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MODELLING OF THE ATMOSPHERIC DISPERSION OF SULPHUR DIOXIDE IN THE URBAN AREA REFERRED TO THE CRACOW AGGLOMERATION

The multiple-source Gaussian model is presented. Its verification is based on the data from the MONAT-84 experiment carried out in the Cracow Agglomeration. The model has been tested by different statistics. The results of analysis have indicated that in the future research input data should be determined more precisely and calibration of the model should be carried out.

1. INTRODUCTION

Mathematical models of air pollution dispersion are very useful in solving problems of the environmental protection. In order to ensure the correctness of decisions based on the results of the model calculations, this model should correspond to the complex processes of the dispersion pollution occurring in atmosphere. Thus, the model should be verified to show its validity.

In the available literature a single criterion of the quality of models is not given, thus it seems that such a criterion does not exist at all. That is why the different statistics are used in models verification.

In this paper an attempt has been made to verify the URFOR-2 (URban FORecast) model. This model has been developed for the Cracow Agglomeration as a part of the Government Programme PR-8. Its verification has been based on the data obtained in the MONAT-84 (MONitoring of the ATmosphere) experiment conducted on 1st to 29th February 1984. The purpose of the model is to forecast the short-term ground-level concentration of gas pollution in the city. It has an universal character in the sense that it can be used in any urban agglomeration.

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2. DESCRIPTION OF THE MODEL

The URFOR-2 model is a multiple-source Gaussian model. The basic dispersion formula used in the model is the following:

$$C(x, y) = \frac{E(x)}{\pi \bar{u} \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \sum_{n=-\infty}^{\infty} \exp\left[-\frac{(H + 2nL)^2}{2\sigma_z^2}\right] \tag{1}$$

where:

$C(x, y)$ – short-term ground-level concentration of gas pollution at receptor point located at (x, y) and produced by a steady point source,

σ_y and σ_z – Pasquill diffusion coefficients,

H – effective height of source,

L – mixed depth,

$\bar{u}$ – mean wind speed,

x – downwind distance between the receptor and source,

y – horizontal cross-wind distance between the receptor and the plume centreline,

$E(x)$ – intensity of pollution flow through the cross-wind plane located at the distance x from the source.

$E(x)$ is given by:

$$E(x) = E \exp\left\{ -\sqrt{\frac{2}{\pi}} \frac{W}{\bar{u}} \int_0^x \frac{1}{\sigma_z} \sum_{n=-\infty}^{\infty} \exp\left[-\frac{(H + 2nL)^2}{2\sigma_z^2}\right] dx - (k_1 + k_2) \frac{x}{\bar{u}} \right\} \tag{2}$$

where:

E – source intensity,

w – deposition rate of dry of air pollutants,

k_1 – coefficient of conversion of air pollutants,

k_2 – coefficient of the wet deposition of air pollutants.

The URFOR-2 model describes approximately the vertical rotation of wind and the vertical rotation of wind and the vertical change of the atmospheric stability by distinguishing 2 layers in mixed depth.

The total concentration of pollution emitted by point and area sources is the sum of pollution emitted by individual sources. The area sources located in the city constitute an appropriate set of source elements and are treated as a multiple source. The area sources located far from the city are replaced by the virtual point sources, using the initial horizontal cross-wind diffusion coefficients, proportional to the size of area source.

The model allows us to identify the sources of emission, thus to determinate their contribution to the atmosphere pollution.

3. DATA SET FOR MODEL VERIFICATION

As has been mentioned earlier, the model URFOR-2 has been verified using the data obtained in the MONAT-84 experiment carried out in Cracow in February 1984. Details of this experiment are presented by NOWICKI [1].

The 30 minute ground-level concentrations of sulphur dioxide were measured twice a day for 29 days at 24 sampling points located in the city.

The meteorological data for the city were supplied by 10 surface stations and by the aerological sounding. Similar data for the area, responsible for the air pollution emission, were determined by the IMGW meteorological stations network located within the radius of 150 km from the centre of Cracow.

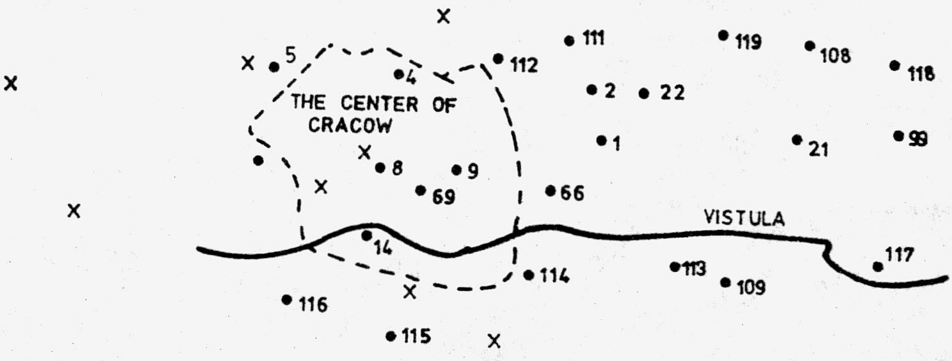

Figure. The localization of SO_2 measuring sites (·) and meteorological stations (x) in the Cracow Agglomeration
Scale 1:200 000

Rysunek. Lokalizacja miejsc pomiaru SO_2 (·) i stacji meteorologicznych (x) w aglomeracji krakowskiej
Skala 1 : 200 000

The localization of the measuring sites and meteorological stations in the Cracow Agglomeration is shown in figure.

4. THEORETICAL BASIS OF MODEL VERIFICATION

The analysis of two concentration sets — observed and calculated ones, each of N el... — served as URFOR-2 verification. In the analysed series either one sampling point and ferent measuring periods or one period and different sites, or different sampling points and different measuring periods can be considered. The analyses give the information about the time correlation, the spatial correlation and time-spatial correlation.

To state the agreement of the model with observations the following measures are used: linear correlation coefficient (R), coefficient of variation (W), absolute difference between the means of the observed and calculated concentrations (ΔC). These statistics are given by the following formulae:

$$R = \sum_{i=1}^{N} (C_{oi} - C_{mo})(C_{ci} - C_{mo}) \Big/ \left[\sum_{i=1}^{N} (C_{oi} - C_{mo})^2 \sum_{i=1}^{N} (C_{ci} - C_{mc})^2 \right]^{1/2} \tag{3}$$

where:

C_{oi} – observed concentration,
C_{ci} – calculated concentration,
C_{mo} – mean of the observed concentrations,
C_{mc} – mean of the calculated concentrations,
N – size of the series.

$$W = \left[\frac{1}{N-1} \sum_{i=1}^{N} (C_{oi} - C_{ci})^2 \right]^{1/2} \Big/ C_{mo}, \tag{4}$$

$$\Delta C = |C_{mo} - C_{mc}|. \tag{5}$$

The correlation between two sets is analysed by $U = 0.5 \ln(1 + R)/(1 - R)$ statistics. According to Fisher it is approximately distributed even for small sizes of N. At different significance levels β, usually $\beta = 5$°/o, and for degrees of freedom $f = N - 2$, the critical value of correlation coefficient R_β should be found. When $R < R_\beta$, the zero hypothesis, i.e. that there is correlation between the characteristics of two sets, cannot be accepted, if, however, $R \geqslant R_\beta$, the alternative hypothesis, i.e. that the significant correlation exists, may be accepted.

The value of the coefficient of variation W for the ideal model is equal to 0. The "good" model has W significantly less than 1.

The comparison of two means C_{mo}, C_{mc} of the observed and calculated concentrations may be based on the assumption that they have normal distributions and that their square deviations S_{oy}, S_{cx} are known. The zero hypothesis is that ΔC does not differ significantly from 0. The alternative hypothesis is that C differs significantly from 0. The difference between two means is normally distributed, the square deviation being

$$S_{xy} = \left(\frac{1}{N}\left(S_{oy}^{\;2} + S_{cx}^{\;2}\right)\right)^{1/2}$$

At different significance level β (usually $\beta = 5$°/o), the critical value of the absolute difference between means, $t_\beta S_{xy}$, should be found. If the absolute value of the difference ΔC between the means is greater than $t_\beta S_{xy}$, the means differ significantly.

5. RESULTS OF MODEL VERIFICATION

Verification of the URFOR-2 model required a number of calculations. The model has been tested in different ways. This paper presents only the tests characterizing directly the model at the present stage of calibration. The analyses can be divided into two groups:

1. Analysis of the total area of the Cracow Agglomeration. It comprised $N = 24 \times 29 \times 2 = 1392$ elements; observed and calculated concentrations at 24 sampling points measured twice a day for 29 days were examined.

2. Analysis of the area of the centre of Cracow. $N = 8 \times 56 = 448$ elements, i.e. the observed and calculated concentrations at 8 sampling points representing this area were examined. In this case, however, 2 periods statistically uncertain have been neglected.

5.1. ANALYSIS OF THE TOTAL AREA OF CRACOW

The time correlation coefficients obtained for the 24 sampling points vary from about 0 to 0.6805. The critical value of R_β at 5°/o significance level for $f = 56$ is 0.2593. The condition $R \geqslant R_\beta$ is satisfied at 9 sites only.

The results for the 58 measuring periods are much better. The critical value R_β at $\beta =$ 5°/o for $f = 22$ is 0.4060. The space correlation coefficients for 34 periods are greater than the critical one.

The comparison of all the observed concentrations and the calculated ones gives a very good time-space correlation. The computed R is 0.2093, while the critical value of R_β at $\beta = 5$°/o for $f = 1390$ is 0.05025. The value of the time-space correlation is significantly greater, even for 0.1°/o significance level for which R_β is 0.0881.

For all of the observed and calculated concentrations the coefficient of variation W is 1.8263, thus it may be regarded as unsatisfactory.

The means of the observed C_{mo} and calculated C_{mc} concentrations are 65 and 72 $\mu g/m^3$, respectively. Their difference ΔC is 7 $\mu g/m^3$. The mean square deviations of the observed and calculated concentrations are: $S_{oy} = 56$ and $S_{cx} = 117$ $\mu g/m^3$. The square deviation of ΔC is $S_{xy} = ((56^2 + 117^2)/1392)^{1/2} = 3.5$ $\mu g/m^3$. At 5°/o significance level the critical value of ΔC is $t_5 \times S_{xy} = 1.96 \times 3.5 = 6.9$ $\mu g/m^3$, being very close to the real one 7 $\mu g/m^3$. At $\beta = 2.5$°/o it is significantly greater and the hypothesis of zero difference between the means cannot be rejected.

5.2. ANALYSIS OF THE AREA OF THE CENTRE OF CRACOW

The 8 sampling points located in/or near the centre of Cracow have been taken as the representatives of that area. According to MONAT-84 they have the following numbers: 4, 8, 9, 14, 62, 69, 112 and 114.

The time correlation R for the 8 points varies from about 0 to 0.6835. The critical value of R_β at 5°/o significance level for $f = 54$ is 0.2638. The time correlation coefficients at 4 sites are greater than R_β. The coefficients R are close to the critical value at 1 point, at 2 sites R are by about 40°/o less than R_β. No time correlation exists at point 1.

The results for the 56 measuring periods are much better. The critical value of R_β at $\beta = 5$°/o for $f = 6$ is 0.707. The condition $R \geqslant R_\beta$ is satisfied for the majority of the periods. The space correlation coefficients for 6 periods range within 0.3–0.4. No spatial correlation exists for 3 periods.

The time-space correlation at 8 sampling points and for 56 measuring periods is very good. The computed R is 0.3707. The critical value of R at 5°/o for $f = 446$ is 0.0927. The condition $R \geqslant R_\beta$ is satisfied even at $\beta = 0.1$°/o for which R_β is equal to 0.1561.

The means of the observed and the calculated concentrations are: $C_{mo} = 92$ and $C_{mc} = 98\ \mu g/m^3$. The square deviation of difference between them is $S_{xy} = ((63^2 + 111^2)\,448)^{1/2} = 6\ \mu g/m^3$. At 5°/o significance level the critical difference is $t_5 \times S_{xy} = 1.96 \times 6.0 = 11.8\ \mu g/m^3$, being significantly greater than the real one. Thus, the difference between the means is inessential and both the observed and calculated sets belong to the same population.

The coefficient of variation W for concentrations at 8 points and 56 periods is 1.15 and it can be regarded as satisfactory.

6. CONCLUDING REMARKS

The results of model verification can be briefly presented as follows:

For the area of the Cracow Agglomeration

the time-space correlation between the observed and calculated concentrations is good;

the calculated mean statistically agrees with the mean of observed concentrations;

the coefficient of variation, having relatively high value, indicates significant local differences between the model results and reality;

the time correlation between the calculated and observed concentrations is unsatisfactory; there are significant differences in concentrations of many receptors;

the space correlation for the area is satisfactory.

For the area of the centre of Cracow

the obtained results are much better than those for the total area of the Cracow Agglomeration;

the time-space correlation between model calculations and reality is very good;

the consistency test for the means of the calculated and observed concentrations gives positive results within the large range;

the coefficient of variation is close to 1 and can be regarded as satisfactory.

The comparison of the means of the observed and calculated concentrations allows us to estimate the balance of emission. If the model obeys the pollution mass conservation law, then for large sets the mean of the calculated concentration, obtained even from the model of limited perfectness, must be close to the mean of the observed concentrations. In the URFOR-2 model the condition of the equality of the means is generally satisfied. The analysis of results for each sampling site or each measuring period indicates that the model gives significant differences for individual receptors. These local differences are not due to the model, especially when there many points for which there are many results are good, but are probably caused by two main reasons:

1. The model is very sensitive to the emitor coordinate's errors, particularly when sources are near the receptors. It seems that such errors occur in the input data, emitor coordinates being determined from different maps of different scales.

2. The calculated concentrations are proportional to the pollution emission. The analysis of results not described in this paper show that emission from "variable" sources may be incorrectly determined in the diurnal cycle.

Other groups of reasons connected with differences between model and reality have a random nature. These are the following: the discretization of the atmospheric stability categories, errors in the determination of wind speed and direction, errors in the determination of the mixed depth and emission fluctuations.

These considerations lead to the conclusion that at the next stage of the research the emissions from "variable" sources and the localizations of sources should be determined more precisely and the URFOR-2 model should be calibrated.

REFERENCES

[1] NOWICKI M., *The searching experiment of the air protection MONAT-84 in Cracow*, Proc. Symp., Książ 1985.

MODELOWANIE DYSPERSJI ATMOSFERYCZNEJ DWUTLENKU SIARKI W OBSZARZE AGLOMERACJI KRAKOWSKIEJ

Przedstawiono wieloźródłowy model Gaussa, który został zweryfikowany na podstawie danych uzyskanych podczas MONAT-u 84. Model przetestowano przy użyciu różnych metod statystycznych.

MODELLIERUNG DER ATMOSPHERISCHEN DISPERSION VON SCHWEFELDIOXID IM BALLUNGSGEBIET VON KRAKAU

Ein Gaussches Modell wird auf Grund der im Project MONAT-84 erhalten Ergebnisse verifiziert. Zur Verifikation werden verschiedene statistische Methoden angewendet.

МОДЕЛИРОВАНИЕ АТМОСФЕРНОЙ ДИСПЕРСИИ ДВУОКИСИ СЕРЫ В РАЙОНЕ КРАКОВСКОЙ АГЛОМЕРАЦИИ

Представлена, основанная на многих источниках,модель Гаусса, которую проверили, опираясь на данные, полученные во время МОНАТ-а 84. На модели провели тесты, пользуясь разными статистическими методами.