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THE GAUSSIAN AIR POLLUTION DISPERSION MODEL WITH VARIABILITY OF THE INPUT PARAMETERS TAKEN INTO ACCOUNT. I. FORMULATION OF THE MODEL

The formulation of the segmented Gaussian plume model for simulation of the transport and dispersion of air pollutants emitted from a group of point sources is presented. The model takes into account the change in time of stack emission parameters and meteorological conditions as well as the spatial variability of topographical conditions and is based on the meteorological data from the routine measurements carried out in Poland. The model development and verification are divided into two parts: formulation of the model and verification of the model. In this paper, the model assumptions, mathematical formulas and model applications are discussed.

1. INTRODUCTION

Mathematical models of air pollution dispersion are the basic tool in air quality assessments.

In Poland, for routine calculations the model based on the Pasquill formula is used. The methodology applied is described in the *Guidance of calculating the atmospheric air contamination* [7]. All data needed for these calculations is available. Meteorological data is collected during the routine measurements carried out at the stations distributed in the whole country. In the model mentioned, it is assumed that the conditions which influence the transport and dispersion of air pollutants are stationary and homogeneous. It means that stack emission parameters and the parameters describing the terrain and meteorological conditions are constant. The model mentioned is one of many Gaussian plume models discussed in literature [2], [7], [12], [22]. These simple models are widely used in practical applications all over the world.

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Another group of models used in air quality calculations is based on the numerical solution of the transport diffusion equation. They are called K-theory models [8], [9], [11], [12], [18]. In these models, the variability of stack emission parameters, terrain and meteorological conditions can be considered in the description of the transport and diffusion of the pollutants. Application of these models requires the meteorological data which cannot be obtained from the routine measurements. These models need much more computing time and computer storage. These last features limit practical applications of the K-theory models.

In the study described below, an attempt is made to develop the air pollution dispersion model which takes into account the change in time of stack emission parameters and meteorological conditions as well as the spatial variability of terrain conditions. At the same time it is postulated that the model should be based on the meteorological data from the routine measurements carried out in Poland and should maintain the simplicity of the Gaussian type models.

The developed model was verified on the basis of data collected during the measurement experiment with the tracer carried out at the Kincaid, Illinois, U.S.A. The model development and its verification are presented in 2 parts:

1. Formulation of the model.
2. Verification of the model.

In this paper, first the assumptions are described. Next, basic mathematical relations are presented. Finally, the model applications are discussed.

2. BASIC ASSUMPTIONS

The developed model is designed to simulate the space distribution of the concentrations of the air pollutants emitted from a single stack or a group of point sources.

The concentrations of pollutants calculated on the basis of the model are averaged over the individual "meteorological episode". The meteorological episode is defined as the period of time Δt, during which stationarity of stack emission parameters and meteorological conditions is assumed. The typical value of Δt is 30 minutes or 1 hour.

The developed model is designed to study the transport and dispersion of the air pollutants in mesoscale, i.e. to the distance of few tens of km from the stack.

The model formulation is based on the concept of the Gaussian plume model. The approach of modelling the air pollutant transport and dispersion phenomenon under complex conditions using the Gaussian equation has been successfully employed in number of works [1], [4], [10], [13], [14], [15], [19], [20], [21], [23]. In the model developed, the following assumptions are accepted:

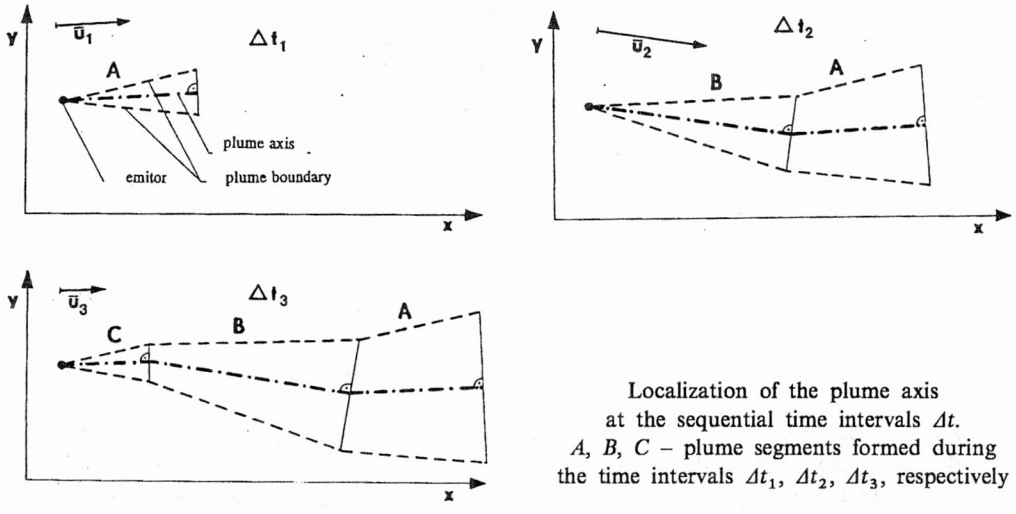
1. Meteorological conditions are spatially uniform. The change of meteorological conditions takes place every time step Δt. The following parameters undergo the

change: atmospheric stability, air temperature, depth of the mixing layer, wind velocity and its direction, intensity of the precipitation.

2. The intensity of emission of pollutants from the stack and the release parameters change in time just as the meteorological conditions, i.e. in every time step Δt, and they are constant over the time interval Δt.

3. The pollutants emitted from the stack during the time interval Δt form the segment of the plume, whose length depends on the wind velocity during this specific episode. The height of the axis of the plume segment is determined by the effective height of the emission. The direction of the segment axis follows the current wind. The distributions of the concentrations in the plume cross-section in the horizontal and vertical directions follow the Gaussian characteristic.

4. The length and height of the plume segment do not change as the plume travels downwind, but the dimensions of the plume increase. Every time step Δt there is a translation of all existing plume segments. The translation vector depends on the wind vector during the specific time interval Δt. The localization of the plume for the sequential time steps Δt is shown in the figure.



Localization of the plume axis at the sequential time intervals Δt. A, B, C – plume segments formed during the time intervals Δt_1, Δt_2, Δt_3, respectively

5. The elevated layer of the temperature inversion reflects the pollutant which is emitted to the atmosphere below the inversion layer.

6. The pollutant present in the atmosphere is not comprised by the inversion layer which falls down. The increase in the mixing layer allows the plume to disperse in the vertical direction.

7. While elevated inversion layer is present, the vertical distribution of the pollutants becomes homogeneous at some distance from the stack. This phenomenon is observed as the plume travels downwind.

8. The possible sinks of the pollution in the atmosphere comprise the following processes: linear chemical transformations, dry and wet deposition.

9. The spatial variability of the terrain is taken into account by introducing the space-dependent roughness coefficient *ZO* and dry deposition velocity *VD*.

10. Every time step Δt, the concentration of the pollutants is calculated based on the Pasquill formula which is extended to describe chemical transformation of the pollutants, wet and dry deposition and the reflection of the plume from the elevated inversion layer. Parameters present in the formula have the same physical interpretation as in the Gaussian plume model.

Each plume segment is defined by the following parameters:

a) coordinates of the plume segment *XS*, *YS* (m, m),

b) segment length: ΔLS (m),

c) height of the plume segment axis: *H* (m),

d) atmospheric diffusion coefficients in the horizontal and vertical directions: *SIGY*, *SIGZ* (m, m),

e) mixing height for the segment: *LMIX* (m),

f) mean wind velocity: *U* (m/s),

g) virtual intensity of the pollutant emission from the stack, i.e. the intensity of the emission lessens due to the removal processes: *EV* (mg/s).

The segment parameters *H*, *SIGY*, *SIGZ*, *LMIX* and *U* are determined for the beginning and the end of each segment. In practice, they are calculated for the end of each segment. The value of the parameter for the beginning of the segment is equal to the value of that parameter for the end of the previous segment. As far as the first segment is concerned, the values of the parameter for its beginning and its end are assumed to be equal.

2.1. MATHEMATICAL DESCRIPTION

2.1.1. STAGES OF THE CALCULATION PROCEDURE

The determination of the space distribution of the pollutants during the considered meteorological episode for a single emission source is a 3-stage procedure. At the first stage, the number of the meteorological episodes which have to be taken into account is calculated. At the second stage, the plume is "defined", i.e. the parameters for the plume segments are determined. The third stage covers the proper calculations, i.e. concentrations of pollutants in receptors are determined.

2.1.2. DETERMINATION OF THE NUMBER OF METEOROLOGICAL EPISODES CONSIDERED

The number of the meteorological episodes, which have to be considered in the calculations, depends on: the stack localization within the area of calculations, the wind velocity and direction during the time interval Δt for which the concentration distribution is determined and the values of these parameters for the earlier episodes.

The calculation algorithm covers the determination of the plume trajectory at the time relevant to $k = 0, 1, 2, \ldots$ episodes in relation to the episode for which the concentration distribution is determined and checking if the plume formed from the $k + 1$ segment covers the calculation area. The calculation area is a rectangular. The geometrical relations are used in the calculation algorithm.

2.1.3. DETERMINATION OF THE SEGMENT PARAMETERS

Coordinates of the beginning of the segment. The coordinates of the beginning of the segments XS_{i+1} and YS_{i+1} at the $i + 1$ time interval Δt of the plume tracing are determined from the relations:

$$XS_{i+1} = XS_i + \Delta LS_{i+1} \sin ALF_{i+1} \quad \text{(m)}, \tag{1}$$

$$YS_{i+1} = YS_i + \Delta LS_{i+1} \sin ALF_{i+1} \quad \text{(m)} \tag{2}$$

where XS_i, YS_i are the coordinates of the beginning of the specific segment at the i time interval (m, m); ALF_{i+1} is the angle between the north direction and the wind direction during the $i + 1$ time interval counted clockwise; ΔLS_{i+1} is the length of the plume segment formed during the $i + 1$ time interval (m).

At the time interval during which the specific segment is formed $XS = XE$ and $YS = YE$, where XE and YE are the emitor coordinates.

Segment length. The segment length ΔLS is determined based on the expression:

$$\Delta LS = UH \Delta t \quad \text{(m)} \tag{3}$$

where UH is the wind velocity at the height H (m/s).

The power law profile is used to describe the vertical change of the wind velocity. The segment lengths are calculated based on the data characteristic of the episode when the segment is formed.

Height of the segment axis. The height of the localization of the plume axis H is determined by the height of the effective emission point:

$$H = h + \Delta h \quad \text{(m)} \tag{4}$$

where h is the geometrical height of the stack (m) and Δh is the plume rise (m).

The plume rise for the stacks for which the heat emission is less than 20 MJ/s is calculated from the well known Holland expression [16], while for the stacks with greater heat emission the CONCAWE formula is used [3].

The effective height of each segment is calculated based on the data from the episode when the segment is formed.

Atmospheric diffusion coefficients. The atmospheric diffusion coefficients $SIGY$ and $SIGZ$ are calculated according to the Nowicki formulas [17]:

$$SIGY = AX^a \quad \text{(m)}, \tag{5}$$

$$SIGZ = BX^b \quad \text{(m)} \tag{6}$$

where X is the distance between the receptor and the stack (m): A and B are the constants which depend on the atmospheric stability, effective height of emission (H) and roughness coefficient (ZO); a and b are the constants which depend on the atmospheric stability.

In the model, the terrain roughness coefficient is allowed to vary spatially. The value of this coefficient at the specific receptor is calculated as the arithmetic mean of the values of ZO on the way of the transport of the pollutants from the stack to the receptor.

In order to allow the meteorological conditions and the roughness coefficient to vary on the way of the transport of the pollutants from the stack to the receptor, the formulas (5) and (6) are modified by introducing a "virtual distance" LV. The value of LV at the time interval Δt is given by:

$$LV_{i+1} = (SIG_i/C_{i+1})^{1/c_{i+1}} \quad \text{(m)} \tag{7}$$

where SIG_i operates for either $SIGY_i$ or $SIGZ_i$; C_{i+1}, c_{i+1} represent A, a or B, b during the $i+1$ time interval of the plume tracing, respectively.

At each time interval Δt, the atmospheric diffusion coefficient for the end of the specific segment is calculated using the virtual distance concept [23]:

$$SIG_{i+1} = C_{i+1}(LV_{i+1} + \Delta LS_{i+1})^{c_{i+1}} \quad \text{(m)}. \tag{8}$$

At the Δt when the segment is formed it is assumed that $LV = 0$.

Limitations of the vertical dispersion of the plume. The dispersion of the plume in the vertical direction is limited by the depth L of the mixing layer. This parameter can change during the transport of the pollutants.

The value of the mixing layer $LMIX_{i+1}$ for the end of each segment at the $i+1$ time interval of plume tracing is determined as follows:

$$LMIX_{i+1} = \begin{cases} LMIX_i & \text{for } LMIX_i \geqslant L_{i+1} \\ L_{i+1} & \text{for } LMIX_i < L_{i+1} \end{cases}, \quad \text{(m)} \tag{9}$$

where L is the mixing layer depth at the $i+1$ time interval of the plume tracing; $LMIX_i$ is the mixing layer depth for the specific segment at the i-th time interval. At the time Δt when the specific segment is formed it is assumed that $LMIX = L$.

Chemical transformation, wet and dry deposition processes. Chemical transformation as well as wet and dry deposition processes reduce the concentration of the pollutants in the atmosphere.

In the model, at the $i+1$ time interval Δt of the plume tracing, the virtual intensity of emission of the pollutant for each segment EV_{i+1}, i.e. the intensity of the emission of the pollutant from the stack reduced due to removal processes, is calculated according to the Zanetti formula [23]:

$$EV_{i+1} = EV_i \exp(-K\Delta t/360\,000) \quad \text{(mg/s)} \tag{10}$$

where EV_i is the virtual intensity of emission of the pollutants for the specific segment at the i-th time interval; K represents the reduction coefficient which covers chemical transformation as well as wet and dry deposition processes (%/h).

Mean wind velocity. The mean wind velocity U, i.e. the wind velocity averaged over the layer bounded by the ground surface and the height of the effective emission, is calculated by the formula:

$$U = [UA/(M+1)](H/HA)^M \quad \text{(m/s)} \tag{11}$$

where UA is the wind velocity at the anemometer height HA (m/s); M is the meteorological coefficient.

Calculation of the pollutant concentration – the basic equation. The concentration of the pollutant is calculated based on the Gaussian formula in which the following processes are taken into account: chemical transformation, wet deposition due to precipitation, dry deposition at the ground surface, and reflections of the plume from the upper inversion layer. For $SIGZ/LMIX \leqslant 1.08$ [5], the formula takes the form:

$$C = \frac{EV}{2\Pi U\, SIGZ\, SIGY} \exp\left(-\frac{R^2}{2\,SIGY^2}\right) \times \sum_{n=-5}^{n=4} \left[\exp\left(-\frac{(z-H+2n\,LMIX)^2}{2\,SIGZ^2}\right) + \exp\left(-\frac{(z+H+2n\,LMIX)^2}{2\,SIGZ^2}\right)\right], \quad \text{(mg/m}^3\text{)}, \tag{12a}$$

while for $SIGZ/L > 1.08$:

$$C = \frac{EV}{\sqrt{2\Pi}\, U\, SIGY\, LMIX} \exp\left(-\frac{R^2}{2\,SIGY^2}\right) \quad \text{(mg/m}^3\text{)} \tag{12b}$$

where R is the distance between the receptor and the plume axis (m).

The values of the parameters: EV, H, $LMIX$, U, $SIGY$, $SIGZ$ for the specific receptor are calculated based on the values of these parameters for the closest segment. It is assumed that the value of the virtual intensity of emission EV is constant for the segment. The values of the height of the effective emission H, the depth of the mixing layer $LMIX$, the mean wind velocity U and the atmospheric dispersion coefficients $SIGY$ and $SIGZ$ are interpolated based on the values of these parameters for the beginning and the end of the segment.

The influence of the turbulence in the buoyant plumes on the increase in the atmospheric dispersion coefficient is taken into account by introducing the Pasquill correction [2]. The corrected atmospheric diffusion coefficient SIG_c is calculated from the relation:

$$SIG_c^2 = SIG^2 + (\Delta h/3.5)^2 \quad \text{(m)} \tag{13}$$

where Δh is the plume rise (m).

3. APPLICATIONS OF THE SPM MODEL

The developed SPM model allows us to simulate the transport and dispersion of the pollutant emitted from a group of the point sources.

The fact that the SPM model takes into account the variability of the input parameters extends its application in comparison to the Pasquill model used in the routine calculations in Poland. In the latter model both stationarity and homogeneity of the input parameters are assumed.

The SPM model just as the Pasquill model can be used to calculate the distribution of pollutant concentration averaged over 30 minutes, 24 hours, and one year as well as the frequencies of the cases when the accepted levels of concentrations are exceeded. However, the SPM model allows us to extend the space scale of the calculation to few tens of km, while the Pasquill model should not be used for the distances greater than 10 km.

The space scale of calculations of the SPM model makes it possible to use this model to simulate the flow of the pollution to the specific region.

The fact that SPM model takes into account the change in time of the stack emission parameters allows us to apply this model in the air quality assessment when the accidental releases take place.

The range of the SPM model applications can be extended to cover the simulation of the transport and dispersion of the air pollutants emitted from the line and area sources by using the algorithms discussed in the paper *Methodology of calculating the air pollution contamination. Line and area sources* [6].

4. SUMMARY

The segmented Gaussian plume model for calculating the transport and dispersion of the pollutants emitted from the group of the point sources is presented. The developed model allows us to take into account the change in time of stack emission parameters and meteorological conditions as well as the spatial variability of the terrain and is based on the meteorological data from the routine measurements carried out in Poland. In this paper, the model assumptions, mathematical formulas and model applications have been discussed. In part II, the model verification, which is based on the data set from the measurement experiment carried out at Kincaid, Illinois, U.S.A., is described.

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GAUSSOWSKI MODEL ROZPRZESTRZENIANIA SIĘ ZANIECZYSZCZEŃ W ATMOSFERZE UWZGLĘDNIAJĄCY ZMIENNOŚĆ PARAMETRÓW WEJŚCIOWYCH CZĘŚĆ I. SFORMUŁOWANIE MODELU

Przedstawiono założenia, podstawy matematyczne i zastosowania segmentowego gaussowskiego modelu smugi (SPM) do symulacji transportu i dyspersji zanieczyszczeń emitowanych z zespołu źródeł punktowych. W części drugiej omówiona będzie weryfikacja doświadczalna modelu SPM.

МОДЕЛЬ ГАУССА РАСПРОСТРАНЕНИЯ ЗАГРЯЗНЕНИЙ В АТМОСФЕРЕ, УЧИТЫВАЮЩАЯ ИЗМЕНЧИВОСТЬ ВХОДНЫХ ПАРАМЕТРОВ. ЧАСТЬ I. ФОРМУЛИРОВКА МОДЕЛИ

Представлены предположения, математические основы и применения сегментной модели полосы Гаусса (SPM) для имитации транспорта и дисперсии загрязнений, эмиттируемых из комплекса точечных источников. Во второй части будет обсуждена экспериментальная проверка модели SPM.