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Software-Supported Visualization of Mathematical Spatial-Time Distribution Models of Air-Pollutant Emissions

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Atmospheric pollution due to emissions of harmful gases from different sources is one of modern society's critical problems. Resolving the consequences of air-pollutants is part of the risk management process aimed at monitoring the crisis, restoration and remediation of the environment, returning to its original state, and removing the risk of a re-emergence of accidents. The need for environmental risk assessment emerged due to increased awareness of the necessity for environmental protection. Modeling air polluter dispersion processes is an essential mathematical tool for exploring pollution's impact on the natural environment. This work describes an analytical and numerical solution to the two-dimensional transport equation of turbulent diffusion in a stationary state. We present a software-based visualization of a numerical model of the harmful gas concentration distribution, depending on weather conditions, terrain configuration, and urbanization.

Keywords: Air pollutants distribution, Emission monitoring, Gaussian model, Mathematical modeling, Maxima

Introduction

Emissions of hazardous gases into the atmosphere, whether by accident due to human negligence, plant failures, natural disasters, or deliberate terrorist attacks, pose a significant danger to the population and infrastructure. Hazard is defined as an action that has the potential to cause damage to human health or the environment.[1]

Physical, chemical, chemo-physical, and electrochemical methods are used to measure the concentration of hazardous gases. The limit value is regulated by law to a particular flow or concentration of harmful and dangerous components at the site of the accident.[2] Measurement results can be shown as mass per unit of the gas volume or as a mass of the flow in the time unit (mg/h, gr/h, etc.). One can use both continuous (over a long time) and discontinuous (measuring concentrations of gases at shorter intervals) methods for hazardous gas emissions estimation in order to assess their impact on the population's health and the environment.[3]

Systems for evaluating the hazardous gas concentration dispersion are based on mathematical models. At first, they were simple, manually calculated models. The development of information technologies has contributed to the accelerated development of more complex dispersion models, calculated based on an increasing number of input parameters. Today, a variety of such systems/models exist.[4] Nevertheless, they mostly provide only a partial solution to the dispersion problem. Many do not work in real-time, with simultaneous acquisition and processing of recorded data, providing only data analysis concentrating on visualization in two dimensions. Estimated zones of different concentrations of hazardous gases they provide are static. They do not consider the dynamics of processes, changes in atmospheric conditions, as well as in the intensity of the source of pollution.[1]

Different parameters are considered while generating models. Hazardous gases transport through the atmosphere, diffusion, chemical transformations, and deposition to the ground are just some of the parameters. As we stated earlier, the gas dispersion model was manually calculated initially, and simple tables and charts were used. Today, software solutions are available with much more complicated analyses of the dispersion models and significantly better pollution visualization. These models describe the cause and consequence between gas emissions, meteorological parameters, atmospheric conditions, physical and chemical characteristics of the

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movement and the proliferation of gas, terrain characteristics, and other factors, having the ability to assess impact and harmfulness of specific processes.[5] These models are the only method that quantifies the deterministic relationship between hazardous gas emission and concentrations. They can be effectively applied to estimate the consequences of observed scenarios and to assess the efficiency of applied strategies for pollution reduction.[6]

Numerous dispersion models (both physical and mathematical) have been developed to evaluate air-pollutants movement and proliferation after they are released into the atmosphere. As the atmosphere is a very complex physical-chemical system, its modeling is exceptionally complex. The process of pollutants' dispersion and their concentration depends on the movement of atmospheric masses (winds), air mixing by altitude, chemical reactions of harmful gases and/or radioactive decay in the atmosphere, and sedimentation speed.[7]

In this paper, modeling of spatial time distribution of air-pollution concentrations is described. A software-based visualization of pollutant concentration in 3-D space is presented after a brief explanation of the mathematical model described by a partial differential adjutant-diffusion equation. A mathematical software package called Maxima is utilized both to resolve numerically and visualize air-pollution concentration modeling. Its effectiveness is presented through a study case.

Method and Data

For modeling, the dispersion of air pollutants is described by a partial differential adjutant-diffusion equation (Eq. 1). Solving this equation results in three possible models: Lagrange, Oiler, and Gaussian. In our experiment, we choose to use the Gaussian model (Eq. 5). The paper's next section gives a detailed description of the initial conditions used to solve the partial differential adjutant-diffusion equation.

We also decided to describe in detail how the Gaussian model can be represented in the ground layers. To simulate atmospheric conditions in order to define the dispersion coefficients, we used Pascuill-Gifford's stability classes. They are found to be a good solution, widely used to classify stability. The way these classes are used to calculate the values of the dispersion functions for the different weather (clear, cloudy), time (day, night), and geographical (urban and rural areas) conditions are also described in the next section of the paper.

As a mathematical tool used to assist our research, a computer algebra system (CAS) Maxima was selected. It is free software that has preferable characteristics and is widely used in science and engineering problems.

A simulation was performed to analyze and visualize sulfur dioxide emissions in the vicinity of the thermal power plant. Detailed presentation of data used for the study case, as well as obtained results, are given in the separate section of this paper.

Modeling Spatial Time Distribution of Air-Pollution Concentrations

Mathematical models describing air pollutants' movement influenced by wind (transmission) and turbulent motion of the atmosphere (diffusion) are called atmospheric models of dispersion. They are divided into theoretical, empirical, and semi-empirical, and also stationary and non-stationary.

In empirical models, the physics of the atmosphere's process is almost entirely not considered or is very roughly included. Today, the best results, tentatively put, are given by semi-empirical models. In this type of model, the empirical model is supplemented by well-developed mathematical-numerical methods that include analyzing the dependency of a large number of observed parameters simultaneously (physical, chemical, geological, meteorological, and others).

The dispersion of pollutants in the air can be described by a partial differential adjutant-diffusion equation.[8] Mathematical models are based on solving this equation, numerically or analytically, or by combining them. As a result, a distribution of pollutant concentrations, taking into account wind sources' distance, using known particle emission speeds from sources and meteorological data, is obtained.[9]

The equation[10,11] describing the construction, advective-turbulent general flow of light pollutants is shown below:

$$\frac{\partial C}{\partial t}+v\frac{\partial C}{\partial x}+u\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}k_x\frac{\partial C}{\partial x}+\frac{\partial}{\partial y}k_y\frac{\partial C}{\partial y}+\frac{\partial}{\partial z}k_z\frac{\partial C}{\partial z}-\varsigma C \qquad \ldots (1)$$

where $u, v, w,$ are wind speeds in the direction of the corresponding axis; $k_x, k_y, k_z,$ are diffusion coefficients along that corresponding axis, and ς is transformation coefficient (chemical changes) of a material.

The initial conditions are given as follows: the current is stationary ($\frac{\partial \mathrm{C}}{\partial \mathrm{t}} = 0$) and the wind is directed along the y axis, so it is taken that $v = 0$ because horizontal movements in the atmosphere are small. Since the z axis is vertical, the speed w has a minus sign for heavy pollutants because it represents the particle's sediment speed. For light pollutants (the case that we will consider in this paper), this speed is taken as $w \approx 0$.

In general, diffusion coefficients in turbulent currents are second-class tensors. Assuming that the grid axis is in the direction of these tensors' main axis, then the non-diagonal components of these tensors disappear, and only the diagonal elements remain non-zero ($\neq 0$) $k_{xx} = k_x, k_{yy} = k_y, k_{zz} = k_z$. Diffusion processes are considerably slower if there is advection, so:

$$u\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial z} k_z \frac{\partial C}{\partial z} - \varsigma C \qquad \dots (2)$$

If we only look at light pollutants that don't have chemical transformations, then it is acceptable to state that $w = 0; \varsigma = 0$.

For all the conditions listed above, the advective turbulent diffusion equation of a particle originating from a stationary point source takes the following form:

$$u(z)\frac{\partial C(y,z)}{\partial y} = \frac{\partial}{\partial z}\left(K(y,z)\frac{\partial C(y,z)}{\partial z}\right) \qquad \dots (3)$$

Due to turbulence, light pollutants do not stay on the ground but return to the atmosphere as if reflected from the ground boundary layer. The boundary conditions for this type of current are:

$$\begin{aligned} &\text{I)}\ -K(y,z)\frac{\partial C(y,z)}{\partial z} = 0\ z \to 0 \\ &\text{II)} -K(y,z)\frac{\partial C(y,z)}{\partial z} = 0\ z \to h \qquad \dots (4) \\ &\text{III)}\quad u(z)C(0,z) = Q\delta(z - H_S) \end{aligned}$$

Here, Q is the power of the source (i.e., the amount of emitted light pollutants in the time unit (kg/s)); δ represents the Dirac's delta function; H_S represents the height of the source emitting pollutants; K states for the turbulent diffusion coefficients, and h the height of the boundary layer of the atmosphere. Considering the particle dispersion process's mathematic description methods, three classes of air-pollution analysis models can be pointed out: Lagrange, Oiler, and Gaussian.

Oiler's model is based on the idea of a fixed reference point through which the air flows, while Langrange's model is based on a reference point that moves with air currents. The Gaussian model is based on the immediate release of pollutants from a point source.[12] Although it cannot be considered state-of-the-art, the Gaussian model has been implemented in most software solutions that are now used and have the most comprehensive practical application due to its relative simplicity.[13] Therefore, it will be more detailed elaborated.

Gaussian Model

The Gaussian model starts from the assumption that the light pollutants emitted by a continuous point source form a smoke column where the symmetrical distribution of particle concentrations relative to the axis of the smoke column is observed. The basic equation of the statistical Gaussian model is composed of two density probability functions with the normal distribution, having the following form:[1,14]

$$C(x,y,\mathrm{z}) = \frac{Qf_F f_W}{2\pi\sigma_y(x)\sigma_z(x)\bar{u}} exp(-\frac{y^2}{2\sigma_y^2(x)})\left\{exp\left[-\frac{(z-h)^2}{2\sigma_z^2(x)}\right] + exp\left[-\frac{(z+h)^2}{2\sigma_z^2(x)}\right]\right\} \qquad \dots (5)$$

where, Q states for the mass flow; C states for the concentration of light pollutants at a given space point; $\sigma_y(x), \sigma_z(x)$ represents the diffusion dispersion in the direction of the appropriate axis — horizontal and vertical respectively (they depends on meteorological conditions and the distance particle have made from source to the point with the coordinate x, under the assumption that direction of the axis $0X$ is same as a direction of the wind vector); $\bar{u}$ states for a medium wind speed (at a measurement level); h is effective source height; and f_F and f_W are adjustments to the reduction of the cloud of light pollutants due to deposition of pollutant particles.[15,16]

The Gaussian model places the base of the coordinate system at the chimney base with the *x-axis* in the wind direction (Fig. 1). The contaminated gas flow (plume) rises from the edge of the chimney of height h and then moves in the direction of the *x, y,* and *z-axis*.[16] The gas flow (plume) rises above the chimney's edge because they are emitted at higher temperatures than the atmosphere’s and at a vertical speed.[14]

Calculations of the plume begin with the assumption that it is emitted at the coordinates (0, 0, H) where H is the effective height of the smoke column, which is calculated by summing the physical height of the chimney and the increase of smoke $(h + \Delta h)$. The smoke emitted at the site is the source of the pollutant emission Q (g/s) and moves in an X-direction with a speed that does not depend on the weather, altitude, or location.[17] The problem is how to calculate the concentration of that source at any point (x, y, z) for x> 0.[18] If the molecular diffusion itself caused the vapors to mix with the surrounding air, the plume would spread slowly as the thin array moves straight along the x-axis.

The Gaussian model (Eq. 5) for ground layer movement can be represented as Eq. 6

$$C(x,y,0) = \frac{Q}{\pi\sigma_y(x)\sigma_z(x)\bar{u}} exp(-\frac{y^2}{2\sigma_y^2(x)})\, exp(-\frac{H^2}{2\sigma_z^2(x)}) \quad \ldots (6)$$

Conditions in the atmosphere define the dispersion coefficients. Pascuill-Gifford's stability classes[19] are most commonly used to classify stability and are shown in Table 1.

The values in the column named ‘Day’ are subdivided as follows:

- a column named ‘Clear’ - refers to a summer day when the sun is more than 60° above the horizon;
- a column named ‘Partly cloudy’ - refers to a summer day with some clouds in the sky or a clear summer day with the sun between 35–60° above the horizon;
- a column named ‘Cloudy’ - refers to the cloudy autumn afternoon, cloudy summer day, or clear summer day with the sun between 15–35° above the horizon;

A column named ‘Night’ is subdivided as follows:

- a column named ‘Cloudy’ - refers to overnight when more than 4/8 of the sky is covered with clouds;

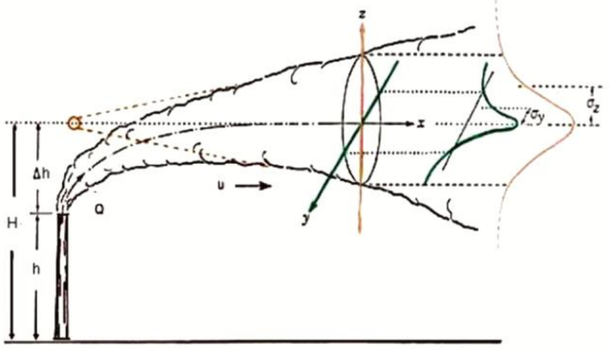


Fig. 1 — Graphical representation of air pollution propagation assumptions in the Gaussian model

Table 1 — Pascuill-Gifford's class of stability

u_{tla} (m/s)	Day			Night	
	Clear	Partly cloudy	Cloudy	Cloudy	Clear
<2	A	A–B	B	E	F
2–3	A–B	B	C	E	F
3–5	B	B–C	C	D	E
5–6	C	C–D	D	D	D
>6	C	D	D	D	D

- a column named ‘Clear’ - refers to a clear night when less than 3/8 of the sky is covered with clouds.

Based on the defined values of Pascuill-Gifford's class of stability (Table 1), corresponding to specific wind speed values and the degree of daytime daily insolation or night cloudiness[20], we calculate the values of the dispersion functions σ_y σ_z for the urban and rural areas[21] as shown in Table 2.

Software Supported Modeling of the Air-Pollutant Concentration Distribution

We used open-source mathematical software called Maxima to numerically resolve and visualize air-pollution concentration modeling. Its possibilities, primarily in the visualization of the results, are best seen in a specific application example. Below we give results obtained in the case of testing air pollution by sulfur dioxide emissions in the thermal power plant's vicinity.

In this paper, we use the centerline and ground-level concentration of sulfur dioxide emitted from a coal-fired power station using values for smokestack height, wind speed, emitted gas and ambient temperature, as well as other variables outlined previously. The emission rate of sulfur can be calculated using the amount of power supplied J_{elec}, the efficiency of the plant, as well as the sulfur concentration per weight J_{therm}.

Table 2 — Values of the dispersion function σ_y , σ_z , depending on stability classes for urban and rural areas

Pasquill categories	$\sigma_y(m)$	$\sigma_z(m)$	Pasquill categories	$\sigma_y(m)$	$\sigma_z(m)$
	Rural areas			Urban areas	
A	$0.22\,x\,(1+0.0001\,x)^{-0.5}$	$0.20x$	A–B	$0.32\,x\,(1+0.0004\,x)^{-0.5}$	$0.024\,x\,(1+0.001\,x)^{0.5}$
B	$0.16\,x\,(1+0.0001\,x)^{-0.5}$	$0.12x$	—	—	—
C	$0.11\,x\,(1+0.0001\,x)^{-0.5}$	$0.08\,x\,(1+0.0002\,x)^{-0,5}$	C	$0.22\,x\,(1+0.0004\,x)^{-0.5}$	$0.20x$
D	$0.08\,x\,(1+0.0001\,x)^{-0.5}$	$0.06\,x\,(1+0.0015\,x)^{-0,5}$	D	$0.16\,x\,(1+0.0004\,x)^{-0.5}$	$0.14\,x\,(1+0.0003\,x)^{-0.5}$
E	$0.06\,x\,(1+0.0001\,x)^{-0.5}$	$0.03\,x\,(1+0.0003\,x)^{-1}$	E–F	$0.11\,x\,(1+0.0004\,x)^{-0.5}$	$0.08\,x\,(1+0.0015\,x)^{-0.5}$
F	$0.04\,x\,(1+0.0001\,x)^{-0.5}$	$0.011\,x\,(1+0.0003\,x)^{-1}$	—	—	—

As an example of calculations, we took a thermal power plant 40% efficiency of 1000MW in which the combustion of coal emits sulfur dioxide SO_2. The assumptions are as follows: the atmospheric conditions are neutral, and winds are blowing at a rate of u = 2.5 m/s; the height of the chimney of the thermal power plant is h = 50 m, and the atmospheric stability class is “C”.

Using the Gaussian model of spreading air pollution, we can calculate the distribution of sulfur dioxide concentrations depending on the chimney's height, on the mass flow rate for neutral atmospheric conditions, as well as the concentration distribution depending on different weather conditions.[22]

The power of a thermal power plant can be calculated as:

Power supplied × efficiency = 1000 MW

$$1000 \times 10^6 \frac{J_{elect}}{s}\left(\frac{J_{therm}}{0.40 J_{elect}}\right) = 2500 \times 10^6 \frac{J_{therm}}{s} \qquad \dots (7)$$

while burning coal consumes energy:
Energy-consuming coal

$$2500 \times 10^6 \frac{J_{therm}}{s} \frac{(1g\_coal)}{28{,}000 J_{therm}} = 89285.71 \frac{g\_coal}{s} \qquad \dots (8)$$

The total amount of sulfur in the coal combustion process is:

Sulfur content

$$89285.71 \frac{(g\_coal)}{s} \frac{3g\_sulfur}{100g\_coal} = 2678.57 \frac{g\_sulfur}{s} \qquad \dots (9)$$

Sulfur dioxide (SO_2) emissions is obtained as:

$$Q = 2678.57 \frac{(g\_sulfur)}{s} \frac{64g\_SO_2}{32g\_sulfur} = 5357.14 \frac{g\_SO_2}{s} \qquad \dots (10)$$

The release of SO_2 into the atmosphere is the result of coal combustion described by the following chemical reaction:

$$S + O_2 \rightarrow SO_2 + Q_{CO_2} \qquad \dots (11)$$

$$1kmol\_S + 1kmol\_O_2 \rightarrow 1kmol\_SO_2 + 298700kJ \qquad \dots (12)$$

$$32kg_S + 32kg_{O_2} \rightarrow 64kg_{SO_2} + 298700kJ \qquad \dots (13)$$

$$32kg\_S + 22{,}4m^3\_O_2 \rightarrow 22{,}4m^3\_SO_2 + 298700kJ \qquad \dots (14)$$

For the complete combustion of 1kg of sulfur, the theoretically required amount of oxygen is 0.7 m^3, i.e., 3.33 m^3 of air, whereby 0.7 m^3 of sulfur dioxide is obtained under normal conditions.

The concentration (C) of sulfur dioxide released from the chimney will be calculated using the Gaussian model for calculating the ground concentration (y = 0 and z = 0) in the wind direction along the x-axis, according to the following formula:

$$C(x,0,0) = \frac{Q}{\pi u \sigma_y \sigma_z}\, exp\left(-\frac{H^2}{2\sigma_z^2}\right) \qquad \dots (15)$$

The dependence of pollutant concentration on atmospheric stability classes at defined emission values Q, wind speed of 2.5 m, and chimney height of 50 m for rural conditions is shown in Fig. 2. It can be observed that the concentration has the highest initial value that declines fastest with the increase of distance from the source for the case when the atmosphere is the most unstable (atmospheric stability A). In contrast, it has the lowest initial value with the

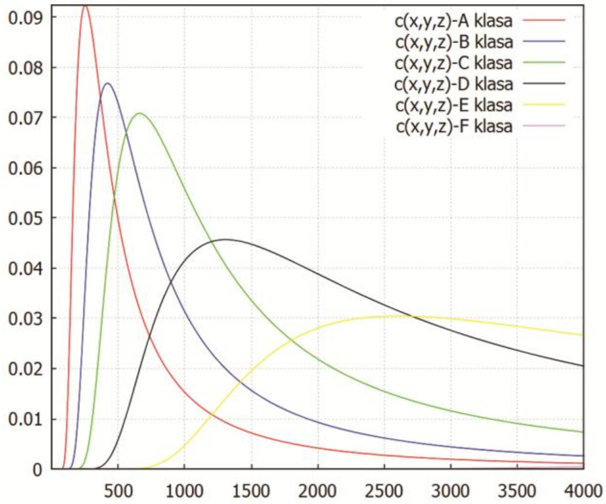


Fig. 2 — Sulfur dioxide (SO_2) concentrations when changing classes of atmospheric stability

slowest decline with the change of distance from the source for the most stable atmosphere (atmospheric stability E and F).

The dependence of the pollutant concentration on the wind speed for the value of atmospheric stability C and chimney height of 50 m is presented in Fig. 3. It can be noticed that for the lowest value of wind speed of 1.5 m/s, we have the highest concentration of pollutants, which decline fastest with increasing distance from the source. An increase in wind speed follows a reduced initial concentration that decreases more slowly with a distance change. At a wind speed of 5 m/s, the initial concentration, in our case, is 30% of the concentration's initial value at a speed of 1.5 m/s.

Pollutant's concentration dependence on chimney height is shown in Fig. 4. A case of inverse proportionality of the concentration's value and the chimney's height at a constant wind speed is noticeable. In our case, the chimney with the lowest height of 50 m releases the pollutant with the highest concentration. The initial concentration of pollutants declines as the chimney's height increases several times.

For the reason of clarity, Table 3 shows the numerical values of the pollutant concentration at different chimney heights and wind speeds at different distances from the pollutant source. It can be concluded from the table that for the lower values of wind speed and chimney height, we have higher concentration values of pollutants that decline with an increase in distance from the source, as we have shown graphically in the previous figures.

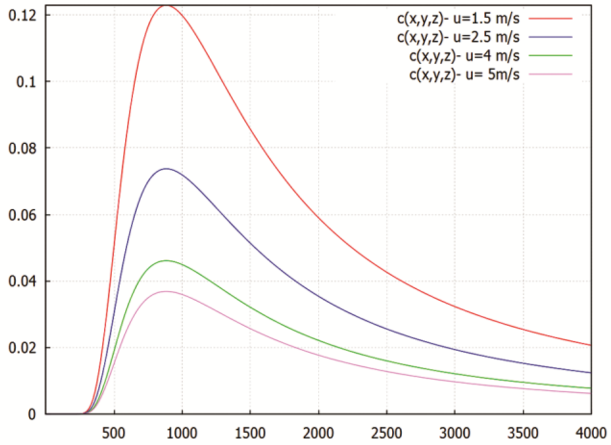


Fig. 3 —Sulfur dioxide (SO_2) concentrations depending on the change in wind speed

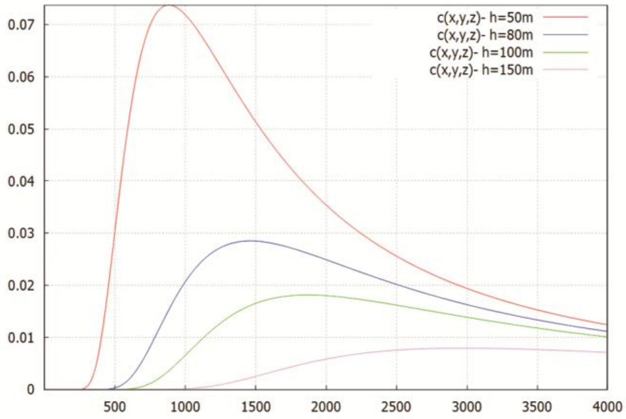


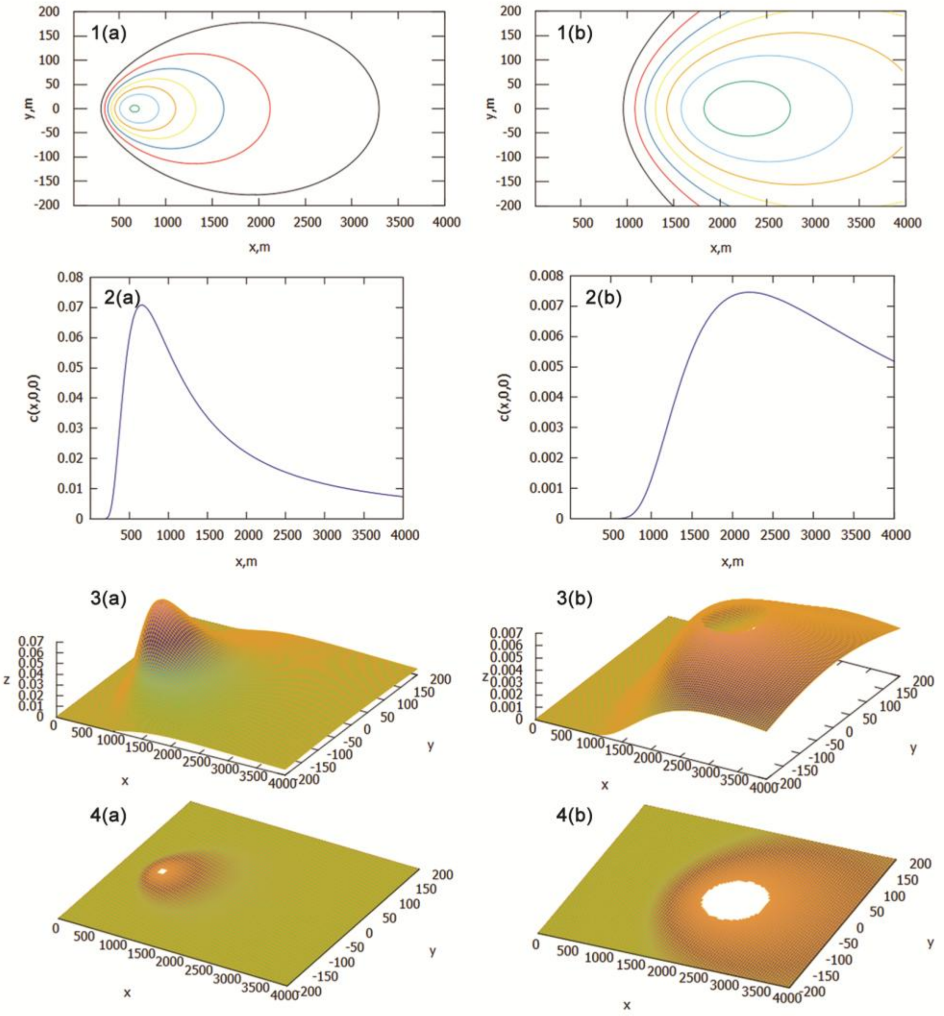
Fig. 4 — Sulfur dioxide (SO_2) concentrations depending on chimney height changes

In order to show in greater detail the results of the concentration dependence on the chimney height, obtained by applying the Gaussian model, Figs 5a and 5b give a graphical representation of the spatial-time distribution in different projections for the cases of chimney height of 50 m and 150 m, respectively. It can be seen that in the case of higher chimney height (h = 150 m), the concentration is lower and declines more slowly with the distance from the source. In comparison, at a lower chimney height (h = 50 m), the concentration is higher and decreases faster with increasing distance from the source. In our case, the value of the concentration is ten times lower at a higher chimney height.

To summarize, the concentration of pollutants decreases as chimney height increases at unchanged wind speed. By increasing the chimney's height, the maximum concentration moves to greater distances from the chimney, and at the same time, the

Fig. 4 — Sulfur dioxide (SO_2) concentrations depending on chimney height changes

chimney height (m)	wind speed (m/s)	distance (m)				
		500	1000	2000	3000	4000
50	1.5	0.118	0.058	0.019	0.010	0.006
	2.5	0.071	0.035	0.011	0.006	0.003
	4.0	0.044	0.022	0.007	0.003	0.002
	5.0	0.035	0.018	0.006	0.003	0.001
80	1.5	0.031	0.041	0.018	0.009	0.006
	2.5	0.018	0.024	0.011	0.005	0.003
	4.0	0.011	0.015	0.006	0.003	0.002
	5.0	0.009	0.012	0.005	0.002	0.001
100	1.5	0.009	0.029	0.016	0.009	0.005
	2.5	0.005	0.017	0.009	0.005	0.003
	4.0	0.003	0.011	0.006	0.003	0.002
	5.0	0.002	0.009	0.005	0.002	0.001
150	1.5	0.000	0.009	0.011	0.007	0.005
	2.5	0.000	0.005	0.006	0.004	0.003
	4.0	0.000	0.003	0.004	0.002	0.001
	5.0	0.000	0.002	0.003	0.001	0,001



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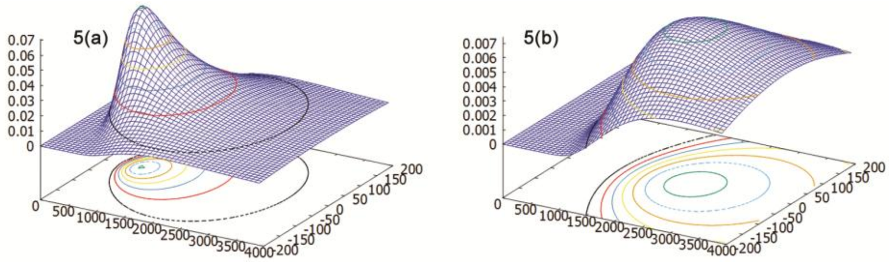

Fig. 5 — Comparative graphical representation in different projections of dispersions of sulfur dioxide concentration (SO_2) when changing the chimney height (a) h = 50 m and (b) h = 150 m

maximum concentration values are lower. The concentration also changes depending on the atmosphere's state, i.e., the class of atmospheric stability, wind speed, the speed of sulfur dioxide at the exit of the chimney, the ambient temperature and temperature at the exit of the chimney.

Conclusions

The processes of particle propagation in the atmosphere are of great importance for many areas of human activity. Understanding the importance of these processes has enabled permanent collection, monitoring, measurement, and data analysis. Based on the obtained data, empirical models are created to analyze pollutants' diffusion processes in the air. Such studies are used to assess and predict the consequences of dangerous particles' spread due to accidents and incidents in possible emergencies. Despite the enormous efforts invested in research, there are no universal models for air pollution analysis. Dispersion models are used to study the effects of different sources on air quality as well as for the possible prediction of pollutant concentrations. Difficulties in modeling pollutants' dispersion are particularly noticeable due to a lack of knowledge of complex turbulent processes in air-pollution. However, by using certain assumptions and approximations, the solutions become consistent with the observed phenomena.

It was proven that the Gaussian model could be utilized to describe the dispersion process effectively. Also, a mathematical software package called Maxima, very useful for modeling (numerical resolution) of air-pollution concentration, show its advantage primarily in the visualization of the results, as was demonstrated in a case study. In further research, we will explore the possibilities of implementing these mathematical models in Geographic Information Systems (GIS) as they have become an integral part of understanding natural hazards. With data obtained by monitoring a specific area near the source of pollution, the concentration and direction of the proliferation of gaseous substances regarding real geo-topographical data can be obtained and used to estimate the endangered zone. Therefore, a powerful tool can be created and used in emergency management to respond to events and mitigate the impact of disasters.

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