

Chlorine Decay Model Calibration and Comparison: Application to a Real Water Network

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Abstract

This work presents a methodology to efficiently calibrate chlorine decay models. The calibration consists in estimating the unknown parameters by comparing the measured and simulated chlorine concentrations at the monitored nodes within the distribution system in a least square sense using a normalized quadratic cost function. Since this function involves a non-explicit expression of the model, a genetic algorithm (GA) is applied to optimize the model parameters by minimizing the difference between the model-predicted values and the field-measured ones. The method is applied to a part of the Barcelona drinking water network.

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1. Introduction

A water quality model is a reliable tool only if it is able to predict the real system behavior (Yi Wu, 2006). In addition, water quality modeling within water distribution systems is not an easy task because a hydraulic model analysis has to be performed previously in order to provide the resulting flow distribution to the water quality module to transport the chlorine through the system. The predicted chlorine concentrations within a distribution system are governed by bulk and wall reaction parameters. Bulk decay coefficients for chlorine depend on the nature of the source water and the treatment it has received while wall decay coefficients depend on the pipe material and its condition. It is generally assumed that chlorine evolution in a water distribution system can be described by a first-order kinetic model. But the bulk decay parameter can also be non first-order and some more reliable alternatives have been presented in some recent works (Clark, 1998; Boccelli et al., 2003).

In water quality model calibration, some of the parameters can be determined by laboratory test and others have to be estimated by field measurements. Since manual trial and error method (Clark et al., 1995) is time consuming, automated calibration procedure for those parameters is expected to perform well. Zeirolf et al. (1998) illustrated the use of input–output models for chlorine transport to estimate the first-order (global and zoned) wall reaction parameter. The model is applicable only for first-order reaction kinetics, and does not incorporate storage tanks and multiple water quality sources. Al-Omari and Chaudhry (2001) used finite difference procedures for the

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determination of the overall first-order chlorine decay coefficient. Munavalli and Mohan Kumar (2003) developed an inverse model, which estimates the various reaction parameters in a multi-source steady-state distribution system.

This work presents a methodology that enables to efficiently calibrate a water quality model such that the field measured water quality values match with the simulated ones. The calibration of the chlorine model consists in estimating the unknown parameters by comparing the measured and simulated chlorine concentrations at the monitoring nodes within the water distribution system in a least square fashion with a normalized quadratic cost function. Since this function involves a non-explicit expression of the model, a GA is applied to optimize the model parameters by minimizing the difference between the model-predicted values and the field-observed ones.

The method is applied to a part of the Barcelona drinking water network and demonstrated that a water quality model can be optimized for managing adequate water supply to consumers and to perform further monitoring tasks (e.g. abnormal chlorine levels) in a more reliable way (Nejjari et al. 2011).

The strategy consists in dividing the area under study in different zones and then estimating the chlorine bulk coefficients taking into account one or two-source water distribution systems. A comparative study taking into account chlorine decay models that are based on first-order decay, second order decay and combined first-second order decay (Chang et al., 2006) have been considered. The methodology represents accurately the process in the network, improving the water quality prediction in the area of study and allowing the establishment of zones where the chlorine decay was significant. The simulations have been performed using the EPANET-MSX software package.

2. Chlorine decay models

In water distribution systems, chlorine decays over time as it reacts with organic materials in the water. A number of models have been developed to predict chlorine decay in drinking water networks (Clark, 1998, Boccelli et al., 2003, Powell et al., 2000). Generally, they can be divided into first order and non first order reaction kinetic models. The first order decay model has been mostly used because of its simplicity and its reasonable accuracy to represent chlorine decay in water systems. The first-order chlorine decay model includes expressions to describe reactions occurring in the bulk fluid and at the pipe wall. The differential form of the decay model is given by:

$$\frac{dC}{dt} = -k \cdot C \quad (1)$$

where k is the decay rate and C is the chlorine concentration at a certain time t .

Clark (1998) developed a second-order chlorine decay model based on the concept of competing reacting substances, while Hua et al. (1999) proposed a semi-empirical combined first-order and second-order model, which provides a good description of the chlorine decay as follows

$$\frac{dC}{dt} = -k_R \cdot C^2 - k_S \cdot C \quad (2)$$

where the decay constants k_R and k_S are the functions of the overall decay constant k and are determined by deriving the best fitting of Eq. (2) with the experimental data. In this work both models have been used and the results of calibration have been compared with the real data.

3. Chlorine decay model calibration

The chlorine decay model has been calibrated by means of solving a least-squares problem that leads to an optimization problem. Since this involves a non-explicit expression of the model, the problem has been solved using Genetic Algorithms (GA). The GA and Direct Search Toolbox included in the Matlab R2009a release have been used in this work. In order to simulate the hydraulic model, public domain EPANET solver has been used while the chlorine evolution simulations have been performed with an extension of this program called EPANET-MSX, which is focused on water quality simulations and allows more detailed settings (e.g. species decay model structure) than classical EPANET water quality solver. Both software packages have been linked through the EPANET-toolkit.

The calibration has been performed by formulating a least-squares problem with the normalized quadratic cost function given by

$$J(\theta) = \frac{1}{N \cdot S} \cdot \sum_{t=1}^N \sum_{s=1}^S (C_s(t) - \hat{C}_s(t, \theta))^2 \quad (3)$$

where θ are the quality parameters (bulk decay coefficients) to be tuned, N is the number of measurements, S is the number of sensors, $C_s(t)$ is the chlorine measurement for a sensor s at a certain instant t and $\hat{C}_s(t, \theta)$ is its estimation using a particular chlorine decay model. To solve the previous least squares problem, the optimization problem in (4) is solved

$$\begin{aligned} & \min_{\theta} J(\theta) \\ & \text{s.t.} \\ & \hat{C}_s(t, \theta) = \text{EPANET_MSX_simulation}(t, \theta) \end{aligned} \quad (4)$$

Notice that since the estimation of the sensor measurement $\hat{C}_s(t, \theta)$ using a particular chlorine decay model requires a simulation using EPANET MSX, the previous optimization problem does not have an analytical expression. Thus, it must be solved using some heuristic approach such as GAs (The MathWorks, Inc. (2009)).

The percentage error is obtained using the validation period of data as follows

$$e_v = \left[1 - \left(\frac{\max(C_{s_v}(t)) - \sqrt{J_v}}{\max(C_{s_v}(t))} \right) \right] \cdot 100 \quad (5)$$

where $\max(C_{s_v}(t))$ is the maximum measured value in the validation period among all the sensors used for calibration and J_v is the cost index in Eq. (3) obtained using validation data.

The performance index (5) is useful in order to compare between different models and to evaluate the fit obtained between a particular calibrated model and the measured data.

4. Network of study

4.1. Network description

The case study in this work (Fig. 1) is a part of the Barcelona water transport network, a vast network of 4480 Km of pipes which is divided in 113 different pressure floors. It corresponds to the floor 55th and has 438 nodes

and 453 pipes. There are two inflows (i.e. Cantàbria and Drassanes) where flow, pressure and chlorine concentration are measured and four outputs (Llull, Àlaba, Passeig Colon and Joan de Borbó) where these variables are monitored as well.

The flow and pressure data of these control points together with the data provided for some relevant demands allow the hydraulic adjustment of the model. Once the hydraulic model is available the chlorine information is used for the chlorine model calibration.

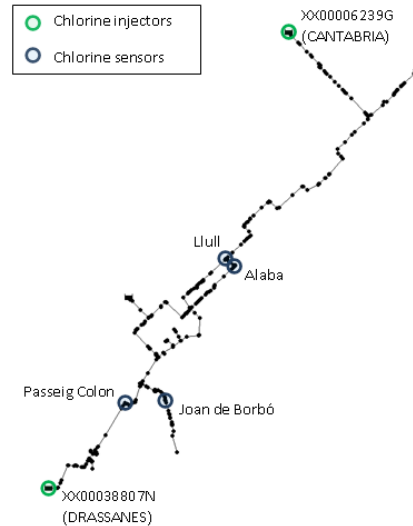


Fig. 1. Pressure floor 55th in Barcelona water transport network

4.2. Hydraulic Model Validation

To achieve a good water quality calibration, a well calibrated hydraulic model is essential before starting water quality calibration. The accuracy of water quality simulation relies on the hydraulic simulation results.

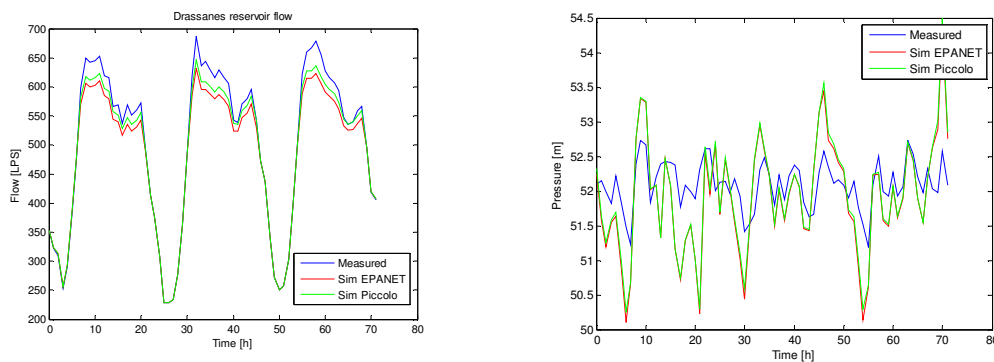


Fig. 2. Comparison between measured and simulated flows and pressures in Drassanes and Cantàbria reservoirs

From the hydraulic point of view, the network selected has two inputs, called Cantàbria and Drassanes, and 21 measured points. In order to simulate it isolated, the boundary conditions have to be fixed. Boundary conditions are pressures and flows that are measured every hour at the network inputs. Pressures are fixed in the reservoir Drassanes and flow in the reservoir of Cantàbria. After the hydraulic simulation, the resulting flows and pressures

at Drassanes and Cantàbria are obtained and compared with the measured values, sampled every hour. In Fig. 2, a comparison between flows and pressures corresponding to the time range from 07/09/2010 (at 00h) to 09/09/2010 (at 23h) in Drassanes and Cantàbria reservoirs is depicted. The results obtained with the EPANET/PICCOLO simulators show a good validation and calibration of the hydraulic model when comparing with the measured data.

5. Chlorine decay calibration

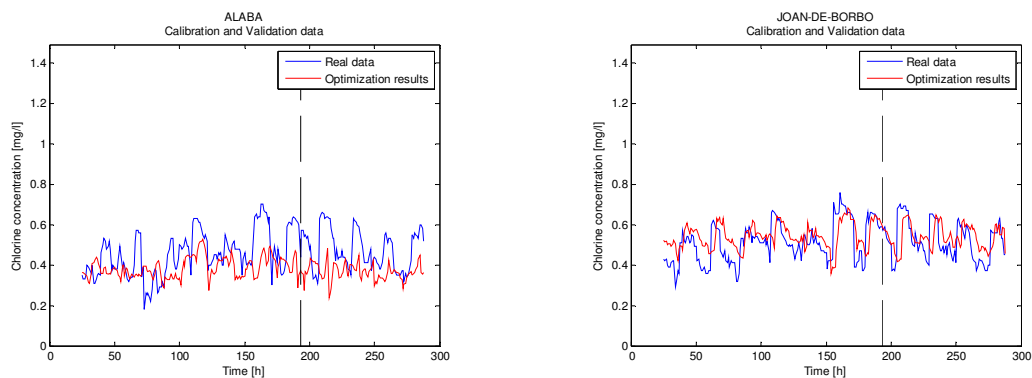
The chlorine concentration data used is hourly sampled, measured from 03/09/2010 (at 00h) to 14/09/2010 (at 23h) in the sensors installed in the actual DMA (Fig. 1). In order to perform the chlorine model calibration, the first 24 hours of data are used to let the chlorine getting stabilized in the DMA. Hence, the data within this period is not used to calibrate the chlorine decay model (from 2010-09-03 00:00:00 to 2010-09-03 23:00:00). The measurements comprised between 2010-09-04 00:00:00 and 2010-09-10 23:00:00 (7 days) have been used to calibrate the chlorine model, and the data comprised between 2010-09-11 00:00:00 and 2010-09-14 23:00:00 (4 days) have been used to validate the model. In this calibration process, real chlorine measurements in Cantàbria and Drassanes have been considered in the simulations as the injected chlorine in the network. These simulations have been used to obtain a chlorine decay model parameters. Measurements in the four current available sensors in Fig.1 have been considered to minimize the cost index (3).

The figures in this section show the results obtained using the whole period of data (i.e. calibration and validation) testing the model obtained in the calibration period (i.e. from 2010-09-04 00:00:00 to 2010-09-10 23:00:00). In all these figures, the boundary between calibration and validation periods is depicted with a dashed line.

Due to a lack of space only the figures that show the results obtained using a combined first and second order chlorine decay model are presented. However the results for the different chlorine decay models are summed up in Table 1.

5.1. Single-Zone Combined First-Second Order Model Calibration

The optimization variable in this case is $\theta = [k_R \ k_S]$. The calibration gave the following optimal chlorine decay constants, $k_R = 2.9319$ [1/day] and $k_S = 0.04688$ [1/day]. The cost value obtained for the calibrated single-zone combined first-second order chlorine decay model is $J = 0.022335$. The corresponding average percentage error is $e = 16.36$ %. As it may be observed from the results obtained and from Fig. 3, the cost obtained and the fit achieved in the measurement points with this particular model are better than the ones attained using the single-zone first-order chlorine decay model (see Table 1).



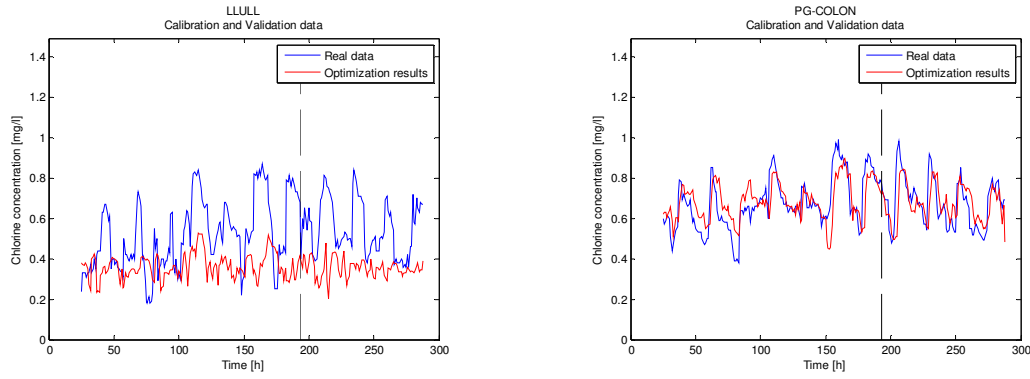


Fig. 3. Validation of a single-zone combined first-second order chlorine decay model in pressure floor 55th network

5.2. Two-Zones vs. Single-Zone approach

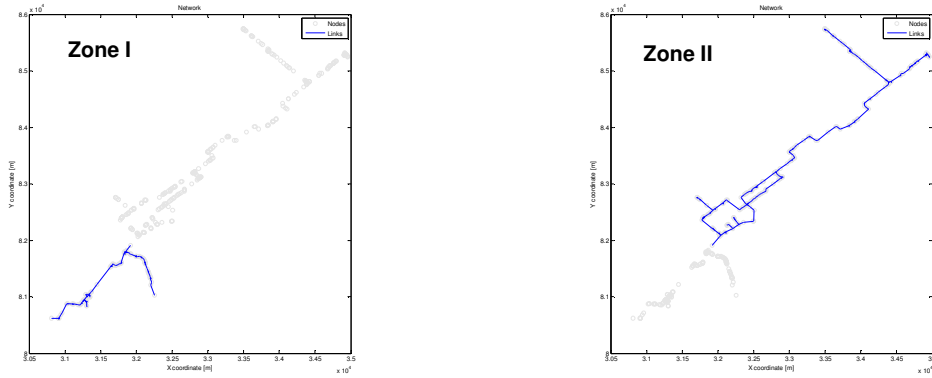


Fig. 4. Two-zones selected in pressure floor 55th network, with different chlorine decay model each

The results presented in this section show how, while in Joan de Borbó and Passeig Colon measurement points a reasonable good fit between real data and the computed values is achieved, in Alaba and Llull measurement points the model fit is not that good. This may happen because Joan de Borbó and Passeig Colon always receive chlorinated water from a single water source whilst Alaba and Llull may receive chlorinated water from two different sources (e.g. Drassanes and Cantàbria) depending on the network demands in a particular time. A possible and more accurate approach to model this behavior is to divide the network in two different zones, southern (Zone I) and northern (Zone II), and assign a different chlorine decay model to each one. The two selected zones are depicted in Fig. 4.

5.3. Two-Zones Combined First-Second Order Model Calibration

The optimization variable in this case is $\theta = [k_{R_1} \quad k_{S_1} \quad k_{R_2} \quad k_{S_2}]$. The obtained optimal chlorine decay constants after the calibration process for the two different zones are presented in Table 1. The cost value obtained for the calibrated two zones using the combined first-second order chlorine decay model is $J = 0.022504$. The

corresponding average percentage error is $e = 16.53 \%$.

It may be observed how the effect of the first order part in Zone I (k_{S1}) is not important while the first order part in Zone II (k_{S2}) seems to be not negligible (see Table 1). In this case, a better fit in *Alaba* and *Llull* measurement points is provided in comparison with previous calibrations, as may be noticed in Fig. 5.

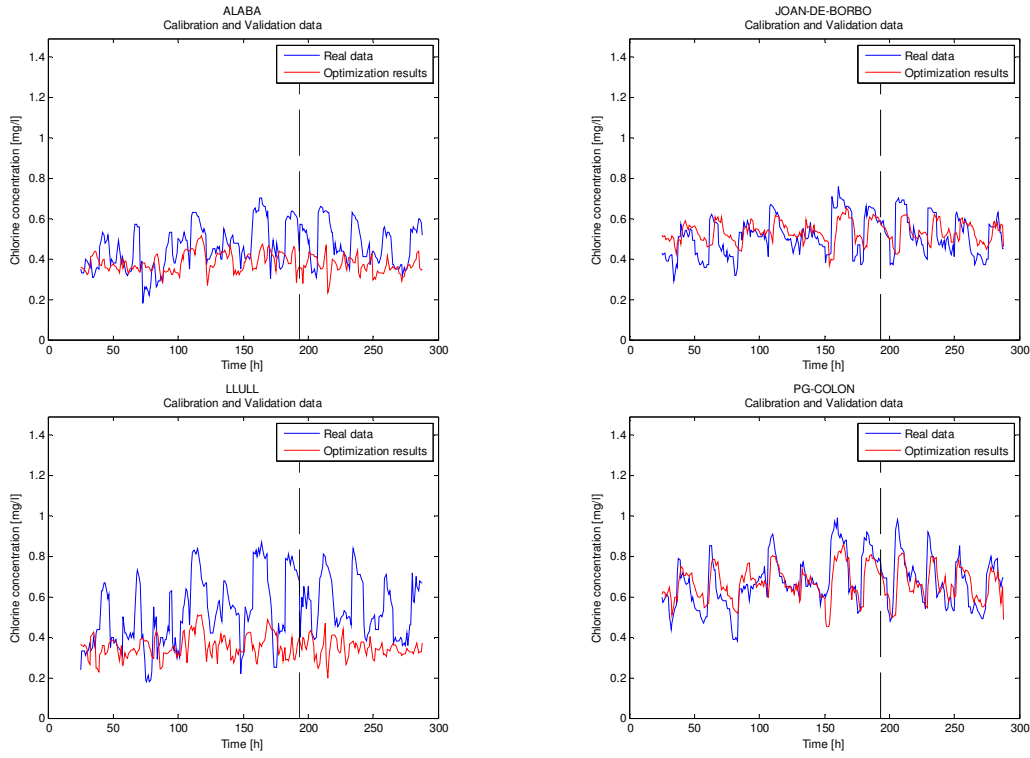


Fig. 5. Validation of two-zones combined first-second order chlorine decay model in pressure floor 55th network

5.4. Three-Zones approach

In this case, an extra zone is added in aims of providing a better model of the chlorine decay through the network in Fig. 1. The new zone distribution considered is shown in Fig. 6.

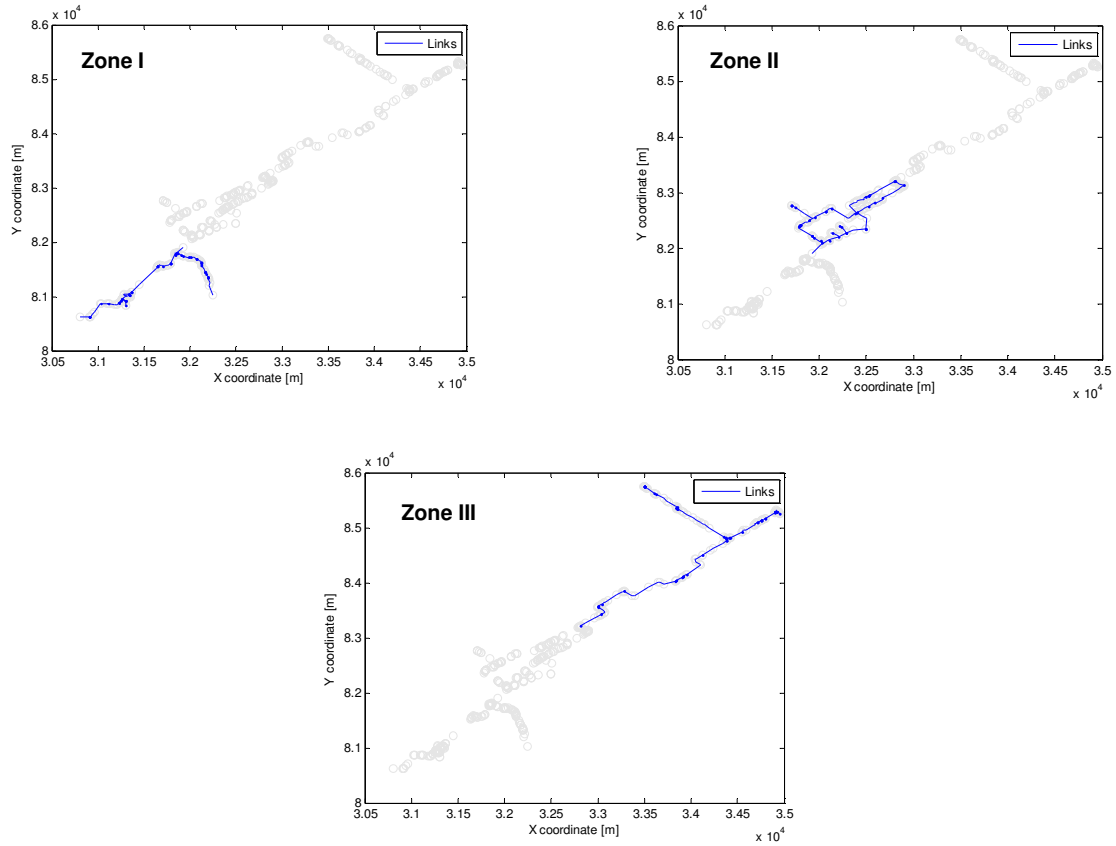


Fig. 6. Three zones selected in pressure floor 55th network, with different chlorine decay model

5.5. Three-Zones Combined First-Second Order Model Calibration

The optimization variable in this case is $\theta = [k_{R_1} \ k_{S_1} \ k_{R_2} \ k_{S_2} \ k_{R_3} \ k_{S_3}]$. In this particular approach, different chlorine decay models have been calibrated for the different zones in Fig. 6. The obtained optimal chlorine decay constants after the calibration process for the three different zones are presented in Table 1. The cost value obtained for the calibrated two zones using the combined first-second order chlorine decay model is $J = 0.017009$. The corresponding average percentage error is $e = 12.78 \%$. This is the best model fit achieved in comparison to the previous chlorine decay models presented. As can be seen in Fig. 7, a better fit in *Alaba* and *Llull* measurement points is provided in comparison with previous calibrations considering one or two zones approaches.

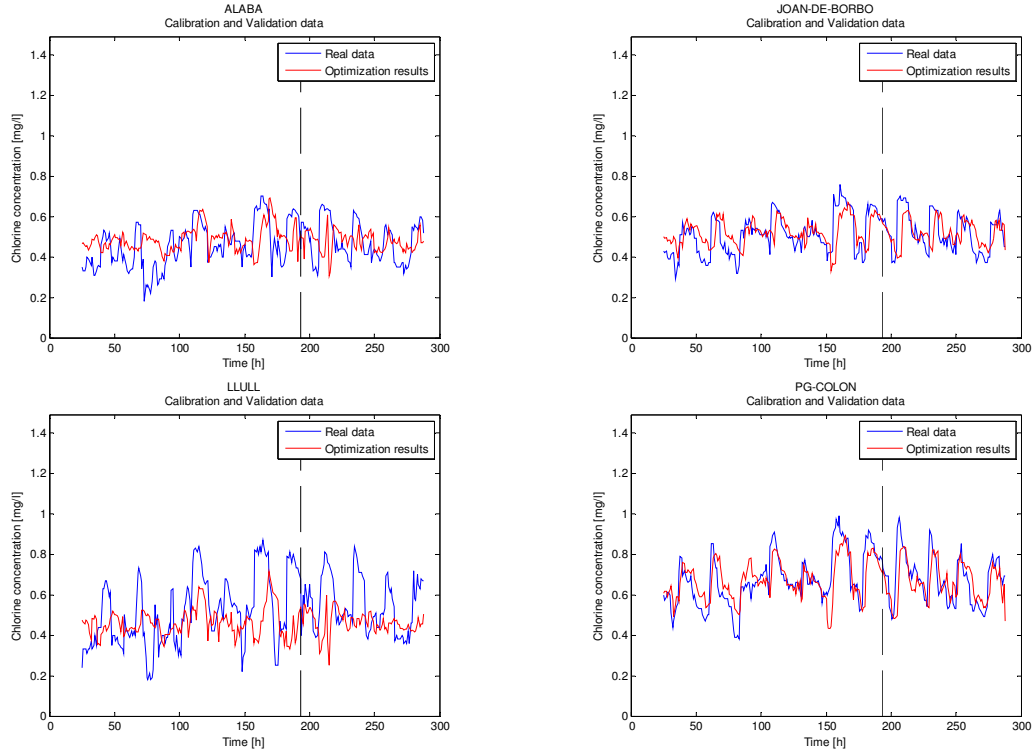


Fig. 7. Validation of a three-zone combined first-second order chlorine decay model in pressure floor 55th network

From Table 1 it may be observed how an important fit improvement has been achieved when comparing the initial first order single zone model (19.41 % of error) with the three-zones combined first-second order model (12.78 % of error).

Table 1. Chlorine decay model calibrations sum up

Model	k_{S1} [d ⁻¹]	k_{R1} [d ⁻¹]	k_{S2} [d ⁻¹]	k_{R2} [d ⁻¹]	k_{S3} [d ⁻¹]	k_{R3} [d ⁻¹]	J	e [%]
Single-zone 1 st order	1.8024	-	-	-	-	-	0.030669	19.4083
Single-zone 1 st - 2 nd order	0.04688	2.9319	-	-	-	-	0.022335	16.3613
Two-zones 1 st order	1.5469	-	1.9213	-	-	-	0.02913	18.6414
Two-zones 1 st - 2 nd order	0.01244	3.2973	-0.48129	3.8365	-	-	0.022504	16.5324
Three-zones 1 st order	2.3544	-	0.56331	-	0.8686	-	0.019871	13.9038
Three-zones 1 st - 2 nd order	0.51034	2.5506	0.00838	1.5385	-0.09283	1.1915	0.017009	12.7773

6. Conclusions

In this article, results achieved with chlorine decay model calibration have been presented for a particular DMA. Good results have been obtained with the suggested alternative models, which managed to improve the original model error from 19.41 % to 12.78 when using the three-zone combined first-second order model. This leads to consider this better approach instead of the original one, in order to achieve more accurate monitoring of the chlorine evolution through the network. The calibration methodology and the different models proposed should help water companies to obtain a better estimation of the chlorine evolution through a particular network by

simulation, and to use this information to perform further monitoring tasks (e.g. chlorine fault detection) in a more reliable way.

Acknowledgments

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