Early warning of changing drinking water quality by trend analysis

Jani Tomperi, Esko Juuso and Kauko Leiviskä

ABSTRACT

Monitoring and control of water treatment plants play an essential role in ensuring high quality drinking water and avoiding health-related problems or economic losses. The most common quality variables, which can be used also for assessing the efficiency of the water treatment process, are turbidity and residual levels of coagulation and disinfection chemicals. In the present study, the trend indices are developed from scaled measurements to detect warning signs of changes in the quality variables of drinking water and some operating condition variables that strongly affect water quality. The scaling is based on monotonically increasing nonlinear functions, which are generated with generalized norms and moments. Triangular episodes are classified with the trend index and its derivative. Deviation indices are used to assess the severity of situations. The study shows the potential of the described trend analysis as a predictive monitoring tool, as it provides an advantage over the traditional manual inspection of variables by detecting changes in water quality and giving early warnings.

Key words | aluminium, drinking water, nonlinear scaling, operating conditions, turbidity, water treatment process

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INTRODUCTION

There is a growing demand to improve water treatment management to ensure high quality water for consumers at as low as possible operating cost. Efficient monitoring and control have a key role in high quality drinking water processing at water treatment plants (WTPs). Many process measurements are available in modern WTPs, but the quality of the processed water is not measured until it is leaving the plant for distribution to consumers and corrective control actions have no effect on water quality. In addition, water treatment processes are very challenging for monitoring, modelling and control because they are complex, nonlinear processes where several (partly unknown) variables affect the functionality and quality of water. Poorly operating WTPs and low quality water may cause health problems to consumers and significant economic losses to a WTP. Health effects can be due to single exposures to microbial pathogens or long-term exposure to chemicals. Economic losses include excessive chemical and energy consumption, cleaning the distribution system, compensation to consumers and process improvements. The contamination of the water can be prevented, reduced or eliminated by the proper control of the process. Successful control, on the other hand, requires accurate monitoring of the process. Specific limits of the operating and quality variables are monitored by on-line or laboratory analysis (WHO (World Health Organization) 2003, 2008).

The quality of drinking water and the efficiency of a WTP can be assessed by many parameters, but the most common are turbidity and residual chemical level. Surface waters are typically treated by a chemical coagulation-based process, and aluminium or iron salts are widely used as coagulants to reduce the organic matter, colour and turbidity of raw water (WHO (World Health Organization) 2008). Aluminium has a good ability to coagulate

doi: 10.2166/wh.2016.330

and flocculate both organic and inorganic compounds, but using aluminium salts in a water treatment process may lead to an increased concentration of residual aluminium in drinking water if the coagulant is overdosed or the water treatment process is dysfunctional. In Finland, for residual aluminium, the maximum target value of the quality recommendation, defined in the Health Protection Act of the Ministry of Social Affairs and Health, is 0.2 mg/litre (FINLEX 2000). If the residual aluminium level in drinking water rises above 0.1–0.2 mg/litre, it is usually noticed by consumers. It has been found that the residual aluminium level in drinking water is affected by, inter alia, the raw water temperature, raw water $KMnO_4$ (potassium permanganate) value, raw water pH, turbidity, Al/$KMnO_4$-ratio, pH of coagulation and silicate concentration (Driscoll & Letterman 1995; Juntunen et al. 2012; Tomperi et al. 2013a). The residual aluminium also increases the water turbidity (WHO (World Health Organization) 2008). The residual aluminium concentration in drinking water can be minimized, for example, by optimizing water pH, avoiding excessive dosing of aluminium, good mixing of coagulants, optimum paddle speed in the flocculation process and efficient floc filtration (WHO (World Health Organization) 2008).

Turbidity is caused by suspended particles, which reduce the clarity of water. Suspended particles usually come from the raw water source due to inadequate water treatment or from the resuspension of sediments in a distribution system. The limit for acceptable drinking water turbidity is around 5 NTU (WHO (World Health Organization) 2008). Higher turbidity indicates problems in the treatment process. Particles that cause turbidity can protect microorganisms from the effects of disinfection and stimulate bacterial growth, which causes health effects for consumers. Thus, the turbidity must be as low as 0.1 NTU for effective disinfection. Among others, the coagulation chemical dose, the turbidity of the raw water, the temperature of the water, the raw water $KMnO_4$ value and water pH affect the turbidity of drinking water (Juntunen et al. 2012). Residual aluminium and turbidity in drinking water have been found to be strongly correlated (Tomperi et al. 2011).

The time series of measurements includes effects of many distinct contributions: slow trends, various equipment faults, periodic disturbances and changing sensor noise (Stephanopoulos & Han 1996). Outliers and structural breaks need to be analysed to find true trends (Metz 2010). Typical reasoning systems have a language to represent the trends, a technique to identify the trends and a mapping from the trends to operational conditions (Dash et al. 2003). The fundamental elements are modelled geometrically as triangles to describe local temporal patterns in

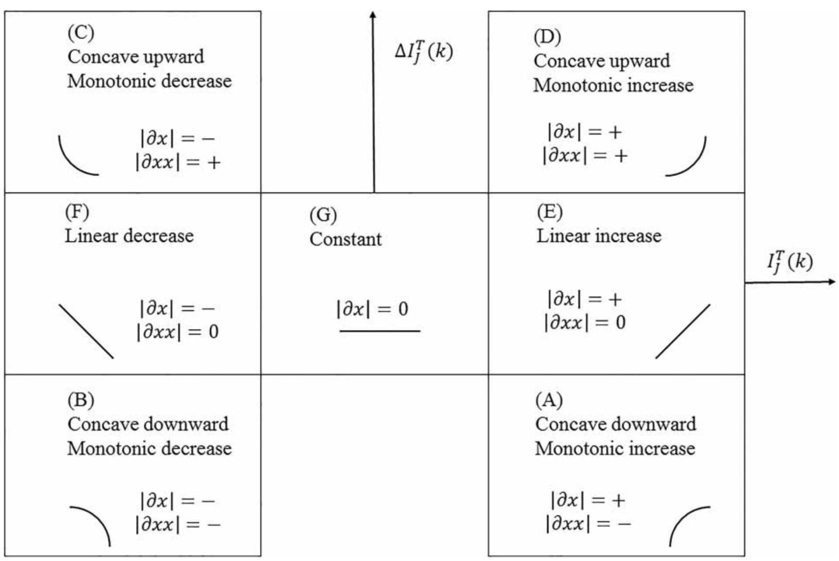

Figure 1 | Triangular episodic representation defined by the index $I_j^T(k)$and the derivative $\Delta I_j^T(k)$: seven basic types of episodes used for interval description, each episode type is denoted by a letter from the set from A to G (redrawn from Kivikunnas 1999; Juuso 2011).

data (Figure 1). The elements, which are also known as triangular episodic representations (Cheung & Stephanopoulos 1990), are defined by the signs of the first and second derivative. These elements have their origin in qualitative reasoning and simulation (Forbus 1984; Kuipers 1985). Temporal reasoning is a valuable tool for diagnosis and control of slow processes. Manual process supervision relies heavily on visual monitoring of the characteristic shapes of changes in process variables, especially their trends. For control system software, detecting such patterns is a difficult problem (Kivikunnas et al. 1996; Kivikunnas 1999). In these cases, the appropriate time window is not always recognized. Detecting changes is important for data compression, process control and fault diagnosis. Linear regression combined with fuzzy reasoning can be used in detecting significant changes up or down in process variables (Poirier & Meech 1993). The episodes shown in Figure 1 provide features for more detailed analysis. Trend extraction methods are based on polynomials (Konstantinov & Yoshida 1992), linear segments, wavelets, B-splines and neural networks. Similarities between trends are analysed, for example, with sequence matching, decision trees, pattern recognition and stochastic hidden Markov models (Maurya et al. 2007). Resolution, fine or coarse, has a strong effect on results (Stephanopoulos & Han 1996).

The qualitative scaling defined by episodes shown in Figure 1 generates a multiscale structure of trend descriptions over different time scales from process data (Stephanopoulos et al. 1997). Generalized norms provide tools for analysing different effects (Lahdelma & Juuso 2011a, 2011b). These norms and the nonlinear scaling approach (Juuso & Lahdelma 2010) are combined with the method introduced in Juuso et al. 2009 to form the trend analysis method presented in Juuso (2011).

In the present study, the described trend analysis is applied to the water quality variables and operating conditions that have been found to affect the water quality. Before the trend analysis, all measurements are scaled to the range [−2, 2] by using a nonlinear scaling approach which is based on generalized norms and skewness. The scaling is necessary to perform the trend analysis, as it uses only values between −2 and 2. The goal is to demonstrate the potential of the presented trend analysis, which shows the direction, speed and severity of the changing situation, as a monitoring tool in a slow water treatment process. The trend analysis can also be applied to various other measurements and processes. Here, the trend analysis is utilized with a short period of water treatment data where the quality of the water changes drastically, as against in our earlier study, in which the trend analysis was applied to fewer variables and proved functional for a longer period (Tomperi et al. 2014). By using a properly tuned trend analysis, the changes in water quality can be forecast in advance, an early warning can be received and it is possible to perform control or proactive actions to avoid the problems.

MATERIAL AND METHODS

The water treatment plant

Data was collected from a Finnish WTP, which uses the surface water of a lake as raw water. The raw water is treated with chemical flotation and filtration. The coagulation chemical is dosed as a function of raw water $KMnO_4$ value. $KMnO_4$ is an oxidizing agent that is used for measuring the chemical oxygen demand (COD) which indicates the amount of organic compounds in water. UV-radiation and sodium hypochlorite are used for disinfection and the pH is adjusted to the optimal value with calcium hydroxide.

Nonlinear scaling

For the trend analysis, the dataset was scaled between [−2, 2] using the nonlinear scaling method based on generalized moments, norms and skewness. Before scaling, the dataset was inspected and incorrect values were deleted and replaced with interpolation. The main concepts used in this section, the feasible range and the membership definition, are presented in Figure 2, which also shows the connection between the membership definition and the corresponding fuzzy membership functions. Membership definitions provide the nonlinear mappings of each variable from the operation area of the (sub)system inside a real-valued interval [−2, 2]. In this way, each variable is scaled between [−2, 2] and they can be compared with each other on a similar basis. Thus, a normal scaling to range [−1, +1] is combined with the handling of warnings and

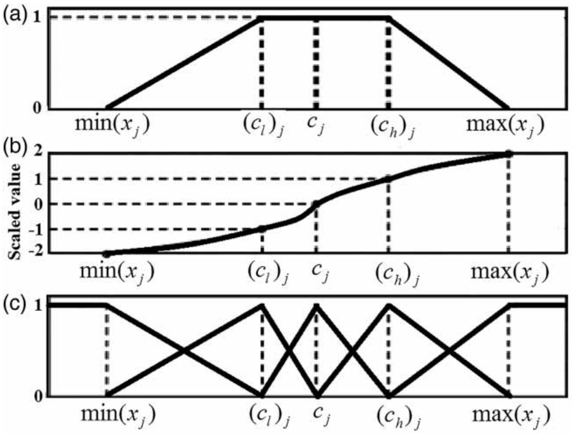

Figure 2 | (a) The feasible range, (b) scaled value and (c) membership functions (redrawn from Juuso 2004).

alarms. A trapezoidal membership function, based on the support and core areas defined by fuzzy set theory (Zimmermann 1992), is used to define the concept of the feasible range. The support area is between the minimum and maximum values of the variable x_j. The central value c_j divides the whole value range of x_j into two parts. The core area, $[(c_l)_j, (c_h)_j]$, is limited by the central points of the lower and upper parts.

The nonlinear scaling consists of two second order polynomials, one for negative values, and one for positive values:

$$\begin{cases} f_j^- = a_j^- X_j^2 + b_j^- X_j + c_j, X_j \in [-2, 0) \\ f_j^+ = a_j^+ X_j^2 + b_j^+ X_j + c_j, X_j \in [0, 2] \end{cases} \tag{1}$$

The coefficients of the polynomials are defined using the corner points of the feasible range:

$$\left\{(\min(x_j), -2), ((c_l)_j, -1), (c_j, 0), ((c_h)_j, 1), (\max(x_j), 2)\right\} \tag{2}$$

As the membership definitions are used in a continuous form, the functions f_j^- and f_j^+ should be monotonic, increasing functions in order to produce realizable systems. In order to keep the functions monotonic and increasing, the derivatives of the functions f_j^- and f_j^+ (Figure 3) should always be positive. Derivatives Dj can be presented in three groups: (1) decreasing and increasing, (2) asymmetric

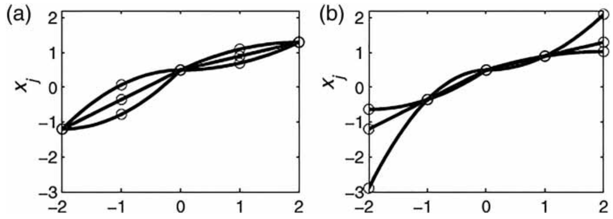

Figure 3 | Feasible shapes of membership definitions fj: (a) coefficients adjusted with core and (b) support (redrawn from Juuso 2009).

linear and (3) increasing and decreasing. The functions are monotonic and increasing if the ratios

$$\begin{aligned} \alpha_j^- &= \frac{c_j - (c_l)_j}{(c_l)_j - \min(x_j)} \quad \text{and} \\ \alpha_j^+ &= \frac{(c_h)_j - c_j}{\max(x_j) - (c_h)_j} \end{aligned} \tag{3}$$

are both in the range [1/3,3]. If needed, corrections are done by changing the core area, the support area or the centre point. The coefficients of the polynomials can be calculated as:

$$\begin{aligned} a_j^- &= \frac{1}{2}(1 - \alpha_j^-)\, \Delta c_j^-, \\ b_j^- &= \frac{1}{2}(3 - \alpha_j^-)\, \Delta c_j^-, \\ a_j^+ &= \frac{1}{2}(\alpha_j^+ - 1)\, \Delta c_j^+ \text{and} \\ b_j^+ &= \frac{1}{2}(3 - \alpha_j^+)\, \Delta c_j^+, \end{aligned} \tag{4}$$

where $\Delta c_j^- = c_j - (c_l)_j$ and $\Delta c_j^+ = (c_h)_j - c_j$. Membership definitions may contain linear parts if α_j^- or α_j^+ is equal to 1 (Juuso 2009).

The typical way to tune the membership definition (based on the generalized skewness) is to define the central value c_j and the core $[(c_l)_j, (c_h)_j]$, the ratios α_j^- and α_j^+ from the range [1/3, 3], and calculate the support $[\min(x_j), \max(x_j)]$. The membership definitions of each variable are configured with four parameters $\{a_j^-, b_j^-, a_j^+, b_j^+\}$ and the central value c_j. The upper and the lower parts of the scaling functions can be convex or concave, independently of each other (Figure 3). Simplified functions can also be used, for example, a linear membership definition requires two parameters and an asymmetrical linear definition requires three. Additional constraints can be taken into account for derivatives, for example, a locally linear function results if the continuous derivative is chosen in the central value (Juuso 2009).

In the analysis of the corner points, the value range of x_j is divided into two parts by the central tendency value c_j, and the core area (Figure 2) is limited by the central tendency values of the lower and upper part. The central point is chosen as the point where the skewness changes from positive to negative. Then the data set is divided into a lower part and an upper part and the same analysis is done for both subsets. The estimates of the corner points, $(c_l)_j$ and $(c_h)_j$, are the points where skewness goes to zero. The iteration is performed with generalized norms. Then the ratios α_j^- and α_j^+ are forced inside the range [1/3, 3] by changing the corner points $(c_l)_j$ and $(c_h)_j$ or the upper and lower limits $\min(x_j)$ and/or $\max(x_j)$. The linearity requirement at the central point c_j is taken into account, if possible (Juuso 2009).

The trend indices applied

In simple terms, the trend episodes and deviation indices resulting from the trend analysis show the direction, speed and severity of the change in the observed variable. Here, they provide warnings of changes in the water quality and environmental conditions that affect the water quality.

For any variable x_j trend index $I_j^T(k)$ is calculated from the scaled values X_j:

$$I_j^T(k) = \frac{1}{n_S+1}\sum_{i=k-n_S}^{k} X_j(i) - \frac{1}{n_L+1}\sum_{i=k-n_L}^{k} X_j(i), \quad (5)$$

which is based on the means obtained for a short and a long time period, defined by window lengths n_S and n_L, respectively. The index value in range [−2, 2] represents the strength of both decrease and increase of the variable x_j (Juuso et al. 2009). The length of the time window in trend analysis depends on the process and the purpose of the analysis. Long time windows are usually applied in monitoring the process and short time windows are more suitable in control, where a faster reaction is demanded. In the present study, the short time period was 24 hours and the long time period was 672 hours.

The derivative of the index $I_j^T(k)$, denoted as $\Delta I_j^T(k)$, is used for analysing triangular episodic representations (Figure 1). The derivative is calculated simply as a difference of subsequent values of the trend index. An increase is detected if the trend index exceeds a threshold $I_j^T(k) > \varepsilon_1^+$ and correspondingly, $I_j^T(k) < \varepsilon_1^-$ for a decrease. The trends are linear if the derivative is close to zero:$-\varepsilon_2^- < \Delta I_j^T(k) < \varepsilon_2^+$. Concave upward monotonic increase (D) and concave downward monotonic decrease (B) are dangerous situations where the situation is bad and it is getting worse at an increasing rate. Concave downward monotonic increase (A) and concave upward monotonic decrease (C) mean that an unfavourable trend is stopping. In process monitoring, the concave upward monotonic increase (D) requires special attention. New phenomena are activated when the system moves from the linear increase to this area. The scaling functions should be defined for the whole operating area. However, a wide range of measurements is only available after failure. Initial estimates are needed at the beginning for the corner points. Parameters for the lower part [−2, 0] are updated when a change to episode D is detected with the trend analysis based on the initial estimates of the scaling functions. Parameters for the upper part [0, 2] can be updated recursively (Juuso et al. 2009).

The severity of the situation can be evaluated by a deviation index

$$I_j^D(k) = \frac{1}{3}\left(X_j(k) + I_j^T(k) + \Delta I_j^T(k)\right). \quad (6)$$

This index has its highest absolute values, when the difference from zero is very large and is getting still larger at a rapidly increasing rate (Juuso et al. 2009).This can be understood as an additional dimension in Figure 1.

Weight factors and parameters for trend analysis affect the accuracy of the trend analysis and its forecasting ability. They are selected separately for every measurement. The trend episodes are visualized step by step during the operation, and thus the sequence of the points is not seen when all the points are presented in the same plot. The direction of the change in the trend episodes at the time of remarkable change is marked with arrows in Figures 5 and 6.

RESULTS AND DISCUSSION

In the present study, trend indices were calculated using scaled measurement values to find trend episodes and deviation indices for a short period and several variables, whereas in our earlier study the trend analysis was performed and proved to be efficient using a 16-month long dataset (Tomperi *et al.* 2014). In the present study, the dataset for trend analysis was a continuous 2,500-hour long period when the potable water quality changed drastically. However, to include seasonal changes and all different conditions available, the scaling was performed using the whole original 16-month dataset, not only the short selected period. The original data was smoothed to delete single spikes and to make presented figures clearer.

In addition to the common quality variables (turbidity, residual coagulation chemical and residual disinfection chemical), important operating condition variables that have been found to affect the water quality and water treatment process efficiency were also selected for the trend analysis. Operating conditions like raw water temperature, raw water $KMnO_4$ value (representing the COD of raw water) or raw water turbidity are not controllable variables, but their values depend on the season of the year, heavy rains, and snow melting, for example. The $KMnO_4$ value indicates the amount of organic matter in water and should be as low as possible. It is typically high in autumn and spring. Decreasing temperature reduces the performance of the coagulation chemical, whereas the higher the temperature is, the better the water treatment coagulation chemical works. However, a water treatment process can be improved by optimizing the coagulation chemical dosage, mixing speed, flow, sodium hypochlorite and calcium hydroxide dosages, for example. The coagulation chemical dose has been found to be a major factor for residual aluminium level (Tomperi *et al.* 2013a).

The scaled values of quality parameters, the variables that have been found to affect the water quality, and some controllable process variables of the WTP are shown in Figure 4(a), 4(b) and 4(c), respectively. Measurements are presented as scaled values for easier comparison and thus the trend analysis requires values between [−2, 2]. The operating conditions (Figure 4(b)) show that before the residual aluminium level in drinking water rises, the $KMnO_4$ value and turbidity of the raw water rise rapidly from the normal level; at the same time the temperature is constantly decreasing and the pH drops. In particular, the change in the $KMnO_4$ value from normal to poor is alarming. Due to the changes in the raw water, the disinfection and especially the coagulation chemical doses rise (Figure 4(c)), which cause the residual values measured from the drinking water (Figure 4(a)) to rise as well. The aluminium level and turbidity of the processed water rise from an acceptable level towards warning and alarming levels. Turbidity returns momentarily to the normal level but rises back to an even higher level, whereas the residual aluminium stays at the high level and even increases slightly. The residual chlorine level in the drinking water also varies during the inspected period.

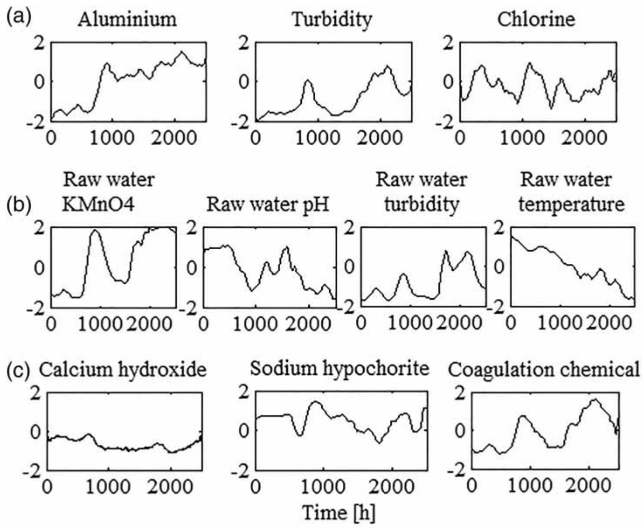

Figure 4 | (a) Drinking water quality variables, (b) operating conditions and (c) controllable water treatment process variables.

Trend episodes and deviation indices for residual aluminium, turbidity and residual total chlorine are shown in Figure 5. The behaviour of the trend episodes in aluminium (A), turbidity (C) and chlorine (E) levels before and during the first rapid change are indicated with arrows. Deviation indices show how severe the changed condition is. Both aluminium and turbidity are at first constant at normal levels but rapidly rise towards the warning limit (here set to 1). The behaviour of chlorine is more unstable during the whole period. The trend episode figures of aluminium and

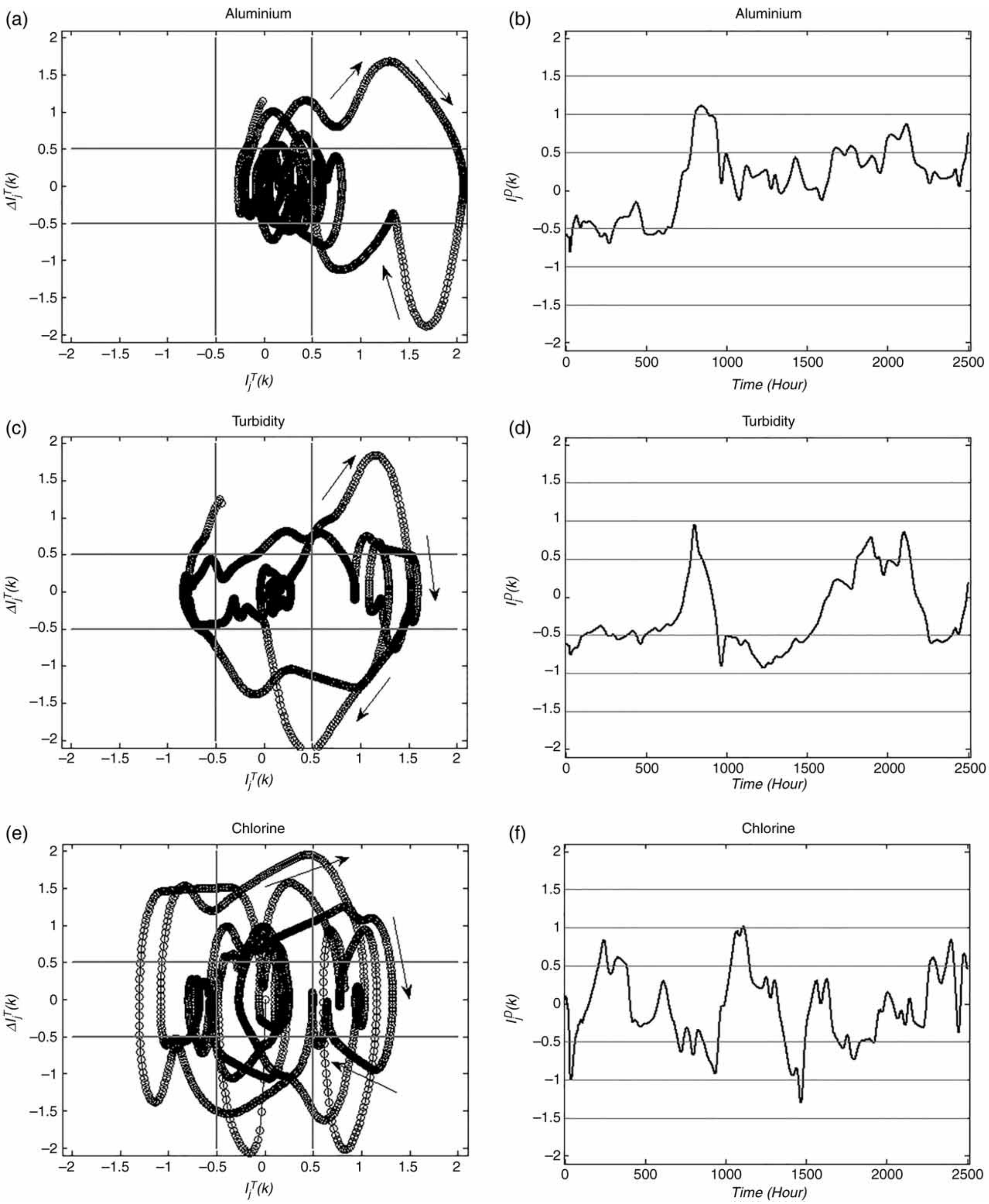

Figure 5 | Trend episodes (left) and deviation indices (right) for quality variables of the drinking water: residual aluminium, turbidity and total residual chlorine.

turbidity show how the constant state changes, through a dangerous concave upward increase, to a linear increase, and to a concave downward monotonic increase, which indicates that the dangerous situation is ending. After that, the trend episode returns to a constant level (and decreased state of turbidity). The deviation index of aluminium shows that the rise begins at time point ~600 hours; the first peak is reached at ~840 hours and the second peak is reached at ~2,115 hours. In the original measurements (Figure 4), the first peak for aluminium is at ~925 hours and the second

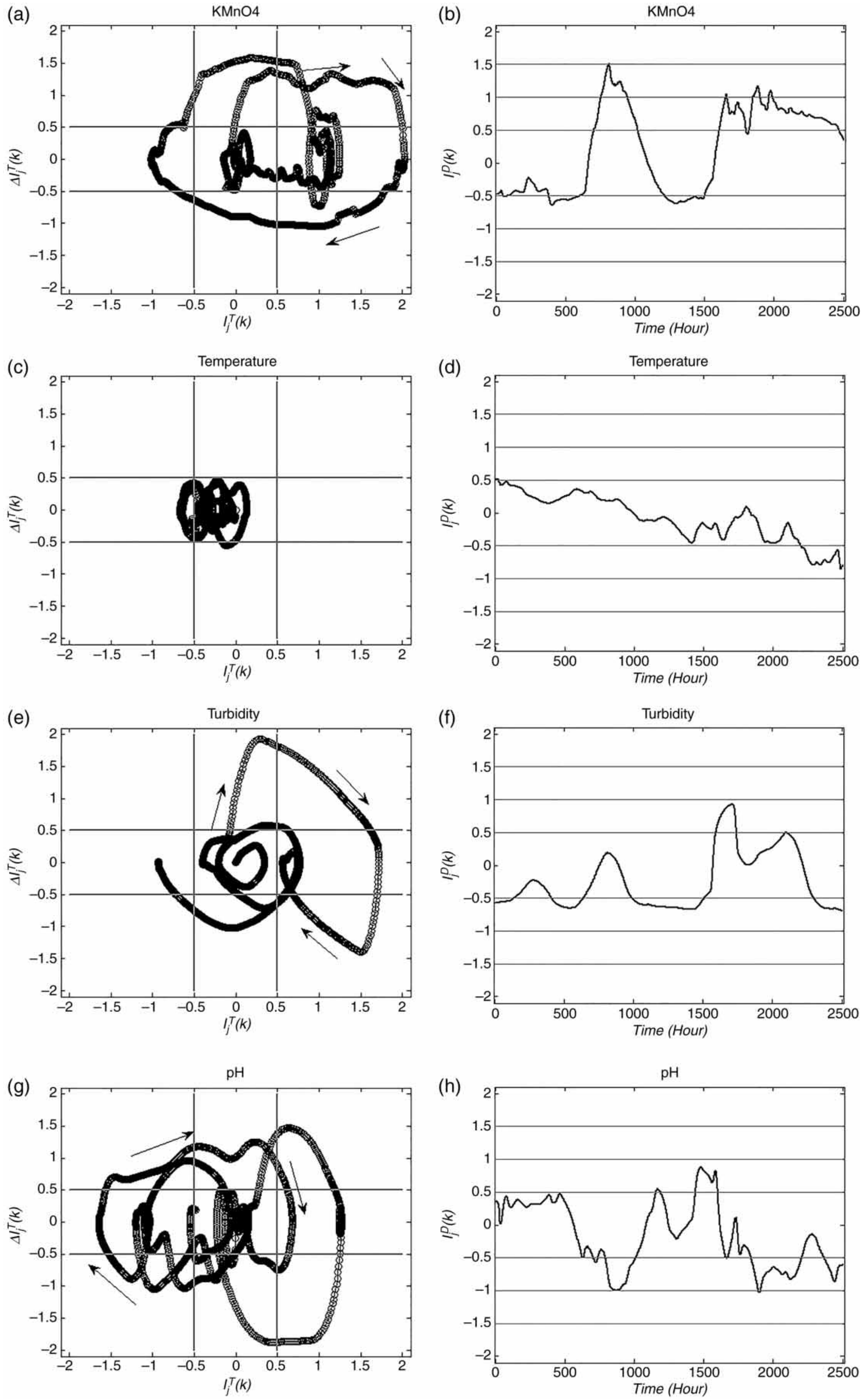

Figure 6 | Trend episodes (left) and deviation indices (right) for operating conditions of water treatment: $KMnO_4$ level, the temperature, turbidity and pH of raw water.

at ~2,130 hours. The deviation index of turbidity shows the first peak is at ~800 hours and the second at ~2,100 hours, whereas in the original measurements, the first peak is at ~815 hours and the second is at ~2,125 hours. Correspondingly, the first peak of total residual chlorine is at ~240 hours in the deviation index and at ~370 hours in the original measurements. Thus, the trend analysis yields a remarkable advance by forecasting upcoming severe situations hours earlier than the original measurements.

The quality of the raw water has a great effect on the water treatment process efficiency and thereby the quality of drinking water. The temperature, turbidity and $KMnO_4$ values, which determine the coagulation chemical dose, can be used to predict the residual aluminium level in potable water (Tomperi *et al.* 2013a). The temperature, turbidity, pH and the $KMnO_4$ values of raw water can be used to predict the turbidity level in potable water (Tomperi *et al.* 2013b). So, assessing the development of these variables shows the upcoming condition of the water treatment process and the quality of drinking water. Figure 6 shows the trend episodes and the deviation indices of raw water measurements that have been found to have an effect on the water quality. The temperature of the raw water decreases almost linearly towards colder levels (Figure 6(d)). However, the $KMnO_4$ value, turbidity and pH have major and rapid changes from normal to more dangerous levels. From a constant state, the $KMnO_4$ value rapidly changes to a dangerous upward increase and through a linear increase, to a concave downward increase before going to the decreased state. According to the deviation index, the $KMnO_4$ value reaches the first peak at ~810 hours. As shown in Figure 4, the peak in the original measurements is not reached until ~900 hours. Trend analysis again reveals the upcoming warning condition in advance, hours before it is shown in the real-time value of $KMnO_4$ or in the quality parameters of the potable water. The deviation index of raw water turbidity also shows that the top of the highest peak is observed hours in advance with trend analysis (~1,710 hours) of the original measurement (~1,725 hours). Raw water pH drops drastically and is at its lowest point at ~880 hours, whereas in the original measurement the lowest point is at ~940 hours. The trend episode shows how the pH changes from the constant state to the dangerous concave downward monotonic decrease. After a while, the decrease becomes steady and changes to the increased state. The information received from the trend analysis can be exploited by proactive control of the water treatment process or by preventing water distribution to consumers. Control actions can be easily addressed to, for example, optimize the coagulation chemical dose or adjust the pH or mixing speed.

CONCLUSION

The accurate monitoring and control of a water treatment process are essential to ensure high quality drinking water. By using proper control, the water treatment process is functional, the quality of potable water remains at the required level, and environmental problems, health effects, excessive energy consumption and financial losses are avoided. However, the control of the process can only be as accurate as the monitoring is. In the present study, the trend analysis presented was used for the most common water quality variables, and some important raw water variables that have been found to affect the drinking water quality and water treatment process functionality. It was shown that using trend analysis for indirect measurements of water quality and the operating conditions, the water quality can be forecast in advance; that is, early warnings of changes can be received and control or other proactive actions such as preventing water distribution to consumers can be performed. The information from trend analysis can be exploited by, for example, optimizing the coagulation chemical dose, and adjusting the pH or mixing speed. The trend analysis of the measured variables gives an advantage compared to the common, approximate examination done by the process operators, as visual monitoring is not efficient in detecting slow changes of process variables, especially if the viewed monitoring period is short.

ACKNOWLEDGEMENTS

The writing of this paper was financially supported by KAUTE Foundation, which is thereby warmly acknowledged. The data used in this study were collected during the project 'Development of a comprehensive water quality management system'.

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First received 29 September 2015; accepted in revised form 7 December 2015. Available online 10 February 2016