Comparative analysis of time-scaling properties about water pH in Poyang Lake Inlet and Outlet on the basis of fractal methods

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ABSTRACT

Detrended fluctuation analysis (DFA) and multifractal methods are applied to the time-scaling properties analysis of water pH series in Poyang Lake Inlet and Outlet in China. The results show that these pH series are characterised by long-term memory and multifractal scaling, and these characteristics have obvious differences between the Lake Inlet and Outlet. The comparison results suggest that monofractal and multifractal parameters can be quantitative dynamical indexes reflecting the capability of anti-acidification of Poyang Lake. Furthermore, we investigated the frequency-size distribution of pH series in Poyang Lake Inlet and Outlet. Our findings suggest that water pH is an example of a self-organised criticality (SOC) process. The results show that it is different SOC behaviours that result in the differences of power-law relations between pH series in Poyang Lake Inlet and Outlet. This work can be helpful to improvement of modelling of lake water quality.

Key words | detrended fluctuation analysis, multifractal, pH, Poyang Lake

INTRODUCTION

pH is often considered the “spider in the web” of biogeochemical reactions in aquatic ecosystems, since almost any process affects pH either directly or indirectly (Sarmiento & Gruber 2006). The future pH changes in aquatic ecosystems may have large impact on biogeochemical processes and organisms. In recent years, a number of modelling approaches have been presented that allow prediction of the time evolution of pH in aquatic ecosystems. These methods, which have been powerful tools to understand pH dynamics of aquatic systems, include simple empirical correlations (Bjerknes & Tjomsland 2001), stochastic approaches (Ahmad et al. 2001), neural network approaches (Moatar et al. 1999) and mechanistic biogeochemical models (Jourabchi et al. 2005) that contain reactive transport descriptions of varying complexity.

Although pH modelling has make great progress, the mechanisms that drive water pH temporal evolutions are not well understood. In a typical aquatic system, there are processes going on vastly different timescales. One group of comparatively fast acid-base reactions (e.g. the carbonate, silicate systems) relaxes on timescales of fractions of seconds up to hours, while another group of rather slow processes relaxes on timescales of days up to years or even longer. This latter group of processes comprises chemical reactions, such as calcium carbonate precipitation or dissolution and organic matter degradation, as well as physical transport processes, for example the exchange of CO₂ with the atmosphere and pollution sedimentation. Inter-relationships between these processes and pH values are complex and nonlinear and many processes associated with water pH are uncertain in nature. Hofmann et al. (2007) consider that it is this complexity that results in the recent pH modelling approaches being not always optimal.

In the study of seemingly complex phenomena such as seismic crisis, rainfall, river flows, DNA sequences, stock market indices and so forth, monofractal and multifractal
analysis techniques, developed to draw qualitative and quantitative information from time series, have been applied recently to the study of a large variety of irregular, nonstationary signals (Matsoukas et al. 2000). And fractal methods by now have proved to be very useful to detect deep dynamical features. To our knowledge, up to now, there are very few studies on application of fractal methods to the study of the temporal evolution dynamics of water pH.

In this paper, Poyang Lake Inlet and Outlet water pH series are chosen as research objects. Poyang Lake (28°22′–29°45′N, 115°47′–116°45′E) is the largest freshwater lake in China (Li et al. 2003). Poyang Lake Inlet and Outlet water quality data are provided freely on the Internet by Ministry of Environmental Protection the People’s Republic of China web site: http://www.mep.gov.cn/. We have used weekly average pH monitoring data of Poyang Lake Inlet and Outlet from 2004 to 2008. The study area and monitoring sections are shown in Figure 1.

In this study, firstly, we investigate the difference of temporal scaling properties about water pH series in Poyang Lake Inlet and Outlet in China by detrended fluctuation analysis (DFA) and multifractal method. Secondly, we discuss the presence of self-organised criticality (SOC) processes in these pH series. At last, based on the SOC theory, we analyse the cause of different scale-free power-law behaviour between pH series in Poyang Lake Inlet and Outlet.

Figure 1 | Location of the study area and monitoring sections. (A) China. (B) Poyang Lake and its vicinity.

METHODS

DFA method

DFA was proposed by Peng et al. (1994), which is an advanced method for determining the scaling behaviour of data in the presence of possible trends without knowing their origin.

The root mean square fluctuation of this integrated and detrended time series \( F(n) \) behaves as a power-law function of \( n \), data present scaling: \( F(n) \propto n^d \). The DFA exponent \( d \) is defined as the slope of the regression line for all points \( \log(n), \log(F(n)) \).

For white noise, the series corresponds to a random walk and \( d = 0.5 \); \( 0.5 < d < 1 \), indicates persistent long-range power-law correlations such that large values are more likely to be followed by large values and vice versa; \( 0 < d < 0.5 \), power-law anti-correlations are present.

Multifractal analysis

We further investigate the possibility that time series generated by certain environmental systems may be members of a special class of complex processes, termed multifractal, which require a large number of exponents to characterise their scaling properties. Multifractal analysis has been applied to several fields of the scientific research. For further detail computation, see Lee et al. (2006).

Three parameters are very important to describe the complexity of the multifractal spectrum (Sun et al. 2001; Shimizu et al. 2002; Shi et al. 2009). Firstly, the width of multifractal spectrum is \( \Delta \alpha (\Delta \alpha = \alpha_{\text{max}} - \alpha_{\text{min}}) \). The higher the \( \Delta \alpha \), the wider the probability distribution as well as the larger the difference between the highest pH and the lowest pH, so the “richer” the signal in structure. Secondly, the difference of the fractal dimensions of the maximum probability subset \( (\alpha = \alpha_{\text{min}}) \) and the minimum one \( (\alpha = \alpha_{\text{max}}) \) is \( \Delta f \) \( (\Delta f = f(\alpha_{\text{min}}) - f(\alpha_{\text{max}})) \). \( f(\alpha_{\text{min}}) \) and \( f(\alpha_{\text{max}}) \) reflect the number of the subset of the maximum and minimum probability, respectively. Thus, \( \Delta f < 0 \) represents that the chance of the pH values lying at the lowest site is more than that at the highest site and vice versa. Thirdly, in order to quantitatively recognise possible differences in Legendre spectra stemming from different
signals, it is possible to fit, by a least square method, the spectra to a quadratic function around the position of their maxima at \( \alpha_0 \), namely \( f(\alpha) = A(\alpha - \alpha_0)^2 + B(\alpha - \alpha_0) + C \). Parameter \( B \) indicates the asymmetry of the curve, which is zero for symmetric, positive for left-skewed and negative for right-skewed shapes (Shimizu et al. 2002). A right-skewed spectrum denotes the relatively strong dominance of high fractal exponents, corresponding to rough structures, and a left-skewed spectrum indicates low ones (more smooth-looking).

RESULTS AND DISCUSSION

DFA method

DFA analysis results exhibit clear power-law scaling relationship at the time scale of 4 years at least (Figures 2 and 3). In the original pH series, as to Lake Inlet, \( d_1 = 0.82 \) with \( r^2 = 0.997 \); while as to Lake Outlet, \( d_2 = 0.99 \) with \( r^2 = 0.994 \). In order to verify that the \( d \) values indeed reflect some information of the temporal variation of pH series, we performed the same analysis on randomly shuffled versions of the original two pH series. We calculate the \( d \) values for each shuffled series, which are shown in Figures 2 and 3 respectively. As to Lake Inlet, \( d_{1s} = 0.52 \) with \( r^2 = 0.983 \); while as to Lake Outlet, \( d_{2s} = 0.51 \) with \( r^2 = 0.991 \). The randomly shuffled series indicate the obvious randomness, which differs significantly from those calculated for the original series. The original pH series indicates high persistence or long-term memory. The high persistence signifies that the water pH fluctuations in Lake Inlet and Outlet, from small time intervals to larger ones (up to 4 years at least), are positively correlated in a power-law fashion. For example, there is a tendency for increase in water pH to be followed by another increase in water pH at a different time in a power-law fashion. This suggests that the correlations between the fluctuations in lake water pH do not obey the classical Markov-type stochastic behaviour (exponential decrease with time), but display more slowly decaying correlations. This implies that the long-term memory should be considered in the trend prediction of water pH as an important factor. However, the data set is only 4 years long. It needs longer series to confirm the critical correlated time scale where power-law scaling is varied.

Moreover, obvious difference between Lake Inlet and Outlet still exist, which can be seen by the relation of \( d_1 > d_2 \). Equilibrium pH calculations indicated that the lake water was buffered well. This buffered system has some capability of anti-acidification and different types of wastewater discharges did not cause obvious change in pH of the lake water. Thus Lake Outlet water pH will be characterised by stronger persistence owing to the lake buffered capability, which can more strongly maintain the “current time interval” tendency in following time interval and reflect long-term trend of pH. Consequently we think that the DFA exponent (\( d \)) of water pH is strongly related to the anti-acidification of aquatic body. Lakes with high \( d \) can maintain fluctuation tendency of water pH even with some acid wastewater input. It is noted that the acid neutralising

![Figure 2](https://iwaponline.com/wst/article-pdf/61/8/2113/448496/2113.pdf)

**Figure 2** DFA performed on the original Poyang Lake inlet pH series and randomly shuffled pH series.

![Figure 3](https://iwaponline.com/wst/article-pdf/61/8/2113/448496/2113.pdf)

**Figure 3** DFA performed on the original Poyang Lake outlet pH series and randomly shuffled pH series.
capacity (ANC) was presented in some aquatic chemistry studies (Rubin et al. 1992). The measurement of ANC is based on aquatic chemistry theory whereas the DFA exponent ($d$) of water pH is based on time-scaling properties of dynamics behaviour. The question is whether there are significant relationships between them. This still needs further research.

**Multifractal analysis**

Multifractal analysis results exhibit the clear difference of multifractality between Poyang Lake Inlet and Outlet in Figure 4. The wide opening of the graph indicates a non-uniform clustering structure of the sequences. Relative to Lake Outlet, the larger $\Delta \alpha$ in Lake Inlet shows that the variation of the water pH values is larger and the multifractality is stronger. The larger $\Delta \alpha$, the richer signal in structure. It is obvious that the shape of $f(\alpha)$ curve for Lake Inlet is like a hook to the right and the relation that $\Delta f < 0$ indicates that for Lake Inlet pH series, the probability of the pH values at the lowest values is more than that at the highest values in the whole 4 years, while the reverse is true for Lake Outlet. A larger $B$ value (positive) for Lake Outlet indicates a left skewed multifractal spectrum shape and a relative dominance of lower fractal exponents corresponding to more smooth-looking structures.

We consider that the multifractal parameters calculated over the whole series are not informative about the dynamical differences between Lake Inlet and Outlet. Thus, what we need is a time-dependent analysis of multifractality. By using the variable window sizes method (Shi et al. 2009), one can calculate the temporal evolution of multifractality. In our case, we consider an original window of 52 events (namely 52 weeks) and we calculate multifractal parameters for this data set. Then, we enlarge the window size by one point toward the right along pH time sequence and again calculate multifractal parameters. This added point will result in the change of multifractal parameters. Iterating this procedure for the data sequence, the window size increases step by step and some local measurements are obtained. Each added point (each new pH value) is associated to the occurrence time of the last event in these windows. So the variability of multifractal parameters can provide some information about the temporal evolution dynamics of pH. Figure 5 provides a comparison between the spectra obtained from Lake Inlet and Outlet pH series. Projecting the points on the three-dimensional coordinate ($\Delta \alpha$, $\Delta f$, $B$), we find a clear discrimination between signals measured in Poyang Lake Inlet and Poyang Lake Outlet. The pH series in Poyang Lake Inlet seems to be well separated from that of Poyang Lake Outlet. Now, it is demonstrated that some methods, such as iterated function systems, are useful in time series predicting based on the fractal scaling feature of the data. Thus, a natural step forward in this line of research would be the use of the different fractal characteristics of Lake Inlet and Outlet pH to develop new interpolation predicting methods.
The differences between these two multifractal spectra indicate that heterogeneity (disordered state) characterises Lake Inlet pH dynamics owing to stream flow, pollutant emission and other related factors; while the lake buffered capability results in Lake Outlet pH being characterised by a dynamical change from heterogeneity (disordered state) toward homogeneity (ordered state). This result also indicates that multifractal approach provides a much deeper insight into data structure than monofractal approach.

**Cumulative frequency-size distribution**

Cumulative frequency-size distributions associated with many natural systems exhibit power law scaling. This is the typical “critical” dynamical behaviour found in the SOC systems (Hergarten 2003). A power law applied to a cumulative distribution has the relation (Turcotte & Malamud 2004)

\[ N = cr^{-\lambda} \]

where \( N \) is the cumulative number of events per unit time with size greater than or equal to the magnitude \( r \), \( \lambda \) is the scaling exponent, \( c \) is a constant.

Noting \( \text{pH} = -\log[H^+] \), Figure 6 shows the number density (\( N \)) of pH events (Lake Inlet and Outlet), with size greater than or equal to some pH value \( r \), respectively. Note the similarity to the Gutenberg-Richter law in the earthquakes study (Turcotte & Malamud 2004). We found that water pH in the Poyang Lake Inlet and Outlet exhibits different power law behaviour. For Lake Inlet, the plot exhibits curvature, showing obviously two different scaling regions with the scaling exponent of 1.01 and 0.50 respectively, while for Lake Outlet, only one scaling region appears with the scaling exponent of 2.08. We note that the power law breaks down in smaller pH magnitude regions. We think that low monitoring frequency of pH series result in the low-size tail of the frequency distribution. Peters & Christensen (2006) have found a similar phenomenon in rainfall.

We think that the fluctuation of pH values does not look very different from avalanches from the point of view of SOC. In order to further explain it, we show an analogy between water pH and the sand-pile. In the complex aquatic ecosystems, pH is affected by the water’s chemistry, photosynthesis, solar radiation, nutrients, temperature, algal biomass, pollution discharge and so on (Stumm & Morgan 1981). All the variables driving the change of pH interact with each other and these inter-relationships are complex, nonlinear. We define the measurement value of water pH as an avalanche event, and the magnitudes of various pH values as avalanche sizes in a granular pile. And the superposition of local \([H^+]\) concentration represents the chain of forces in the sand-pile. When the amounts of microscopic condensed \([H^+]\) reach some threshold magnitude, the \([H^+]\) masses can be transported on microscopic scales by diffusion or convection. They reach a new location, where the local \([H^+]\) concentration is lower, and can be diluted. If the local \([H^+]\) concentration in the neighbourhood is also high, the amount of condensed \([H^+]\) masses will increase. Once the system reaches some critical point by its own internal tuning, any small fluctuation, in principle, can trigger a chain reaction like the avalanches in the sand-pile. It is important to note that the system is “tuned” to a critical state solely by its own internal dynamics rather than external dynamics. Therefore, we may interpret the water pH, which goes through very large fluctuations, as consequences of SOC processes. So the power-law scaling in these pH series is equivalent to that of avalanche size evolution.

In Figure 6, we found two different scaling regions for Lake Inlet and only one scaling region for Lake Outlet. For Lake Inlet, stream flow and pollution discharge change greatly. So we infer that the SOC of water pH and SOC of...
rainfall may independently affect the temporal variation of Lake Inlet pH in different regimes respectively, and it is these compound mechanisms that result in the appearance of two different power-law regions for Lake Inlet. However, for Lake Outlet, owing to the effect of Poyang Lake buffered capability, streamflow and pollution discharge have small fluctuation, the independent effect of rainfall SOC becomes small. Thus the SOC of water pH plays a major role in the temporal variation of Lake Outlet pH. It results in the appearance of only one power-law region for Lake Outlet.

CONCLUSIONS

Based on the DFA and multifractal methods, we have identified that water pH in Poyang Lake Inlet and Outlet exhibits strong long-term memory and multifractal characteristics. The comparison result between Lake Inlet and Outlet shows monofractal (DFA exponent) and multifractal (Δα, Δf, B) parameters can be other quantitative indexes reflecting the capability of anti-acidification of Poyang Lake. These new indexes are based on time-scaling properties of pH dynamics behaviour, which are different from the concept of ANC based on aquatic chemistry theory. The scale-free power-law behaviour is found to govern the statistics of water pH over a range of event size scales. Our findings suggest that water pH is an example of a SOC process. The analysis shows that for Lake Inlet, the SOC of water pH and SOC of rainfall may affect the temporal variation of Lake Inlet pH in different regimes respectively; while for Lake Outlet, owing to the lake buffered capability, the SOC of water pH plays a major role in the temporal variation of Lake Outlet pH. The comparison result between Lake Inlet and Outlet pH series can be helpful to the further understanding of Poyang Lake ecological buffered function and improvement of modelling of lake water quality.

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REFERENCES


