sensors

Supplementary Materials

Chlorine Concentration Modelling and Supervision in Water Distribution Systems

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1. Calculation of added chlorine concentration

The concentration of the chlorine added in the network refereed to free chlorine (Cl_2) was calculated from the concentran of the reagent used, which was NaClO at 15 % as shown in the following equation:

$$Cl_{reagent} = \frac{15gNaClO}{100g\ water}\frac{1\ g\ water}{1\ ml\ water}\frac{1000ml}{1l}\frac{1molNaCLO}{74.45gNaClO}\frac{1molCl_2}{1molNaClO}\frac{70.9gCl_2}{1molCl_2} = 143gCl_2/l \qquad (1)$$

This equation is based on the following reaction:

$$Cl2(g) + H2O \rightarrow HOCl + HCl \qquad (2)$$

2. Algorithm for on-line decay constant calibration

The algorithm for the on-line calibration of the chlorine decay constant described in section 2.2 (article) are provided in pseudocode in Table 1. Varibles are consistent with those in section 2.2 (article).

Table S1. Pseudocode to estimate the decay chlorine constant.

$Weekly\ Decay\ constant\ estimation$	
Require: $V_1, V_2, \Delta V_{Cl}, Q_1, Q_2, L, \emptyset, Cl_{reagent}$	Return: K_b
1: For $i = 1 : N_{weeks}$ do:	
2: *Evaluate* $\overline{V_1} = mean(V_1(week = i))$	
3: *Evaluate* $V_{pipe} = L \cdot \pi \cdot \left(\frac{\emptyset}{2}\right)^2$	
4: *Evaluate* $\overline{Q_1} = mean(Q_1(week = i))$	
5: *Evaluate* $\overline{RT_1} = \frac{\overline{V_1}+V_{pipe}}{\overline{Q_1}}$	
6: *Evaluate* $\overline{V_2} = mean(V_2(week = i))$	
7: *Evaluate* $\overline{Q_2} = mean(Q_2(week = i))$	
8: *Evaluate* $\overline{Q_2} = mean(Q_2(week = i))$	
9: *Evaluate* $\overline{RT_2} = \frac{\overline{V_2}}{\overline{Q_2}}$	
10: *Evaluate* $\overline{Cl_{added}} = \frac{\Delta V_{Cl}(week=i) \cdot Cl_{reagent}}{\int Q_2(week=i)}$	
11: *Evaluate* $\overline{Cl_1} = mean(Cl_1(week = i))$	
12: *Evaluate* $\overline{Cl_2} = mean(Cl_2(week = i))$	
13: *Evaluate* $K_b(i) \mid \overline{Cl_2} = \overline{Cl_1} e^{-K_b(\overline{RT_1}+\overline{RT_2})} + \overline{Cl_{added}} e^{-K_b(\overline{RT_2})}$	
12: End for	
14: Return: K_b	

3. Algorithm for decay constant estimation in the distribution network

The algorithm for the calibration process of the chlorine decay constant in the distribution network described in section 2.3 (article) are provided in pseudocode in Table 2.

Table S2. Pseudocode to estimate the chlorine decay constant in the distribution network.

Decay constant estimation for distribution network	
Require: K_b, Cl_{Sample}, *WDN Model*, ε *(finalisation criterion)*	Return: μ
1: *Initialise* μ 2: While: $\Delta MSE > \varepsilon$ 3: *Simulate WDN Model with* $K_w^{dist} = K_b^{dist} = \mu \cdot K_b$ 4: *Evaluate* $Cl_{Simulation}$ 5: *Evaluate* $MSE = \frac{1}{N}\sum_N \left(Cl_{Sample} - Cl_{Simulation}\right)^2$ 6: $\mu = \mu + \Delta\mu$ 7: End while 8: Return: μ	