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Use of on-line water quality monitoring data to predict bacteriological failures

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Abstract

Variations in continuously monitored on-line water quality data were investigated to establish whether they could be linked to coliform detections at regulatory monitoring points. We focussed on chlorine residual, turbidity and flow rate at water treatment works (WTW)-A. Archived on-line monitoring data from WTW-A were analysed using cross-correlation and self-organising maps in MATLAB® to identify trends in the data running up to coliform detections. The results show that these tools could be developed to help manage WTWs to reduce the number of bacteriological failures. A fingerprint of WTW conditions relating to coliform failures was identified for this case study.

Keywords: Bacteriological water quality; data analysis; monitoring data; pro-active failure prevention

1. Introduction

The goals of bacteriological quality monitoring are to assure the safety of drinking water for consumers and to monitor the performance of treatment processes. Water samples are routinely collected from water treatment works (WTWs), service reservoirs and customers' taps. Monitoring focuses on indicator organisms because bacteriological pathogens are rarely isolated from drinking water due to their low numbers under normal circumstances. The principal bacteriological indicators are coliforms, *Escherichia coli*, Enterococci and

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Clostridium perfringens (Standing Committee of Analysts, 2002). Positive results in analyses for these microorganisms are indicative of environmental or faecal contamination of treated water and all four parameters have prescribed values of 0 cells per 100 ml (Council of the European Communities, 1998). Heterotrophic plate counts (HPCs) per ml are also monitored; they represent a common indicator of the general microbiological quality of water (Standing Committee of Analysts, 2012).

This work focuses on WTW-A, which produces 120 Ml d^{-1}. WTW-A is owned and operated by Severn Trent Water Ltd. (STW), UK. It treats surface-water using the process outlined in Fig. 1:

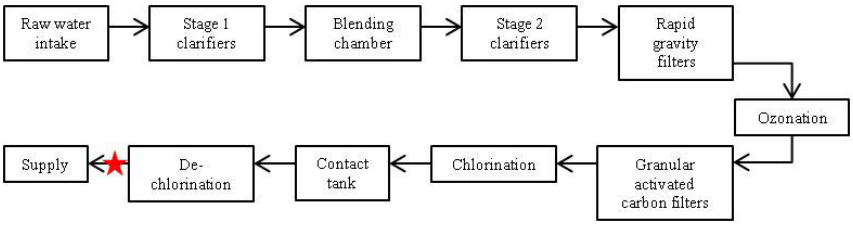

Fig. 1. Process flow diagram for WTW-A; ★ marks the location of the on-line monitors and final spot-sampling point.

Monitoring at WTW-A final sampling point detected a single coliform in March 2011 and March 2012. Despite extensive investigations, neither of these failures had causes identified. This is the outcome for approximately two thirds of all failure investigations (Ellis et al., 2013). Since no cause was identified, these failures were selected for the data analysis in this work. The supply network for WTW-A is extensive and it is important to STW to determine the causes of these non-compliances so that they can protect their consumers.

In our previous work (Ellis et al., 2013) we observed that there were weak correlations between the presence of indicator organisms in drinking water samples and other data relating to spot samples: free and total chlorine and water temperature amongst others. The reliance on spot-sampling data was a weakness of this study. Work by Codony et al. (2005) observed that discontinuous chlorination affected the efficacy of disinfection as demonstrated by HPCs. Their work involved neutralising the chlorine in a test reactor for periods of several days. This project seeks to identify whether short-term variations in archived on-line residual free chlorine, turbidity and flow could have impacted bacteriological water quality at WTW-A.

Nomenclature

CFU	colony forming units
DPD	diethyl-p-phenylene diamine
HPC	heterotrophic plate count
HPC22	heterotrophic plate count at 22 °C
HPC37	heterotrophic plate count at 37 °C
NTU	nephelometric turbidity units
SOM	self-organising map
STW	Severn Trent Water Ltd.
WTW	water treatment works

2. Methods

2.1. Data collection

Spot-sampling occurs daily at WTW-A final sampling point. There were two coliform detections: one in March

2011 and one in March 2012. The following results were extracted from STW's data handling software for the periods 1st January to 30th June 2011 and 1st January to 30th June 2012: coliforms, colony forming units (CFU) 100 ml^{-1}; HPCs at 22 °C and 37 °C (HPC22 and HPC37), CFU ml^{-1}; free chlorine, mg l^{-1}; and water temperature, °C. In addition, for the same time periods, the following archived monitoring data for WTW-A final monitoring points were requested from STW's Asset Creation Data Team: free chlorine, mg l^{-1}, Sigrist AquaScat WTMA (Sigrist, Germany); turbidity, nephelometric turbidity units (NTU), Capital Controls® TVU/CC1930 (Severn Trent Services, Philadelphia); and flow, Ml d^{-1}, Marsh Multi-Mag™ 285L (Marsh-McBirney Inc., Maryland). Free chlorine data were archived every 1 min and turbidity and flow data were archived every 15 min. The final sampling point and the on-line monitors are all situated after de-chlorination and before the storage tank from which water is pumped to supply (Fig. 1).

2.2. Routine sample collection and HPC and coliform analyses

STW samplers collect routine quality samples using the following procedure:

- WTW sample taps are kept constantly running. Aliquots of water are collected and analysed for free and total chlorine using the diethyl-p-phenylene diamine (DPD) colorimetric standard method (Standing Committee of Analysts, 2010). The water temperature is measured using a digital thermometer.
- WTW sample taps have simple spouts with no additional flow modifiers. The outer surfaces of the tap are sprayed with 10,000 mg l^{-1} chlorine solution and a 2 min contact time is allowed for disinfection.
- A 500 ml bacteriological sample is collected in a sample bottle dosed with sufficient sodium thiosulphate to neutralise free and combined residual chlorine in concentrations not exceeding 5 mg l^{-1} (Standing Committee of Analysts, 2010).

Samples are transported in refrigerated containers to the laboratory and microbiological analyses occur within 24 h of collection. HPCs are enumerated on yeast extract agar using the pour plate method (Standing Committee of Analysts, 2012). Coliforms are enumerated on membrane lactose glucoronide agar following the manufacturer's protocol (Oxoid, 2012), which conforms to Methods for the Examination of Water and Associated Materials (Standing Committee of Analysts, 2009). At the end of the incubation period the number of colonies is counted. HPCs are recorded as CFU ml^{-1}; coliforms are recorded as CFU 100 ml^{-1}.

2.3. Data manipulation

All datasets were imported into MATLAB® R2012a (The MathWorks Inc., Massachusetts). 2011 and 2012 data were treated separately throughout. The date field was converted to date-number format during the import.

The analyses required that all columns contain the same number of rows. Thus linear interpolation and zero padding were applied. Linear interpolation was used on the turbidity monitor, flow monitor, chlorine spot and temperature spot data, using the date-number field from chlorine monitor data. For HPC22, HPC37 and coliforms all gaps were filled with zeros to ensure that when colonies were recorded, the results remained as integers.

Full outer joins were used to create time-aligned datasets with 1 min time intervals, one for 2011 and one for 2012.

2.4. Cross-Correlation

Cross-correlation is a measure of the similarity of two variables (signals) as a function of a time lag between them (Bracewell, 1965). It achieves this by aligning peaks (or troughs) across the two signals at different lags and hence can be used to determine the time delay between two signals. Twenty-seven cross-correlations were applied to both joined datasets, as detailed in Fig. 2, using the un-biased XCORR function in MATLAB®. The output from this process was a data table of time lags between peaks in data for the first factor (across the top of Fig. 2) and peaks in data for the second factor (down the side of Fig. 2).

	Chlorine monitor	Flow monitor	Turbidity monitor	Temperature spot	Chlorine spot	HPC22	HPC37
Chlorine monitor		x	x	x			
Turbidity monitor		x		x			
Chlorine spot	x	x	x	x			
HPC22	x	x	x	x	x		
HPC37	x	x	x	x	x	x	
Coliforms	x	x	x	x	x	x	x

Fig. 2. Cross-correlations applied to joined datasets for 2011 and 2012.

To extract results from the data table of time lags, equations 1 to 3 were used and a dataset of final results compiled. The MAX function was used to find the highest correlation between the two factors. A subset of this dataset was created containing only the cross-correlations where the time lags were both positive and <24 h. Positive time lags mean that peaks in the first factor occurred before peaks in the second factor and could have impacted them. A time lag of <24 h was selected because the spot sampling was conducted daily.

$$[\text{Peak height}, \text{Lag time}] = \max(\text{XCORR result}) \quad (1)$$

$$\text{Zero lag} = (\text{size of series} + 1)/2 \quad (2)$$

$$\text{Time lag}, \text{hours} = (\text{Zero lag} - \max(\text{XCORR result}))/60 \quad (3)$$

2.5. Self-Organising Maps

The Self-Organising Map (SOM) is an artificial neural network model which draws inspiration from biological processes. The Map evolves localised response patterns to input vectors. The prototype vectors are positioned on a regular low-dimensional grid in a spatially ordered fashion helping to improve visualisation. SOMs can aid in the identification of correlations among more than two parameters. Complex datasets can be clustered and the output is a visual representation of the statistical pattern found by the SOM algorithm (Kangas and Kohonen, 1996; Kohonen, 1998). SOMs have been used for analysis and modelling of water resources as reviewed in Kalteh and Hijorth (2008). Mounce et al. (2012) proposed their use in data mining microbiological and water quality data from a pilot-scale pipe rig.

The analysis was carried out using the MATLAB® SOM Toolbox version 2.0 (Laboratory of Computer and Information Science, Finland). For both 2011 and 2012, the SOM analysed nine parameters: chlorine monitor, turbidity monitor, flow monitor, chlorine spot, temperature spot, HPC22, HPC37, coliforms and month number (1 = January through to 6 = June). The SOM algorithm first normalised the datasets and conducted rough training on these to learn the global structure. After which, fine training was completed before producing the SOM plots. The default settings of linear initialisation and batch training were selected. Each variable (such as turbidity) is represented by a colour-coded rectangular plot called a component plane; the same point in one plot is related to all corresponding plots enabling an understanding of how parameters change one with another.

2.6. Records of monitor interventions

When operators make un-scheduled adjustments to equipment, for example re-calibrating a monitor, a record is

made. These records can be used to check whether changes in data trends are genuine or the result of an intervention. If an un-scheduled adjustment has been made, this could be indicative of changes to the quality of water passing through the monitors.

The records pertaining to WTW-A final monitors were requested from operational staff.

3. Results

3.1. Cross-correlation

Of the 54 cross-correlations conducted, 13 yielded positive time lags between 0 and 24 h (Table 1). Where the results were 0 h, this showed that the two parameters changed respective to one another and there was no time lag between them. This was true for both years for the following cross-correlations: chlorine monitor x chlorine spot, flow monitor x chlorine spot, temperature spot x chlorine monitor, and temperature spot x chlorine spot. These results provide confirmation of good chlorine monitoring by both on-line monitors and samplers and also confirm the variation of chlorine with temperature. However, the variation of chlorine spot data with flow monitor data suggests that chlorine concentration could rise and fall with flow rate.

The cross-correlations of turbidity monitor with chlorine spot and chlorine monitor produced interesting results. In 2011, a time lag was identified for both correlations: 5 h for chlorine monitor and approximately 16 h for chlorine spot. This suggests that changes in turbidity impacted the chlorine concentration of the water. The difference in time lag could be a function of the different frequency of sampling for the two sets of chlorine data. In 2012, the cross-correlation between turbidity monitor and chlorine spot showed no time lag; and between turbidity monitor and chlorine monitor the result did not meet the positive criterion. This means that peaks in turbidity occurred after peaks in chlorine monitor data and could not be considered causative. There were two other occasions where the cross-correlation time lags did not meet the criteria for both years: temperature spot x turbidity monitor and HPC22 x HPC37. In both cases, the time lag was 0 h for 2012 and differed for 2011 with lags of -136 h and 1339.5 h, respectively. Even if both time lags had been positive, such large time lags are not considered to be relevant due to the sampling frequency at WTW-A.

Table 1: Principal cross-correlation results for 2011 and 2012.

Cross correlation inputs		Year	
Input 1	Input 2	2011	2012
Chlorine monitor	Chlorine spot	0	0
Flow monitor	Chlorine spot	0	0
Turbidity monitor	Chlorine monitor	5	(-0.2)
Turbidity monitor	Chlorine spot	16.3	0
Temperature spot	Chlorine monitor	0	0
Temperature spot	Turbidity monitor	(-136)	0
Temperature spot	Chlorine spot	0	0
HPC22	HPC37	(-1339.5)	0

3.2. Self-Organising Maps

The SOMs for 2011 and 2012 are presented in Fig. 3. There are two parts to the SOM output. They are the summary U-matrix and the component planes for the individual parameters. The U-matrix allows examination of the overall cluster patterns in the input dataset after the model has been trained. In the component planes for each parameter, the colouring corresponds to actual numerical values for the parameters as shown in the scale bars next

to each plot. Blue shades show low values and red corresponds with high values. The ranges for the bacteriological parameters have been adjusted by the algorithm as a result of the zero-padding; the SOM output is blue where the result was 0 CFU ml^{-1}/100 ml^{-1}; for the maximum results the resulting colour is red.

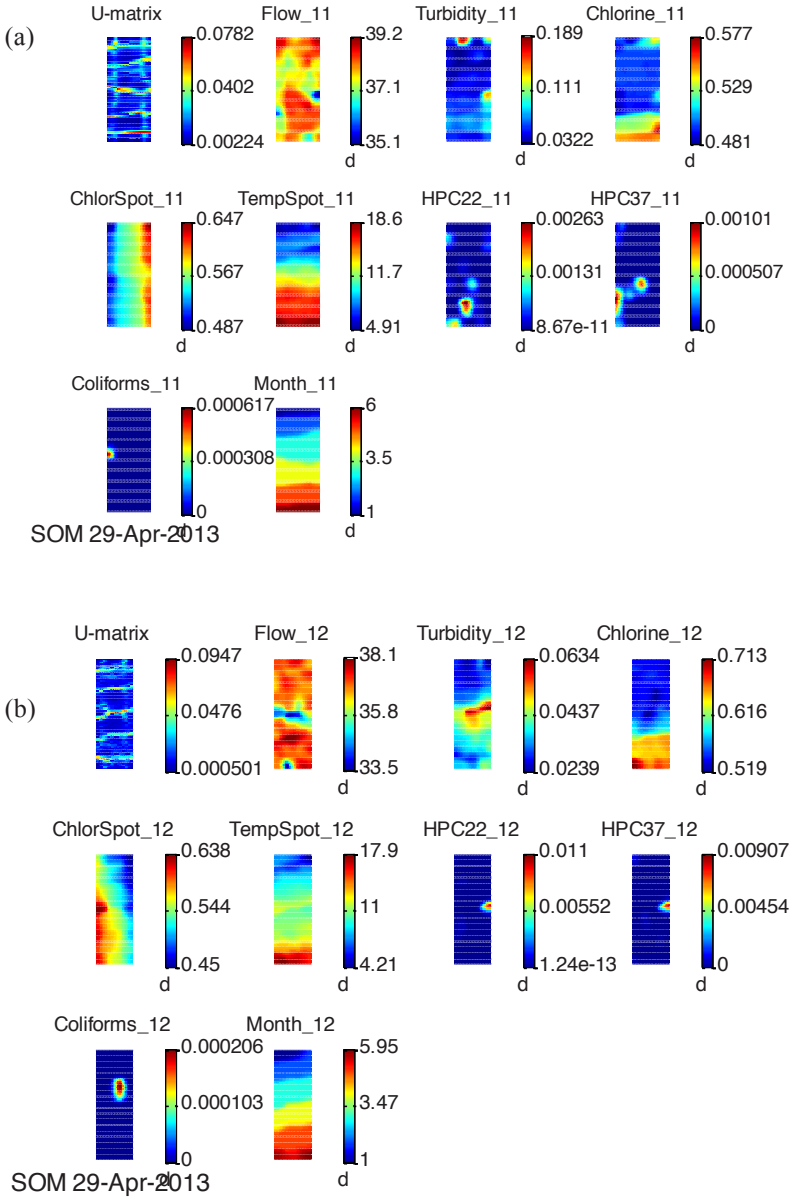

Fig. 3. Self-organising maps for (a) 2011; and (b) 2012.

The plots for month and temperature have similar patterns for both years and the higher the month number, the warmer the water temperature. The minimum (4.2 °C) and maximum (17.9 °C) water temperatures in 2012 were 0.7 °C cooler than those for 2011.

The flow plot for 2011 shows a spread of flow rates with high (37.8 – 39.2 Ml d^{-1}; dark orange) and medium (36.5 – 37.8 Ml d^{-1}; green) flow rates being more prevalent, whereas the one for 2012 shows high (36.6 – 38.1 Ml d^{-1}; dark orange) and low (33.5 – 35.0 Ml d^{-1}; blue) flow rates dominating.

The turbidity plots also differ in their patterns. In 2011, the turbidity monitor recorded predominantly low (0.03 – 0.08 NTU; blue) turbidities. There was a patch of high (0.14 – 0.19 NTU; red) turbidity and a patch of medium (0.08 – 0.14 NTU; yellow) turbidity. In comparison, the plot for 2012 has an upper and a lower portion of low (0.02 – 0.04 NTU; blue) turbidity and a patch of medium (0.04 – 0.05 NTU; yellow) to high (0.05 – 0.06 NTU; red) turbidity across the middle.

Chlorine monitor data (Chlorine_11 and Chlorine_12) show broadly similar patterns, with the majority of each plot showing low (0.48 – 0.51 mg l^{-1}, 2011; 0.52 – 0.58 mg l^{-1}, 2012; blue) chlorine and a lower portion of medium (0.51 – 0.55 mg l^{-1}, 2011; 0.59 – 0.65 mg l^{-1}, 2012; green) to high (0.55 – 0.58 mg l^{-1}, 2011; 0.65 – 0.71 mg l^{-1}, 2012; dark orange/red) chlorine.

The chlorine spot plots show the chlorine concentrations in approximately vertical stripes. In 2011, the concentrations run low (0.49 – 0.54 mg l^{-1}; blue) to high (0.59 – 0.65 mg l^{-1}; red) from left to right, whilst in 2012, the pattern runs high (0.58 – 0.64 mg l^{-1}; red) to low (0.45 – 0.51 mg l^{-1}; blue).

The numbers of HPC bacteria at 22 and 37 °C varied between the two years. In 2011, there were 19 detections of HPC22 ranging from 1 – 15 CFU ml^{-1}; in 2012, there were 10 detections ranging from 1 – 22 CFU ml^{-1}. In 2011, there were 10 detections of HPC37 ranging from 1 – 5 CFU ml^{-1}; in 2012, there were 9 detections ranging from 1 – 18 CFU ml^{-1}. These results are reflected in the variations of the SOM plots for these parameters. The 2011 plots show several areas of HPC detections, all of which occurred in the lower portions of the plots. In 2012, there was one area of HPC detections on each plot located half-way down on the right side. The HPC results have different fingerprints for the two years. In 2011, detections tended to occur with high flow rates (37.8 – 39.2 Ml d^{-1}), low turbidity (0.03 – 0.08 NTU), medium to high chlorine monitor values (0.51 – 0.58 mg l^{-1}), low to medium chlorine spot values (0.49 – 0.59 mg l^{-1}), high temperature (14.0 – 18.6 °C) and high month number (May – June). In 2012, detections tended to occur with low to medium flow rates (33.5 – 36.6 Ml d^{-1}), high turbidity (0.05 – 0.06 NTU), low chlorine monitor values (0.52 – 0.58 mg l^{-1}), low chlorine spot values (0.45 – 0.51 mg l^{-1}), medium temperature (8.8 – 13.3 °C) and medium month number (March – April). There was no correlation between HPC results and coliform detections.

One coliform CFU 100 ml^{-1} was detected in each year. The detection was plotted just above the middle of the plot for both years; in 2011 this was on the left side of the plot; in 2012 it was further to the right. The coliform results produced similar fingerprints for the two years. The detections occurred with low chlorine monitor values (0.48 – 0.51 mg l^{-1}, 2011; 0.52 – 0.58 mg l^{-1}, 2012) and low chlorine spot values (0.49 – 0.54 mg l^{-1}, 2011; 0.45 – 0.51 mg l^{-1}, 2012), medium temperature (9.5 – 14.0 °C, 2011; 8.8 – 13.3 °C, 2012) and medium month numbers (March – April). In 2011, the flow rate was medium (36.5 – 37.8 Ml d^{-1}) and turbidity was low (0.03 – 0.08 NTU), whilst in 2012, the flow rate was medium to high (35.0 – 38.1 Ml d^{-1}) and the turbidity low to medium (0.02 – 0.05).

3.3. Cross-correlation and SOM results

Few of the cross-correlation results that met the selection criteria also had observable correlations in the SOMs. Chlorine monitor x chlorine spot, flow monitor x chlorine spot, turbidity monitor x chlorine spot, temperature spot x turbidity monitor and temperature spot x chlorine spot showed no clear patterns in the SOMs for both years. The SOM results representing the cross-correlations for turbidity monitor x chlorine monitor show no pattern in 2012, but for 2011, low turbidity and low chlorines were apparent in the top portions of their SOM plots. The

temperature spot x chlorine monitor results in the SOMs showed agreement for both years: low chlorine concentrations correlated with high water temperatures. In 2011, the HPC22 x HPC37 results in the SOM did not have similar patterns, whereas in 2012, the patterns were alike.

3.4. Monitor interventions

The reports of un-scheduled actions taken to restore correct function to monitors showed 20 interventions in 2011 and 11 interventions in 2012. Of these, 14 and 9 respectively were for the turbidity monitors and 6 and 2 were for un-specified interventions. Most of the reports commented on erratic turbidity readings or high alarms and the principal action taken was to increase the flow through the monitor to achieve a more stable reading. This suggests that fouling of the sensor was occurring between scheduled maintenance visits, but that no major faults were implicated in the variability of the on-line monitoring data.

4. Discussion

4.1. Comparison of the results from cross-correlation and self-organising maps

The cross-correlation analyses only assessed the relationship between the two selected parameters and the output referred solely to the highest correlation from the results. This means that the results are over-simplified and do not relate to the dataset at large. Only 24 % of cross-correlations yielded results that met the selection criteria: time lags that were both positive and <24 h. In contrast, the SOM incorporates all the data in the final output. In the SOMs, time is dealt with in an invariant manner and the time parameter is lost except for the inclusion of the month number.

Turbidity negatively impacts chlorine residual and thus its disinfection efficacy (LeChevallier et al., 1981; Sawyer et al., 2003). The cross-correlation results showed that these parameters changed one with another; the SOM results did not clearly reflect this. The occurrence of coliforms with both low chlorines and low turbidities suggests that the relationship among chlorine, turbidity and indicator organisms is more complex than ‘turbidity affects disinfection efficacy’. Particle size and particle type can be important parameters in influencing the effectiveness of disinfection processes (Templeton et al. 2008). Deborde and von Gunten’s review (2008) observed that there was a difference in the impacts of inorganic and organic turbidities on chlorine stability. Farooq et al. (2008) found that disinfection was more effective in the presence of inorganic turbidity in comparison with organic turbidity. They also noted a weak inverse correlation between chlorine residual and coliforms in drinking water. The results from WTW-A concur with this observation; however, the turbidities were low in both datasets. Particle size and type and turbidity composition are not routinely determined in drinking water. Chlorine concentrations were correlated with water temperature and this may have had a greater effect than the low amount of turbidity.

Both methods showed that there was no relationship between HPCs and coliforms. This observation was also noted in Ellis et al. (2013) for the whole STW region. It is generally accepted that HPCs represent an overview of the bacteriological quality of water (Standing Committee of Analysts, 2012; McCoy and Olson, 1986; Francisque et al., 2009), i.e. the greater the number of HPCs the higher the likelihood of detecting indictor organisms. The lack of correlation between the numbers of HPCs and the detection of indicator organisms suggests this may only be true in cases of acute contamination. No cross-correlation results meeting the selection criteria were found for coliform detections, suggesting that no contamination event occurred in 2011 or 2012.

4.2. Operational value of the results from the two methods

Both methods are useful for identifying relationships among a variety of water quality parameters. Cross-correlation provides a simple time lag output; however, the tendency for qualifying results to be 0 h merely highlights the tendency for parameters to change respective to one another. However, the results from this method did not include correlations with coliform data. The SOMs provide a broader understanding of the water quality at

the final sampling point under all given conditions. They can therefore help in the development of a water quality fingerprint that results in a coliform failure.

Neither method is directly useful to operators on a day-to-day basis as their outputs need interpretation prior to use. It is beneficial to be able to see the general water quality factors that led to coliform occurrences; the cross-correlation results alone show a lack of time lag in which to act upon changes in water quality to prevent a failure. In order to enable the use of these tools it is important to find parameters that give a time lag sufficient for preventive action to be taken (for example by collecting on-line monitoring data from alternative locations within the WTW) and to develop simpler outputs from the analytical tools.

5. Conclusions and Further Work

5.1. Conclusions

This project used cross-correlation and SOMs to determine whether on-line water quality monitoring data could be used to predict bacteriological failures during spot-sampling. Two datasets from WTW-A were examined. They represented 6 months of monitoring data from January to June in 2011 and 2012. There was a single coliform detection in March of both years.

Cross-correlation results that were considered for further analysis were positive and <24 h. Only 13 of the 54 cross-correlations met both criteria; of those, the following four had time lags of 0 h for both years, showing that the factors changed one with another: chlorine monitor x chlorine spot, flow monitor x chlorine spot, temperature spot x chlorine monitor, and temperature spot x chlorine spot. These results show good chlorine monitoring by on-line monitors and samplers and also confirm the variation of chlorine with temperature. The variation of chlorine spot data with flow monitor data suggests that chlorine concentration could rise and fall with flow rate.

The SOMs for the HPC results differed and the following summarises the conditions that correlated with their detection at WTW-A:

- Low to high flow: 33.5 – 39.2 Ml d^{-1}
- Medium to high water temperature: 8.8 – 18.6 °C
- Low turbidity: 0.03 – 0.08 NTU
- Low to high residual chlorine: 0.51 – 0.58 mg l^{-1} (monitor) and 0.45 – 0.59 mg l^{-1} (spot sample)

The detection of coliform bacteria at WTW-A was not correlated with HPC22 or HPC37. They were correlated with the following conditions:

- Medium to high flow: 35.0 – 38.1 Ml d^{-1}
- Medium water temperature: 8.8 – 14.0 °C
- Low turbidity: 0.02 – 0.08 NTU
- Low residual chlorine: 0.41 – 0.58 mg l^{-1} (monitor) and 0.45 – 0.54 mg l^{-1} (spot sample)

The small number of non-compliant coliform tests available for this case study means that definitive WTW conditions cannot be asserted for WTW-A (or any other site) at this time.

5.2. Further work

- In order to increase the confidence in the conditions leading to a bacteriological failure, more historical data needs to be collected and examined using the same protocols.
- It is important that the final output of this research is of use to operators in their work to maintain water quality. One of the key requirements would therefore be to develop an output that recommends timely interventions, for example, ‘increase chlorine residual concentration by X mg l^{-1} or reduce flow rate through WTW by X Ml d^{-1} within a suitable time-frame’. Such a system could be based on an artificial neural network which uses lagged time-series monitoring signals (with time-lags identified by cross correlation) for predicting operational conditions.
- To increase the time lag available between a change in water quality and the detection of a bacteriological failure, it would be beneficial to test data from earlier in the WTW process train. Collecting data from after the

rapid gravity filters or the granular activated carbon filters (Fig. 1) may provide greater insight into the complex relationships between the different parameters under examination.

- The bacteriological quality of water is known to decline with distance from the WTW (Levi, 2004). Using the cross-correlation and SOM tools to determine whether actions at the WTW could have prevented a failure at a service reservoir would be valuable.

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