Journal of Hydroinformatics | 15.1 | 2013

Automated parameter optimization of a water distribution system

Maikel Méndez, José A. Araya and Luís D. Sánchez

ABSTRACT

The hydraulic model EPANET was applied and calibrated for the water distribution system (WDS) of La Sirena, Colombia. The Parameter ESTimator (PEST) was used for parameter optimization and sensitivity analysis. Observation data included levels at water storage tanks and pressures at monitoring nodes. Adjustable parameters were grouped into different classes according to two different scenarios identified as constrained and unconstrained. These scenarios were established to evaluate the effect of parameter space size and compensating errors over the calibration process. Results from the unconstrained scenario, where 723 adjustable parameters were declared, showed that considerable compensating errors are introduced into the optimization process if all parameters were open to adjustment. The constrained scenario on the other hand, represented a more properly discretized scheme as parameters were grouped into classes of similar characteristics and insensitive parameters were fixed. This had a profound impact on the parameter space as adjustable parameters were reduced to 24. The constrained solution, even when it is valid only for the system's normal operating conditions, clearly demonstrates that Parallel PEST (PPEST) has the potential to be used in the calibration of WDS models. Nevertheless, further investigation is needed to determine PPEST's performance in complex WDS models.

Key words | calibration, EPANET, model, optimization, parameter, sensitivity

Maikel Méndez (corresponding author)
José A. Araya
Centro de Investigaciones en Vivienda y Construcción (CIVCO), Escuela de Ingeniería en Construcción,
Instituto Tecnológico de Costa Rica,
APDO 159-7050,
Cartago,
Costa Rica
E-mail: *mamendez@itcr.ac.cr*

Luís D. Sánchez
Instituto Cinara,
Universidad del Valle - Facultad de Ingeniería,
Cali,
Colombia

INTRODUCTION

Water distribution system (WDS) models can be used for a variety of purposes including design, management, maintenance, planning and scenario studies. Nevertheless, in order to be reliable, a model must adequately predict the behavior of the actual system under a wide range of conditions and for an extended period of time (Machell *et al.* 2010). This can be accomplished by calibrating the model using a set of field measurements or observations, mainly water storage tank (WST) levels, nodal pressures and flow rates. The calibration of a WDS model is carried out by optimizing the values of physical and conceptual parameters involved in the model, including pipe roughness-coefficients, minor losses, demand pattern factors, nodal demands, control valves and pump characteristics (USEPA 2005; Koppel & Vassiljev 2009).

Calibration is also referred to as an inverse problem, since observed values are quantitatively compared to model predictions until the optimum set of parameters is found (Gallagher & Doherty 2007). A model is considered to be calibrated for one set of operating conditions if it can predict outcomes with reasonable agreement. Nevertheless, this does not necessarily imply calibration in general. Models should be calibrated over a wide range of operating conditions so that the modeler can rely on model predictions (Walski 1986). As models are only approximations of the actual systems that are being represented, the reliability of model predictions depends on how well the model structure is defined and how well the model is parameterized (Hogue *et al.* 2006).

A critical step in model calibration relates to the quality and density of observation data which may contain significant measurement errors. Even small measurement errors can lead to large errors in estimated parameters

doi: 10.2166/hydro.2012.028

(Goegebeur & Pauwels 2007). As observation data accuracy might be in the same order of magnitude of the measurement errors, including this kind of data in the calibration process will most likely produce misleading results. Only accurate observation data should be used for calibration. Walski *et al.* (2004) suggest that very high quality field data (e.g. pressure and elevation data) would be accurate to 0.1 m. Good quality field data are considered accurate to 1 m. Model predictions would significantly deteriorate when field data are accurate to 3 m, which reflects poorly collected data. On the other hand, sufficient observation data may be infrequent and only collected at select locations (Kang & Lansey 2009). This is particularly true in developing countries where severe limitations constrain the scope and success of public sector projects, particularly water supply and water quality (Lee & Schwab 2005).

Calibration by parameter optimization is a highly underdetermined problem as the number of unknowns is greater than the number of observations (Walski *et al.* 2006). In a real system, there can be hundreds of unknowns and only a relatively small number of observations. As the number of unknowns greatly exceeds the number of observations, there is little confidence in the model predictions. There can be too many solutions that yield equally good results in terms of a predefined objective function within the model's parameter space (Duan *et al.* 1992). This situation has resulted in the development of the concept of 'equifinality' which recognizes that alternative sets of control parameters within a model are capable of producing reasonable estimates of the system response as measured by objective functions defining the goodness of fit (Beven & Binley 1992; Fang & Ball 2007). This ambiguity has serious impacts on parameter and predictive uncertainty and consequently limits the applicability of a model. To reduce the number of unknowns and improve reliability on model predictions, the parameter space must be constrained (Walski *et al.* 2004).

An obvious constraint for any model would be grouping parameters into classes of similar characteristics (e.g. groups of same internal diameter, material, demand sector, etc.). If all parameters within a model are open to adjustment, modelers might end up doing what Walski (1986) calls 'Calibration by compensating errors'. An error in the estimated roughness can be compensated for by an error in demand. Compensating errors can take over the calibration process and produce numerically correct, but physically meaningless, solutions. Under these circumstances, a model would be matching observations rather than determining the system's optimal parameters. On the other hand, only those parameters sensitive to field observations should be included in the calibration process. If insensitive parameters are included, the parameter space would increase and model predictions will have little chance of improving the goodness of fit (Zaghloul & Abu Kiefa 2001).

Model calibration has traditionally been a trial-and-error process. In this approach, values of selected parameters are individually adjusted in a systematic manner until correlation between observed and modeled values no longer improves. Calibration by trial-and-error is a time-consuming and difficult task, as the large number of potential unknowns makes it impossible to analytically solve all calibration parameters (Walski *et al.* 2006). When a trial-and-error optimization approach is followed, the goodness of fit of the optimized model is essentially based on the modeler's judgments and experience (Ibrahim & Liong 1992; Khu *et al.* 2006). Since the judgment involved is subjective, it is difficult to explicitly assess the confidence of the model predictions (Kumar *et al.* 2009). As deviations between observed and modeled values might be outside the acceptable tolerance range, a much more 'tuned' optimization may be required. In this case an automated optimization approach may be used.

In an automated optimization approach, parameters are adjusted automatically according to a specified search scheme and quantitative numerical measures of the goodness of fit (Skahill & Doherty 2006). The development of automated optimization procedures has mainly focused on using a series of objective functions to evaluate the goodness of fit of the optimized model. Algorithms try to minimize the deviations between the observed and modeled values in order to find the global minimum of the selected objective function (Savic *et al.* 2009). Nevertheless, as calibration is a highly underdetermined problem, it is impossible to know whether any automated or manual calibration approach is actually correct. This situation might worsen if an automated calibration approach is followed, as calibration algorithms might contain little knowledge of the physical laws that govern a model's structure.

Several automated techniques have been used to calibrate WDS models including genetic algorithms (Jamasb *et al.* 2008; Nicklow *et al.* 2009; Kovalenko *et al.* 2010), Bayesian-type procedures (Kapelan *et al.* 2007) and Markov Chain Monte Carlo simulations (Peng *et al.* 2009). Various calibration tools have been incorporated into commercially available software packages including WaterGEMS's Darwin-Calibrator (Wu *et al.* 2002; Walski *et al.* 2006), H2ONET Calibrator (Wu *et al.* 2000) and InfoWater Calibrator (de Schaetzen *et al.* 2010). Although these applications are robust and well proven, little attention has been paid to end-user applications and product development (Abe & Cheung 2010). This is particularly true in the context of free and open source software applications. Water utilities in developing countries might not have access to commercial packages due to budget restrictions. Still the use and proper calibration of WDS models is a necessity.

The parameter estimator package PEST; an acronym for Parameter ESTimation (Doherty 2005) might eventually be used to calibrate a WDS model such as EPANET (Rossman 2000). PEST offers several strategic advantages to modelers. Firstly, PEST is a model-independent application. This avoids changes to the original code as it communicates with a model through its own input and output files. Secondly, PEST has successfully been used to calibrate numerous types of models including, groundwater models (Doherty 2005; Christensen & Doherty 2008), hydrological models (Arabi *et al.* 2007; Immerzeel & Droogers 2008; Bahremand & de Smedt 2010), soil layer and soil moisture analysis (Tischler *et al.* 2007) and hydraulic models (Koppel & Vassiljev 2009; Maslia *et al.* 2009). Thirdly, PEST can be used to carry out various predictive and exploratory tasks including sensitivity, correlation and uncertainty analysis. Fourthly, PEST is freely available to the public and is user-oriented. As modeling of WDSs is just emerging in developing regions, particularly in small water supply systems (municipalities and rural communities), it would be of great importance to explore the possibility of using available free and open source software applications in this context. This would gradually promote a 'modeling culture' which may generate demand for more comprehensive, commercially available tools.

The aim of this study is to determine if model independent parameter estimator PEST can be used to develop a fully calibrated extended-period model for a WDS using the public domain model EPANET.

METHODOLOGY

La Sirena's WDS was used as a case study to examine the advantages of using a fully automated optimization approach versus a trial-and-error optimization. La Sirena is a rural community located in the department of Valle del Cauca, Municipality of Cali, Colombia (Figure 1).

The system is served by a single multi-stage filtration (MSF) water treatment plant which produces approximately 0.012 $m^3 s^{-1}$ and consists of small diameter PVC pipes, ranging from 20 to 85 mm (Table 1). The system contains four ground WSTs that create four different pressure zones (Figure 1). Each WST is equipped with a Float Actuated Valve (FAV) that controls flow admission and prevents overflow. Isolation valves prevent flows among pressure zones. A complete topographic survey of the system was performed using a total station which allowed elevation data to be accurate to 0.02 m.

Since the system consists mainly of small diameter pipes and minor losses could have a significant impact, the number of fittings for each individual pipe was carefully identified. The types of fittings included tees, elbows, bends, contractions, expansions and fully open isolation valves. Minor loss coefficients (K) were assigned to these fittings based on typical values found in the literature (Mays 2000).

Observation data for the calibration process included water levels in the four storage tanks and nodal pressures in seven nodes (Figure 1). A period of 7 consecutive days (168 hr) was used for observations recording. Observations were taken during normal operating conditions and therefore, considered highly representative. Pressure gauges used to record nodal pressures were accurate to 1 m while pressure sensors at WSTs were accurate to 0.1 m. The time interval of water level and nodal pressure observations was 60 min, sparsely distributed throughout the entire recording period. In most cases, these observations represent discrete values recorded at the top of the hour. As recommended by Walski *et al.* (2001), when possible, nodal pressure observations were performed at maximum head

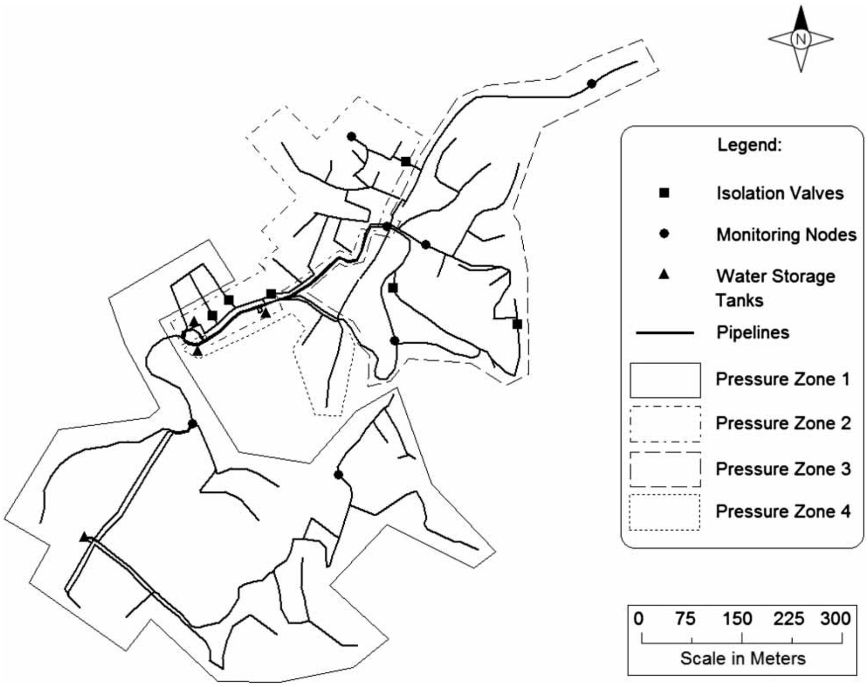

Figure 1 | La Sirena's water distribution system model.

Table 1 | Town of La Sirena's water distribution system characteristics

Component	Quantity
Number of nodes	325
Number of pipelines	279
Float Actuated Valves (FAVs)	5
Internal pipe diameter range (mm)	20–85
Total pipeline length (m)	9,554
Water storage tank, elevation ([a]MASL) and capacity (m^3)	
Tank 1	1,178; 56
Tank 2	1,113; 79
Tank 3	1,112; 200
Tank 4	1,097; 54

[a]Meters above sea level.

loss, which also corresponded to the system's highest water demand.

At the time the field data were collected, there was a total of 851 consumers registered in the Water Utility records. Each consumer was supplied with a flow meter which was read once a month. This information was used to estimate and allocate water demand per consumer. A period of 12 months between 2009 and 2010 was analyzed for this purpose. Nearly 96% of water demand was classified as residential. The remaining 4% was classified as commercial and/or industrial. A point-based method was used for nodal demand allocation. This required a detailed field survey to determine the precise number of households that were connected to the WDS.

As actual flow meter locations were known, a spatial function was used to assign each meter to the closest demand node (Cabrera *et al.* 1996). To include unaccounted for water, field measurements of production and metered consumption were recorded and compared during a period of 24 hr and then added proportionally to nodal demands. Estimations of leakage for each pressure zone were prepared from night flow and water level measurements. Nevertheless, severe inconsistencies regarding consumption records and unaccounted-for-water estimations were detected. Therefore, nodal demand exhibits the highest input data uncertainty for this case study.

This situation has been identified in the literature (Lansey & Basnet 1991; Kenward & Howard 1999; Zhou *et al.* 2000) and solutions such as on-line implementation of Supervisory Control and Data Acquisition (SCADA) systems have been suggested to improve knowledge of water demand temporal variation (Kang & Lansey 2009; Machell et al. 2010). However, SCADA systems are beyond the reach of most water utilities in developing countries. In recent years, researchers have identified the necessity to include uncertainty in the calibration of WDS models including pipe roughness coefficients and nodal demands (Alvisi & Franchini 2010; Giustolisi & Berardi 2011). Uncertainty quantification of model parameters such as nodal demands implies a profound knowledge of the system and the availability of sufficiently long time series data. Again, this might not be the case for many water utilities.

Demand patterns for each WST and their respective pressure zones were constructed by analyzing diurnal dynamics of water demand. These temporal variations were measured for various consumers of each pressure zone. The effect of the day of the week on the demand patterns was also analyzed. Since significant differences between weekday and weekend consumption were detected, two 24-hr diurnal demand patterns (with a temporal resolution of 1 hr) were constructed for each pressure zone; one known as weekday demand pattern (Monday to Friday) and the other known as weekend demand pattern (Saturday and Sunday). In total, eight 24-hr demand patterns for the entire system were constructed. As this project faced budget limitations, it was not possible to obtain an independent set of data that could have been used for model validation.

Parameter optimization

Calibration and sensitivity analysis of EPANET were performed using PEST, a nonlinear parameter estimation and optimization package, which offers model independent optimization routines (Doherty 2005). PEST is based on the Gauss-Marquardt-Levenberg algorithm (GML) which searches for the optimum values of the model parameters by minimizing the deviations between field measurements (observations) and modeled values (predictions). PEST uses the sum of the squared deviations PHI (ϕ) as its objective function (Skahill 2009) and can be mathematically expressed as:

$$\phi = \frac{\sum_{i=1}^{n} w_i (O_i - M_i)^2}{n} \tag{1}$$

where n equals the total number of observations, O_i the observed value on timestep i, M_i is the modeled value on timestep i and w_i is the relative weight attached to each observed value.

At the beginning of each iteration timestep, the relationship between model parameters and modeled output values is evaluated for the current set of parameters. For instance, the derivatives of all observations with respect to all adjustable parameters must be calculated. These derivatives are stored as the elements of a Jacobian matrix used for sensitivity analysis.

During each iteration timestep, PEST varies each adjustable parameter incrementally from its currently estimated value and re-runs the model. The ratio of modeled output differences to parameter differences approximates the derivative. For greater accuracy in derivatives' calculation, parameter values can be both increased or decreased until the objective function PHI is minimized. PEST determines whether additional iterations are required by comparing the parameter change and objective function improvement achieved through the current and previous iterations (Skahill & Doherty 2006).

PEST also calculates a composite relative sensitivity for each adjustable parameter which measures the sensitivity of all observations with respect to a relative change in the value of that specific parameter. The sensitivity of a parameter describes the effect that a variation on that specific parameter has over the whole model generated values. Sensitivity is a useful indicator for assessing the degree to which a parameter is capable of estimating the variables on the basis of the observation dataset available for model optimization (Doherty 2005).

PEST communicates with a model through the model's own input and output files. For PEST to be able to take control of the model, the model itself must be executable from the command line. Hence, the optimization of a model can be carried out without the requirement for the model to undergo any changes in its original structure.

To couple EPANET with PEST, several input files must be prepared (Figure 2). In the case of EPANET, the model's master input file has a suffix 'inp' (Rossman 2000). This ASCII-file contains all the necessary information to run EPANET from the command line using the EPANET2D.EXE

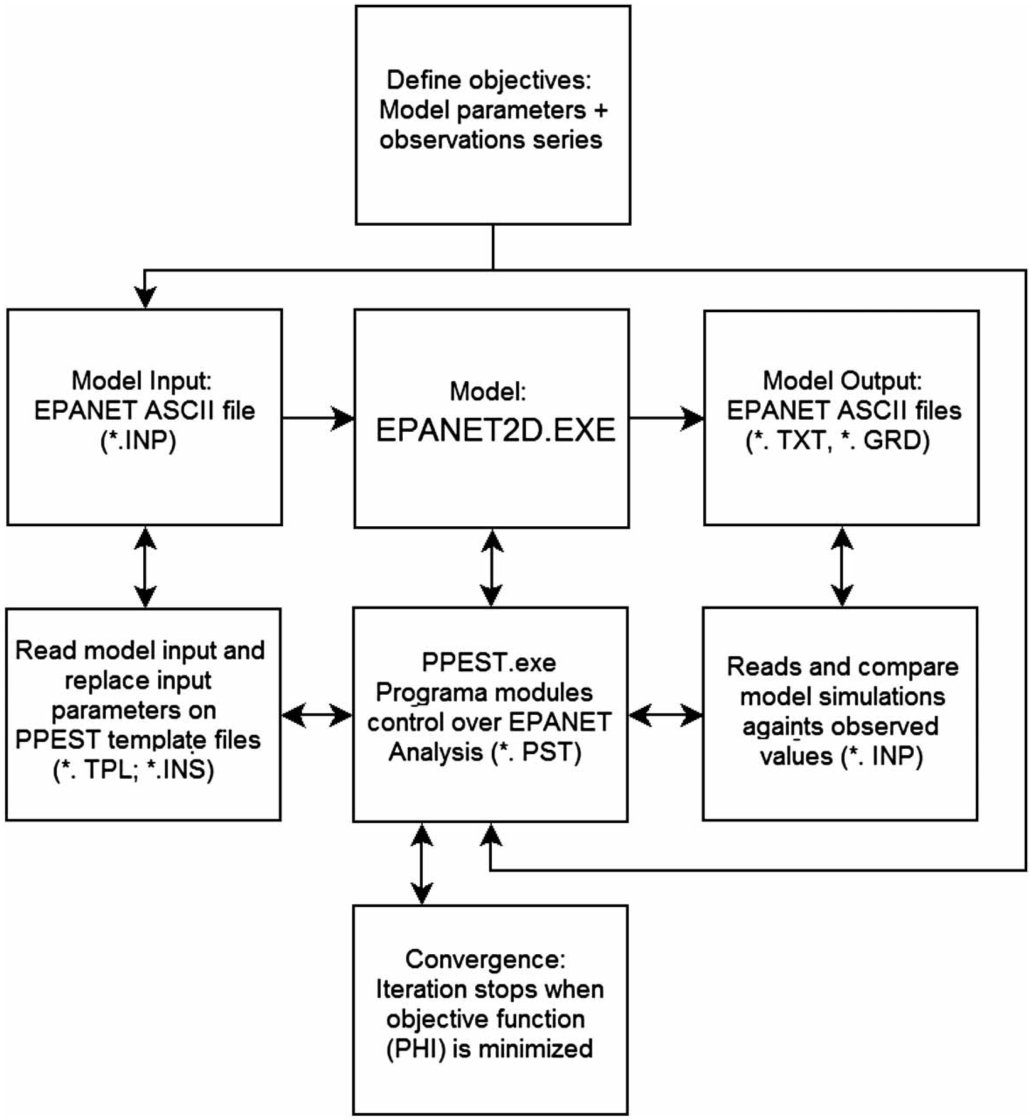

Figure 2 | Coupling schematics of EPANET and PEST.

extension. After EPANET is run, ASCII and binary files with the suffixes 'txt' and 'grd' are respectively created. For PEST, three types of input files must be created; a template files (with suffix 'tpl') which is basically a copy of the 'inp' input-file, a control file (with suffix 'pst') which contains all the PEST's control and numeric parameters, and finally an instruction file (with suffix 'ins'), which allows PEST to properly read observations from the EPANET's 'txt' output-files. In the course of the optimization process, PEST creates several output files which are stored for later inspection (Doherty 2005).

In most cases, the bulk of PEST's run time is consumed in running the model itself. Therefore, a special version of PEST known as Parallel PEST (PPEST) was used instead. PPEST does not only have all the functionalities of PEST but also facilitates a dramatic enhancement in the optimization performance by allowing PEST to run in parallel. This is particularly useful when the amount of adjustable parameters and the model run-times are large. It also allows modelers to take full advantage of the most recent and powerful multi-core processors, significantly reducing the time needed to achieve convergence.

Model setup

Model optimization for the La Sirena's WDS was achieved in two steps. In the first step, a trial-and-error approach was followed. Values of the selected parameters were individually modified in a systematic manner until correlation between observations and modeled values no longer improved. Three groups of parameters were taken into account for this step: demand pattern factors [–], nodal demands (L/s) and (C-factors) [–].

In the second step, an automated parameter optimization process was executed by linking EPANET with PPEST. Two different scenarios identified as 'constrained' and 'unconstrained' were established to evaluate the effects of parameter space size and compensating errors over the PPEST calibration process. In both scenarios, 12 parameter groups were created and they included: demand pattern factors [–], nodal demands (L/s), local losses [–], (FAVs) [–] and C-factors [–] (Table 2).

For the constrained scenario, a total of 24 adjustable parameters were declared. Demand pattern factors were fixed to their original values as sufficient confidence was obtained during their derivation. Nodal demands were aggregated into four different demand groups, one for each pressure zone. The same demand multiplier was assigned to each node within each demand group. Therefore, all nodes experienced a proportionally equal change in demand within each specific pressure zone. Minor loss coefficients (K) for fittings were not adjusted either. FAVs loss coefficients were adjusted as significant differences between manufacturer's curves and field behavior were detected. Throttle Control Valves (TCVs) were used in EPANET to simulate FAVs. TCVs are commonly used to simulate a partially closed valve by adjusting the minor head loss coefficient of the valve (Rossman 2000). C-factors were classified into groups of the same pipe diameter. No distinction was made regarding the age of the pipes as the entire system was constructed of relatively young PVC.

For the unconstrained scenario, a total of 723 adjustable parameters were declared, which accounted for the 12 parameter groups mentioned above. Each parameter within these groups was individually adjusted by PPEST. Nevertheless, a unique C-factor was used for all pipes in the system.

Observations in both scenarios, which included water levels and nodal pressures, were grouped in five observation groups, four for WSTs and one for monitoring nodes. Since observations were of two different types, the objective function relative weight attached to each observation, varied according to its relative importance in the overall parameter estimation process. Consequently, greater weights were assigned to water level observations since they were considered more reliable than those of the nodal pressures.

Concerning the ranges for parameter adjustments, a ±30% variation for demand patterns factors was allowed for the unconstrained scenario (Table 3). As severe inconsistencies regarding consumption records and unaccounted-for-water estimations were detected, a ±30% and ±50% variation in nodal demands multipliers were assigned to

Table 2 | Set of control settings used for PPEST

	Scenario	
Item	**Constrained**	**Unconstrained**
Number of adjustable parameters	723	24
Number of fixed parameters	0	192
Number of tied parameters	0	507
Number of observation groups	5	5
Number and type of parameter groups		
Demand patterns factors	8	8
Nodal demands	1	1
Minor loss coefficients (Ks)	1	1
Float Actuated Valves (FAVs) loss coefficients	1	1
C-factors	1	1

Table 3 | Ranges for parameters adjustments

	Ranges of parameters values per scenario	
Parameter group	**Constrained**	**Unconstrained**
Demand patterns factors (%)	Not applicable	±30%
Nodal demands multiplier (%)	±30%	±50%
Minor loss coefficients (Ks) (–)	Not applicable	0–20[b]
Float Actuated Valves (FAVs) loss coefficients (–)	0–350	0–350
C-factors (–)	130–150[a]	130–150[a]

[a]Walski et al. (2001).
[b]Mays (2000).

the constrained and unconstrained scenarios, respectively. Minor loss coefficients (K) for pipe fittings were allowed to vary from 0 to 20 based on typical values found in the literature (Mays 2000). FAVs loss coefficients (K) were allowed to vary from 0 to 350 based on manufacturer's pressure drop curves and field measurements. Two flow tests conducted in 69 mm PVC showed C-factor values of 130 and 134 correspondingly. For instance, a lower value of 130 was selected for C-factors in each scenario while a feasible upper value of 150 was obtained from the literature (Walski *et al.* 2001).

Even when observations were recorded every 60 min a hydraulic timestep of 1 min was used for the entire 168-hr simulation period regardless of the optimization approach (trial-and-error or PPEST). This is due to the fact that many observations (mainly nodal pressures) were sparsely and manually recorded throughout the entire recording period and no specific timing for field measurements was possible.

An Intel® Core™ i7-930, 2.80 GHz multi-core processor with 24 GB of RAM memory was used to run PPEST by controlling one master and eight slaves (two for each of the four cores of the i-7 processor). PPEST was run in estimation mode which means that PPEST continued with the iteration procedure until the global minimum was found. All other PPEST numerical parameters were assigned typical values as noted in the PEST manual (Doherty 2005).

Efficiency of the model optimization process was assessed according to two indicators (Maslia *et al.* 2009): the Pearson correlation coefficient (R),

$$R = \frac{\sum_{i=1}^{n}(O_iM_i) - (n\bar{O}\bar{M})}{\sqrt{\left[\sum_{i=1}^{n}\left((O_i^2) - n(O_i^2)\right)\right]\left[\sum_{i=1}^{n}\left((M_i^2) - n(M_i^2)\right)\right]}} \quad (2)$$

and the root mean square error (RMSE),

$$\mathrm{RMSE} = \left(\frac{\sum_{i=1}^{n}(O_i - M_i)^2}{n}\right)^{1/2} \quad (3)$$

where n equals the total number of observations, O_i is the observed-value on timestep i, $\hat{O}$ is the average of the observed values, M_i is the modeled-value on timestep i and M is the average of the modeled values.

R serves as an indicator of the correlation degree between observed and modeled values. A value of 1 yields perfect correlation whereas a value of 0 indicates that data are uncorrelated. The RMSE provides information on the average error between observed and modeled values.

RESULTS AND DISCUSSION

RMSE and R for modeled values of water levels and nodal pressures were obtained from the two optimization approaches: trial-and-error and PPEST. Overall, both PPEST optimization scenarios resulted in lower RMSE and higher R than those obtained by trial-and-error. Nevertheless, little variation in RMSE and R between PPEST scenarios can be seen (Table 4).

This is more evident for water levels in WSTs as RMSE remains within the 0.1 m accuracy expected for pressure sensors. In the trial-and-error approach, RMSE for water levels remains over the 0.1 m accuracy except for WST 2 (0.06 m). Still, RMSE values obtained by trial-and-error are considered acceptable if limitations in observation data acquisition are taken into account.

WSTs 1, 3 and 4 experienced the highest RMSE reductions, 54.8, 31.2 and 32.8%, respectively for the PPEST constrained scenario. Very similar values (57.6, 41.4 and 36.7%) were obtained for the PPEST unconstrained scenario. WST 2 is the exception for both PPEST scenarios since its RMSE increased rather than decreased with respect to the trial-and-error approach.

As mentioned, PPEST attempts to globally minimize the objective function PHI taking into consideration the contributions of the available observation groups. Since the relative weight of the water level observation group was the same for all tanks, it appears that PPEST allowed for higher deviations in WST 2 in order to compensate for errors in the remaining WSTs and pressure monitoring nodes. Maslia *et al.* (2009) obtained similar results in their EPANET-PEST analysis of the Holcomb Boulevard WDS, with RMSE reductions between 26.5 and 91.4%. Their study included four WSTs, one of which experienced an increase in RMSE after the optimization with PEST.

In our case, correlation coefficients increased in both PPEST scenarios, with WST 1 presenting the highest R

Table 4 | RMSE and *R* modeled values of water levels and nodal pressures for the town of La Sirena's water distribution system model

Optimization approach	Trial-and-error		Constrained PPEST scenario				Unconstrained PPEST scenario			
	Objective function		Objective function		Percentage change		Objective function		Percentage change	
Component	RMSE (m)	*R* (–)	RMSE (m)	*R* (–)	RMSE (m)	*R* (–)	RMSE (m)	*R* (–)	RMSE (m)	*R* (–)
Water levels in Tank 1	0.134	0.821	0.061	0.965	−54.781	17.548	0.057	0.975	−57.617	18.707
Water levels in Tank 2	0.064	0.895	0.068	0.917	6.438	2.429	0.073	0.911	13.633	1.796
Water levels in Tank 3	0.116	0.946	0.080	0.982	−31.194	3.733	0.068	0.987	−41.437	4.252
Water levels in Tank 4	0.158	0.879	0.106	0.940	−32.825	6.979	0.100	0.947	−36.713	7.777
Nodal pressures	4.678	0.981	1.852	0.998	−60.407	1.732	1.545	0.999	−66.976	1.776

increase, 17.6 and 18.7% for the constrained and unconstrained scenarios, respectively. In the case of nodal pressures, PPEST significantly reduced RMSE with respect to the trial-and-error approach as it passed from 4.7 to 1.9 m for the constrained scenario and 1.5 m for the unconstrained scenario. In all cases, RMSE for nodal pressures was higher than the 1 m accuracy expected for pressure gauges. The difference of roughly 0.4 m in RMSE between the two PPEST scenarios might seem trivial, but it does have profound implications in the optimization process.

As the method used in EPANET to solve the flow continuity and headloss equations is driven by nodal demands and energy losses (Rossman 2000), small measurement errors and large parameter spaces can lead to large errors in estimated parameters. This is clearly the case of the PPEST unconstrained scenario, where every single parameter was declared adjustable in PPEST (Table 3). These conditions defined an unmanageable parameter space of 723 parameters, which implied the optimization of every single nodal demand, demand pattern and minor loss coefficient in the system. The conditions stated for this scenario evidently forced PPEST to calibrate the model by compensating for errors as suggested by Walski (1986). Errors in nodal demands were most likely compensated by errors in demand patterns, minor loss coefficients, C-factors and pretty much any other adjustable parameter. The problem is aggravated by the fact that nodal demand is still the most uncertain and variable parameter in this case study. The large parameter space and considerable compensating errors resulted in a 1.5 m RMSE for nodal pressures, but also required considerable change in the individual nodal demands.

After the PPEST optimization, all nodes experienced some level of change in demand (Figure 3) with an absolute average change of 34.2%. Several nodes were pushed towards the predefined upper and lower demand bounds (Table 3). Over 40 nodes exhibited a −50% change in demand and over 50 nodes experienced a +50% change in demand. The parameter space was too big for PPEST to search effectively.

Total water demand for the system changed only slightly, as it passed from 10.58 to 10.47 ls^{-1} after the PPEST unconstrained optimization. This represents a percentage change in total water demand of around 1%. This reaffirms once more the presence of considerable compensating errors. In this respect, PPEST is most likely producing a numerically correct but physically meaningless solution. Furthermore, PPEST is possibly matching observations rather than determining the system's optimal parameters as there is an excessive number of parameter groups and insufficient observation data. Baranowski (2007) encountered similar conditions when calibrating nodal demands in two experimental EPANET networks using PEST and Newton-Raphson algorithms. Both methods maximized hydraulic and water quality standards but also required significant change in the nodal demands. C-factors had little chance to actively participate in the optimization process as one unique parameter was defined for all pipes.

An optimized C-factor value of 137 was found for all pipes that remain close to the C-factor values found for the two flow tests conducted in 69 mm PVC (130 and 134 correspondingly). At the end of the optimization process, the percentage change between trial-and-error and PPEST optimized values was 2.1% for local losses and 8.5% for

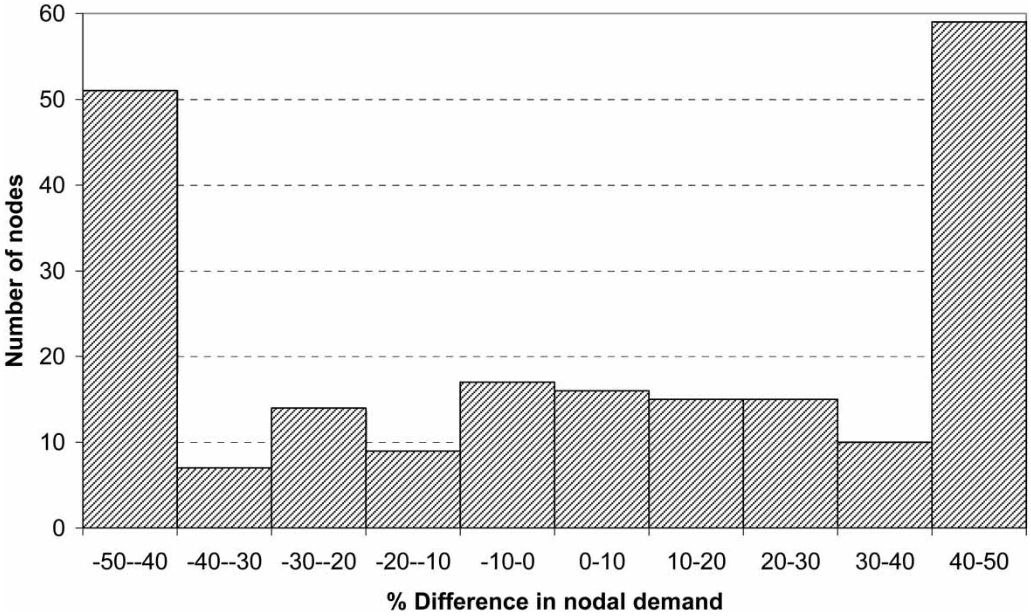

Figure 3 | Percent change for nodal demand after PPEST unconstrained optimization scenario.

FAVs. These percentages could seem small compared to those experienced by nodal demands or demand pattern factors; however, it is relative to the overall sensitivity of each adjustable parameter.

In the case of the PPEST constrained scenario, only 24 adjustable parameters were declared (Table 3). The remaining parameters were either fixed or tied to other parameters. In PEST, a tied parameter represents a parameter that is linked to a master parameter. In this case, only the master parameter is optimized and the tied parameters are simply varied with this parameter, maintaining a constant ratio, through the calibration process.

This represents a much smaller parameter space. Nodal demands were aggregated into four different demand groups, one for each pressure zone. Since demand pattern and minor loss coefficients were fixed, the solution of the parameter space was limited to four nodal demands (four parameters), four FAV valves (12 parameters) and eight C-factors (eight parameters). In this case, the absolute average change of nodal demand was 13.4%, much lower than the 34.2% found for the unconstrained scenario. None of the nodes were pushed towards the predefined upper and lower demand bounds. This would appear to be the result of compensating errors from the C-factors group (Table 5).

Table 5 | Optimized C-factor values after PPEST constrained optimization scenario

Pipe internal diameter (mm)	Initial C-factor	PEST optimized C-factor
84	136	136
69	136	137
57	136	136
45	136	142
40	136	142
31	136	136
25	136	142
19	136	136

Nevertheless, almost all diameter groups remained in the lower bound of 130. Only pipes with internal diameters of 69 and 45 mm were moved to higher values (138 and 150, respectively). Since demand patterns and minor loss coefficients were fixed, compensating errors for this scenario are considerably lower than those of the unconstrained scenario. For instance, this solution is more physically correct as PPEST had a higher chance to find the optimum set of parameter values. Still, no validation data exist to sustain this statement. Maslia *et al.* (2009) experienced comparable results in their analysis of Holcomb Boulevard WDS as PVC C-factor change from its original 145 proposed value to an optimized range of 147–151 optimized values. This is more likely to be a consequence of the inherent smoothness of plastic materials and low relative sensibility as compared to other materials such as cast iron or steel which are greatly affected by age, corrosion and deposition processes (Koppel & Vassiljev 2009).

Total system water demand also changed only slightly, as it passed from 10.58 to 10.50 ls^{-1} for the PPEST constrained scenario. Regarding temporal variation of water levels at WSTs, a closer match between observed and modeled values can be appreciated for the PPEST scenarios (Figure 4). This is particularly true for WSTs 1 and 3 (Figure 4(a),(c)), whereas little difference can be seen for tanks 2 and 4 (Figure 4(b),(d)) regardless of the optimization approach. The PPEST unconstrained scenario was partly based on the adjustment of the demand pattern factors (Table 3).

PPEST optimized weekday demand factors are generally in good agreement with those initially obtained by analyzing diurnal dynamics of water demand, particularly for WSTs 1 and 3 (Figure 5(a),(c)).

There are, however, local differences that show a larger variation around the hours of higher water demand, between 0900 and 1400 hr, principally for WSTs 2 and 4 (Figure 5(b),(d)). This could be attributed to the relative sensitivity of those pattern factors. Nonetheless, little confidence can be attributed to these patterns as compensating errors are very high for the PPEST unconstrained scenario.

Parameter sensitivity

As calculated by PPEST, the WDS model is mostly sensitive to nodal demands since this group of parameters exhibits the highest average composite sensitivities for both constrained and unconstrained scenarios, 2.86 and 2.26×10^{-1}, respectively (Table 6). As discussed above, EPANET is controlled by water

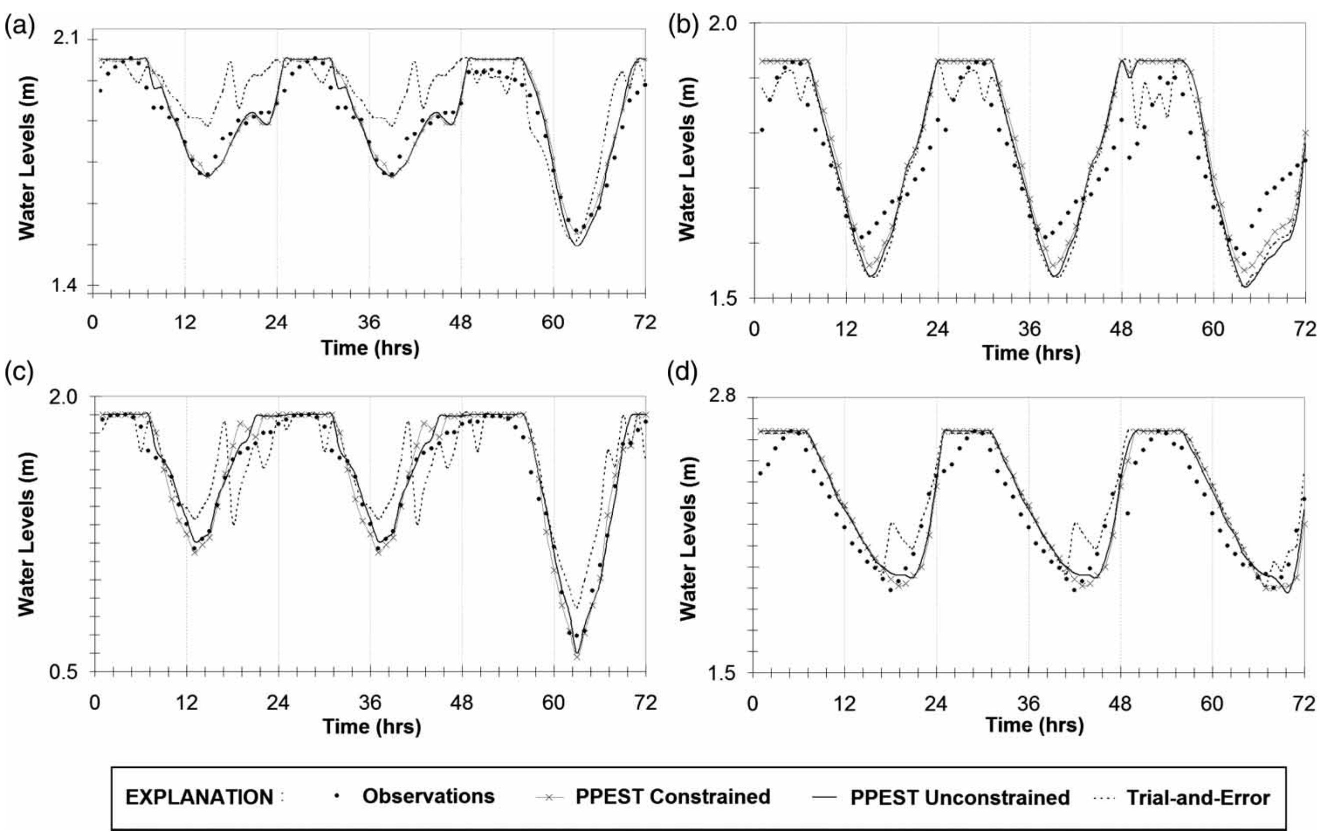

Figure 4 | PPEST optimized water-level values for a time lapse of 72-hr.

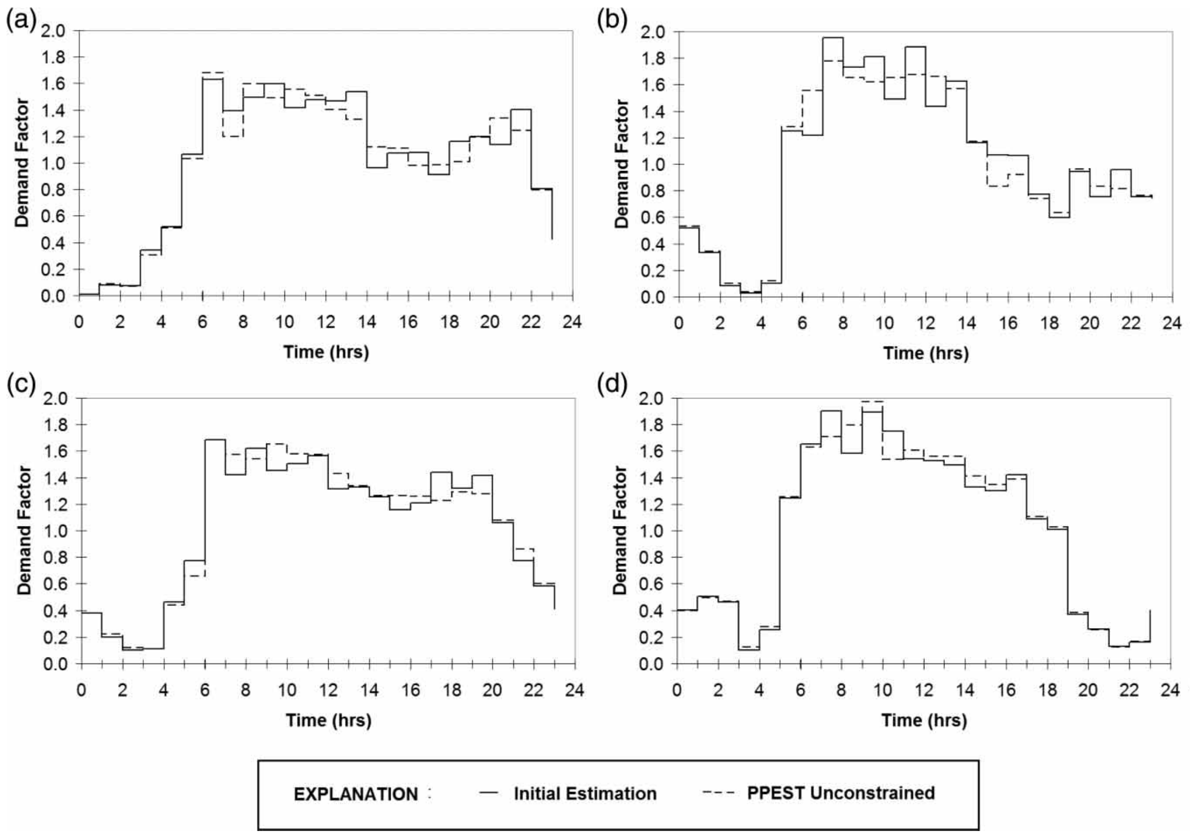

Figure 5 | Initially estimated versus PPEST unconstrained optimized weekday demand pattern factors.

Table 6 | Average composite sensitivity per parameter group for PPEST constrained and unconstrained scenarios

Parameter group	Average PPEST composite sensitivity Constrained run	Unconstrained run
Demand patterns factors	Not applicable	4.62×10^{-3}
Nodal demands multiplier	2.86	2.26×10^{-1}
Minor loss coefficients (Ks)	Not applicable	5.09×10^{-3}
Float Actuated Valves (FAVs) loss coefficients	1.80×10^{-2}	2.59×10^{-2}
C-factors	1.37×10^{-4}	2.54×10^{-4}

demand and energy losses and it is therefore predictable that nodal demand represents the most sensitive group of parameter.

The FAVs loss coefficients represent the second most sensitive group of parameters, as their average composite sensitivity reach values of 1.80×10^{-2} and 2.5980×10^{-2} for the constrained and unconstrained scenarios, respectively. This is also expected since FAVs strongly control flow admission to WSTs. In the case of the unconstrained scenario, demand pattern factors and minor loss coefficients have very low composite sensitivities, 4.6280×10^{-3} and 5.0980×10^{-3}, respectively. However, they represented a group of 471 insensitive adjustable parameters that clearly introduced significant compensating errors in the optimization process. This suggests once more that only sensitive parameters should be taken into consideration.

Finally, the C-factors exhibited an extremely low sensitivity, with both scenarios in the order of 1.3780×10^{-4} and 2.5480×10^{-4}, almost four orders of magnitude less important than nodal demands. Again, this is probably due to the inherent low roughness of PVC. Walski *et al.* (2004) have demonstrated that roughness associated to C-factors are only determinant if sufficient head loss is experienced across the WDS. This is clearly not our case, as velocities and head losses are quite small most of the time.

Objective function

From a practical standpoint, it is essential to assess the number of model calls that PPEST required to minimize its objective function PHI (Φ). For the unconstrained scenario, PPEST needed to run EPANET 6507 times in order to find what PPEST considers to be the global minimum.

This global minimum was found after the fifth iteration, achieving a PHI reduction of nearly 77%, as its initial value was reduced from 7.77 to 1.817 m^2. As stated by Goegebeur & Pauwels (2007), even when PHI differs from RMSE, the minimization of this function also leads to a minimization of the RMSE (Table 4).

After running in estimation-mode, PPEST executed four additional iterations after the global minimum was found, just to ensure that it did not encounter a local minimum. A total of 10,845 EPANET calls were needed to complete the optimization process, which lasted for 13.2 hr, clearly indicating a high computational burden. If PEST instead of PPEST had been used in this case, an estimated 90.4 hr run would have been needed to accomplish the same result. This is quite predictable as PEST's final report states how long it needs to complete one EPANET's run.

For the more realistic and physically correct constrained scenario, PPEST completed the whole optimization process in 0.74 hr, almost 18 times faster than the unconstrained scenario and with similar outcomes as PHI was reduced from its original trial-and-error value of 7.77–2.065 m^2.

The most time consuming part of PPEST's operations is related to the calculation of the Jacobian matrix through partial derivatives, which requires two model calls for each adjustable parameter. Nonetheless, the calculation of the Jacobian matrix permits PPEST to derive important by-products such as relative and absolute sensitivity, correlation, uncertainty and Eigenvectors which are of great importance in post-optimization analysis.

On the other hand, PPEST is capable of fixing parameters based on a given sensitivity threshold. This could help improve PPEST's performance through modeler intervention (Doherty 2005). Finally, it is important to note that EPANET is a fully distributed complex hydraulic solver which demands a great deal of computational resources by itself. This clearly increases the time lapse needed for PPEST to achieve convergence.

CONCLUSIONS

The feasibility of using the model independent parameter estimator PPEST to develop a fully-calibrated extended period model for a WDS using EPANET was investigated. It was found that the results from a fully automated calibration technique like PPEST should be used with caution.

As calibration is a highly underdetermined problem, PPEST may produce numerically correct but physically meaningless solutions if insufficient restrictions are applied. The two PPEST scenarios analyzed in this study further emphasize this situation.

The unconstrained scenario showed that if all parameters are open to adjustment, considerable compensating errors are introduced into the optimization process. Under these circumstances, PPEST was capable of matching observations but incapable of determining the optimum set of parameters for the system. As the number of unknowns was much greater than the number of observations, the parameter space was simply too large for PPEST to find a proper solution. It was demonstrated that including insensitive parameters significantly deteriorates model's solutions and imposed a heavy computational burden on the whole optimization process.

On the other hand, the constrained scenario represents a more properly discretized and therefore, more reliable scheme as parameters were grouped in classes of similar characteristics and insensitive parameters were fixed. This had a profound impact on the parameter space as adjustable parameters were reduced from 723 in the unconstrained scenario to 24 in the constrained scenario. In this regard, the computational requirements were much lower as the whole optimization process took 0.74 hr as compared to the 13.2 hr needed for the unconstrained scenario.

The model was mainly sensitive to nodal demands as average composite sensitivities for both constrained and unconstrained PPEST scenarios reached 2.86 and 2.26×10^{-1}, respectively. The FAVs loss coefficients represented the second most sensitive group of parameters as their average composite sensitivity reached values of 1.8080×10^{-2} and 2.5980×10^{-2} for the constrained and unconstrained PEST scenarios, respectively. The remaining groups of parameters, including C-factors, showed very low sensitivities, two to three orders in magnitude lower than that of nodal demands. A considerable RMSE reduction was obtained for the constrained scenario, particularly for nodal pressures as its value decreased from 4.68 to 1.85 m.

The constrained solution, even when it is valid only for the system's normal operating conditions, clearly demonstrates that PPEST has the potential to be used in the calibration of WDS models.

FUTURE WORK

Further investigation is needed to determine PPEST's performance in complex WDS models over a wide range of operating conditions. This may include the evaluation of control valves, pump curves, control rules and water quality issues. An EPANET-PEST utility software could be developed to facilitate communication between both packages. This would allow users to run PEST directly in a graphical environment, where many of the variables and outcomes of the calibration process could be viewed and externally manipulated.

ACKNOWLEDGMENTS

The authors wish to thank Junta Administradora del Acueducto La Sirena, La comunidad de la Sirena, Estación de Investigación y Transferencia de Tecnología de Puerto Mallarino and Cinara-Universidad del Valle for their help and guidance in the development of this project.

REFERENCES

Abe, N. & Cheung, P. B. 2010 Epanet Calibrator – an integrated computational tool to calibrate hydraulic models. *Int. Water Syst.* **V**, 129–133.

Alvisi, S. & Franchini, M. 2010 Pipe roughness calibration in water distribution systems using grey numbers. *J. Hydroinf.* **12**, 424–445.

Arabi, M., Govindaraju, R. S. & Hantush, M. M. 2007 A probabilistic approach for analysis of uncertainty in the evaluation of watershed management practice. *J. Hydrol.* **333**, 459–471.

Bahremand, A. & de Smedt, F. 2010 Predictive analysis and simulation uncertainty of a distributed hydrological model. *J. Water Res. Manage.* **24**, 2869–2880.

Baranowski, T. 2007 Development of Consequence Management Strategies for Water Distribution Systems. Doctoral Dissertation, Graduate School of Vanderbilt University, Nashville, Tennessee, USA.

Beven, K. & Binley, A. 1992 The future of distributed models: model calibration and uncertainty prediction. *Hydrol. Process.* **6**, 279–298.

Cabrera, E., Espert, V., Garcia-Serra, J. & Martinez, F. 1996 *Ingenieria hidráulica, Aplicada a los sistemas de distribución de agua*. Universidad Politecnica de Valencia, Spain.

Christensen, S. & Doherty, B. 2008 Predictive error dependencies when using pilot points and singular value decomposition in groundwater model calibration. *Adv. Water Resour.* **31**, 674–700.

de Schaetzen, W., Hung, J., Clark, S., Gottfred, C., Acosta, B. & Reynolds, P. 2010 How much is your uncalibrated model costing your utility? Ten lessons learned from calibrating the CRD Water Model. In *Proc. Water Distribution System Análisis* (A. Z. Tucson, ed.). USA, Sept. 12–15, pp. 1053–1065.

Doherty, J. 2005 *PEST: Model Independent Parameter Estimation Users Manual*. Watermark Numerical Computing, Brisbane.

Duan, Q., Sorooshian, S. & Gupta, V. K. 1992 Effective and efficient global optimization for conceptual rainfall runoff models. *Water Resour. Res.* **24**, 1163–1173.

Fang, T. & Ball, J. E. 2007 Evaluation of spatially variable control parameters in a complex catchment modelling system: a genetic algorithm application. *J. Hydroinf.* **9**, 163–174.

Gallagher, M. R. & Doherty, J. 2007 Parameter interdependence and uncertainty induced by lumping in a hydrologic model. *Water Resour. Res.* **43**, 1–18.

Giustolisi, O. & Berardi, L. 2011 Water distribution network calibration using enhanced GGA and topological analysis. *J. Hydroinf.* **13**, 621–641.

Goegebeur, M. & Pauwels, R. N. 2007 Improvement of the PEST parameter estimation algorithm through Extended Kalman Filtering. *J. Hydrol.* **337**, 436–451.

Hogue, T., Gupta, H. & Sorooshianc, S. 2006 A 'User-Friendly' approach to parameter estimation in hydrologic models. *J. Hydrol.* **320**, 202–217.

Ibrahim, Y. & Liong, S. Y. 1992 Calibration strategy for urban catchment parameters. *ASCE J. Hydraul. Eng.* **118**, 1550–1570.

Immerzeel, W. W. & Droogers, P. 2008 Calibration of a distributed hydrological model based on satellite evapotranspiration. *J. Hydrol.* **349**, 411–424.

Jamasb, M., Tabesh, M. & Rahimi, M. 2008 Calibration of EPANET using Genetic Algorithm. In *Proc. 10th Annual Water Distribution Systems Analysis Conference*, Kruger

National Park, South Africa, August 17–20th, 2008, pp. 881–889.
Kang, D. & Lansey, K. 2009 Real-time demand estimation and confidence limit analysis for water distribution systems. *ASCE J. Hydraul. Eng.* **135**, 825–837.
Kapelan, Z., Savic, D. A. & Walters, G. A. 2007 Calibration of water distribution hydraulic models using a Bayesian-Type procedure. *ASCE J. Hydraul. Eng.* **133**, 927–936.
Kenward, T. C. & Howard, C. D. 1999 Forecasting for urban water demand management. In *Proc. Annual Water Resources Planning and Management Conf.*, ASCE, Tempe, Arizona, USA. June 6–9th, 1999, ch. 9A188, pp. 1–15.
Khu, S. T., di Pierro, F., Savic, D., Djordjevic, S. & Walters, G. A. 2006 Incorporating spatial and temporal information for urban drainage model calibration: an approach using preference ordering genetic algorithm. *Adv. Water Res.* **29**, 1168–1181.
Koppel, A. & Vassiljev, A. 2009 Calibration of a model of an operational water distribution system containing pipes of different age. *Adv. Eng. Softw.* **40**, 659–664.
Kovalenko, Y., Gorev, N. B., Kodzhespirova, I. F., Álvarez, R., Prokhorov, E. & Ramos, A. 2010 Experimental analysis of hydraulic solver convergence with Genetic Algorithms. *ASCE J. Hydraul. Eng.* **136**, 331–335.
Kumar, S. M., Narasimhan, S. & Bhallamudi, S. M. 2009 Parameter estimation in water distribution networks. *J. Water Res. Manage.* **24**, 1251–1272.
Lansey, K. E. & Basnet, C. 1991 Parameter estimation for water distribution networks. *ASCE J. Water Res. Plann. Manage.* **117**, 126–144.
Lee, E. J. & Schwab, K. J. 2005 Deficiencies in drinking water distribution systems in developing countries. *J. Water Health* **3**, 109–127.
Machell, J., Mounce, S. R. & Boxall, J. B. 2010 Online modelling of water distribution systems: a UK case study. *Drink. Water Eng. Sci.* **3**, 21–27.
Maslia, M. L., Suárez-Soto, R. J., Wang, J., Aral, M. M., Faye, R. E., Sautner, J. B., Valenzuela, C. & Grayman, W. M. 2009 *Analysis of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions*. Agency for Toxic Substances and Disease Registry. US Department of Health and Human Services, Atlanta, Georgia.
Mays, L. W. 2000 *Water Distribution Systems Handbook*. McGraw-Hill, New York.
Nicklow, J. W., Reed, P., Savic, D. A., Dessalegne, T., Harrell, L., Chan-Hilton, A., Karamouz, M., Minsker, B., Ostfeld, A., Singh, A. & Zechman, A. 2009 State of the art for genetic algorithms and beyond in water resources planning and management. *ASCE J. Water Res. Plann. Manage.* **136**, 412–432.
Peng, S., Wu, Q. & Zhuang, B. 2009 Parameter identification by MCMC method for water quality model of distribution system. In *Proc. 3th International Conference on Bioinformatics and Biomedical Engineering*, Beijing, China, June 11–13th, 2009, pp. 1–5.
Rossman, L. A. 2000 *EPANET 2 Users Manual*. National Risk Management Research Laboratory, Office of Research and Development. US Environmental Protection Agency, Cincinnati, Ohio, USA.
Savic, D. A., Kapelan, Z. & Jonkergouw, P. 2009 Quo vadis water distribution model calibration? *Urban Water J.* **6**, 3–22.
Skahill, B. E. 2009 More efficient PEST compatible model independent model calibration. *J. Environ. Model. Softw.* **24**, 517–529.
Skahill, B. E. & Doherty, J. 2006 An advanced regularization methodology for use in watershed model calibration. *J. Hydrol.* **327**, 564–577.
Tischler, M., Garcia, M., Peters-Lidard, C., Moran, M. S., Miller, S., Thoma, D., Kumar, S. & Geiger, J. 2007 A GIS framework for surface-layer soil moisture estimation combining satellite radar measurements and land surface modeling with soil physical property estimation. *J. Environ. Model. Softw.* **22**, 891–898.
USEPA 2005 *Water Distribution System Analysis: Field Studies, Modeling and Management: A Reference Guide for Utilities*. Office of Research and Development. National Risk Management Research Laboratory, Water Supply and Water Resources Division, Cincinnati, Ohio, USA.
Walski, T. M. 1986 Case study: pipe network model calibration issues. *ASCE J. Water Res. Plann. Manage.* **112**, 238–249.
Walski, T., DeFrank, N., Voglino, T., Wood, R. & Whitman, B. E. 2006 Determining the accuracy of automated calibration of pipe network models. In *Proc. 8th Annual Water Distribution Systems Analysis Symposium*, Cincinnati, Ohio, USA, August 27–30th, 2006, pp. 1–18.
Walski, T., Wu, Z. & Hartell, W. 2004 Performance of automated calibration for water distribution systems. In *Proc. World Water and Environmental Resources Congress*, Salt Lake City, Utah, USA, June 27th–July 1st, 2004, pp. 1–10.
Walski, T. M., Chase, D. V. & Savic, D. A. 2001 *Water Distribution Modeling*. Haestad Press, Waterbury.
Wu, Z. Y., Boulos, P. F., Orr, C. H. & Ro, J. J. 2000 An efficient genetic algorithms approach to an intelligent decision support system for water distribution networks. In *Proc. Hydroinformatics 2000 Conference*, Iowa, IW, USA, July 23–27th, 2000.
Wu, Z. Y., Walski, T. M., Mankowski, R., Herrin, G., Gurrieri, R. & Tryby, M. 2002 Calibrating water distribution model via genetic algorithms. In *Proc. AWWA IMTech Conference*, Kansas City, Missouri, USA, April 14–17th, 2002, pp. 1–10.
Zaghloul, N. A. & Abu Kiefa, M. A. 2001 Neural network solution of inverse parameters used in the sensitivity-calibration analyses of the SWMM model simulations. *Adv. Eng. Softw.* **32**, 587–595.
Zhou, S. L., McMahon, T. A. & Lewis, W. J. 2000 Forecasting daily urban water demand: a case study of Melbourne. *J. Hydrol.* **236**, 153–164.

First received 8 February 2012; accepted in revised form 19 May 2012. Available online 11 September 2012