Cyclic variations of quality characteristics in river water in an industrial region

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ABSTRACT

River water in industrial regions is a dynamic medium defined by random variables that cannot be described by linear equations. However, some water quality characteristics, e.g., pollutant concentrations, which look chaotically distributed are largely governed by deterministic laws resulting in periodic variations of water chemistry. Understanding this process will enable the researchers to analyse the history of the characteristics involved and to predict their future values. We provide further evidence of predictable, cyclic concentration behavior from the Iset River flowing through a heavily industrialized area in the Ob River basin, Ural Federal District, Russia. In particular, we found that the concentration of copper and nitrate can be characterized by pronounced fractals and quasi-cycles with predominant lengths of 7–8 and 4–5 months, respectively. Our results can improve forecast reliability and water use efficiency. Results from the Iset River could be potentially applicable to virtually any other river in the world, at least in temperate climate areas.

Key words | fractal analysis, phase analysis, quality of river water in industrial region, sustainable water use, water management

HIGHLIGHTS

- Time series (TS) of pollutants in river flows are determined.
- Dynamics of copper and nitrogen oxide concentration in the Iset River (Russia) is fractal.
- The memory depth for TS for different pollutants is different.
- It is advisable to simultaneously apply the fractal and phase analysis in studies of the dynamics of TS.
- The results obtained are not related to the seasonality of changes in water quality.

INTRODUCTION

The problem of sustainable water use is gaining in importance as the economy and the quality of life become more dependent on the chemistry and properties of natural water. The high instability of these characteristics and the unpredictability of pollution events at large scale cause unacceptable economic damage to plants that have to operate under uncertain conditions. The problem can be solved by studying the natural processes and incorporating this knowledge in strategies, rather than ‘mastering the nature’ (Danilov-Danilyan & Rozental 2019). The choice of the methods required to do this is determined by the fact that the characteristics to be controlled, which look random, still follow some laws, the understanding of which is a prerequisite of the sound water management (Lobanova et al. 2015; Rozental & Alexandrovskaya 2018). This assumption is based on experience, which shows that even considerable irregularities in natural systems contain some elements of regular structure (Mandelbrot 1982; Kondepudi & Prigogine 1998; Fulcher et al. 2015; Rozental & Tambieva...
In particular, cyclic processes often take place in the Earth’s lithosphere and biosphere, reflecting the basic principles of environmental development (Kuznetsov et al. 1991; Polishchuk & Yashchenko 2001). Therefore, it is reasonable to assume that the idea of spontaneous leveling of concentrations is true only for a eustatic (stationary) medium. Conversely, definitions such as deterministic chaos and dissipative systems (Kondepudi & Prigogine 1998) are gaining in popularity, and the signs of self-organization processes in solutions (Chashechkin & Rozental 2019), including river water in industrial regions, become more common. Therefore, it would be unreasonable to assume that the redistribution of solute particles in water bodies is governed by completely stochastic forces, or that deterministic factors have no effect at all. The consideration of these factors makes it possible to predict the water composition with a certain degree of probability and makes it possible to develop the software for automatic set-up of water consumption and treatment systems.

**METHODS**

Identification of cyclicity by phase analysis

The assumption regarding the cyclic character of the chemistry and properties of river water in industrial regions was checked using data on the Iset River (the Ob basin), the most heavily polluted water body in the Ural Federal District and one of the dirtiest rivers in Russia. Data on river water chemistry and properties, provided by the Ural Department of Hydrometeorology and Environmental Monitoring, have shown that Iset water contains a lot of nitrogen compounds, manganese, phosphorus, and heavy and non-ferrous metals.

The preliminary analysis of these data has shown some signs of periodicity in variations of pollutant concentrations. The most vivid example is given in Figure 1. It shows distinct cyclic variations of the concentration of copper, which in this section is regarded as most difficult to forecast because of the heterogeneity of the geochemical composition of the territory and the discharges of copper-bearing pollutants by industry. As can be seen from Figure 1(a), the alternating phases, i.e., periods of either positive or negative changes in the concentration, are very similar. Figure 1(b) shows also that the change in concentration $C_i$ ($i$ is the month number) in the same period is similar to a cyclic process with a constant period. However, nothing of this kind can be seen in longer time series (TS). No periodicity can also be seen in the envelope line for the time series of Cu (TS $Cu$, Figure 2), nitrate (TS $NO_3$, Figure 3), and water discharge (TS $D$, Figure 4) from January 25, 2001, to December 23, 2009, at a gage 19.1 km downstream of Yekaterinburg. Even TS $D$ shows no distinct dependence on spring flood and winter low-water season, likely due to the intense water consumption and disposal in the industrial zone.

This required a rigorous analysis, which was carried out with the use of approaches based on phase and fractal analysis. The data used in the analysis were obtained from monitoring with monthly intervals and can be not fully representative. Therefore, the authors also carried out fractal and phase analyses of some other monitored characteristics, which gave basically similar results.

The phase analysis is among the most powerful methods of nonlinear dynamics, which is widely used in the forecast analysis to identify the cyclicity of TS (Zhang 1993; Peters 1996). In this case the nonstochastic processes, which are subject to the effects of either deterministic or stochastic factors, can show not fully periodic behavior, and form quasi-cycles, a quantitative characteristic of which is their length, and a qualitative characteristic is their configuration.
A series \((w_i, w_{i+1}, \ldots, w_{i+k})\) from a total series
\((w_1, w_2, \ldots, w_{n-1})\), containing \(n - 1\) points, in a phase
space \(\varphi_{p-1}(C) = \{w_i\}, w_i = (C_i, C_{i+1}), i = 1, 2, \ldots, n - 1\)
with dimension \(p = 2\) form a cycle (quasi-cycle), if in the inter-
val \([w_i, w_{i+k}]\) segments \((w_i, w_{i+1})\) and \((w_{i+k-1}, w_{i+k})\) intersect
to form the first intersection of the phase trajectory. If the
phase trajectory in the interval \([w_i, w_{i+k}]\) tends to self-intersec-
tion but starts moving away before this self-intersection takes
place, the end of the quasi-cycle is taken to be the point \(w_{i+k}\),
for which \(\rho(w_i, w_{i+k}) = \min_j \rho(w_i, w_{i+j}) < \rho(w_i, w_{i+k+1})\),
\(j = 1, k\); i.e., the distance between \(w_i\) and \(w_{i+k}\) is minimal in
the interval \([w_i, w_{i+k}]\). In this case, \(k + 1\) is the length of the
quasi-cycle.

Figure 5 gives examples found with the use of phase analysis of typical quasi-cycles for the observation series of
TS Cu given in Figure 1.

Note that in some cases, phase analysis clearly shows
nesting of a shorter cycle into another, longer cycle
(Figure 6(a) and 6(b)).

The fuzzy sets of the lengths of quasi-cycles for TS Cu,
NO\(_3\) and \(D\), identified with the use of phase analysis, are
given in Tables 1–3. One can see that only TS \(D\) shows
the predominance of quasi-cycles with a length of half a
year, though the distribution of this characteristic is diffuse,
perhaps because of the non-strict correspondence between
the within-year variations of water regime phases and the
alternation of seasons. It can be seen also that quasi-cycles with a length $d = 7 \pm 1$ dominate for TS $Cu$ and those with $d = 4$ and $d = 5$ dominate for TS $NO_3$. The mechanisms underlying these regularities require special water–environmental studies, but the fact that the total contribution of these TS to the cyclic structure reaches 70% allows the users to forecast the expected chemistry of river water in industrial regions with appropriate reliability.
expected water quality can be evaluated with the use of the membership function $\mu(d)$ of the constructed fuzzy set $M = \{d, \mu(d)\}$ (see Tables 1–3). In the calculation of this characteristic, the lengths of the quasi-cycles with the largest contribution $\nu(d^+) = \max \{\nu(d)\}$ are assigned the values $\mu(d^+) = 0.9$, while the other values of the membership function are evaluated taking into account their contributions as

$$\mu(d) = \frac{0.9 \cdot \nu(d)}{\max \{\nu(d)\}} = \frac{0.9 \cdot \nu(d)}{\nu(d^+)}$$

**Observation of the cyclicity of water chemistry variations with the use of fractal analysis**

This part of the study was carried out to specify the obtained data on the cyclicity of water quality characteristics.

### Table 1 | Quantitative assessment of the reliability of the expected water quality (the length of a quasi-cycle in the form of a fuzzy set $M = \{d, \mu(d)\}$ for TS $Cu$

| Quasi-cycle length $d$ | Number of quasi-cycles $m(d)$ | Contributions of quasi-cycles $\nu(d)$ | Membership function $\mu(d)$ |
|-----------------------|------------------------------|---------------------------------|--------------------------------|
| 3                     | 1                            | 0.059                           | 0.225                          |
| 4                     | 2                            | 0.118                           | 0.45                           |
| 5                     | 2                            | 0.118                           | 0.45                           |
| 6                     | 3                            | 0.176                           | 0.675                          |
| 7                     | 4                            | 0.235                           | 0.9                            |
| 8                     | 3                            | 0.176                           | 0.675                          |
| 9                     | 2                            | 0.118                           | 0.45                           |

### Table 2 | Quantitative assessment of the reliability of the expected water quality (the length of a quasi-cycle in the form of a fuzzy set $M = \{d, \mu(d)\}$ for TS $NO_3$-

| Quasi-cycle length $d$ | Number of quasi-cycles $m(d)$ | Contributions of quasi-cycles $\nu(d)$ | Membership function $\mu(d)$ |
|-----------------------|------------------------------|---------------------------------|--------------------------------|
| 3                     | 6                            | 0.156                           | 0.54                           |
| 4                     | 10                           | 0.227                           | 0.9                            |
| 5                     | 10                           | 0.227                           | 0.9                            |
| 6                     | 4                            | 0.09                            | 0.36                           |
| 7                     | 5                            | 0.114                           | 0.45                           |
| 8                     | 5                            | 0.114                           | 0.45                           |
| 9                     | 2                            | 0.045                           | 0.18                           |
| 10                    | 0                            | 0                               | 0                              |
| 11                    | 1                            | 0.022                           | 0.09                           |
| 12                    | 1                            | 0.022                           | 0.09                           |

### Table 3 | Quantitative assessment of the reliability of the expected water quality (the length of a quasi-cycle in the form of a fuzzy set $M = \{d, \mu(d)\}$ for TS $D$

| Quasi-cycle length $d$ | Number of quasi-cycles $m(d)$ | Contributions of quasi-cycles $\nu(d)$ | Membership function $\mu(d)$ |
|-----------------------|------------------------------|---------------------------------|--------------------------------|
| 3                     | 1                            | 0.059                           | 0.225                          |
| 4                     | 2                            | 0.118                           | 0.45                           |
| 5                     | 3                            | 0.176                           | 0.675                          |
| 6                     | 4                            | 0.235                           | 0.9                            |
| 7                     | 3                            | 0.176                           | 0.675                          |
| 8                     | 2                            | 0.118                           | 0.45                           |
| 9                     | 2                            | 0.118                           | 0.45                           |

Fractals or self-similar objects, which, notwithstanding their irregularity at different scales, look nearly the same, are difficult to describe analytically because of the diversity of the dynamic factors that form them. However, fractal or $R/S$ analysis can be used to determine their presence, thus improving the reliability of the above conclusion or refuting it.

The $R/S$ analysis involves observation of the values of the variable in question and the assessment of deviations of these from random values (Sukhorukov 2011). The random walk is described by Brownian law, according to which the mean-square increment $R_0$ of the examined characteristic is directly proportional to the square root of the current time: $R_0 \sim t^{1/2}$. In the presence of deterministic factors, the exponent changes and a more general case of random walk takes place; as applied to the problem in question, it is described by the law (Mandelbrot 1982; Palma 2007):

$$R(i) = A^{H(i)}$$

where the time is replaced by the number of TS term and

- $A$ is a constant, which can be evaluated as the constant term of the regression equation;
- $S(i)$ is the standard deviation $S(i) = \sqrt{\frac{1}{i-1} \sum_{k=1}^{i} (C_k - \bar{C})^2}$
- $\bar{C}_i = \frac{1}{i} \sum_{k=1}^{i} C_k$ is the current arithmetic mean concentration of the substance in water, $k = 3, 4, \ldots, i$;
- $R(i)$ is the standardized range of variation $R(i) = \frac{\max (\hat{C}_{ij}) - \min (\hat{C}_{ij})}{1 \leq k \leq i, 1 \leq j \leq T}$, i.e., the difference between the maximal and minimal accumulated deviations $\hat{C}_{ij} = \sum_{k=1}^{T} (C_k - \bar{C})$, and $j = 1, T$;
- $H$ is Hurst exponent, a characteristic governing the behavior of TS (Butakov & Grakovskiy 2005; Lepikhin & Perepelitsa 2016).
Figure 7 | R/S- and H-trajectories for TS Cu no. 7, 20 and 40: (a) TS Cu no. 7 with a clearly seen quasi-cycle with a length of 6; (b) TS Cu no. 20; (c) TS Cu no. 40.
At $H > 0.5$ (black-noise domain), the series in question shows long-range correlation between the characteristics referred to as persistence, suggesting the presence of long-term memory in TS (Geweke & Porter-Hudak 1985; Palma 2007). In the problem under consideration, this means that the chemistry and properties of water in the past are closely related with their current and future characteristics. This feature of TS also demonstrates its fractal character. At $H = 0.5$ (the domain of white noise) all variables have the same variance and each value has zero correlation with all other values in the series. At $H < 0.5$ the time series is nonpersistent, tending to return toward the mean, such that an increase in the characteristic in some period will, most likely, give place to its decrease in the following period, again followed by an increase (Peters 1996; Perepelitsa & Popova 2001; Perepelitsa et al. 2005).

$R/S$ analysis is a multistep process. It is first carried out for the entire TS (Yamaguchi et al. 1987) (in this case, since December 25, 2001), and next repeated for series obtained from the original by successive elimination of the initial terms of the series. The Hurst exponent is successively evaluated at $A = 0.5$:

$$H(i) = \frac{\log (R(i)/S(i))}{\log (i/2)}$$

until the number of remaining TS terms becomes approximately equal to the supposed memory depth, if it exists. The total number of steps (the main and truncated) for all TS was 90 by data for the same time interval from January 25, 2001, to December 23, 2009.

The Hurst exponent was found to reach 0.8–0.9 for 82% of the truncated TS $Cu$, suggesting a long memory (from 6 to 20 periods). Typical results are given in Figure 7(a)–7(c). In some cases, $R/S$-trajectories were found to abruptly drop from the black-noise into the white-noise domain (from the deterministic into the stochastic state, as given in Figure 7(a)). In other cases, they remained in the black-noise domain (Figure 7(b)), and it was only in 8% of cases that the passage into the white-noise domain was smooth (Figure 7(c)).

**RESULTS AND DISCUSSION**

In all cases, the fractal analysis of TS $Cu$ shows the presence of long memory all over the length of the series, though its depth in many cases is not distinct (Figure 7(b) and 7(c)). At the same time, the results of fractal and phase analysis of TS $Cu$ are not contradictory. This can be seen, for example, from the comparison of Figures 5(a) and 7(a), presenting the results of the visualization of the phase trajectory and $R/S$- and $H$-trajectories, for the same segment of TS $Cu$ (starting from the point $C_7$ (July 2001)). This follows from the comparison of Figures 6(a) and 7(b) for a segment of TS $Cu$ starting from the point $C_{20}$ (August 2002).

Regularities in the variations of the cyclic component of water quality characteristics, obtained with the use of fractal and phase analyses for TS $Cu$ are given in Figure 8(a) and Table 4. It can be seen that the most common length of quasi-cycle ($q$) is $7 \pm 1$ months. Figure 8(a)–8(c) show a graphic representation of the fuzzy sets of memory depth ($q$, $\mu(q)$) of the time series $Cu$, $NO_3$, and $D$, respectively. Here $q$ is the detected length of the quasi-cycle, and $\mu(q)$ is the membership function of this set (Peters 1996; Perepelitsa & Popova 2001; Perepelitsa et al. 2005).

In the case of TS $NO_3$ and TS $P$, fractal analysis also suggests the presence of long memory, as can be seen from Figure 8(b) and 8(c) and Tables 5 and 6.

This leads to a general conclusion that the seemingly chaotic variations of water quality characteristics at the analysed gages during the chosen period show obvious elements of ordering. This can be seen from the results of fractal and phase analyses. Such data, obtained timely by many plants withdrawing water from the Iset River, would improve the stability of water use.

**Figure 8** Graphic image of a fuzzy set memory depth (the length of quasi-cycles) ($q$, $\mu(q)$). (a) The lengths of quasi-cycles identified in TS $Cu$ with the use of fractal and phase analysis. (b) The lengths of quasi-cycles identified in TS $NO_3$ with the use of phase analysis. (c) The lengths of quasi-cycles identified in TS $D$ with the use of phase analysis.
CONCLUSIONS

The joint application of fractal and phase analysis to water quality in the Iset River in Sverdlovsk oblast showed elements of periodicity in the structure of TS for the monitored characteristics and quasi-cyclic TS character. The presence of cyclic variations suggests the possible manifestation of self-regulation mechanisms. Such effect is of undoubted scientific interest for understanding the dynamic characteristics of river flow. This is also of practical importance, as it allows assessment of the dependence of the future values of the monitored characteristics on their previous values and forecasting of water quality.

The examined hydrometeorological data were used to identify the effects of the deterministic factors on water chemistry and to assess the memory depth for various TS. In the case of copper, this value is 6–8 months in almost 70% of cases, and in the case of nitrate, it is 4–6 months in 60% of cases. The cyclic component derived from the fractal and phase analyses is the same in the majority of series fragments with distinct quasi-cycles.

The obtained quantitative results are not related to seasonal variations of water quality and suggest the existence of external factors, which, most likely, are of anthropogenic nature and which have to be taken into account in planning the regime of water consumption and treatment by the numerous users in the industrial region.

DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

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