as circles. In a) the roughness iterations are plotted ; in b), the inset shows the principle of the dual model, where the pressure measurements are replaced by the combination of a valve and a virtual reservoir whose head is equal to the measured head h_i ; the dual model transforms h_i into virtual leakage flows q_{v_i} ; in (c) the pressure residuals are shown for the first week of 2018; and finally, in (d) the minimum, maximum, and root mean square errors (RMSE) are shown in increasing RMSE order.

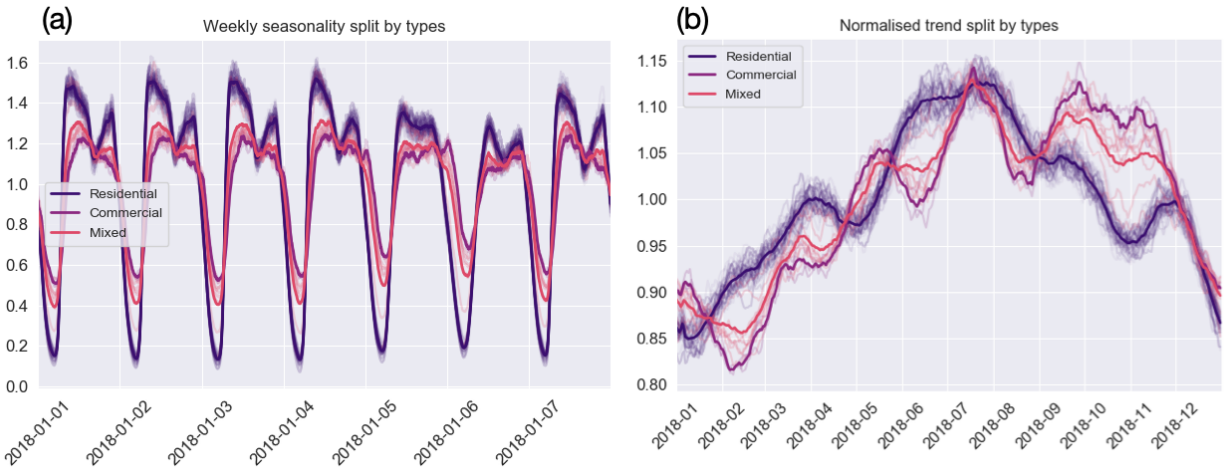


Fig. 3. Weekly seasonality (a) and yearly trend (b) extracted from the AMR measurements for the different customer types (Residential and Commercial) and nodes consisting of a mix of them (Mixed).

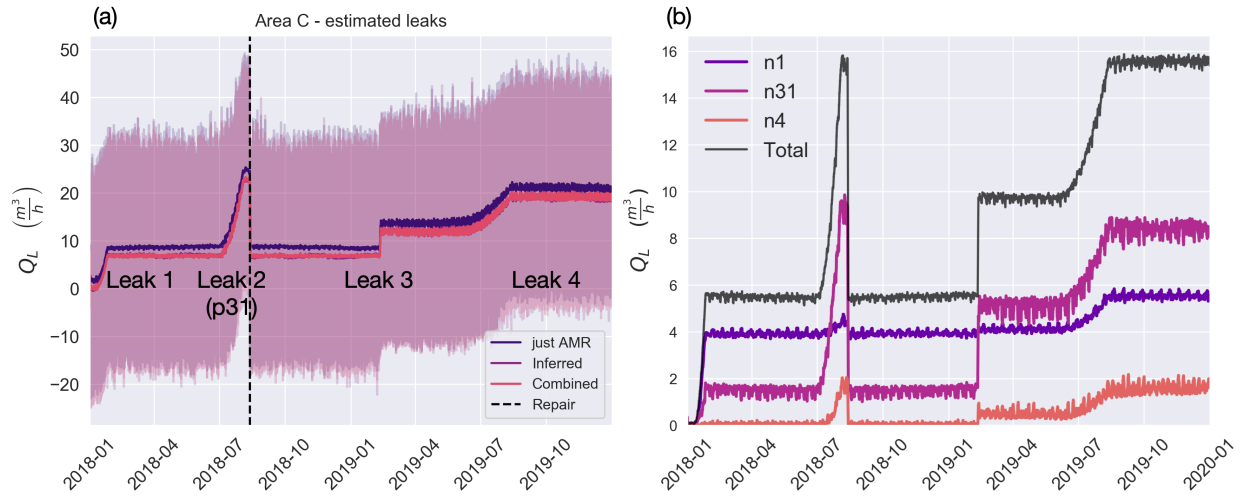


Fig. 4. Leakage outflow in Area C (a) estimated by comparing the “virtual” inflow measurement and the demand model and (b) as provided by the dual model.

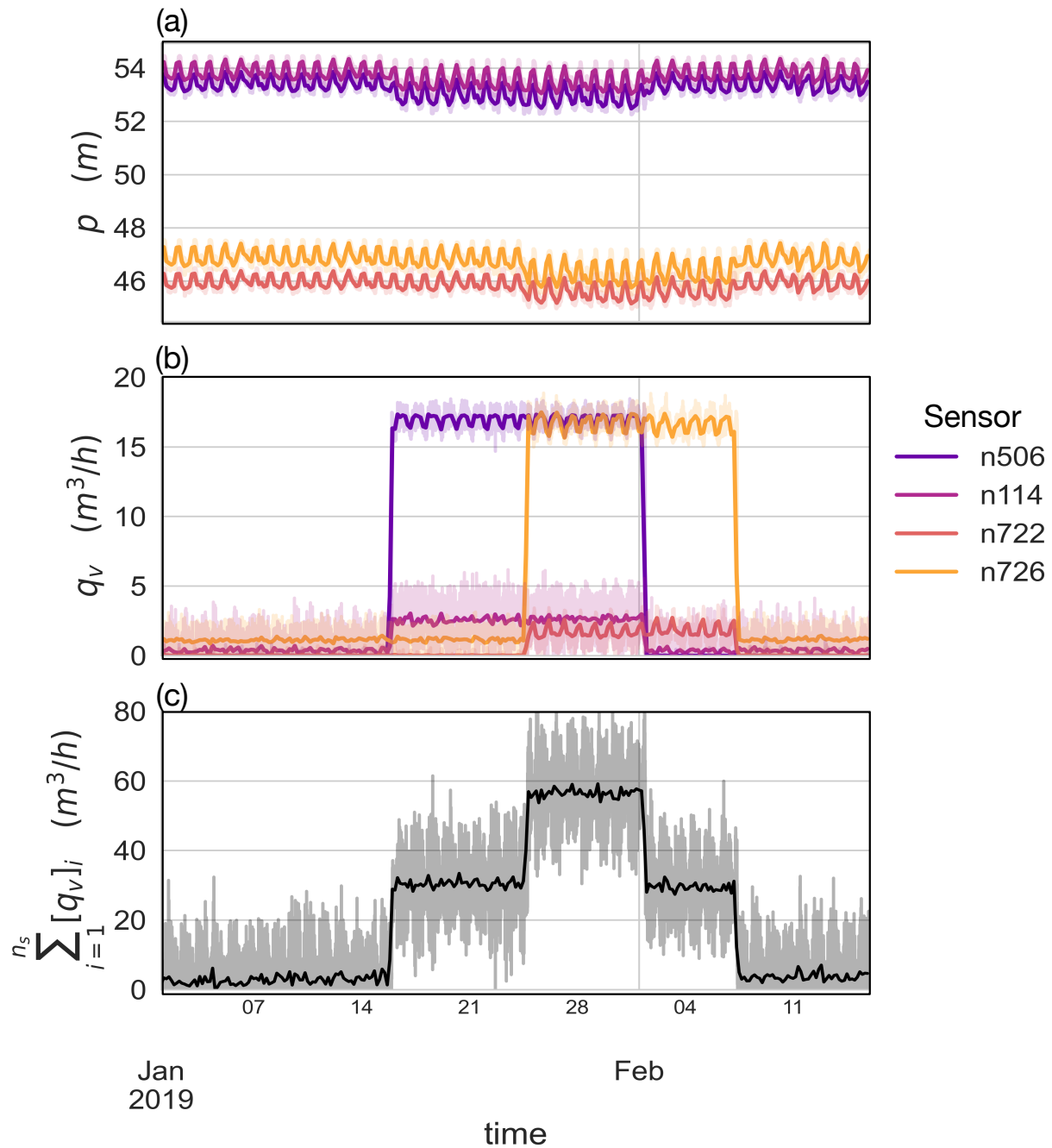


Fig. 5. Dual model signals for first two leaks in Area A in 2019 (location at pipes p827 and p523 with magnitudes of approximately $27 m^3/h$ each). (a) Pressure measurements p over time, (b) sharp and localized signal of the virtual leak outflows q_v over time calculated by the dual model at the same measurement locations, (c) the sum over all virtual leak flows in the dual model serves as good estimates for leak size.

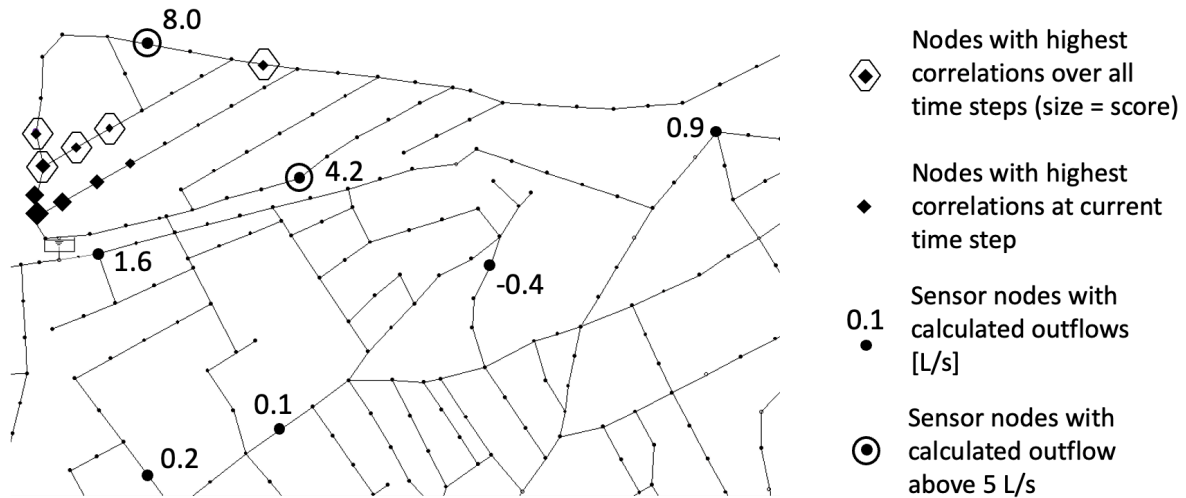


Fig. 6. Snapshot of the leakage isolation tool: calculated outflows at virtual reservoirs of sensor nodes and correlation results: small diamonds for current time step and large diamonds for sum of all time steps (the size represents the score).

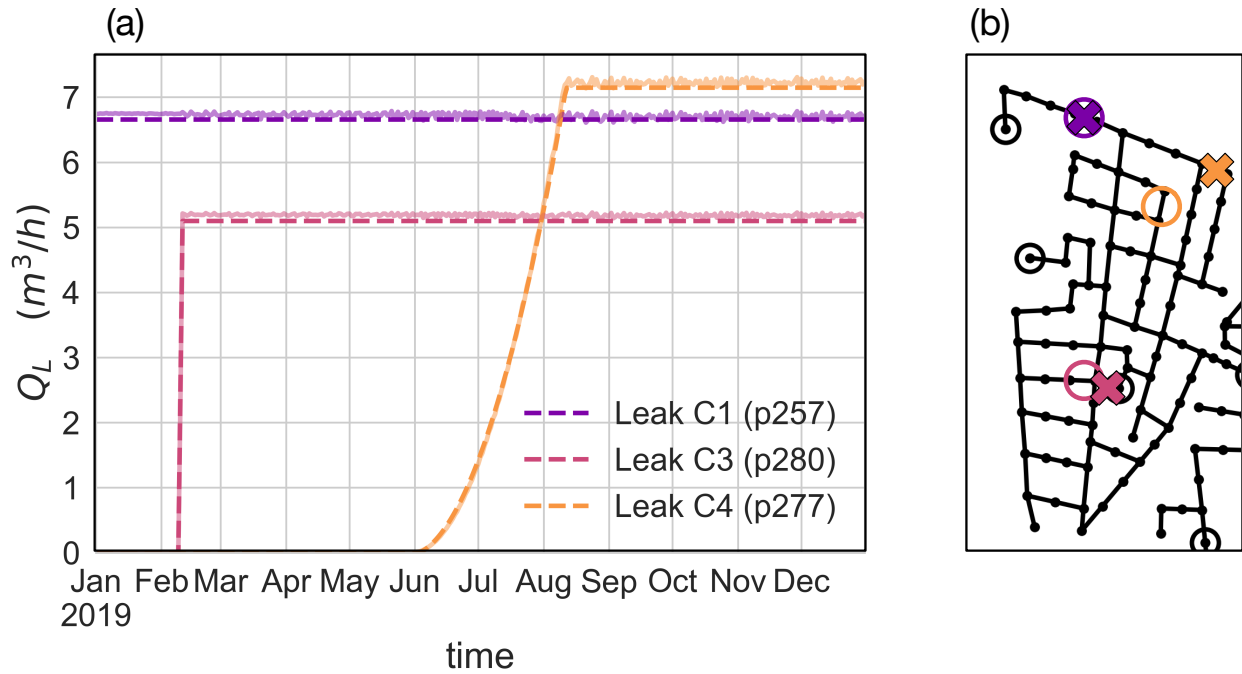


Fig. 7. Results of leak detection and localization for the unknown leaks in Area C in 2019: (a) Identified leakage outflows over time and (b) estimated locations of the leaks. Crosses are the estimated leak locations, circles indicate the real locations.

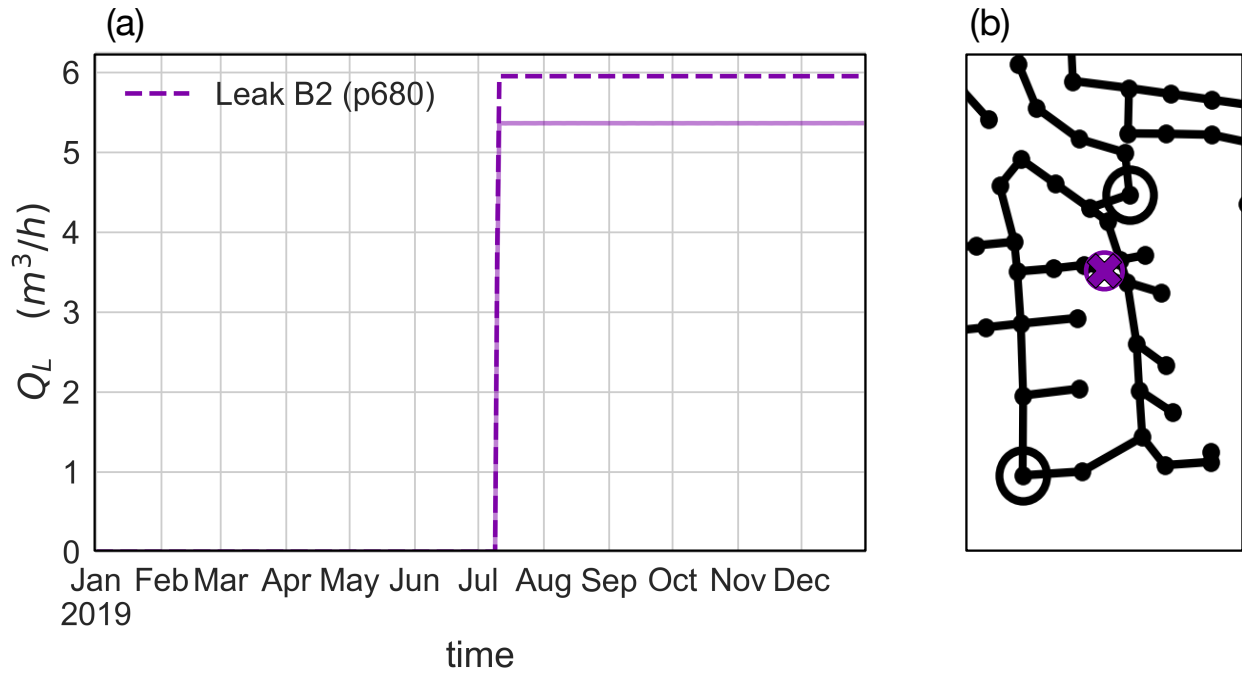


Fig. 8. Results of leak detection and localization for the unknown leaks in Area B in 2019: (a) Identified leakage outflows over time; and (b) estimated locations of the leaks. The Cross is the estimated leak location, the circle indicates the real location.

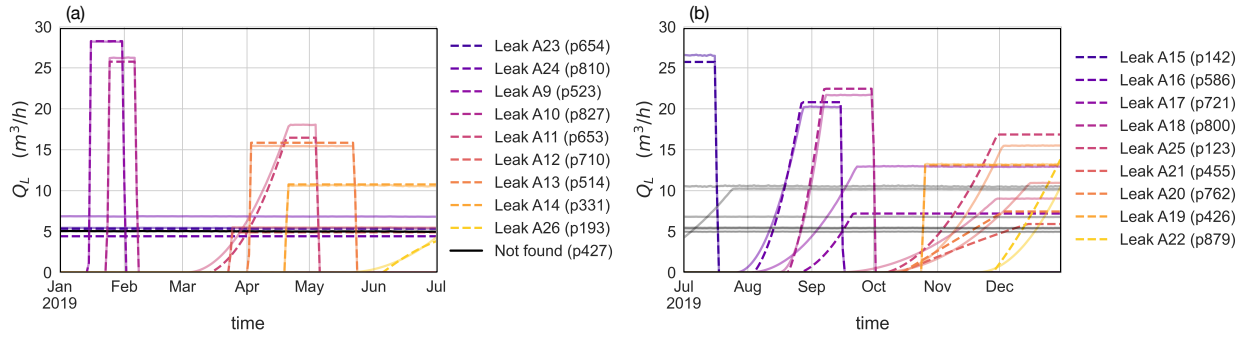


Fig. 9. Results of leak detection for the unknown leaks in Area A in 2019: (a) Leakage outflows for the first half of the year / leaks, and (b) for the second half of the year / leaks. The second half also includes the ongoing leaks from (a) as shaded lines. Additionally, the missed detected leak at pipe p427 is shown in (a).

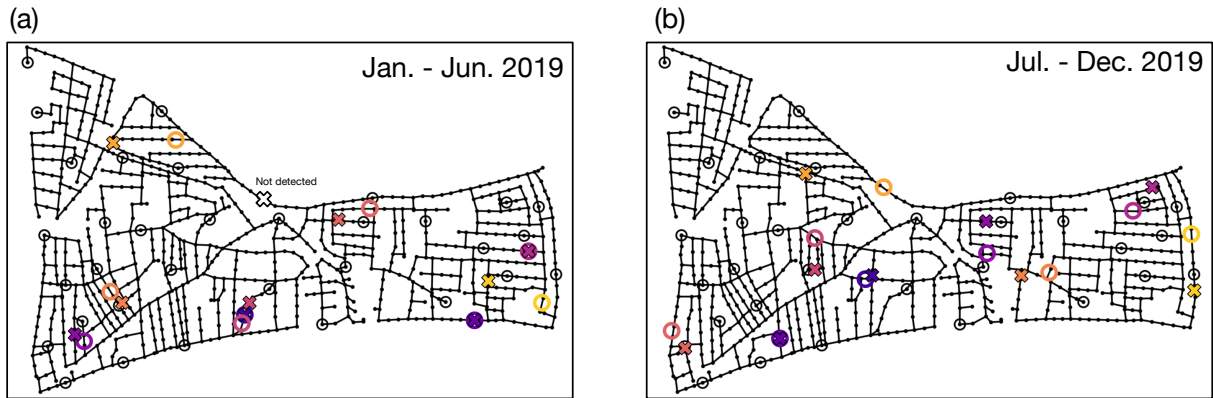


Fig. 10. Results of leak localization for the unknown leaks in Area A in 2019: (a) First half of the year from January to June, and (b) for the second half of the year from July to December. The not detected leak at pipe 427 is shown as a white cross in (a). Crosses are the estimated leak locations, circles indicate the real locations.