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A simple approach for statistical modelling of ice phenomena in the Curonian Lagoon, the south-eastern Baltic Sea

Viktorija Rukšėnienė, Inga Dailidienė, Kai Myrberg, Kęstutis Dučinskas

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Abstract The paper addresses the possibilities of spatio-temporal statistical modelling of basic hydrophysical and meteorological parameters of sea surface layer in the south-eastern Baltic Sea, Curonian Lagoon. The aim of the paper is to compare two methods (multivariate linear regression and regression kriging) for the analysis of changes and trends of ice phenomena, their dependence on changes in the air temperature, sea surface temperature and water salinity. The prediction of ice conditions for several locations at different distances from the reference sites shows that spatial information is an extremely important factor in making forecasts. The application of the regression kriging is more efficient than the multivariate linear regression for predicting the ice phenomena in semi-enclosed basins and lagoons.

Keywords *• ice phenomena • sea surface temperature • air temperature • water salinity • multivariate linear regression • regression kriging*

✉ *Viktorija Rukšėnienė (viktorija.rukseniene@gmail.com), Inga Dailidienė, Kęstutis Dučinskas, Faculty of Natural Sciences and Mathematics, Klaipėda University, H. Manto Str. 84, 92294 Klaipėda, Lithuania; Kai Myrberg, Finnish Environment Institute / Marine Research Centre, P.O.Box 140, FI-00251 Helsinki, Finland*

INTRODUCTION

Water temperature and ice phenomena are the basic physical characteristics describing properties of sea surface. They have a direct impact on the aquatic ecosystems, for the navigation and fishery. While monitoring the status and properties of the sea water, the sea surface water should be considered as an important part of comprehensive analysis of spatial-temporal variability within existing marine data of the Baltic marine environment monitoring programme. This analysis is used to determine the current environmental status, trends and prognosis foreseen in the requirements of European Parliament and of the Council formulated in the Marine Strategy Framework Directive (MFSD) (MSFD 2008).

To obtain reliable spatial statistics, it is essential to provide a full hydrophysical and hydrochemical analysis of the data and to compare the observed results with the estimated values of different statistical models. Presently, statistical methods are widely used to validate various models. Such methods could be found in any quantitative science, including ecology and environmental studies. According to Cressie (1993) there is a need for new statistical models and approaches that address new questions arising from both old and novel technologies. The application of mathematical models for investigations of marine ecosystems often yields substantial scientific merits (Renk 1989). Marine hydrodynamic processes are among the most changeable, non-linear ones owning a multitude of scales in space and time. Thus, it is a complicated task to describe various changes in water parameters and interactions among them.

The complicated behaviour of climatic systems requires the usage of mathematical models with increasing complexity. There is a continuous need to improve these models and make them applicable for various purposes. In the recent decades, one of the main priorities for scientific research has been climate variability, particularly because of the observed global warming. The global sea surface temperature has risen by approximately 1°C in 140 years. This increase is one of the primary physical impacts of climate change (Coppini *et al.* 2007). The sea surface temperature (SST) in European seas is increasing more rapidly than in the World Ocean on average. In this context, the coastal lagoons are most vulnerable to direct impacts of climate change (Dailidienė *et al.* 2011). They serve as links and mediators between terrestrial ecosystems and the open sea (Schiewer 2002). Among the requirements of the MFSD (MSFD 2008), there are the diverse conditions, problems and needs of various marine regions or subregions that host specific marine environment and that require different and specific solutions. A comprehensive knowledge of the trends in the parameters of the hydrological regime is relevant for not only the knowledge of the processes of climate change but also for the development of strategies of adaptation to the consequences of these processes.

Spatial data about various properties of the sea often have a limited resolution and the observation points are distributed irregularly. Collecting data in a certain period of time may thus cause many irregularities. Solution of the "spatial" problem is generally based on various ways to interpolate the data or to estimate the average quantities. The data collected in a certain time interval are often used to predict the future trends or to investigate seasonal processes. In many occasions, various spatio-temporal projections are required. A straightforward solution is to analyse collected spatial data at a single time instant, ignoring the temporal changes. Alternatively, it is possible to work with the time layers at different points, to predict, extrapolate and evaluate the values at locations outside the sampling area. In general, it is necessary to take into account both spatial and temporal correlations and to establish the interrelations between them (Dučinskas, Šaltytė-Benth 2003). Another problem is a choice of the statistical model. If the data have been collected spatially, it is common to start from empirical semivariogram techniques for the estimation of isotropic model parameters such as nugget, sill and range. The weighted least squares (WLS) method is often used for estimation of above-mentioned parameters (Dučinskas, Šaltytė-Benth 2003).

While investigating the characteristics of the spatial distributions of various properties in the natural environment or their temporal changes, we often face the lack of data. For example, monitoring of various sea parameters is often carried out just once or a few times per season. As an example, according to the Lithuanian State Environmental Monitoring Programme (Ministry of Environment of the Republic of Lithuania 1998), in Lithuanian territorial waters national monitoring takes place 4–6 times per year in the open Baltic Sea, whereas in the Curonian Lagoon monitoring is carried out 1–2 time per month.

This paper is devoted to the analysis of the changes in physical processes in the Curonian Lagoon. The main purpose is to analyse changes in the ice phenomena, their dependence on the related changes in the air temperature, sea surface temperature (SST) and water salinity in the Lithuanian part of the Curonian Lagoon. We employ spatio-temporal analysis of hydrophysical data using multiple linear models. This method assists in determining whether the network of monitoring stations is adequate and optimal, and helps to integrate regression coefficients into various models (Verfaillie, Lancker, Meirvenne 2006).

MATERIAL AND METHODS

The semi-enclosed and shallow Curonian Lagoon (Fig. 1), a large shallow coastal water body situated in the south-eastern (SE) part of the Baltic Sea, is like a model of a small continental sea having an ecosystem that is sensitive to both internal and external pressures. The lagoon is separated from the open Baltic Sea by the relatively narrow sandy Curonian Spit and is connected to the sea only through the Klaipėda Strait (width of 0.3–0.6 km) located at the northern end of the lagoon. The Curonian Lagoon has a total area of approximately 1584 km^2. The northern part of the lagoon, that takes about 413 km^2 (26 %) of the total area (Ministry of Environment of the Republic of Lithuania 1998), belongs to the Lithuanian territory. The southern and central parts of the lagoon have almost fresh water due to discharge from the River Nemunas (on average 22 km^3 year^{-1}) and other smaller rivers (about 1 km^3 year^{-1}). The salinity in the lagoon ranges from <0.5 ‰ till 7.5 ‰ (Dailidienė, Baudler, Chubarenko, Navrotskaya 2011). The duration of ice season has decreased by about one month in the south-eastern part of the Baltic Sea, including the Curonian Lagoon. This change is related to the rise of the mean air and water temperatures (Dailidienė, Davulienė, Kelpšaitė, Razinkovas 2012). The hydrological regime and the ice phenomena in the lagoon are mostly controlled by wind patterns, air temperature, water temperature and salinity variations.

To project the mean ice phenomena in the Curonian Lagoon, we use multivariate linear regression (MLR) and regression kriging (RK). The focus is on two locations in central part of the lagoon (sites 12A and 14 in Fig. 1). The first target point is situated in the northern part (site 5) of the lagoon and the second one in the Klaipėda Strait (3 and 3A). Ice phenomena at these points are predicted according to the air temperature, sea surface temperature (SST) and water salinity data from the monitoring stations (1, 2, 3B, 8, 10, 12; Fig. 1).

We used water temperature (SST), salinity and ice phenomena data collected in the Curonian Lagoon monitoring stations operated by the Department of Marine Research of the Environmental Protection Agency. Observations of air temperature, sea water salinity and water temperature are carried out once a month. The measurements are not carried out when the lagoon is completely covered by ice. The records thus represent the time when the ice is melting, drift ice periods or without the ice periods. Throughout the sampling of data in 1993–2013, the ice phenomena were collected in the Lithuanian monitoring stations only in 2009–2012. Thus, the data set has been composed for this period.

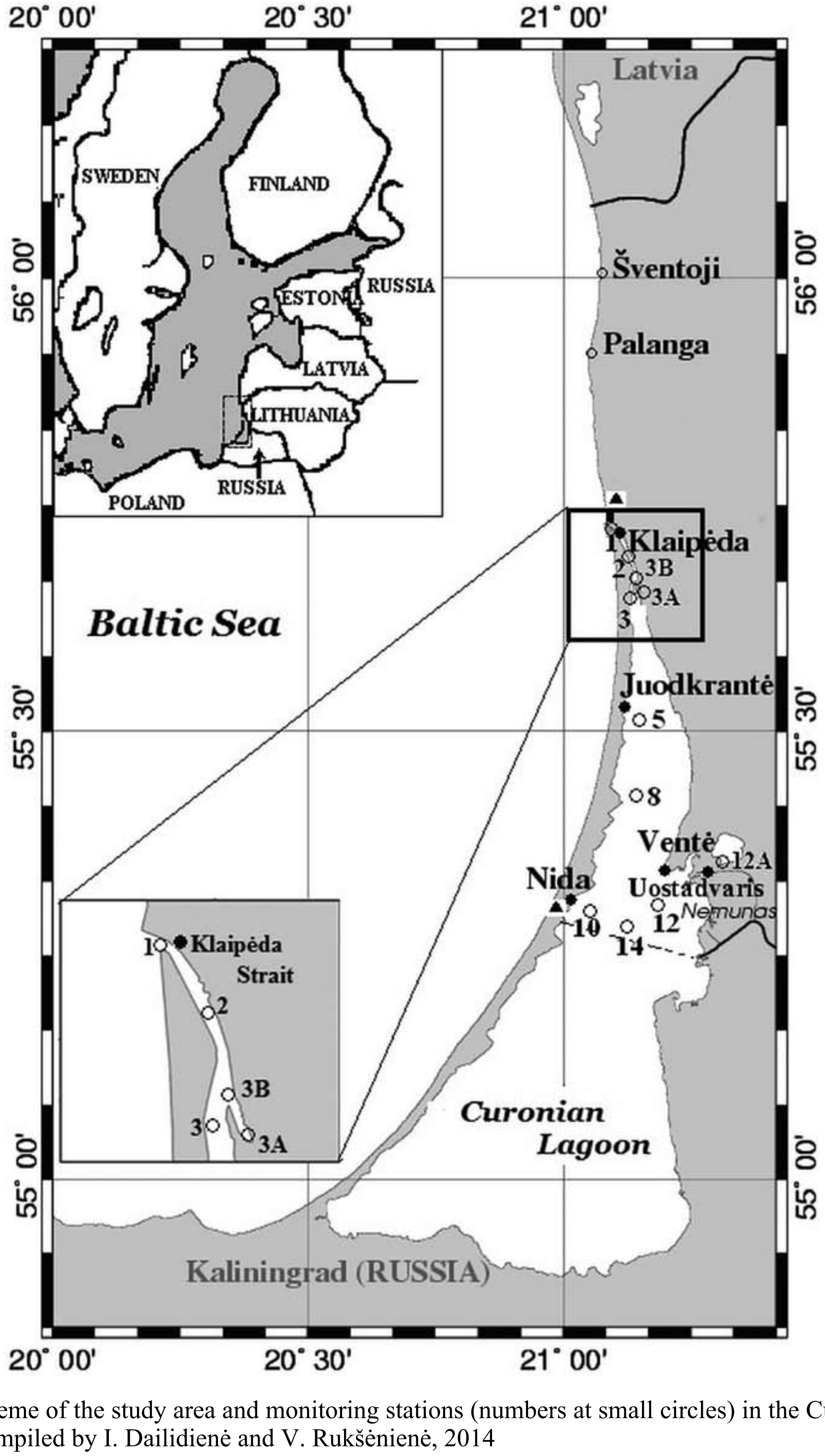

Fig. 1 Location scheme of the study area and monitoring stations (numbers at small circles) in the Curonian Lagoon and Klaipėda Strait. Compiled by I. Dailidienė and V. Rukšėnienė, 2014

We compare two methods: multivariate linear regression (MLR) and regression kriging (RK), in order to clarify the dependence of ice phenomena formation and air temperature, SST and salinity variation as well as the dependence of spatial dispersion of ice phenomena on these parameters variations and distance from the sea port gate to the lagoon.

A well-known approach consists of modelling the relation between the ice formation and air temperature, SST and salinity using a linear function

$$I^* = b_0 + b_1 T + b_2 T_W + b_3 S_W, \quad [1]$$

where I^* quantifies the ice formation scoring from 1 to 10 points at location s, b_0 is a constant that characterises the value of the intercept, b_1, b_2, b_3 are the slope constants; T (°C) is the measurement of the air temperature at location s, T_W (°C) is the measurement of the SST at location s and S_W (‰) is the measurement of the salinity at location s.

Equation [1] converts the values of air temperature, SST and salinity into a quantity that characterises ice formation. This type of regression has the major shortcoming that the ice formation is only derived from air temperature, SST and salinity at a single location s, regardless of the surrounding values (Verfaillie, Lancker, Meirvenne 2006).

The use of geostatistical interpolation techniques (generally known as kriging) often provide more options for spatio-temporal projections than deterministic techniques like trend surfaces. Their advantage is the ability of systematic use of the spatial correlations between neighbouring observations to predict values at unsampled places (Goovarts 1999). The use of geostatistical techniques requires a relation (like Eq. [1]) between the predicted variable (e.g. ice phenomena) and secondary variables (e.g. air temperature, SST and salinity). It is possible to include this secondary information into the interpolation.

A well-known approach consists of modelling the relation between the ice phenomena and the air temperature, SST, and salinity using spatial linear models with covariates in trend and stationary Gaussian random error at location s and time moment t:

$$I^* = \beta_0^{(t)} + \beta_1^{(t)} T + \beta_2^{(t)} T_W + \beta_3^{(t)} S_W + \varepsilon^{(t)}(s), \quad [2]$$

where I^* quantifies the ice phenomena scoring from 1 to 10 points, $\beta_0^{(t)}$, $\beta_1^{(t)}$, $\beta_2^{(t)}$ and $\beta_3^{(t)}$ are unknown trend parameters, T (°C) is the measurement of air temperature, T_W (°C) is the measurement of sea surface water temperature, S_W (‰) is the measurement of sea surface water salinity and $\varepsilon^{(t)}(s)$ is random error with parametric semivariogram denoted by $\gamma(h, \theta)$.

Suppose $\hat{\beta}^{(t)} = \left(\hat{\beta}_0^{(t)}, \hat{\beta}_1^{(t)}, \hat{\beta}_2^{(t)}, \hat{\beta}_3^{(t)}\right)$ are ordinary least squares methods (*OLS*) estimators of $\beta^{(t)} = \left(\beta_0^{(t)}, \beta_1^{(t)}, \beta_2^{(t)}, \beta_3^{(t)}\right)$. Then the estimated residual is $\hat{\varepsilon}^{(t)}(s) = I^* - \hat{\beta}_0^{(t)} - \hat{\beta}_1^{(t)} T - \hat{\beta}_2^{(t)} T_W - \hat{\beta}_3^{(t)} S_W$.

The parameter of semivariograms θ is estimated by fitting the model to the values of empirical semivariogram given by the following equation:

$$\hat{\gamma}^{(t)}(h) = \frac{1}{2|N(h)|} \sum_{\{i,j: i,j=1,\ldots,n; |s_i - s_j| = h\}} \left(\hat{\varepsilon}(s_i) - \hat{\varepsilon}(s_j)\right)^2, \quad [3]$$

where $N(h)$ is the number of data pairs separated by a distance h, $\hat{\varepsilon}(s_i)$ and $\hat{\varepsilon}(s_j)$ are the estimated residuals at locations s_i and s_j that are separated by distance h. The *WLS* estimator of θ is $\hat{\theta} = \left(\hat{\sigma}^2, \hat{\tau}^2, \hat{\varphi}\right)$.

The fitting of a theoretical semivariogram (a curve) is an important step in the analysis. The “sill” (σ^2) is the total variance of the variable, the “range” (τ^2) is the maximal spatial extent of spatial correlation between observations of the variable and the “nugget” (φ) is the random error (Verfaillie, Lancker, Meirvenne 2006). The exponential, Gaussian and spherical models were fit to the sample semivariograms. The semivariogram models with the smallest ordinary least squares estimates were selected to describe the spatial dependencies.

The model presented by Eqs. [1] and [2] has been applied using open-source programming language R (http://www.r-project.org/), which provides a wide variety of statistical (linear and nonlinear modelling, classical statistical tests, time-series analysis, classification, clustering) and high level graphical techniques, a programming language, interfaces to other languages and debugging facilities. Prediction of I^* values at unsampled locations has been made by kriging, using estimators of the model given by Eq. [2] as described above.

Several indices are suitable to evaluate the interpolation. In essence, they all are a measure of estimation error that is the difference $I^*(S_\alpha) - I(S_\alpha)$ between the estimated and observed values. The mean estimation error *MEE* has to be about zero for unbiased estimators:

$$MEE = \frac{1}{n} \sum_{\alpha=1}^{n} \left(I^*(s_\alpha) - I(s_\alpha)\right). \quad [4]$$

The mean square estimation error (*MSEE*) has to be as low as possible. This measure is useful for the comparison of different procedures. The root mean square estimation error (*RMSEE*) is expressed in the same units as the variable in question. This parameter has to be compared to the variance or the standard deviation of the dataset:

$$MSEE = \frac{1}{n} \sum_{\alpha=1}^{n} \left(I^*(s_\alpha) - I(s_\alpha)\right)^2. \quad [5]$$

The mean absolute estimation error (*MAEE*), which is analogous to the *MSEE*, but less sensitive to extreme deviations.

$$MAEE = \frac{1}{n}\sum_{\alpha=1}^{n}\left|I^{*}(s_{\alpha}) - I(s_{\alpha})\right|. \quad [6]$$

The Pearson correlation coefficient (*R*) between $I^*(s)$ and $I(s)$ indicates the degree of linear correlation between the observed and estimated values. This value has always to be considered in combination with the *MEE*. The correlation coefficient is itself a measure of the proportion of variance explained, hence it is related to the *MSEE* (Verfaillie, Lancker, Meirvenne 2006).

RESULTS

The Curonian Lagoon is totally ice-covered 1–3 times per year in the cold period (from October till April). Ice phenomena (from the first appearance of ice and until the final disappearance of sea and coastal ice) can repeatedly appear inside the lagoon. The lagoon's hydrological regime and the associated ice phenomena are mostly controlled by physical factors such as air temperature, water temperature, and salinity. The correlation coefficient between ice cover (at the observation points) and salinity was the highest ($r = -0.97$; $p < 0.05$). The presence of ice cover has also a strong and statistically significant correlation with air temperature ($r = -0.79$; $p < 0.05$) and SST ($r = -0.70$; $p < 0.05$)

During the period of 1993–2013, the analysis of the changes and trends of the ice phenomena, their dependence on changes in the air temperature, SST and salinity in the Klaipėda Strait and in the central and northern parts of the Curonian Lagoon shows that application of the regression kriging method is more efficient to predict the ice cover than the multivariate linear regression.

Using model [1] the relation between the ice formation (I^*) and air temperature (T, °C), SST (T_W, °C), and salinity (S_W, ‰) was modelled as:

$$I^* = 6.198 + 0.014 \cdot T - 0.974 \cdot T_W - 3.628 \cdot S_W. \quad [7]$$

For the period of 2009–2012, we assessed empirical semivariogram parameters. According to the minimised sum of squares (MSS) criteria, the spherical semivariogram model is the optimal one (Table 1). Figure 2 presents a comparison of the calculated semivariogram values (dots) with the experimental semivariogram.

Using the semivariogram model (we applied the *variofit* function in the R language) and the procedure described above, the following values of the trend parameters were obtained: $\hat{\beta}_0 = 5.4081$, $\hat{\beta}_1 = -0.2732$, $\hat{\beta}_2 = -1.0622$, $\hat{\beta}_3 = -0.4963$.

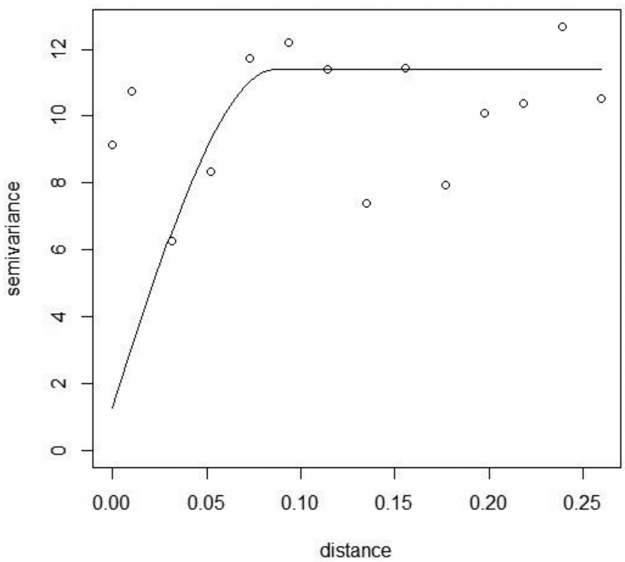

Fig. 2 Empirical semivariogram points and the optimal spherical model (solid line). Compiled by V. Rukšėnienė, 2014

The observed data and the described model were applied for the ice conditions prediction using the MLR and RK methods. The stations chosen for the prediction are located in other parts of the Curonian Lagoon: central part (stations 12A and. 14), northern part (station 5) and Klaipėda Strait (stations 3 and 3A). At these locations the changes in the air temperature, SST, salinity and ice forming were fixed in 2009–2013. The predicted values of the average ice cover (scoring from 1 to 10 points) and their mean squared prediction error (MSPE) are presented in Table 2. The ice cover is measured in a scale (*P*) from 0 (there is no ice in the observed area) up to 10 (the area is 100 % ice-covered) points.

A comparison of the two prediction methods based on the minimum mean squared prediction error (*MSPE*) indicates that the RK method provided more accurate predictions than the MLR approach. The results show that the ice cover formation is most

Table 1 Parameters of semivariograms and minimised sum of squares (MSS) value. Compiled by V. Rukšėnienė, 2014

Estimators	$\hat{\tau}^2$	$\hat{\sigma}^2$	$\hat{\varphi}$	MSS
Exponential	9.15	10.98	1.49	44.18
Gaussian	0	10.02	0	48.59
Spherical	9.17	842.27	185.81	44.18

Table 2 Results of predicted ice cover in points (I^*) and their mean squared prediction error (MSPE). P stands for the average scoring (from 1 to 10) at selected points. Compiled by V. Rukšėnienė and I. Dailidienė 2014

Stations	Latitude	Longitude	Locations	Linear regression			Regression kriging		
				I^*	*P*	*MSPE*	I^*	*P*	*MSPE*
3	55°40'N	21°08'E	Strait	1.0624	1	5.64	1.5353	2	3.62
3A	55°38.8'N	21°09.8'E	Strait	0.0555	0	4.23	0.1725	0	0.03
5	55°31.8'N	21°08.2'E	Northern part	1.4105	1	10.73	3.3552	3	1.78
12A	55°20.8'N	21°18.1'E	Central part	5.3073	5	1.73	4.1646	4	0.03
14	55°15.8'N	21°04.7'E	Central part	4.9247	5	24.25	4.1663	4	17.36

accurately described by the air temperature, SST and salinity changes in the central part of the lagoon (station 12A) and in the Klaipėda Strait (station 3A). The maximum extension of ice cover during the winter period is expected to occur in the central part of the lagoon.

The results suggest that the ice cover in the lagoon may be scored by 4 points in the monitoring stations 12A and 14 (Fig. 1, Table 2) in 2009–2013. Station 14 is the most remote from the stations that were included into the sample (Fig. 1). The MSPE for this station is the largest according to both methods. This shows that in order to get more accurate predictions, it is important to take into account the spatial distribution of the observations.

The validation is applicable when the primary goal is the prediction. It helps to determine how well the proposed model describes the analysed data. At first, useful information is provided by scatter plots (Fig. 3) of the observed and the estimated values.

The validation indices are presented in the Table 3. The scatter plot is related to the Pearson correlation coefficient. The values of the validation indices suggest that the error is larger for the multivariate linear regression than for the regression kriging, except for the mean estimation error (MEE). Moreover, the MEE of the multivariate linear regression is lower than for regression kriging. For the multivariate linear regression method the correlation coefficient is much lower than for the regression kriging method. Other validation indices may provide additional information about the accuracy of the used models.

Table 3 Validation indices for multivariate linear regression (MLR) and regression kriging (RK): the mean estimation error (MEE), the mean square estimation error (MSEE), the root mean square estimation error (RMSEE), the mean absolute estimation error (MAEE), Pearson correlation coefficient (R). Compiled by V. Rukšėnienė, 2014

	MLR	RK
MEE	0.116	0.254
MSEE	8.468	4.562
RMSEE	2.910	2.136
MAEE	2.788	1.548
R	0.031	0.325

As Eqs. [1] and [2] were used for modelling the relation between the ice phenomena and the air temperature, SST and water salinity, it is important to consider several functions of semivariogram in order to thoroughly evaluate the quality of estimates. In general, different models of semivariogram mean different values of the minimised sum of squares (MSS). The smallest MSE indicates the single model that fits

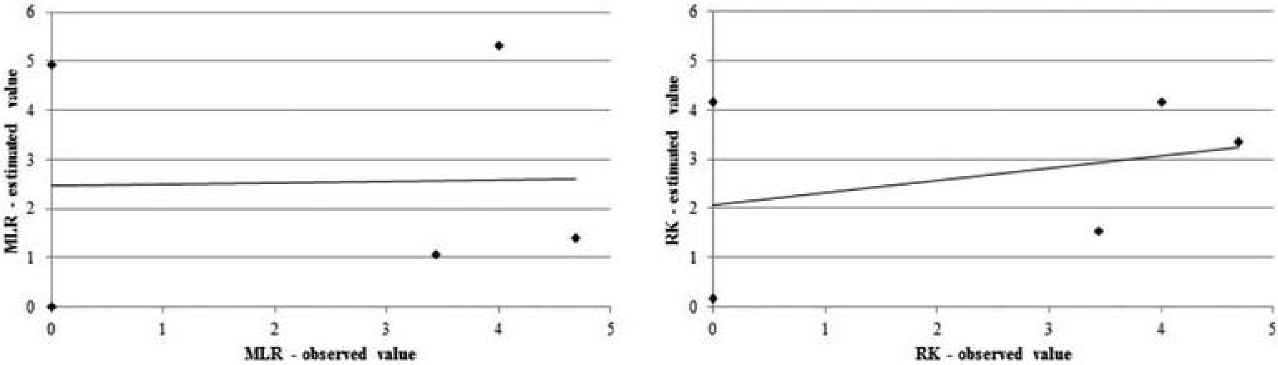

Fig. 3 Scatter plot of observed ice cover (points in the 0–10 scale) and estimated values using multivariate linear regression (MLR, left) and regression kriging (RK, right). Compiled by V. Rukšėnienė, 2014

the best model of semivariogram. The calculated values of σ^2, τ^2 and φ in semivariograms [3] (Table 1) illustrate the exponential, Gaussian and spherical semivariogram models with values of minimized sum of squares. The spherical semivariogram is an optimal model for the problem in question. As discussed above, a longer distance means a reduced amount of spatial information and thus a less accurate forecast (Dučinskas & Šaltytė-Benth 2005). The predictions carried out in the stations with different distances underline the importance of spatial information in such projections.

CONCLUSIONS

Regression kriging and multivariate linear regression methods have been used in order to clarify the dependence of ice phenomena formation on variations in the air temperature, SST and salinity in the Curonian Lagoon. The discussed dependence is not always straightforward because of the transit nature of the lagoon system. In such water bodies, there is a particularly complicated task to predict ice formation as air temperature, SST and salinity often vary in time depending on meteorological and hydrodynamic conditions, and wind impact or wave fields may play a large role in the formation of the ice cover in the coastal areas of the Baltic Sea (Zaitseva-Pärnaste, Soomere 2013). While designing the models, it is important to assess the weight of the variable parameters. Often, the monitoring stations selected in water basins can not be used in models, as measurements carried out there do not completely describe the status of water basin.

Often spatial data sets are limited and the observation points are distributed irregularly, so the data are not always available. Suitable mathematical models and an optimal selection of the monitoring stations would partly solve the problem. The most difficult task is to choose the appropriate methods in transit zones between the sea and river mouths, as there occurs in this case of the Curonian Lagoon.

The performed analysis shows that application of the regression kriging is more efficient for predicting the ice cover in such almost closed basins as the Curonian Lagoon comparing to the multivariate linear regression. A comparison and validation of these two approaches supports the conjecture that the regression kriging is a better interpolation method. In the discussed example, it becomes evident that the air temperature, SST and salinity variability describe the formation of the ice coverage in the central part of the lagoon in a more reliable way. In the northern part of the lagoon and Klaipėda Strait the ice cover formation could be also predicted, however, the used methods are related too much larger uncertainties and prediction errors, as most likely these parts are more exposed to marine water inflow. During the cold period, the larger amount of saline and warmer water entering the lagoon from the Baltic Sea proper may prevent the formation of a stable ice cover.

This feature vividly demonstrates the problems related to the adequate calculation and interpretation of the role of existing conditions when the environmental interface of air temperature, water temperature and salinity varies and cannot be exactly calculated by the geophysical environmental models. This is an intrinsic component of the dynamics of the northern part of the lagoon that functions as the transition zone between the rest of the lagoon and the open Baltic Sea. In particular, intense hydrodynamic patterns in this zone often prevent the formation of a stable ice cover.

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