SPATIAL DISTRIBUTION OF EXCEEDANCE OF EC OZONE THRESHOLD VALUES - METHODS OF CALCULATION

Artur Gzella and Jerzy Zwoździak
Wroclaw University of Technology, Faculty of Environmental Engineering**,**
Institute of Environment Protection Engineering, Poland

INTRODUCTION

Proper and quick forecasting of surface ozone concentrations as well as the possibility of risk analysis for the exceedance of the air quality standards plays an important role in air quality control and monitoring systems. Most of the analysis of surface ozone distribution gives a set of maps with ozone concentrations isolines as a result. However for vegetation and human health protection the most valuable information is to show where and when the ozone air quality standards were exceeded. The rest of the data (concentrations below the thresholds) can be treated as an information noise and in some cases, like i.e. for warning purposes, should be neglected. In the reports of the European Environment Agency overviews of the exceedances of EC ozone threshold values during the summer seasons can be found. EEA shows in those reports the European areas which are exposed to high ozone concentrations in the meaning of number of days with exceedances observed on respective monitoring stations *(Fiala, J. et al,* 2003). The purpose of this paper is to propose other methods for the estimation and graphical presentation of the exceedance of surface ozone air quality standards in advance. The methods are leaned on geostatistical model which is shortly presented in this paper and on the EU standards (Ozone Directive 2002/3/EC).

SURFACE OZONE AIR QUALITY STANDARDS

On the 12th February 2002 the European Parliament and the Council adopted a new EU Directive 2002/3/EC relating to ozone in ambient air *(Official Journal,* 2002). For the protection of human health and vegetation the levels were established which should be attained where possible over a given period ('target values') and the levels which should be attained in the long term ('long term objectives'). For the protection of vegetation the standard of AOT40 was established which means the accumulated exposure for exceedance of 80 $\mu gO_3/m^3$. For the protection of human health the maximum daily 8-hour mean, selected by examining 8-hour running averages was established. It is calculated from hourly data and updated each hour. The maximum which should not be exceeded is 120 $\mu gO_3/m^3$ (on more than 25 days per calendar year averaged over three years, until 2010). The Ozone Directive established also information threshold (1 hour average, 180 $\mu gO_3/m^3$) and alert threshold (1 hour average, 240 $\mu gO_3/m^3$).

SURFACE OZONE MODELING AND FORECAST

Geostatistical model for predicting hourly surface ozone concentrations at the mesoscale was developed as an alternative to photochemical model of ozone dispersion. It can be described as 'linear regression with collocated cokriging of the residuals'. The model is based on an equation derived using simple and ordinary collocated cokriging estimators:

$$Z^*(x_0) = m_Z(x_0) + w_0\,(S(x_0) - m_S(x_0)) + \Sigma^n_{\alpha=1}[w_Z^{\alpha}(\, Z(x_\alpha) - m_Z(x_\alpha)) + w_S^{\alpha}(\, S(x_\alpha) - m_S(x_\alpha))]$$

where: the index "0" means estimated point (here: the point where no measurement of ozone concentration is carried out, the term 'point' is here understood also as the time step), the index "α" is the measurement point (here: the point where measurement of ozone concentration is performed) and: $Z^*(x_0)$, $Z(x_\alpha)$ – target variable, $S(x_0)$, $S(x_\alpha)$ – auxiliary variable, $m_Z(x_0)$, $m_Z(x_\alpha)$– local mean values for the target variable, $m_S(x_0)$, $m_S(x_\alpha)$ – local mean values for the auxiliary variable, w_Z^α – weight coefficient for the target variable, w_0, w_S^α – weight coefficients for the auxiliary variable. The estimator allows model calibration and maximal application of the knowledge about values of the auxiliary variable. The weight coefficients are calculated according to the method used for ordinary block cokriging *(Wackernagel, H.,* 1998). In such a model ozone data and auxiliary data from the last 48 or 24 hours for the forecast calculation (48 hours in advance) are indispensable. Auxiliary variable is a result of PCA reduction of meteorological parameters and topography. The meteorological parameters were calculated using the model of boundary layer MEMO *(Kunz, R. and N. Moussiopoulos,* 1995). The surface ozone model was tested for the ozone episode which occurred on August 14th, 1997 in the so-called 'Black Triangle' region. Forecasted and measured values of ozone concentration were in agreement.

METHODOLOGY

Vegetation and human health protection

For the estimation and presentation of the exceedances of the vegetation and human health protection threshold values simply 8-hour running average were applied. For calculation of 8-hour running averages for every point of the area of interest, the results of abovementioned forecast were used. The results of surface ozone forecast had the time step of 3 hours. Therefore the 8-hours running averages were estimated with the 3-time steps moving window. As the result of averaging only these area were shown for which the exceedance of the value for the protection of human health occurred.

Information and alert threshold

RMSE analysis

The minimize of cokriging variance during the modelling leads on the one hand to the reduction of value estimation error of the given parameter but on the other hand causes smoothing of modelled spatial and temporal distributions. It means that the cost for the optimal value estimation of the given parameter is the loss of its entire variability information for analysed area and time period. The model presented above did not gain the level equal or greater than 180 $\mu gO_3/m^3$ (the highest forecasted surface ozone concentration was 177 $\mu gO_3/m^3$, the highest observed value: 221 $\mu gO_3/m^3$). For the analysis of the risk of the 180 $\mu gO_3/m^3$ exceedance can be used the positive correlation between the RMSE (root square mean error) value and the ozone concentrations. On the basis of RMSE values and the averaged ozone concentrations from several monitoring stations and test periods a regression analysis was done resulting with following equation:

$$RMSE = 7.13 + 0.19*O_3,$$

where O_3 means the surface ozone concentration.

In the figure 1 the relationship between RMSE and ozone level is presented, together with the line of RMSE values which are foreseen on the basis of the above equation. The equation was then used for the calculation of RMSE values for entire analysed area. After that the forecasted ozone concentrations and RMSE values were added and the highest possible surface ozone levels which could occur in the region were obtained.

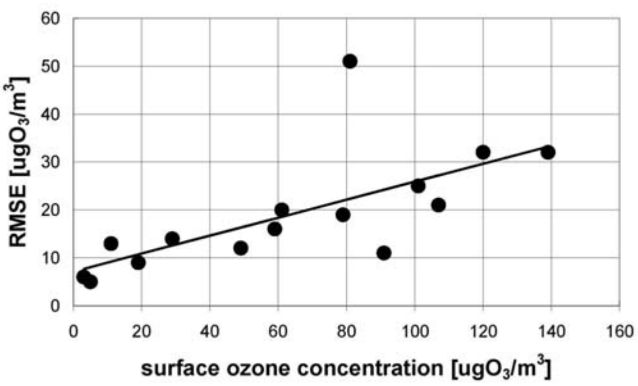

Fig. 1; Relationship between RMSE and ozone level.

"Turning bands" simulation

An alternative approach to the interpolation and forecasting problem is called the simulation and relies on the reconstruction of the variability of the given parameter by the loss of estimation accuracy that means – by the increase of estimation variance. The aim of the simulation method is then the calculation of the spatio-temporal distributions which characterize the same histogram and variogram like the observed values. The simulation method which is adequate to cokriging, that means – which has the feature of exact interpolation and take into account more than one variable, is called conditional co-simulation. It reconstructs the histograms of all analysed variables and also their variograms and cross-variograms. One of the most popular simulation method is the „turning bands" method. It was proposed by *Matheron, G.* (1973), as the simulation method of non-conditional random fields. One of the first applications of the „turning bands" method in the conditional form occurred in hydrology *(Delhomme, J.P.,* 1979). The way of conditioning of „turning bands" method is described in the work by *Dutter, R.* (1985). In analyzed case, because the surface ozone data fit very well to the normal distribution, the Gaussian anamorphosis modelling was omitted. In the simulation the same cross variogram and the neighbourhood parameters were used like in the predictive geostatistical model.

RESULTS AND DISCUSSION

Vegetation and human health protection

In the figure 2 the spatial distribution of the exceedance of the value 120 $\mu gO_3/m^3$ as the 8-hour mean, for 15:00 (daily maximum) and for 18:00, on 14th August 1997 is presented. The worst situation was surveyed in the South-Western part of the analysed area. The highest values of exceedance were observed along the German-Czech border and at most at the Ore mountains. The high values of the 8-hour mean lasted there also the longest time. Similar method can be used for AOT calculation and the value for the protection of vegetation monitoring and control. Instead of 8-hour mean calculation the addition of the exceedance of 80 $\mu gO_3/m^3$ should be undertaken.

Information and alert threshold

RMSE analysis

In the figure 3 the spatial distribution of the exceedance of the value 180 $\mu gO_3/m^3$, for 15:00 and for 18:00, on 14th August 1997 is presented. The areas of exceedance of 180 $\mu gO_3/m^3$

value are distributed similar as the exceedance of the value 120 $\mu gO_3/m^3$ as the 8-hour mean what suggests the correctness of the method.

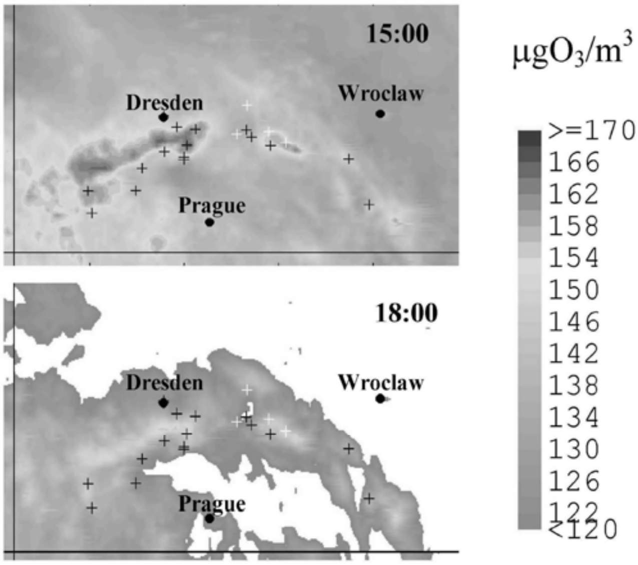

Fig. 2; Spatial distribution of the exceeding of the value 120 $\mu gO_3/m^3$ as the 8-hour mean, for 15:00 (daily maximum) and for 18:00, on 14th August 1997.

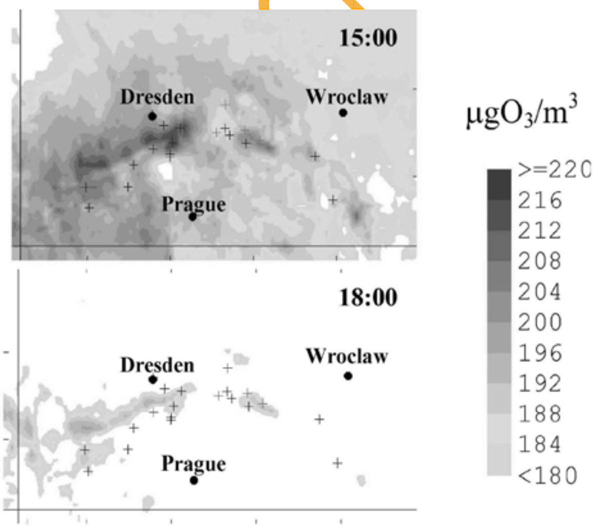

Fig.3; Spatial distribution of the exceeding of the value 180 $\mu gO_3/m^3$, for 15:00 and for 18:00, on 14th August 1997.

"Turning bands" simulation

In the figure 4 the spatial distribution of the probability of the 180 $\mu gO_3/m^3$ value exceedance, for 15:00 and for 18:00, on 14th August 1997 is presented. The probability of the 180 $\mu gO_3/m^3$ value exceedance is for the most of the analysed area small and does not exceed 0.1. The places where the probability is higher (up to about 0.48) overlie the places where the previous analysis showed the highest possible surface ozone concentrations. Similar method of risk assessment can be used for the alert threshold (240 $\mu gO_3/m^3$).

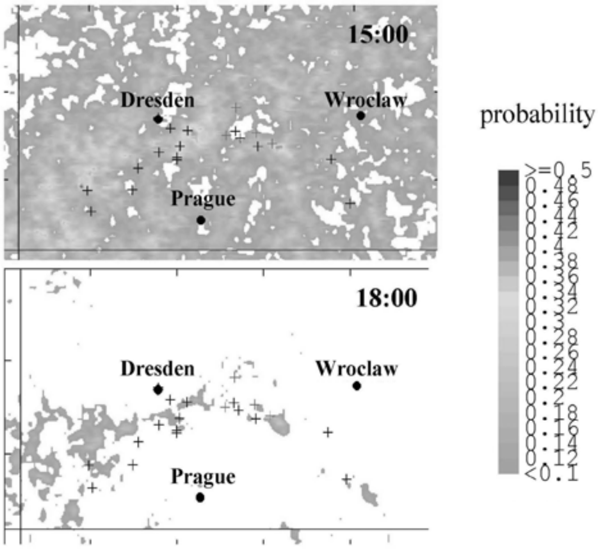

Fig. 4; Spatial distribution of the probability of the 180 $\mu gO_3/m^3$ value exceeding, for 15:00 and for 18:00, on 14th August 1997.

CONCLUSIONS

In this paper several methods of analysis and visualization of the risk connected with the surface ozone were presented. All of them result from the predictive geostatistical model and are its valuable supplement but can also be implemented together with other forecasting models. They make possible a more precise indication of the areas which can be exposed for losses following the ozone impact on vegetation and human health. Together with a prognostic model they constitute an effective tool for surface ozone air quality standards control and can be easily brought in the institutions which are responsible for that kind of activity on a regional level.

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