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Particle Filter-Based Model for Online Estimation of Demand Multipliers in Water Distribution Systems under Uncertainty

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25 integrating online observation data. The standard particle filter and an improved particle filter
26 method, which incorporates the evolutionary scheme from genetic algorithms into the resampling
27 process to prevent particle degeneracy, impoverishment and convergence problems, are
28 investigated to implement the predictor-corrector approach. Uncertainties of model outputs are
29 also quantified and evaluated in terms of confidence intervals. Two case studies are presented to
30 demonstrate the effectiveness of the proposed particle filter model. Results show that the model
31 can provide a reliable estimate of demand multipliers in near real-time contexts.

32

33 *Keywords: Particle filters, sequential Monte Carlo method, real-time demand estimation, water*
34 *distribution systems, uncertainty.*

35 **Introduction**

36 Water distribution systems (WDS) are constructed to supply water for domestic, industrial and
37 commercial consumers. The design, operation and management of these distribution systems is
38 usually supported by the application of hydraulic models, which are built to replicate the behavior
39 of real systems. These conventional models simulate flows and pressures of a WDS either under
40 steady state conditions (constant demands and operational conditions) or under a short term
41 extended period simulation (time-varying demands and operational conditions), for example a day
42 or a week (USEPA 2005). The outputs from hydraulic models, therefore, usually represent the
43 distribution system behavior during the sampling period (Preis et al. 2009). This leads to an
44 inadequate understanding of the full range of operational states in the water system.

45 The installation of sensor devices as well as the Supervisory Control and Data Acquisition
46 (SCADA) systems within the WDS can provide information on the status of some components in
47 the system. However, the use of this additional data is currently limited to computing gross

48 differences between the model outputs and reality (Kang & Lansey 2009). Modification of the
49 hydraulic models to maintain the consistency between observed data and simulated data is still a
50 challenge that needs to be dealt with. Estimation of the model states/parameters, hence, is required
51 so that the model is able to represent the real system.

52 Estimation is the process of fitting the outputs from the computer model, usually the pressures and
53 flow rates at particular locations in the water network, with the field measurements, in order to
54 calculate unknown variables of interest. Initial estimation studies in WDSs were pioneered by
55 Rahal et al. (1980), Walski (1983) and Bhave (1988) with the proposal of the ad hoc (trial-and-
56 error) calibration schemes, in which an iterative process to update unknown model parameters was
57 implemented. Due to the slow convergence rate, this method is only applicable to small water
58 networks. Later, explicit calibration methods were introduced (Ormsbee & Wood 1986; Boulos &
59 Wood 1990; Boulos & Ormsbee 1991). These methods solved an even-determined set of water
60 network equations where the number of unknown parameters is grouped to be equal to the number
61 of measurements. As the measurement errors were also neglected, these methods usually did not
62 represent real-world practical outputs. Therefore, explicit calibration models were often used to
63 analyse historic events in water systems (Savic et al. 2009). Subsequently, implicit methods were
64 developed using either mathematical techniques or evolutionary optimization techniques, for
65 example: Complex Method (Ormsbee 1989), Weighted Least Squares approaches (Lansey &
66 Basnet 1991; Datta & Sridharan 1994), Singular value decomposition (SVD) method (Sanz &
67 Pérez 2015) or Genetic Algorithms (GA) (Preis et al. 2009; Abe & Peter 2010; Do et al. 2016).
68 These methods have drawn a high degree of attention from researchers. However, these models
69 are mostly impractical due to either a requirement for a large quantity of ‘good’ observation data
70 (Savic et al. 2009) or ignoring model uncertainties. Furthermore, few approaches have attempted

71 to estimate model parameters and model states in conjunction with model uncertainties. Bargiela
72 and Hainsworth (1989) found that a good approximation of pressure uncertainty bounds can be
73 obtained by a linearization of the mathematical network model. Piller (1995) and Bush and Uber
74 (1998) used a sampling design method to estimate the model parameters and approximate the
75 uncertainties. Lansey et al. (2001) applied a first-order approximation method to identify pipe
76 roughness uncertainty. Nagar and Powell (2002) applied a linear fractional transformation and
77 semi-definite programming method to estimate the pressure heads and their confidence bounds. In
78 addition, some probabilistic methods (Xu & Goulter 1998; Kapelan et al. 2007; Hutton et al. 2013)
79 have also been investigated for the estimation of model parameters. Due to the complexity of the
80 uncertainties, estimation methods associated with uncertainty quantification are still a continuing
81 research area, especially for real-time estimation purposes.

82 The complexity of uncertainties in WDS modeling has been addressed in Hutton et al. (2012b), in
83 which the uncertainty is divided into three categories: (1) structural uncertainty, (2) parameter
84 uncertainty and (3) measurement/data uncertainty. Structural uncertainty derives from the
85 mathematical representation of the real system, such as network skeletonization and model
86 aggregation. Skeletonized and/or aggregated models are predominantly used instead of all-pipes
87 models to reduce the complexity of the network being analysed as well as to increase
88 computational speed. It has been shown that skeletonized/aggregated network models can closely
89 resemble the behaviour of full sized systems under steady state conditions (e.g. Perelman et al.
90 (2008) and Preis et al. (2011)). The second category, parameter uncertainty, refers to the errors of
91 the parameters used to represent system components (e.g. pipe roughnesses, pipe diameters).
92 According to Kang and Lansey (2009), these parameters are time invariant or vary slowly over
93 time. Hence, this source of uncertainty can be neglected for real-time estimation problems. Finally,

94 measurement/data uncertainty is the uncertainty from measurement devices and, more importantly,
95 uncertainty from the inability to capture the temporal and spatial variation of consumer demands.
96 Because of their high impact on model uncertainty during short periods of time (or in real-time),
97 nodal demands are therefore usually selected as the time varying parameters to be estimated.
98 The issue of short term demand forecasting and real-time demand estimation under uncertainties
99 can be found in some recent studies. Note that the short-term demand forecasting and demand
100 estimation are two different problems. The former focuses on predicting future demands (e.g.
101 Cutore et al. (2008), Hutton and Kapelan (2015) and Alvisi and Franchini (2017)). The latter
102 focuses on estimation of the current demands, which is also the main interest of this paper. This is
103 useful, as demand estimation can be used at regular time steps to verify the accuracy of the
104 predicted value and update the system operations. The problem of near real-time demand
105 estimation has been studied using different approaches. Shang et al. (2006) applied an extended
106 Kalman filter, an iterative linear algorithm for nonlinear state estimation, to approximate water
107 demand patterns. In that paper, water demand patterns were predicted by an ARIMA time series
108 model and were refined using real-time observations. Similarly, Hutton et al. (2012a) introduced
109 a particle filter method and an ensemble Kalman filter for the estimation of a single district meter
110 area, which was assumed to follow a linear time series model. The particle filter model was
111 implemented with and without measurement error to show its effect on the demand prediction
112 uncertainty. An alternative for the demand estimates can be found in Kang and Lansey (2009). In
113 their paper, two comprehensive methods for the demand estimation problem were introduced, the
114 Kalman filter and the tracking state estimator (TSE). For the Kalman filter model, the water
115 demand patterns were also assumed to follow a linear time series model, while the TSE model
116 involved recursively computing the sensitivity matrix (i.e. the Jacobian matrix of the measurement

117 vector with regards to the change in the state vector). The uncertainties of the demand estimates
118 were suggested to be quantified by applying the first-order second moment formula. The two
119 models were then tested on a case study (116 pipes, 90 nodes, 1 source and 1 tank) with an
120 assumption that 19 flow measurement sites and 5 pressure measurement sites were available. It
121 should be noted that the demand estimation problem is sensitive to the locations and types of the
122 measurements (Do et al. 2016). Demand estimation models usually perform better with flow
123 measurements rather than pressure/head measurements. However, due to the cost and difficulty of
124 installing flow measurement devices compared to pressure measurement devices, flow
125 measurement devices are usually not as commonly used as pressure measurement devices in real
126 WDS networks.

127 In summary, water demands in WDS studies are usually assumed to be known and varied based
128 on a diurnal curve. However, this assumption might lead to large approximations of WDS states
129 in real-time due to the unpredictable variation of the water demands. Some efforts have been
130 focused on the real-time demand estimation. By assuming that the water demand follows a linear
131 time series prediction model, these models approximated the water demand patterns with some
132 linear algorithms such as the Kalman filter or extended Kalman filter. Given the nonlinear
133 stochastic nature of the water demands as well as the need for practical applicability, real-time
134 estimation modeling of WDS still requires much research effort.

135 This paper presents a model framework for the online (near real-time) demand estimation of a
136 WDS, which is named the *DMFLive* model. A predictor-corrector methodology is adopted in the
137 *DMFLive* model to predict the hydraulic behaviors of the water network based on a nonlinear
138 demand prediction sub-model, and to correct the prediction by using online pressure observation
139 data. A particle filter method is applied to implement the predictor-corrector approach. The typical

140 problems of the particle filter approach (particle degeneracy, impoverishment and particle
 141 convergence) are investigated by two different resampling schemes: systematic resampling (SR)
 142 algorithm and systematic resampling integrated with a genetic algorithm process (SRGA).
 143 Uncertainties of model outputs are quantified and evaluated in terms of confidence intervals.
 144 The paper is structured as follows. First, an explanation of the state estimation problem and its
 145 conceptual solution is introduced. Second, the basic concepts of particle filter methods to solve the
 146 estimation problem are explained. This is followed by a detailed description of the particle filter
 147 methodology applied for water demand state estimation in WDS. Two case studies are then used
 148 to evaluate the model. Finally, conclusions and suggestions for future work are given.

149 **State estimation problem and its conceptual solution**

150 The problem of state estimation involves finding a target state vector x_k that evolves according to
 151 a discrete time stochastic model (Ristic et al. 2004):

$$x_k = f_{k-1}(x_{k-1}, u_{k-1}) \quad (1)$$

152 where k is the index of discrete time steps; f_{k-1} is a known, possibly nonlinear function of the
 153 previous state and u is the process noise sequence. The value of x_k can be found from
 154 measurements z_k , which are related to x_k via the measurement equation:

$$z_k = h_k(x_k, w_k) \quad (2)$$

155 where h is a known implicit or explicit, possibly nonlinear function and w is the measurement
 156 noise sequence. The noise terms u_k and w_k are usually assumed to be white noise and independent.
 157 From a statistical and probabilistic perspectives, the state model can be represented by a probability
 158 density function (pdf). The state estimation problem, therefore, becomes a process of recursively
 159 quantifying some degree of belief in the state x_k given the measurement series $Z_k (z_i, i=1, \dots, k)$ up

160 to time k . This process can be obtained by two stages: prediction and correction/update. The
 161 prediction stage involves applying the system model to predict the prior pdf of the state:

$$p(x_k|Z_{k-1}) = \int p(x_k|x_{k-1})p(x_{k-1}|Z_{k-1})dx_{k-1} \quad (3)$$

162 where $p(x_k|x_{k-1})$ is the probabilistic model of the state model, or the transitional probability
 163 density function, which is defined by the system equation Eq. (1) with the known statistics of v_{k-1} ;
 164 and $p(x_{k-1}|Z_{k-1})$ is the pdf of the model at time $k-1$, which is supposed to be known.

165 The correction/update stage implements Bayes' rule to compute the posterior probability density
 166 of the state model when the measurement z_k becomes available:

$$p(x_k|Z_k) = \frac{p(z_k|x_k)p(x_k|Z_{k-1})}{\int p(z_k|x_k)p(x_k|Z_{k-1})dx_k} \quad (4)$$

167 where $p(z_k|x_k)$ is the likelihood function, defined by the measurement equation (Eq. (2)) with the
 168 known statistics of w_k .

169 According to Ristic et al. (2004), the recursive propagation of the posterior pdf shown in Eq. (3)
 170 and Eq. (4) is only a conceptual solution that cannot be analytically solved. The solution requires
 171 the storage of a fully non-Gaussian pdf, corresponding to an infinitive dimensional vector. Since
 172 the true solution is too complex and almost impossible to compute, an implementation of
 173 approximation techniques or suboptimal Bayesian algorithms is developed. The following section
 174 introduces an approximation technique, namely the particle filter, to solve the aforementioned state
 175 estimation problem.

176 **Particle filters**

177 Over the last decade, particle filters have been successfully applied to the state and parameter
 178 estimation of complex system models in various environmental engineering fields, such as
 179 hydrology (Moradkhani et al. (2005), Weerts and El Serafy (2006)), hydraulic (Hutton et al. 2012a)
 180 and geoscience (van Leeuwen (2010)). Unlike the Kalman filter (for linear problems), extended

181 Kalman filter (which requires a linearization of the nonlinear problems) or the unscented Kalman
 182 filter (which uses a small number of deterministically chosen samples), the particle filter can use
 183 a large number of Monte Carlo samples to estimate fully nonlinear, possibly non-Gaussian target
 184 states. The key concept of a particle filter is to approximate the posterior pdf of states, defined in
 185 Eq. (4), by an ensemble of samples (N_p), each of which contains an associated weight (w_k^i), and
 186 to compute estimates based on these samples and weights:

$$p(x_k|Z_k) \approx \sum_{i=1}^{N_p} w_k^i \delta(x_k - x_k^i) \quad (5)$$

$$w_k^i = w_{k-1}^i \frac{p(z_k|x_k^i)p(x_k^i|x_{k-1}^i)}{p(x_k^i|x_{k-1}^i, z_k)} \quad (6)$$

187 where δ is the Dirac delta function; i is the particle index; and $p(x_k^i|x_{k-1}^i, z_k)$ is the importance
 188 density function. In order to simplify the weight update of the particle, the importance density
 189 function is usually chosen as the transitional density function, $p(x_k^i|x_{k-1}^i, z_k) =$
 190 $p(x_k^i|x_{k-1}^i)$, which yields with scaling:

$$w_k^i = \frac{p(z_k|x_k^i)}{\sum_{i=1}^{N_p} p(z_k|x_k^i)} \quad (7)$$

191 These equations form the basis of most particle filters. However, it has been shown by Doucet et
 192 al. (2000) that the variance of the weights will increase over time if the particle filtering process is
 193 limited at executing only these equations. Since the particles drift away from the “truth” as well as
 194 obtain negligible weights (Moradkhani et al. 2005), the model will fail to estimate the real states
 195 of the system. To avoid this problem, a resampling process, which replaces samples with low
 196 importance weights by the samples with high importance weights, is added to the procedure of
 197 particle filter models. In this paper, the systematic resampling method, also called the stochastic
 198 universal resampling, introduced by Kitagawa (1996), is selected for the resampling procedure of
 199 the particle filter model. A comprehensive explanation of the systematic resampling and the full

200 review of particle filtering methods are described in (van Leeuwen 2009). In addition, an improved
201 resampling method which integrates the evolutionary scheme from genetic algorithms into the
202 resampling process, is also proposed to improve the efficiency of the particle filter model.

203 **Particle filters applied for water demand state estimation in WDS**

204 In this study, the predictor-corrector approach implemented by a particle filter model for the
205 estimation of water demands in real-time is proposed, namely the *DMFLive* model. The demand
206 prediction sub-model presented by van Zyl et al. (2008) has been applied to predict the water
207 demand multipliers (DMF) in a WDS. The hydraulic EPANET toolkit (Rossman 2000) which
208 solves the hydraulic equations was used to compute the model equivalent of the measurement data
209 (i.e. the nodal pressures, flow rates at measurement locations or the final tank levels at the end of
210 each time step). These computed values then were integrated with the corresponding field
211 measurements in order to correct/update the particle weights. Particles were, thereafter, resampled
212 (with either SR or SRGA) and subsequently used as input for the prediction model.
213 Simultaneously, the estimated demand multipliers were computed and selected for uncertainty
214 quantification. The uncertainties of the demand multipliers caused by the errors from measurement
215 devices were computed using the first-order approximation formula. The flowchart of the
216 *DMFLive* model is shown in Figure 1.

217 ***Initialization of particles***

218 The *DMFLive* model starts with a creation of an ensemble of the particles (N_p). The particles are
219 the demand residuals, driven by the demand prediction model to predict the demand multipliers.
220 In addition, each particle is assigned an initial weight equal to $1/N_p$.

221 ***Demand prediction sub-model***

222 The initial particles (for the first iteration) or the particles after resampling (from the second
 223 iteration onwards) are transferred to the demand prediction sub-model. Demand residual
 224 information carried by the particles is used to track the states and predict the demand multipliers
 225 via the following equations (van Zyl et al. 2008):

$$\ln x_k^j = \sum_{i=1}^m \phi_i^j \ln x_{k-i}^j + \ln v_k^j \quad (8)$$

226 where x_k^j is the demand residual state at time step k of the j^{th} DMF; i is the lag counter; m is the
 227 number of autocorrelation lags (for the state estimation problem $m=1$ as referred to Eq. (1)); ϕ_i is
 228 the auto-regression coefficient for lag i and $v_k(0, \sigma_h)$ is the white noise with mean zero and standard
 229 deviation σ_h .

230 The j^{th} DMF is calculated as:

$$DMF_k^j = C_k^j x_k^j \quad (9)$$

231 where C_k^j is the value at time k of a typical diurnal demand pattern of the j^{th} DMF. The C value
 232 can be identified based on meter information of different water users (e.g. in Beal and Stewart
 233 (2014)).

234 ***Real-time hydraulic data***

235 In practice, hydraulic data can be captured in real-time via the SCADA system or sensor devices.
 236 For the *DMFLive* model, two types of real-time hydraulic data are required. First are the tank
 237 levels, pump and valve statuses, and second are the nodal heads and pipe flow rates at measurement
 238 locations. Tank levels, pump and valve statuses are used as boundary conditions for the hydraulic
 239 simulation of the water network model while the observations at measurement locations are used
 240 to correct/update the weight of the particles.

241 In order to validate the performance of the proposed model as well as its practical applicability to
 242 real WDS networks, all case studies in this research are assumed to have pressure measurements

243 only. The input data sets to evaluate the *DMFLive* model are synthetically generated based on
 244 deterministic models, where the water network parameters are fully known, as follows: (1) known
 245 demand patterns are assigned to nodal demands; (2) EPANET is run to record tank levels, pump
 246 statuses, and pressures at selected measurement locations; (3) to introduce the measurement errors,
 247 a normal distributed random error in an allowable range ($\pm\Delta^{\text{meas}}$) is added to each nodal pressure.

248 ***Simulator***

249 The hydraulic behavior of the water distribution network at each time step is simulated using an
 250 EPANET steady state simulation. The inputs are the predicted DMFs, tank levels, and pump and
 251 valve statuses. The water network characteristics such as pipe lengths, diameters, roughness
 252 coefficients, node elevations, pump curves, etc. are assumed to be known and constant. The outputs
 253 from the EPANET hydraulic solver is the model equivalent of the observations, i.e. the simulated
 254 nodal heads and pipe flow rates at measurement locations.

255 ***Corrector***

256 The weights of the particles are corrected/updated by associating the simulated heads and flows
 257 with the actual observations via Eq. (7) where the likelihood function is assumed to be Gaussian:

$$p(z_k | x_k^i) = \frac{1}{\sqrt{2\pi|R|}} e^{\left(-\frac{1}{2}[z_k - h(x_k^i)]^T R^{-1}[z_k - h(x_k^i)]\right)} \quad (10)$$

258 where $h(x_k^i)$ is the model equivalent of the observations z_k (simulated nodal heads and flow rates),
 259 and R is the covariance matrix of the observation errors, which in general is caused by errors from
 260 two main sources: forward model error and measurement device error. The forward model error,

$$\Delta^{\text{true}} = Z^{\text{true}} - h(x^{\text{true}}) \quad (11)$$

261 is the difference between the true observation vector, Z^{true} , and the corresponding vector output
 262 from the hydraulic simulation model EPANET using the true state x^{true} . The true observation vector

263 is a theoretical vector that represents observations measured by perfect measurement devices. It
 264 is linked to the actual measured values via the expression:

$$Z = Z^{true} + \Delta^{meas} \quad (12)$$

265 The observation error covariance matrix, therefore, can be estimated as $R = R^{true} + R^{meas}$, where
 266 R^{true} and R^{meas} denote the covariance of the forward model error and the covariance of measurement
 267 error, respectively (see Waller (2013) for a detailed explanation and calculation of the observation
 268 error covariance matrix). To produce good estimates of the model state in real case studies, the
 269 error covariance matrix must be well understood and properly calibrated. As previously mentioned
 270 in this paper, the measured data in all case studies were synthetically generated from the EPANET
 271 model based on “true” demand patterns. The forward model error, therefore, equals to zero. The
 272 covariance matrix R , as a result, is the diagonal matrix where the diagonal elements are the
 273 variances of the measurement errors, since observations are independently measured at different
 274 locations of the network by different measurement devices. The measurement errors **with specified**
 275 **ranges** are assumed to be known so that the covariance matrix R can be identified. **Resampling**
 276 Resampling is applied to create new ensembles of particles from the posterior pdf of the previous
 277 step. In this paper, two alternatives of resampling are tested: systematic resampling algorithm (SR)
 278 and systematic resampling integrated with the GA operators (SRGA).

279 The SR algorithm generates a random number u_s from the uniform density $U[0, 1/N_p]$, and
 280 consequently creates N_p ordered numbers (Hol et al. 2006):

$$u^i = \frac{i-1}{N_p} + u_s \quad (i = 1, \dots, N_p) \quad (13)$$

281 New particles are then selected that satisfy Eq. (14):

$$x_{new}^i = x(F^{-1}(u^i)) \quad (14)$$

282 where F^{-1} denotes the generalized inverse of the cumulative probability distribution of the
 283 normalized particle weights.

284 To reduce the convergence problem of the particles (i.e. all the particle weights are equal to zero)
 285 when applying the model for large networks with multiple demand patterns, the SRGA method is
 286 also applied. Three GA operators of selection, crossover and mutation are responsible for
 287 modifying the predicted demands before computing the weight of a particle by Eq. (10). In the
 288 selection step, particles are compared to each other through tournament selection and the best
 289 particles are selected as parents. Parent particles are then paired and go through crossover and
 290 mutation to generate offspring solutions. While the details of GA can be found in Nicklow et al.
 291 (2010), it is important to know that new parameters need to be introduced: the probability of
 292 crossover P_c , the probability of mutation P_m and the number of generations N_{gen} .

293 ***Demand multiplier outputs and uncertainty quantification***

294 The estimate of the state x_k is obtained by taking the mean of the particle filter sample set (Salmond
 295 & Gordon 2005):

$$\hat{x}_k \approx \frac{1}{N_p} \sum_{i=1}^{N_p} x_k^{i*} \quad (15)$$

296 where x_k^{i*} is the state updated based on the posterior analysis of the model weights.

297 For particle filter models, the uncertainty of the model output can be computed by taking the
 298 variance of the samples:

$$var(x_k) \approx \frac{1}{N_p} \sum_{i=1}^{N_p} (x_k^{i*} - \hat{x}_k)(x_k^{i*} - \hat{x}_k)^T \quad (16)$$

299 For the demand multiplier estimation problem, it should be noted that a small change in the demand
 300 multiplier can cause a large change in nodal demands (for nodes with large base demands) and
 301 consequently result in large variations of nodal pressures, especially at nodes that are sensitive to

302 nodal demands. Most of the demand forecasting models are required to capture both peak-demand
 303 hours and off-peak demand hours, with a demand multiplier factor that can vary from 0 to 4 (Chin
 304 et al 2000). The weight of the particles via Eq. (10) can, therefore, easily approach zero which
 305 leads to either particle degeneracy or particle non-convergence. Using a larger number of particles
 306 can prevent this problem, however, if the dimension of the state vector increases, the required
 307 number of particles increases exponentially. One way to solve these issues is to incorporate the
 308 covariance of the forecasting nodal heads/ pipe flow rates into the likelihood function:

$$p(z_k|x_k^i) = \frac{1}{\sqrt{2\pi|R^*|}} e^{\left(-\frac{1}{2}[z_k-h(x_k^i)]^T (R^*)^{-1}[z_k-h(x_k^i)]\right)} \quad (17)$$

309 where $R^* = R + \Sigma$, Σ is the covariance matrix of the forecast nodal heads or pipe flow rates,
 310 computed based on the forecast demands. This covariance matrix can be estimated by running the
 311 demand forecasting model multiple times to obtain the range of forecast demand multipliers, then
 312 applying these values into the hydraulic model to compute the variance of simulated nodal heads
 313 and pipe flow rates at measurement locations.

314 Although the method can ensure some of the particles always contain weights to avoid particle
 315 non-convergence and degeneracy, this would increase the noise of the output model. The variance
 316 of the model output (i.e. the uncertainty of the model output) is required to be computed by a
 317 different method instead of using Eq. (16).

318 Another way to overcome the convergence and degeneracy issues is to integrate the GA operators
 319 into the resampling process as mentioned in the previous sections. The integrated GA approach
 320 can prevent the model from experiencing these problems by exploring the state-space region and
 321 selecting the best particles (including the replication of good solutions). However, it might lead to
 322 another problem for the particle filter, referred to as particle impoverishment. The distribution of

323 the state model, because of the particle impoverishment, is poorly represented by only one or a
 324 few particles which significantly reduces the variance of the model state.
 325 To ensure reliable outputs from the particle filter model, it is proposed to approximate the
 326 uncertainty of the model state by an independent method, such as the first-order approximation
 327 (FOA) method adopted from Piller (1995). This also has the advantage of significantly decreasing
 328 the computational time, as it will be shown in the case studies. The model outputs, therefore, are
 329 the estimate of the demand multipliers computed by Eq. (15) and the confidence intervals
 330 computed by FOA method. For example, the 95% confidence interval of the estimated demand
 331 multiplier (i.e. the range in which the true demand multipliers are expected to be 95% of the time)
 332 can be obtained by the following expression:

$$\|\Delta DMF_k\| \leq 1.96(W^{\frac{1}{2}}J)^{\dagger} \quad (18)$$

$$|\Delta DMF_k^j| \leq 1.96 \sum_{j=1}^m |S_{ij}|, \text{ with } S = (W^{\frac{1}{2}}J)^{\dagger}$$

333 where J is the Jacobian matrix of flows and heads with respect to the water nodal demand at time
 334 k ; W is the weight matrix where the diagonal elements are the reciprocals of the variances of
 335 measurement errors ($W=R^{-1}$); superscript \dagger represents the pseudo-inverse operator. The derivation
 336 of Eq. (18) is explained in detail in Appendix A.

337 By considering the Jacobian (sensitivity) matrix, the uncertainty of the output model from FOA
 338 method can provide meaningful information about the sensitivity of the pressure with respect to
 339 the change in the nodal demand. This information can be used to guide where to place
 340 measurement stations. However, the method requires calculation of the sensitivity matrix, which
 341 may be time consuming when applied to large and complex networks.

342 ***Summary of assumptions and input requirements for the DMFLive model***

343 Several assumptions are made for this study: (1) the model of the water distribution network
 344 perfectly represents the real system with known network characteristics (e.g. pipe roughness

345 coefficients, length and diameters, etc.), and only demand multipliers are required to be estimated;
346 (2) typical demand patterns for different homogeneous demand groups in WDS are assumed to be
347 known. The homogeneous demand groups can be identified based on a multi-criteria demand
348 zones clustering algorithm presented in Preis et al. (2010). There is uncertainty of the model
349 outputs associated with demand groupings, but this is not considered here. Therefore, (3) the
350 source of uncertainty is only from the errors from measurement devices; (4) the errors of the
351 measurement devices are assumed to be known and to follow a Gaussian distribution; (5) the
352 observation data for the online (near real-time) estimation model is available every 10, 15 minutes,
353 1 hour or larger time steps. The influence of slow transients (mass oscillations) are, therefore,
354 ignored in this context.

355 The inputs required for the *DMFLive* model consist of the number of particles, the inputs for the
356 demand prediction sub-model, inputs for the hydraulic simulation model (EPANET), input for the
357 correction step and the parameters for the integrated GA operators (P_c , P_m and N_{gen}). The prediction
358 sub-model requires the data of typical demand patterns, the auto-regression coefficient (ϕ_l) and the
359 variance of noise of demand residuals (σ_h^2). These parameters are calibrated independently based
360 on historical demand data for specific networks, for example $\phi_l = 0.7$ and $\sigma_h^2 = 0.13^2$ as in van
361 Zyl et al. (2008). The EPANET model requires the known data of tank levels, pump and valve
362 statuses. The correction step requires the observation data at measurement sites. Note that the
363 particle filter model associated with the GA process can only be applied to networks with multiple
364 demand patterns (e.g. the second case study in this paper). Two-point crossover operator with the
365 probability of crossover $P_c=0.7$, bitwise mutation with the probability of $P_m = 1/N_{DM}$ (N_{DM} is the
366 number of demand patterns in the network, $N_{DM} = 5$, corresponding with $P_m=0.2$ for the second
367 case study) and the number of generations $N_{Gen} = 50$ were selected for the GA process.

368 Case study 1

369 The first case study used to evaluate the model is shown in Figure 2. The network has 9 nodes (8
370 nodes with demands), 12 pipes, one tank and one reservoir. The network characteristics can be
371 found from the EPANET example, namely the Net1 network. Three pressure measurements (with
372 a precision of $\Delta^{meas} = \pm 0.2$ m, consistent with a standard deviation of $\sigma^{meas} = 0.1$ for the
373 measurement error at 95% confidence interval) are assumed to be placed at three random locations
374 (nodes 13, 22 and 31). All nodal demands are assumed to follow a single demand pattern that
375 varies every 15 minutes, (represented by the continuous line in Figure 2.b). The demand pattern is
376 a random daily demand pattern (from a yearly demand pattern) for 100 households obtained from
377 the BESS model (Thyer et al. 2011). The *DMFLive* model is required to track this demand pattern
378 using the three pressure measurements, which are also obtained every 15 minutes.

379 In this case study, the default demand pattern given in the Net1 example (represented by the dashed
380 line in Figure 2.b) was selected as the typical demand pattern. Different values of the auto-
381 regression coefficient (ϕ) as well as variance of noise (σ_h^2) were applied for the demand prediction
382 sub-model.

383 The accuracy of the demand estimates from the *DMFLive* model were evaluated in terms of the
384 coefficient of determination (R^2) and the root mean squared error (RMSE). For a number of
385 particles $N_p = 100$, the results of the demand estimates from the *DMFLive* model are presented in
386 Table 1.

387 The *DMFLive* model performed very well when the auto-regression coefficient was selected in the
388 range of $0.3 \leq \phi \leq 0.9$ and the noise variance was selected in the range of $0.25 \leq \sigma_h^2 < 0.64$. Due
389 to the large difference between the typical demand value and the actual demand value at each time
390 step (Figure 2.b), the selection of small values of the auto-regression coefficient and noise variance

391 resulted in relatively poorer performance of the model (e.g. $R^2 = 0.465$ and $RMSE = 0.198$ for
392 $\phi=0.3$ and $\sigma_h^2=0.04$). The best output of the *DMFLive* model was obtained at $\phi=0.7$ and $\sigma_h^2=0.25$,
393 with $R^2 = 0.988$ and $RMSE = 0.028$, respectively.

394 For this best estimated demand pattern, the confidence intervals and the scattergram between
395 actual demand multipliers and estimated demand multipliers are plotted in Figure 3.a.

396 In Figure 3.a, the estimated demand pattern yields a very good match with the actual demand
397 pattern during the time period (24 hours, corresponding to 96 time steps). The actual demand
398 pattern is entirely covered by the range of the 95% confidence intervals calculated from FOA
399 method. This confidence interval range, which is expected to bracket the “true” demand multipliers
400 in 95% of the cases, represents the uncertainty magnitude of the estimated demand due to the error
401 from measurement devices.

402 The model has also been run with the number of particles $N_p=100$ and $N_p=20$ to provide a
403 comparison between the FOA method (i.e. Eq. (18)) and the posterior analysis (i.e. Eq. (16)) for
404 uncertainty quantification, as shown in Figures 3.b, 3.c and 3.d. Figures 3.a and 3.c show the
405 uncertainty quantified by the FOA method while Figures 3.b and 3.d shown the uncertainty
406 quantified by the variance of particles. For $N_p= 100$ particles, the 95% confidence intervals from
407 both methods are comparable to each other, which demonstrates that the FOA method can provide
408 reliable results compared to the variance of the particle filter samples.

409 A good estimate of the demand multipliers ($RMSE=0.047$) is obtained by the *DMFLive* model
410 even when the number of particles is reduced by a factor of five ($N_p=20$), as seen in Figures 3.c,
411 and 3.d. The uncertainty boundary calculated by the FOA method in Figure 3.c has a similar range
412 to the case with $N_p=100$ particles and covers most of the actual values. On the other hand, the
413 uncertainty bounds calculated by Eq. (16) in Figure 3.d are collapsed into single value at some

414 time steps due to an insufficient number of the particles. Application of Eq. (16) for uncertainty
415 quantification, therefore, requires an in-depth evaluation of the number of particles in the model if
416 it is selected for the uncertainty quantification.

417 The range of demand multipliers predicted in time according to the evolution of the particles is
418 presented in Figure 4.a. The predicted values range from $DMF_{min} = 0.1$ to $DMF_{max} = 7.0$,
419 indicating that the demand prediction sub-model can predict a large range of demand multipliers,
420 and cover the range $0 \leq DMF \leq 4$ suggested by Chin et al. (2000). Figure 4.b plots the scattergrams
421 of the actual demand multipliers versus the predicted demand multipliers (i.e. the mean of the
422 prediction) and actual demand multipliers versus estimated demand multipliers. The scattergram
423 shows a constant and strong correlation between actual demand multipliers and estimated demand
424 multipliers over time with R^2 being close to unity. Due to large difference between the typical
425 demand pattern and the actual demand pattern, the forecasting model does not provide good
426 prediction, resulting in weak and skewed correlation between the actual values and the predicted
427 values. Despite this, the *DMFLive* model is still capable to provide very good estimates of the
428 demand multipliers.

429 ***Effects of tank level update on the estimation***

430 In extended period simulations of most hydraulic solvers (including EPANET), the nodal demands
431 are considered to be constant during the time step. The levels of the tanks in the network at the end
432 of the time step are consequently computed based on this assumption and are used as the initial
433 tank level for the next step. Due to continuously unpredictable change of the water demand in
434 practice, the actual tank level at the end of the time step is usually different to the tank level
435 computed by the model. As a result, the estimated total volume of water used during the time step
436 is also different from the actual volume of water used in practice. This issue can be overcome by

437 minimizing the difference between actual tank levels at the beginning of the time step and the final
438 estimated tank level at the end of the previous step. The demand estimation model, however, will
439 be delayed until the information of the tank level at the beginning of the next time step becomes
440 available. In other words, the model outputs will be the estimates of the demand multiplier at the
441 previous time step.

442 In order to evaluate the effect of including tank level information at the end of every time step, an
443 additional test is conducted. Instead of assuming that the observations are available at every 15
444 minutes, in this test it is assumed that the data can be obtained every hour and the model is required
445 to estimate the demand pattern at each hour time step (while the actual demand pattern is varied
446 every 15 minutes).

447 Figure 5 plots the two estimated demand patterns with and without tank level information (herein
448 referred to as *DMF-WTLive* and *DMFLive*). Note that the *DMF-WTLive* model is the modified
449 version of *DMFLive* model at which the final tank level information is taken into account.

450 It can be seen that the estimates for both cases are matched with the actual demand pattern at every
451 hour time step. The inclusion of tank information only causes a slight difference between two
452 estimated demand patterns at some of the time steps. The root mean squared errors between
453 estimated demand multipliers and actual demand multipliers at every hour step indicates that the
454 *DMFLive* model obtained slight better results than the *DMF-WTLive* model (RMSE =0.046
455 compared to RMSE =0.080, respectively). However, the total estimated water usages tabulated in
456 Table 2 shows that the *DMF-WTLive* model is more accurate in predicting the volume of water
457 delivered to the users.

458 The total estimated water usage during the 24-hour simulation period from *DMFLive* model was
459 5942.43 m³/day, 46.81 m³/day (or 0.78%) less than the actual water usage. On the other hand, total

460 estimated water usage from *DMF-WTLive* model was 6007.31 m³/day, only 18.07 m³/day (or
461 0.30%) more than the actual value. Therefore, if the estimation can be delayed one time step, the
462 final tank level information should be included into the model to improve the accuracy of the
463 estimated total volume of water used.

464 **Case study 2**

465 In order to evaluate the performance of the proposed model in large networks that contain more
466 than one demand pattern, the C-Town network from Ostfeld et al. (2011) is selected as the second
467 case study. The network consists of 429 pipes, 1 reservoir, 7 tanks, 5 pump stations (with a total
468 of 11 pumps), 4 PRV valves and 388 nodes (334 nodes with demands), which are divided into five
469 district demand areas. Each district demand area follows a different hourly demand pattern. As the
470 data of the demand patterns is available for seven days, the first 24 hours of these demand patterns
471 are assumed to be the typical demand patterns for the demand prediction sub-model. The
472 performance of the particle filter model is then evaluated by estimating the remaining 6-day hourly
473 demand patterns.

474 It is assumed that there are 14 pressure measurement sites (from P1 to P14) that are randomly
475 located at 14 places. These pressure measurements, again, are assumed to have a measurement
476 error of $\Delta^{meas} = \pm 0.2$ m. The inputs for the real-time demand estimation model are, therefore, the
477 pressures at these locations, the tank levels of seven tanks and the pump statuses of 11 pumps at
478 each hour time step. The topology and measurement locations of the C-Town network are shown
479 in Figure 6. Five different demand prediction sub-models were used to predict the five demand
480 patterns. The parameters of the five demand prediction sub-models were assumed to have the same
481 values of $\phi = 0.7$ for the auto-regression coefficients and $\sigma_h^2 = 0.16$ for the variances of noise.

482 The standard particle filter model (i.e. using systematic resampling), herein referred as the
483 *DMFLive-I* model, provides good results only if $N_p \geq 25,000$ particles. The estimates of five
484 different demand patterns for 6 days (from 25h to 168h) are shown in Figure 7. It is seen that the
485 estimated demand patterns closely match the actual demand patterns, especially for DMF 2 (RMSE
486 = 0.021), DMF 3 (RMSE = 0.024), DMF 1 (RMSE = 0.029) and DMF 4 (RMSE= 0.036). The
487 estimated demand pattern DMF 5 is less accurate, with the root mean squared error of RMSE =
488 0.061.

489 Figure 7 also plots the 95% confidence intervals for calculated by the FOA formula. The intervals
490 for the estimated DMF 1, DMF 2 and DMF 3 (in Figure 7.a, 7.b and 7.c, respectively) are narrow
491 and they cover almost the entire set of the actual demand multiplier values. The actual values of
492 DMF 4 are also within the confidence interval of estimated DMF 4 (Figure 7.d) for most of the
493 time. However, due to the locations of the measurements (P7 and P9 - Figure 6), the confidence
494 interval of estimated DMF 4 pattern is relatively large compared to the others. The effect of
495 measurement locations on the confidence intervals of the estimates is discussed later in the paper.
496 In Figure 7.e, approximately 37% of the actual demand values of the demand pattern DMF 5 are
497 outside the 95% confidence intervals, which is caused by the relatively poor estimates for DMF 5.
498 Figure 8 displays the scattergrams and coefficients of determination of the five predicted demand
499 patterns, as well as the estimated demand patterns versus their actual values.

500 The predicted DMFs in this case show an average correlation to the actual DMFs with the R^2
501 ranging from 0.69 to 0.74, while the estimated DMFs are strongly correlated to the actual ones
502 with all R^2 values being close to unity. The estimation for these five DMFs are also reliable during
503 the simulation period (six days), as the spreads of the scattered dots are close to bisector lines.

504 ***Improving DMFLive model performance by SRGA and modified likelihood function***

505 The *DMFLive-I* model can only perform well with a large number of particles ($N_P \geq 25,000$).
506 Smaller numbers of particles result in weak estimates of the DMFs due to particle collapse at some
507 steps. Since increasing the number of demand patterns requires an exponentially increasing
508 number of particles, it is necessary to improve the efficiency of particle filter model so that it can
509 be applied to complex systems.

510 Two methods have been investigated as mentioned previously in the paper: (1) incorporating the
511 variance of the forecasting nodal heads into the likelihood function. The weights of particles in the
512 model, referred as *DMFLive-II* model, are then calculated by the modified likelihood function (Eq.
513 (17)); and (2) by the integration of a GA process into the systematic resampling of the model,
514 herein referred as *DMFLive-III* model.

515 Table 3 presents results (in terms of the RMSE of each demand pattern) of running these models
516 with $N_P=1000$ and $N_P=5000$ for *DMFLive-I, II* and with $N_P^{GA} = 20$ and $N_P^{GA} = 100$ for *DMFLive-*
517 *III*. It may be seen that for both N_P values, the *DMFLive-I* gives very poor estimates of the DMFs.
518 On the other hand, the *DMFLive-II* model only requires $N_P=1000$ (corresponding to $1.43 \cdot 10^5$
519 evaluations for 143 hours) to provide fairly good results, while the *DMFLive-III* performs well
520 when $N_P^{GA} = 100$. The results of *DMFLive-II* ($N_P=5000$) and *DMFLive-III* ($N_P^{GA} = 100$) give
521 similar to the results of *DMFLive-I* running at $N_P=25,000$ (corresponding to total evaluations of
522 $3.575 \cdot 10^6$). This means the computation can be reduced by approximately a factor of five times.

523 Figure 9 shows the DMF 1 uncertainty ranges from 25 to 49 hours of the three models *DMFLive*
524 *I, II* and *III* computed by FOA method and by variance of the particles Eq. (16). As can be seen
525 from Figures 9.a and c, due to particle impoverishment, the uncertainty computed by particle
526 variance, represented by the dashed lines, is merged into a single line at almost all of the time

527 steps. The uncertainty in Figure 9.b computed by this method is wide due to the incorporation of
528 the forecasting nodal heads into the likelihood function.

529
530 On the other hand, the uncertainties by FOA method, which are directly computed from the
531 sensitivity matrix and the measurement errors, show consistent ranges in both cases. Given good
532 estimates of the demand multipliers (as in Figures 9.b and c) these ranges can cover the actual
533 values most of the time.

534 ***Effect of the locations of measurements on the quantification of demand uncertainty***

535 As discussed in a number of studies such as in Piller (1995) and Do et al. (2016), the locations of
536 the measurements have a strong impact on the results of the demand estimation models.
537 Furthermore, the selection of measurement locations also affects the confidence intervals of the
538 estimation outputs.

539 From the mathematical point of view, the uncertainty of estimated demands depends on the
540 sensitivity of the flows/heads at measurement locations in relation to the change in the water nodal
541 demands. This sensitivity is represented by the sensitivity matrix J (Eq. (18)), which is, in this case
542 study, the Jacobian matrix of the heads with respect to the demand multipliers. The sensitivity of
543 the heads with respect to the change of the demand multipliers depends on two factors: (1) the
544 position of the nodes in the network and (2) the base demands at the nodes. In fact, the nodes close
545 to fixed-head nodes (tanks or reservoirs) are less sensitive than the ones far from the fixed-head
546 nodes. This is because of a change in nodal demands will result in a smaller change in the pressures
547 of the closer nodes than the farther nodes. In a similar way, small base demands in the same pattern
548 will result in small friction losses and consequently small changes in pressures. Therefore, nodes
549 selected in these regions may cause large uncertainty in demand multiplier estimation. The
550 sensitivity matrix takes into account these two factors. Small values in the sensitivity matrix values

551 mean that the nodes are less sensitive to the demands and the estimation might have large
 552 uncertainty. Therefore, the uncertainty of the estimated DMFs can be reduced by selecting the
 553 more sensitive locations in the network.

554 Let us conduct an additional test to evaluate the effect of the measurement locations on the
 555 uncertainty of the estimated demand multipliers, for example the uncertainty of the estimated DMF
 556 4. For this test, the locations of measurements P7 (with the base demand of $D_7^0 = 0.50$ L/s) and P9
 557 ($D_9^0 = 0.59$ L/s) are relocated to P7A ($D_{7A}^0 = 1.33$ L/s) and P9A ($D_{9A}^0 = 1.13$ L/s). The *DMFLive*
 558 model was implemented with the same conditions and the other measurement locations are fixed
 559 at the same places as the original test.

560 Figure 10 shows the sensitivity matrixes J_0 (for the original test) and J^A_0 (for the modified test)
 561 corresponding to a set of estimated values DMFs = [0.46; 0.54; 0.65; 0.47; 0.62]

562 It is seen that, for this network, the heads at measurement locations are only sensitive to the change
 563 of the DMF that they belong to. For example, the variation in the DMF 4 pattern only affects the
 564 sensitivity of the heads at measurement locations P7 and P9 (for original test) and at measurement
 565 locations P7A and P9A (for the modified test). The non-zero values in the sensitivity matrices,
 566 therefore, correspond to the measurement locations. For the sensitivity of the heads, the new

567 locations P7A ($\frac{\partial H}{\partial DMF4} = 5.31$) and P9A ($\frac{\partial H}{\partial DMF4} = 11.76$) are considerably more sensitive than the
 568 locations P7 ($\frac{\partial H}{\partial DMF4} = 2.59$) and P9 ($\frac{\partial H}{\partial DMF4} = 2.55$). As a result, the confidence intervals of the

569 estimated DMF 4 for the modified test, as shown in Figure 11, are much narrower than the
 570 confidence intervals of the estimated DMF 4 for the original test presented in Figure 7.d. Note that
 571 in this network case study, the demand patterns are well geographically distributed. The heads at
 572 measurement locations are, therefore, affected by independent demand patterns, which results in a
 573 narrow uncertainty range for the estimate. For non-geographically distributed DMF networks, the

574 sensitivity of the heads at measurement locations are required to be accounted and accumulated
575 for all the related DMFs. This might cause much larger uncertainty and likewise bring difficulty
576 for the estimation of the demand multipliers, as has been addressed in Sanz and Pérez (2014).

577 The relocation of the pressure measurements also improves the estimation of DMF 4, with a RMSE
578 = 0.028 for the modified test, compared to a RMSE =0.036 of the original test. The placement of
579 the two new measurement sites also causes a slight difference in the results of other estimated
580 DMFs due to the change in the particle weights. However, the results of the four remaining DMFs
581 are still very good and similar to the estimated values of the original test.

582 To sum up, the uncertainty of estimated demand multipliers caused by the errors of measurement
583 devices is influenced by the measurement locations. It is suggested to choose the locations that are
584 more sensitive to the demand multipliers (see Do et al. (2016) for an example of optimal
585 measurement location). However, it has also been shown that the *DMFLive* model can be used to
586 estimate the demand multipliers even when the measurement devices are located at some less
587 sensitive places. The uncertainty of the estimated demand multipliers can be used to identify which
588 measurement locations need to be improved. This is another advantage of the *DMFLive* model.

589 **Conclusions and recommendations**

590 Real-time demand estimation under uncertainties is exceptionally difficult due to the unpredictable
591 stochastic behavior of the water demand as well as the nonlinearities of hydraulic systems. In this
592 paper, the *DMFLive* model framework has been introduced, which can be used to estimate the
593 demand multipliers of a WDS in near real-time. A predictor-corrector approach has been adopted
594 and solved by a particle filter method. A nonlinear demand prediction model is applied to predict
595 water demand multipliers at each time step, while the online pressure observations are used to
596 correct the prediction. Output uncertainty caused by the measurement errors has also been

597 quantified by the first-order approximation formula. The performance of the *DMFLive* model is
 598 evaluated by two WDS case studies. The results showed that the nonlinear demand prediction
 599 model combined with the particle filter method used in the paper are well suited for the near real-
 600 time demand estimation problem.

601 Within the first case study, the benefits of having additional information about the tank level of
 602 the next time step have been explored. If the estimation of the demand multipliers can be delayed
 603 one time step, the tank level at the beginning of the next time step can be used by the model to
 604 improve the estimation of the total volume of water used.

605 Within the second case study, three versions of the *DMFLive* model were developed to be used in
 606 large networks with multiple demand patterns. All versions provided good results, showing that
 607 the models are capable to be used in large networks. Finally, the effect of the measurement
 608 locations on the uncertainty of the estimated demand multipliers has been explored. Results
 609 showed that the uncertainty can be used to identify which measurement locations need to be
 610 improved. Future work involves considering adding additional uncertainties into the *DMFLive*
 611 model. Moreover, testing the model for non-geographically distributed demand networks is also
 612 necessary to show its capability when applied in practice.

613

614 **Appendix**

615 The problem of demand calibration involves finding the demands of the network hydraulic model
 616 to best fit the data set. Consider the nonlinear regression equation:

$$y_i^{Meas} = y_i(x) + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma_i) \quad (A1)$$

617 where x is the n_d by 1 vector of parameters to calibrate (the demand multiplier factors that depend
 618 on time); $y_i(x)$ is the scalar multivariate function of predictions from the network hydraulic model,
 619 given the parameter x ; ε_i is the residual between model prediction and observation, which is

620 assumed to be Gaussian with mean of zero and standard deviation of σ_i ; y_i^{Meas} is the i^{th}
 621 measurement site in the data set.

622 The demand calibration can be formulated as a box-constrained Least Squares problem that
 623 minimizes the differentiable criterion at each time step:

$$f(x) = \frac{1}{2} \sum_{i=1}^m \left(\frac{y_i(x) - y_i^{Meas}}{\sigma_i} \right)^2 = \frac{1}{2} \sum_{i=1}^m \varepsilon_R^2 \quad (A2)$$

s. t $x^{min} \leq x \leq x^{max}$

624 where m is the number of measurement sites, ε_R is the reduced residual, which is the residual
 625 divided by the corresponding standard deviation, $\varepsilon_R \sim N(0,1)$.

626 The gradient of f at x^0 is:

$$\nabla f_0 = J(x^0)^T W (y(x^0) - y^{Meas}) \quad (A3)$$

627 where W is the weight matrix where the diagonal elements are the reciprocals of the variances of
 628 measurement errors; $J(x^0)^T = \partial_x y(x^0)^T$ is the transposed Jacobian matrix of the prediction
 629 function at $x = x^0$.

630 The Hessian approximation takes the simple form of the symmetrical, positive semi-definite
 631 matrix:

$$H_0 = J(x^0)^T W J(x^0) \quad (A4)$$

632 It is essential for the Jacobian to be full rank of the size of x , so that H_0 is invertible and a definite
 633 matrix.

634 An approximation of function f to minimize Eq. (A2) by a quadratic function at x^0 leads to the
 635 approximation of x :

$$x = x^0 - (H_0)^{-1} \nabla f_0 \quad (A5)$$

636 By replacing Eq. (A2) and Eq. (A3) into Eq. (A5), the approximation of x can be expressed as:

$$x = x^0 - (J(x^0)^T W J(x^0))^{-1} J(x^0)^T W (y(x^0) - y^{Meas})$$

637 Using Eq. (A1):

$$x(\varepsilon) = x^0 + (J(x^0)^T W J(x^0))^{-1} J(x^0)^T W \varepsilon \quad (\text{A6})$$

638 The influence of the measurement errors with regards to the parameter estimates, therefore, can be

639 obtained at the first-order of Eq. (A6):

$$\Delta x = (J(x^0)^T W J(x^0))^{-1} J(x^0)^T W \varepsilon = (W^{\frac{1}{2}} J(x^0))^{\dagger} W^{\frac{1}{2}} \varepsilon = (W^{\frac{1}{2}} J(x^0))^{\dagger} \varepsilon_R \quad (\text{A7})$$

640 The uncertainty in term of confidence limits can be expressed as:

641 - For 99% confidence intervals ($|\varepsilon_i| \leq 2.58\sigma_i$):

$$\|\Delta x\| \leq 2.58 \left\| (J(x^0)^T W J(x^0))^{-1} J(x^0)^T W^{\frac{1}{2}} \right\| = 2.58 \left\| (W^{\frac{1}{2}} J(x^0))^{\dagger} \right\| \quad (\text{A8})$$

642 - For 95% confidence intervals ($|\varepsilon_i| \leq 1.96\sigma_i$):

$$\|\Delta x\| \leq 1.96 \left\| (W^{\frac{1}{2}} J(x^0))^{\dagger} \right\| \quad (\text{A9})$$

$$|\Delta x_i| \leq 1.96 \sum_{j=1}^m |S_{ij}|, \text{ with } S = (W^{\frac{1}{2}} J)^{\dagger}$$

643

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Table 1: Coefficient of determination (R^2) and root mean squared error (RMSE) of demand estimates corresponding to different parameter values of the demand prediction model for case study 1

No	Auto-regression coefficient (ϕ)	Variance of demand residual (σ_h^2)	R^2	RMSE
1		0.04	0.465	0.198
2	0.3	0.25	0.986	0.030
3		0.64	0.983	0.033
4		0.04	0.528	0.189
5	0.5	0.25	0.986	0.030
6		0.64	0.987	0.029
7		0.04	0.982	0.033
8	0.7	0.25	0.988	0.028
9		0.64	0.986	0.031
10		0.04	0.987	0.029
11	0.9	0.25	0.986	0.031
12		0.64	0.985	0.031

778 *Bold – Best estimated result

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Table 2: Actual and estimated total volume of water usage during calculated period

Cases	Total (m^3/day)	Difference (m^3/day)	% Difference (%)
Actual daily water usage	5989.25		
Estimated water usage with <i>DMFLive</i>	5942.43	46.81	0.78
Estimated water usage with <i>DMF-WTLive</i>	6007.31	18.07	0.30

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Table 3: Performance of DMFLive model with SR (I), modified likelihood function (II) and SRGA (III)

Model type	DMFLive-I		DMFLive-II		DMFLive-III ($N_{Gen}=50$)	
	$N_p=1000$	$N_p=5000$	$N_p=1000$	$N_p=5000$	$N_p^{GA}=20$	$N_p^{GA}=100$
No. Particles						
No. Eval.	$1.43 * 10^5$	$7.15 * 10^5$	$1.43 * 10^5$	$7.15 * 10^5$	$1.08 * 10^5$	$5.43 * 10^5$
RMSE _{DMF1}	0.386	0.405	0.050	0.027	0.107	0.030
RMSE _{DMF2}	0.365	0.422	0.026	0.021	0.067	0.025
RMSE _{DMF3}	0.416	0.237	0.029	0.027	0.068	0.023
RMSE _{DMF4}	0.385	0.229	0.043	0.038	0.086	0.032
RMSE _{DMF5}	0.366	0.246	0.074	0.049	0.190	0.050

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