Analysis of long-term variations in physico-chemical parameters of seawater in the southern Baltic Sea; an approach to incomplete data series

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Abstract

Long-term trends in the variations of physical and chemical parameters characterising seawater were analysed by a method, originally used in climatology, allowing detection of optimal cycles of these variations in incomplete (intermittent) data time series.

The method was used to analyse measurements of water temperature, salinity, density, oxygen saturation and nutrient concentrations (phosphate, nitrate and silicate) from station BMP L1 (P1) in the Gdańsk Deep region obtained between 1979 and 1996.

All parameters revealed a pattern of regular cycles, the spectrum of the cycles being dependent on the parameters and water layer.

As regards reconstruction and forecasting in the deterministic-stochastic model, statistically significant correlation coefficients in the 0.57–0.97 range were obtained between the calculated and empirical data for all the parameters examined. The correlation was poorest in the case of silicate.

Linear regression trends calculated in the deterministic-stochastic model were in relatively good agreement with those obtained using Hirsch's non-parametric test.

1. Introduction

Hydroclimatic elements, like precipitation, air temperature or riverine outflow, vary naturally with time. The daily, seasonal, annual and long-term oscillations are caused mainly by the rotation of the Earth, its motion around the Sun, also by the motion of the Moon, and by centennial changes in the Sun's activity. These oscillations are additionally affected by changes resulting from man's activities, *e.g.* elevated quantities of dust in the atmosphere (absorption of solar radiation, multiple nuclei for vapour condensation, the carbon dioxide problem), the control of water levels in water basins, land reclamation or heavy urbanisation.

Since the sea is exposed to the influence of air-temperature, atmosphericpressure and humidity fields, natural periodic variations are also found in the hydrochemical parameters characteristic of seawater.

Variations of this kind were analysed in data time series from the southern Baltic of seawater temperature, salinity, density, oxygen saturation and nutrient concentrations. Boryczka's method (1981, 1984, 1993), introduced in climatology, was applied to study periodic changes in these variables. This method has proved successful in the detection of optimal (real) periods and trends in meteorological fields (Boryczka 1981). It has also been applied in stochastic-deterministic modelling (Boryczka 1984), and to reconstruct and forecast the elements of the water balance (Gutry-Korycka & Boryczka 1990). Moreover, it has been found useful in the analysis of long-term variations of salinity in Baltic Sea water (Cyberski 1995).

In this method, a concealed period of optimal sinusoids (*e.g.* in Fourier analysis the *n*-th, n/2-th, n/3-th... periods are assumed by dividing the chronological data series into two, three, ..., *n* parts and do not correspond to real periods) is found by solving the regression plane equation

$$y = a_0 + \alpha x_1 + \beta x_2$$

with respect to variables $x_1 = \sin \frac{2\pi}{\Theta} t$ and $x_2 = \cos \frac{2\pi}{\Theta} t$, where

t – time,

 Θ – real period,

the amplitude (b) in the formula is

$$b = (\alpha^2 + \beta^2)^{1/2},$$

the phase displacement (c) is

$$\operatorname{tg} c = \frac{\beta}{\alpha},$$

and the angle c satisfies the conditions $\alpha = b \cos c$, $\beta = b \sin c$.

Hence, the optimal periods Θ_j at the minima of the residual variance ε^2 correspond to the maxima of the multiple correlation coefficient

$$R_a = \left(1 - \frac{\varepsilon^2}{s^2}\right)^{1/2},$$

where s is the standard deviation of variable y.

By using regression sinusoids, dense oscillation spectra are obtained with a period even longer than that of the experimental data series, which allows respective variations to be forecast. Simultaneously, the missing data in the time series are approximated with arbitrary discretion. The reconstruction of a time series is of particular importance in the analysis of long-term fluctuations of oceanographic parameters measured at random time intervals.

Once the optimal periods Θ_j have been determined, the linear trend can be calculated from the final equation

$$y = f(t) = \underbrace{a_0 + at}_{\text{linear changes}} + \underbrace{\sum_{j=1}^k b_j \sin\left(\frac{2\pi}{\Theta_j}t + c_j\right)}_{\substack{\text{periodic variations}}} + \underbrace{\varepsilon_j}_{\substack{\text{stochastic component}}}$$

In this study the method was applied in the form of a computer programme prepared at the Department of Oceanography at Gdańsk University (Cyberski 1995).

2. Material and methods

The analysis was carried out with the experimental data from station BMP L1 (P1) situated in the Gdańsk Deep (Fig. 1) from the years 1979–1996. The hydrochemical data in the oceanographic data base of the Maritime Branch of the Institute of Meteorology and Water Management ($IMGW - data \ base$) were collected within the framework of a) the Helsinki Commission's Baltic Monitoring Programme, financed in Poland by the National Inspectorate for Environmental Protection, b) the IMWM's statutory oceanographic service, and c) various research projects subsidised by the Polish State Committee for Scientific Research.

The data were collected during research cruises using the same methods of measurement and chemical analysis throughout the period under consideration (HELCOM 1988, Lysiak-Pastuszak *et al.* 1998). The time lapse between the cruises was scheduled at 1–2 months but circumstantial irregularities in the measurements are evident in the data series.



Fig. 1. Location of station BMP L1 (P1) in the Gdańsk Deep

The following data were analysed: seawater temperature, salinity and density ($ca\ 200$ results), water saturation with oxygen ($ca\ 160$) and nutrient concentrations – phosphate, nitrate and silicate (130–100), in the 0–24 m, 25–44 m, 45–54 m, 55–64 m, 65–74 m, 75–84 m and 85 m-to-bottom water layers. The lowest level, usually 2 m above the bottom, was at 107 or 108 m. The data were not validated before processing.

The computations based on the Boryczka method consisted of three steps:

- calculations of concealed periods within the 0.01–5 year time range with a 0.01 year discretisation;
- visualisation and determination of residual variance minima (optimal period detection);
- calculations using the model: reconstruction of missing data, hindcasting, forecasting and linear trend determination.

Wisła river runoff values and nutrient (phosphate and nitrate) concentrations in the riverine water from 1987–1996 were kindly supplied by Dr. E. Niemirycz from the IMWM's Department of Riverine Water Protection. The precipitation figures at the land stations were taken from the IMWM's weather records.

The trend functions calculated with the Boryczka model were compared with the long-term trend analysis using Hirsch's non-parametric test, based on Kendal's τ (Helsel & Hirsch 1992). The software was worked out by Sandén (1994) and distributed among the Baltic laboratories for the statistical processing of hydrographic data for the purpose of the Third Periodic Assessment of the State of the Marine Environment of the Baltic Sea (HELCOM 1997).

3. Results and discussion

3.1. Analysis of periodic variations

Periodic variations were detected in all the hydrochemical parameters examined in the present project. Figs. 2a–g illustrate the optimal periods found in the variations of the parameters in particular water layers.

The number of cycles in the spectrum and their duration depends on the parameter and water layer analysed. In all cases there appears a 1-year period which is especially intensive from the surface layer down to 50-60m. Furthermore, there is a well-marked half-yearly cycle in the variations in water saturation with oxygen (Fig. 2d) and nitrate concentrations (Fig. 2g) in the 0-24 and 25-44 m layers. This cycle, presumably related to the growing season, is less obvious in the phosphate and silicate concentrations (Figs. 2e,f). A fairly distinct band of about 2 weeks' duration is present in the spectra of phosphate, nitrate and silicate variations in the $0-24\,\mathrm{m}$ water layer (Figs. 2e–g). An attempt was undertaken to relate the observed periodic variability of hydrochemical parameters to the river outflow rate, the nutrient concentrations in river water and the precipitation (from the rainfall records at the Gdynia and Hel weather stations). Analysis of this data by Boryczka's method revealed a similar 2-week period, this time a much more clearly discernible one, in the Wisła runoff and nitrate concentrations in the river water (Fig. 3) and in the precipitation (Fig. 4). The illustration of phosphate concentration fluctuations in the river water shows that there are no periodic changes. This is understandable, bearing in mind the entirely different routes by which nitrogen and phosphorus compounds enter the river system.

The increasing number of factors affecting the hydrochemical parameters of seawater is reflected in the proliferating periodic fluctuations, especially in water layers with a steep salinity gradient and below the halocline. In the layers beneath the halocline, each parameter is characterised by a slightly different spectrum of periods, though there are obvious similarities in the salinity and density spectra (Figs. 2b,c) as well as in oxygen saturation and phosphate concentrations (Figs. 2d,e).

The well-pronounced quasi 2-year cycles present in deeper water layers are also observed in the troposphere, manifesting themselves as an increase in air temperature and a summer decrease in precipitation. It is very probable that the fluctuations in the physical parameters of seawater are related to climatic changes. An analogous explanation can be applied to



Fig. 2. Optimal periods (local minima of residual variation) detected in the variations of hydrochemical parameters in various water layers: temperature (a), salinity (b), density (c), oxygen saturation (d), phosphate (e), silicate (f), nitrate (g)



Fig. 2. (continued)



Fig. 2. (continued)



Fig. 2. (continued)



Fig. 2. (continued)



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Fig. 2. (continued)



Fig. 2. (continued)



Fig. 3. Optimal periods detected in the Wisła river runoff and in nutrient concentrations



Fig. 4. Optimal periods detected in the precipitation [mm] at the Gdynia and Hel weather stations

the ~ 3.5 -year periods, conspicuous in the salinity and density spectra. Cycles of precisely this duration were found in the 90-year (1901–1990) hydrological series of the monthly mean Wisła outflow rates and the total riverine outflow into the Baltic Sea (Cyberski 1995). Periods of similar length have also been detected in the mass and energy exchange relationships in the North Atlantic system (Kullenberg 1981).

3.2. Long-term trend analysis

Boryczka's mathematical method can be used for calculating these parameters in the deterministic-stochastic model with an arbitrary discretisation, because the method also approximates an incomplete data series by regression sinusoids (periodic variations in the final equation). Figs. 5a–e illustrate the fit between the modelled and experimental values in two opposed water layers – surface (0–24 m) and near-bottom (85 m–bottom).

The approximations were verified by the Fisher-Snedecor test (Doerffel 1989) and Student's *t*-test of correlation (Oktaba 1980). The modelled values were found to be in good agreement with the experimental data, because the correlation coefficients fell within the 0.57-0.97 range, depending on the parameter and water layer, and they were all statistically significant at the 0.01 and 0.05 confidence levels. Generally speaking, the correlation of the physical parameters was better (Figs. 5a,b) than that of the nutrient concentrations (Figs. 5c–e). The modelled silicate concentrations displayed the poorest fit to the field data (Fig. 5e). Moreover, the approximations were better in the upper part of the water column than below the halocline.



Fig. 5. Approximation of hydrochemical parameters by Boryczka's deterministic and stochastic model: salinity (a), oxygen saturation (b), phosphate (c), silicate (d), nitrate (e)



Fig. 5. (continued)



e





Fig. 5. (continued)

This good agreement between calculated and field data suggested the possibility of extrapolating the time series and trend function as a forecast and hindcast. An example of the extrapolation results for the time span 1975–2010 is shown in Fig. 6; the measurement series is from 1979–1996.

The coefficients of trend functions calculated in the Boryczka model (linear changes in the final equation), indicated by the broken line in Figs. 5a–e and 6, were compared (Table 1) with those obtained using Hirsch's non-parametric test (Helsel & Hirsch 1992).

The marked characters in the Hirsch trends denote statistically significant values. In the case of conservative parameters, both methods show good agreement as regards the direction and magnitude of changes, and

Table 1. Linear trend coefficients calculated by Boryczka's method (B_0) and by the Mann-Kendall method according to Hirsch's non-parametric test (slope)

Layer [m]	$\begin{array}{c} \text{Temperature} \\ [^{\circ}\text{C year}^{-1}] \end{array}$		Sal [PSU	inity year ⁻¹]	Density $[\delta \text{ year}^{-1}]$	
	B_0	slope	B_0	slope	B_0	slope
$\begin{array}{c} 0-24\\ 25-44\\ 45-54\\ 55-64\\ 65-74\\ 75-64\\ \end{array}$	$\begin{array}{c} 0.058 \\ 0.087 \\ 0.111 \\ 0.111 \\ 0.087 \\ 0.046 \end{array}$	0.086 0.031 0.110 0.106 0.061	$\begin{array}{c} -0.039 \\ -0.043 \\ -0.043 \\ -0.049 \\ -0.066 \\ 0.072 \end{array}$	$\begin{array}{r} -0.038 \\ -0.039 \\ -0.039 \\ -0.052 \\ -0.084 \\ 0.001 \end{array}$	$\begin{array}{r} -0.043 \\ -0.043 \\ -0.044 \\ -0.048 \\ -0.066 \\ 0.065 \end{array}$	$\begin{array}{r} -0.044 \\ -0.035 \\ -0.041 \\ -0.048 \\ -0.080 \\ 0.072 \end{array}$
75–84 85–bottom	$\begin{array}{c} 0.046 \\ 0.007 \end{array}$	$\begin{array}{c} 0.030 \\ 0.003 \end{array}$	$-0.073 \\ -0.025$	- 0.081 -0.040	$-0.065 \\ -0.031$	- 0.072 -0.037

a) physical parameters

b) chemical parameters

Layer [m]	Oxygen $[\% \text{ year}^{-1}]$		Phosphate		Silicate $[mmol m^{-3} year^{-1}]$		Nitrate]	
	B_0	slope	B_0	slope	B_0	slope	B_0	slope
0-24	0.261	0.213	0.002	0.002	0.135	0.162	-0.031	0.005
25 - 44	0.277	0.384	-0.003	-0.001	0.009	0.111	-0.020	0.016
45 - 54	0.251	0.454	-0.003	-0.002	-0.121	-0.165	-0.038	-0.027
55-64	0.844	0.759	0.000	-0.006	-0.169	-0.201	-0.029	0.005
65 - 74	1.216	1.377	-0.004	0.011	-0.159	-0.108	-0.016	-0.045
75 - 84	0.884	1.589	0.033	-0.015	-0.248	-0.688	-0.112	0.011
85-bottom	0.694	0.941	-0.090	-0.078	-0.856	-1.279	-0.048	0.102



Fig. 6. Extrapolation of data time series of water temperature in selected water layers and the trend function illustrated by the Boryczka model

acceptable discrepancies in magnitude in the case of water saturation with oxygen. However, the further use of Boryczka's method requires thorough statistical validation of the results.

4. Conclusions

- The physico-chemical parameters characterising seawater are subject to periodic variations.
- The number and length of optimal periods detected in the variables studied depends on the parameter and depth. All the parameters displayed a pronounced annual cycle in the upper part of the water column. Longer periods were found in deeper water layers.
- The detected cycles in the fluctuations of physico-chemical parameters can be related to the periodic variations in meteorological elements and also to hydrological factors, *e.g.* river outflow rates.

- The deterministic-stochastic model introduced by Boryczka in climatology to analyse meteorological fields gives a good approximation of the elements studied. Statistically significant correlation coefficients lie within the 0.57–0.97 range.
- Trend analysis by Boryczka's method showed relatively good comparability with the results achieved using the Hirsch test, though further statistical validation is required.

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