

Robert Cichowicz

**Łódź University of Technology, Institute of Environmental Engineering and Construction Installations
90-924 Łódź, Al. Politechniki 6, robert.cichowicz@p.lodz.pl**

Marta Bratkowska

**Łódź University of Technology, Institute of Environmental Engineering and Construction Installations
90-924 Łódź, Al. Politechniki 6, bratkowskamarta90@gmail.com**

MODELING THE DISPERSION OF POLLUTION IN THE ATMOSPHERE ACCORDING TO THE STANDARDS USED IN GERMANY

Abstract

Environmental monitoring involves environmental quality studies, observation and assessment of the environment's condition, and the changes taking place within it. The analysis accounts for sources of linear, surface, and point emission that have an adverse impact on the environment through pollutants. Point source emissions mainly represented by power plants spread harmful substances even for several dozen kilometers. Dispersion modeling is used to track atmospheric pollutants and to plan future emission sources, minimizing their impact on the environment. One of the newest modeling methods is the Lagrange model, currently used in Germany in AustalView software. The article presents the stages of the calculation of atmospheric dispersion of pollutants, according to German standards based on the example of the Schkopau power plant in Germany. This makes it possible to analyze the degree of air pollution depending on the distance from the source, and the information obtained may be useful for locating newly designed power plants through the location system, where the highest pollutant concentrations are recorded.

Key words

Dispersion, modeling, air pollution

Introduction

According to L. Łobocki [1], the methods of modeling the processes of atmospheric pollutant spreading should be changed in Poland to consider all existing pollutants in a given area, define areas of high concentrations, determine specific pollution episode times, determine the accuracy requirements for results, and as a consequence, utilize the results in the recovery plans.

Current simulations of pollutant dispersion present in Poland are based on the Gauss and the Euler models. The most popular systems and programs for this purpose are:

- The Polyphemus system, which is a program containing 4 numerical models [2]:
 - the Gaussian stream model,
 - the Gaussian cloud model,
 - the Eulerian chemical-transport model called Polair 3D,
 - the Eulerian chemical model called Castor;
- The Aria system, which is a simulation tool with a wide range of applications from continental to local, used for analyzing all types of pollutants and their impact on air quality. Depending on the needs, various mathematical dispersion models can be used, from simple Gaussian models to complex Lagrangian or Eulerian models. With the program, the user can perform graphical data processing, prepare animations, and/or 3D concentration maps to provide a clear visualization of the modeling results [3];
- The OPA03 system, which provides modeling of air pollution from point, linear, and surface sources, in which the calculation algorithm complies with the Ordinances of the Minister of the Environment: Journal of Laws from 2008, no. 47, item 281 [4], Journal of Laws from 2010, no. 16 item 87 [5] and Journal of Laws from 2014, item 1546 [6]. The system consists of the programs: Opa03 Kotły03, Opa03_VOC and Maps [7].

Since Poland and Germany are members of the European Community, the common guidelines for permissible concentrations of pollutants set out in Directive 2008/50/EC of the European Parliament and of the Council from May 21, 2008 on air quality and cleaner air for Europe apply [8]. Simulation calculations of atmospheric dispersion of pollutants in Germany are carried out using the Lagrange model, which is more accurate than the Gauss model, most commonly used in Poland (Table 1).

Table 1. Comparison of pollution dispersion modeling systems in Poland and Germany

No.	Characteristic	Poland - Gauss model	Germany - Lagrange model
1.	The main national model for the atmospheric dispersion of pollutants.	The Gauss model, which assumes: - flat terrain without obstacles in the form of buildings; - constant wind speed at a specific height (14 m)	The Lagrange model, which assumes: - different speeds at specific heights - the inclusion of obstacles to the flow of the stream of pollutants, e.g. in the form of buildings - creating wind fields according to each case considered
2.	Determination of atmospheric stability in pollution dispersion calculations in commonly used software	There are 36 meteorological situations resulting from 6 atmospheric equilibrium states that correspond to wind speed ranges at a height of 14 m	Stability of the atmosphere is indicated by the Monin - Obukhov length, if the value is unknown, it is determined according to the Klug/Manier dispersion classes depending on the length of the terrain roughness
2.	Division of the dust fraction	Division into PM10 (particle diameter 10 μm) and PM2.5 (2.5 μm particles)	Division into 4 classes: - class 1 - particles smaller than 2.5 μm ; - class 2 - 2.5 to 10 μm - class 3 - 10 to 50 μm - class 4 - greater than 50 μm
3.	Dust drop criterion	The dust drop criterion considers the emission of all dust substance fractions, including suspended particulates	The dust drop criterion is divided according to the size of its particles per class and the corresponding deposition velocity
4.	Division into wind speed classes	None	Division into 9 classes of wind speed: - class 1 <1.4 m/s - class 2: 1.4 - 1.8 m/s - class 3: 1.9 - 2.3 m/s - class 4: 2.4 - 3.8 m/s - class 5: 3.9 - 5.4 m/s - class 6: 5.5 - 6.9 m/s - class 7: 7 – 8.4 m/s - class 8: 8.5 – 10 m/s - class 9: up to > 10 m/s
5.	Determination of terrain roughness in the area of the emission source - range	50 heights of the emission source	10 heights of the emission source
6.	Performing calculations for emitter groups	Calculations performed for one substitute emitter containing the parameters of the other ones	Performing a simulation that includes all the defined emitters (no substitute emitter creation)

Source: Author

One of the tools for modeling dispersion of pollutants in the atmosphere in Germany is the Austal View program (Fig. 1), which is a graphical module for the specialist Austal 2000 software and is used by the German Federal Environmental Protection Agency. It was developed in accordance with the German Air Pollution Control Regulation TA Luft (Technische Anleitung zur Reinhaltung der Luft) [9] and its work consists of tracking pollutant particles in the atmosphere based on the Lagrange model, to which a mobile coordinate system is introduced, and the observer moves along with the air at a given velocity and keeps in contact with the same air molecules over a given length of time. Through the process of dispersion of the abstract particles introduced into the model, a neutral balloon of density that moves with the wind is tracked. During the simulation of the pollution

dispersion, the program develops its own wind field diagnostics model (TALdia), considering the influence of the terrain shape [10].

The integrated graphical user interface combines graphical tools, such as sources, buildings, monitoring points, and networks into a single automated model. The scope of the simulation involves an area with a radius equal to the height of the emission source, such as for a chimney height of 250 m or the area to be simulated is within a radius of 25 km from the emission point. At the same time, several types of pollutants can be modeled and their spread in the atmosphere can be monitored. An important point in this case is the introduction of meteorological data. The model accepts hourly meteorological data in AKT, AKTerm, and AKS formats. The first two formats contain hourly data for wind direction, wind speed, and stability class according to Klug/Manier [9]. In turn, the AKS file includes wind direction, wind speed, and dispersion class statistics. An example of an AKS file is shown in Fig. 2, where statistics on winds occurring in Leipzig (Germany) are shown [9, 11].

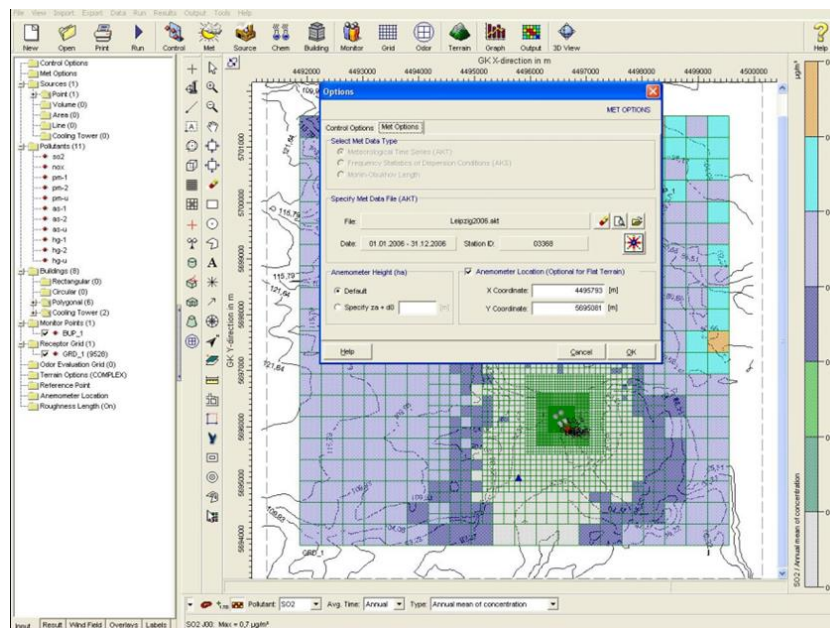


Fig. 1. The main interface window of Austal View
Source: Author's findings.

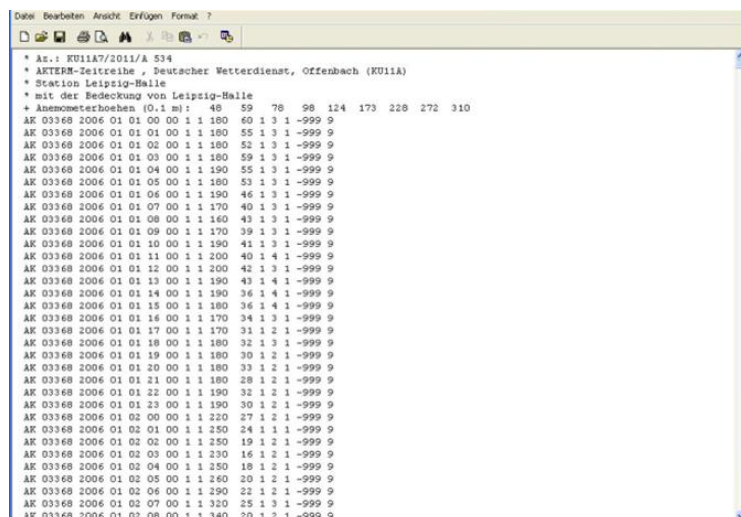


Fig. 2. AKS meteorological data for Leipzig
Source: Author's findings.

The simulated terrain can be treated as flat or as terrain with proper shaping. The type of output results depends on the pollutants that are modeled. The results are obtained in the form of [11] average annual concentration, average annual deposition, maximum daily average "n" of exceedances, maximum hourly with "n" exceedances, estimation of statistical uncertainty, and a series of time-based hourly concentrations (monitor point areas only).

The program allows for receiving automatic result reports, such as "Source Parameters", "Monitoring Point Results" and "Maximum Calculated Results". An example of such a report is shown in Fig. 3, in which a "period" is the emission time in hours, and the "emission rate" is the share of classes of pollutants in relation to their total quantity.

Source Emissions					
Source: SRC_1 - source 1					
	AS	HG	NOX	PM	SO2
Period [hours]:	8735	8735	8735	8735	8735
Emission Rate [kg/h or MOU/h]:	6,030E-04	5,027E-02	5,662E+02	1,237E+01	8,099E+02
	46,8% as-1	25,3% hg-1		19,6% pm-1	
	38,2% as-2	20,7% hg-2		57,7% pm-2	
	15,0% as-u	54,1% hg-u		22,6% pm-u	
Total Emission [kg or MOU]:	5,267E+00	4,391E+02	4,945E+06	1,081E+05	7,075E+06
Total Emission [kg or MOU]:	5,267E+00	4,391E+02	4,945E+06	1,081E+05	7,075E+06
Period [hours]:	8735				

Fig. 3. The Source Emissions Report
Source: Author's findings.

Austal View software also includes the Austal Meteo module, which allows for making a compass rose layout based on meteorological data. You can freely modify the appearance of the compass rose in terms of color, size of the "petals" (columns), and the grid of sectors. It also has the option of 3D visualization from the entire modeling area. Sources, buildings, and modeling results are displayed together with the surrounding terrain of different shape. The wind rose and the diagrams made in Austal Meteo are shown in Fig. 4 and 5.

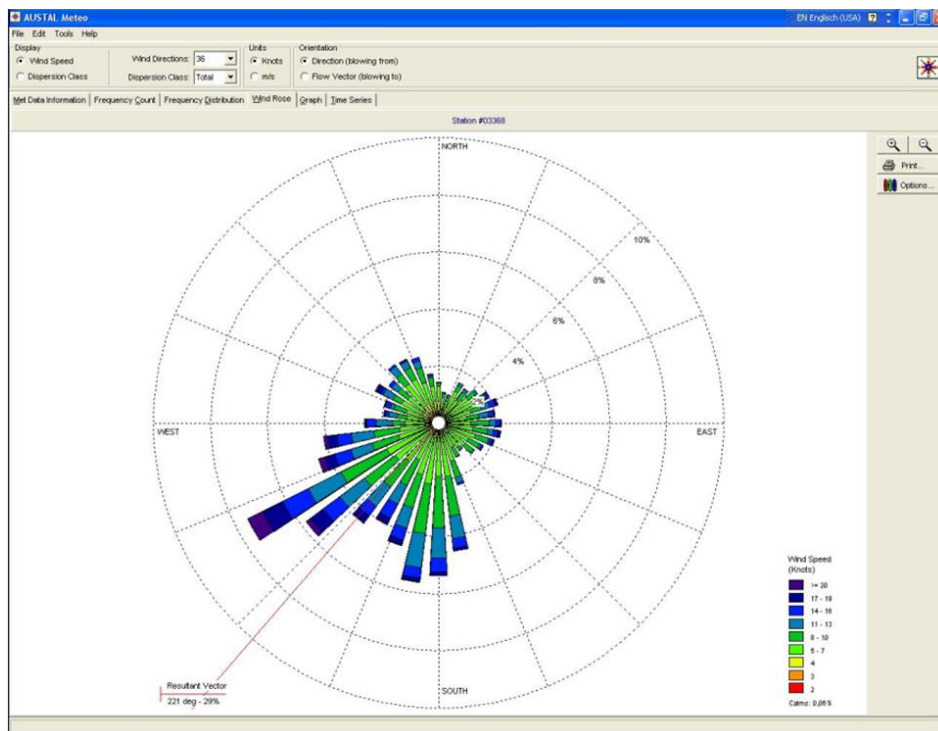


Fig. 4. Compass rose - Austal Meteo, based on meteorological data for Leipzig, Germany
Source: Author's findings.

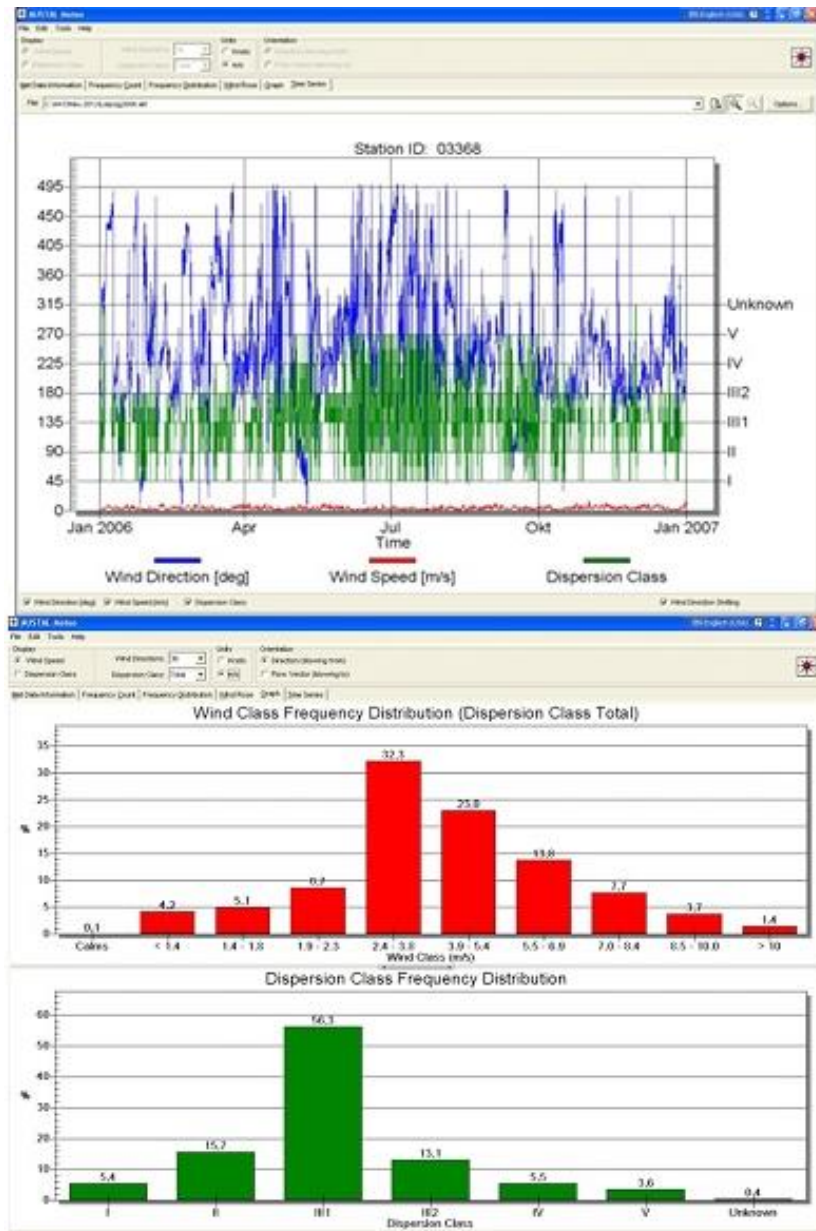


Fig. 5. The meteorological data prepared using the AUSTAL-Meteo program based on meteorological data for Leipzig, Germany
 Source: Author's findings.

The methodology for calculating atmospheric dispersion of pollutants

When performing simulation calculations alongside maps and meteorological data in a suitable format, one should begin with gathering the necessary information about the source and the terrain near the emission point. Gauss-Krueger or UTM system coordinates of the source itself, as well as of the surrounding buildings, which are to be included in the analysis, are necessary. It is important for each object specification to be defined in the same coordinate system, including the reference point.

The basic steps in performing the calculations for the simulation of atmospheric dispersion of pollutants include defining objects for the preparation of the so-called "wind field". At this stage, one should consider the buildings located near the source. A chimney is usually a part of a complex of buildings that can interfere with the flow of wind in the lower layer and change the dispersion of gases emitted. Therefore, first and foremost, one should define the objects, considering their height and shape. Typically, one selects the highest buildings. If too many buildings are included in the simulation, the preparation time of the wind field will be significantly longer (Fig. 6):

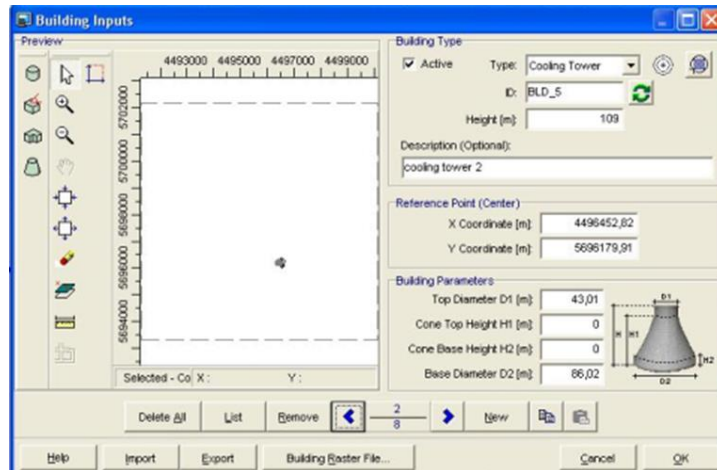


Fig. 6. Building data on the example of the power plant cooling facilities
Source: Author's findings.

- Supplement for the source data. Essential information for modeling is:
 - The height of the chimney [m],
 - The flow of pollutants from the chimney [m^3/h],
 - The temperature at emitter outlet [$^{\circ}\text{C}$],
 - The thermal output of the source [MW],
 - The cross-sectional area of the chimney at the outlet [m^2],
 - The chimney diameter [m],
 - The exhaust gas velocity at the outlet [m/s],
 - The emitter's work time [h/year],
 - The amount of individual pollutants emitted [kg/h].

If all data is not available, the program offers the possibility to calculate some parameters based on other information, considering the basic equations and formulas for calculating them (Fig. 7).

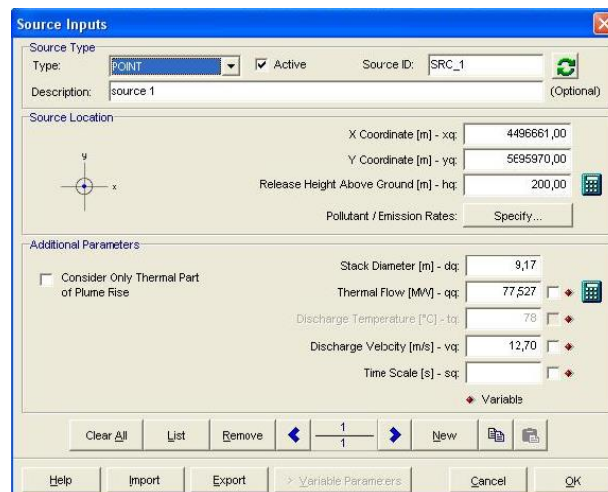


Fig. 7. Calculation of source data
Source: Author.

- Calculating pollutant emissions, using the "Specify" function in the pollution data window, one can enter the necessary information for the simulation, including the emitted substances mass data. You can choose which pollutants are to be included in the analysis. The data on impurities are entered in [kg/h] or [g/s]. It is possible to assign different pollutant values separately for each source when dealing with more than one emitter ("Select Chemicals"). One can also specify a given emission for the given date and time ("Variable Emissions"). An example of this type of data being entered for one emission source is shown in Fig. 8:

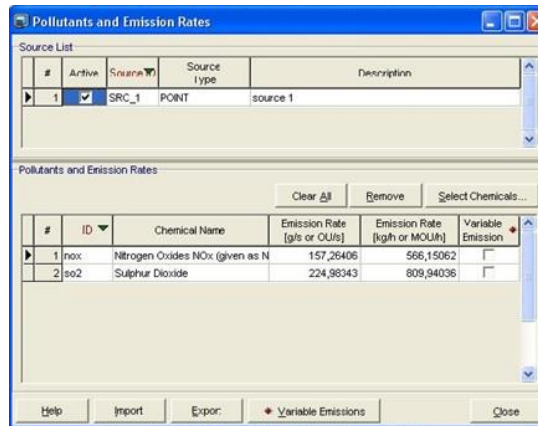


Fig. 8. Entering emissions data

Source: Author.

- Determining the average terrain roughness length. The roughness, or terrain shape is defined by the so-called average roughness length z_0 . In Germany, it is defined according to the soil classes indicated by CORINE [9]. This parameter should be set for the area located in the circle of the chimney with a radius equal to 10 times the emitter's construction height. It can be set independently and entered as input data or if the given area is composed of groups with different terrain roughness, the average roughness is calculated by the program as the arithmetic mean in regard to the proportions of the given surface and then rounded to the nearest value from Table 2:

Table 2. The average length of terrain roughness according to CORINE classes in Germany

z_0 [m]	Classes of soil according to CORINE
0.01	beaches, sand dunes, sandy plains, water reservoirs
0.02	pastures, scarcely overgrown areas, swamps, estuaries, water courses, landfills
0.05	mineral mining sites, sports and leisure sites, non-irrigated farmland, glaciers and areas of eternal snow, coastal lagoons
0.10	airports, inland swamps, peat bogs, seas and oceans
0.20	road and rail networks, urban greenery, vineyards, land occupied by agriculture, peat bogs and heaths, naked rocks
0.5	ports, fruit trees and berry plantations, transitional forests and scrubs
1.0	industrial or commercial facilities, buildings, coniferous forests
1.5	deciduous forests, mixed forests
2.0	urban areas

Source: [9]

- Calculating the size of the area and applying the grid to the map. The calculation area for a single emission source is in its circumference with a diameter of 50 times the chimney height. If other sources are added to the load, the calculation area consists of several calculation areas for each source. However, in non-standard terrain, it is necessary to mark a larger area for calculation. Usually a single grid is used when there are no defined buildings. It can be entered by the user or automatically generated by the program. For calculations that include buildings or a source system with varying heights, the buildings and low sources require a small grid, while at the same time other high sources are covered with a large area grid. If small grids are used over long distances, this may result in large statistical uncertainties in the modeled concentrations. Nested grids are used to avoid this. In the surroundings of the buildings and for low sources, grids with small cells are used, and further to the outside a larger grid is used. However, keep in mind that each nested grid must be subject to constant rules, in that an appropriate multiplier should be considered [11];
- Selection of the accuracy level of the calculations. The level of quality of the simulation results obtained determines the class and speed of analysis. The program offers a scale from -3 to 3. Changing one level doubles the number of the particles used in the simulation and it reduces the statistical uncertainty by $1/\sqrt{2}$. At the same time, this is reflected in the time of simulation analysis (Fig. 9) [11].

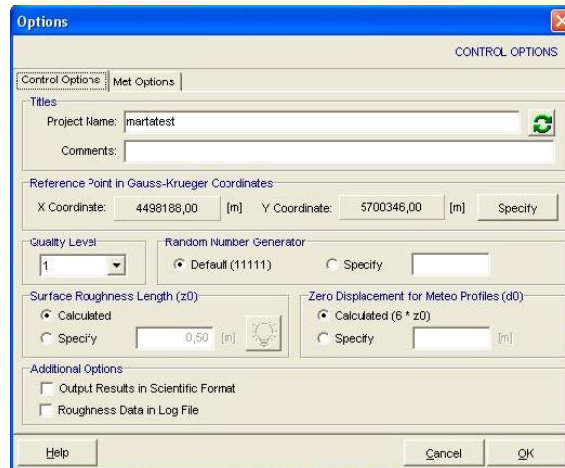


Fig. 9. Selection of the accuracy level of the simulation of the atmospheric dispersion of pollutants
Source: Author.

Calculation of pollutant dispersion for the Schkopau power plant in Germany

The Schkopau power plant is fed with brown coal and its total net power is 900 MW (2 x 450 MW). It provides electricity to the residents, but also supplies nearby plants associated with the chemical industry and the German railways. The power plant burns up to six million tons of brown coal per year.

The following project assumptions were adopted for the calculation:

- Chimney height: 200 [m];
- System flow: 1508953 [m³/h];
- Temperature at the outlet of the chimney: 78 [C°];
- Thermal output: 77.5266 [MW];
- Cross-sectional area of the chimney at the outlet: 66 [m²];
- Diameter: 9.1693 [m];
- Exhaust gas velocity at the outlet: 12.70 [m/s];
- Work time: 7200 [h/year].

The calculations were carried out with the assumption that the nearest buildings are about 130 m tall and that there are two chimneys with a height of 109 m in the immediate vicinity (Fig. 10 and 11).

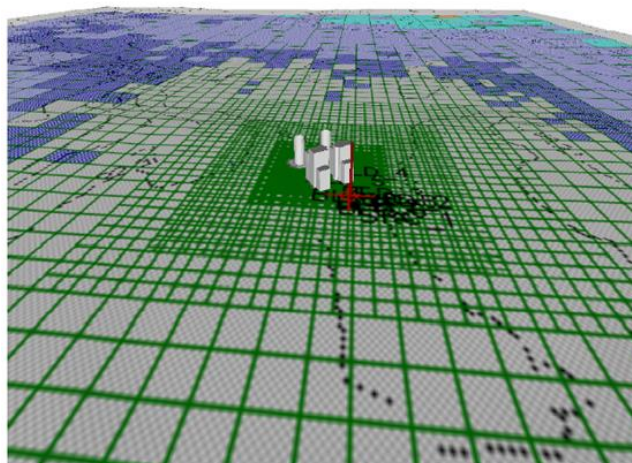


Fig. 10. The defined buildings in 3D visualization
Source: Author's findings.

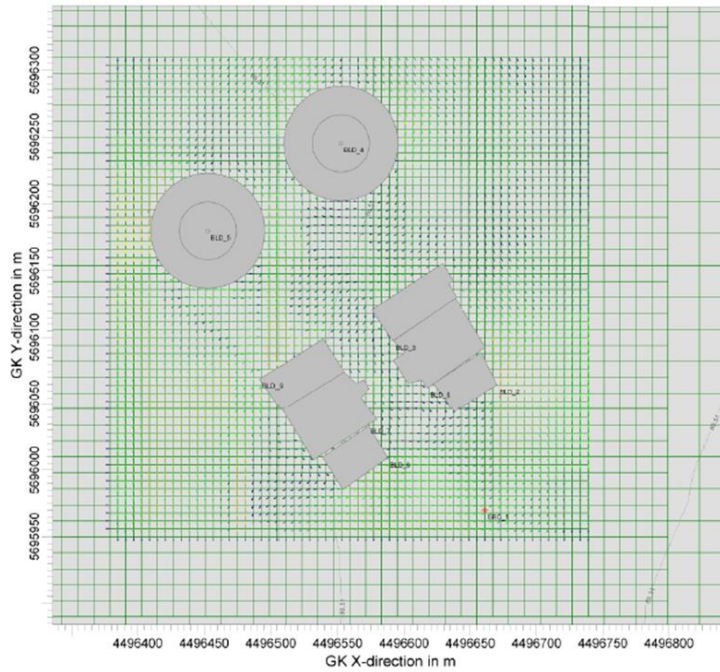


Fig. 11. The defined buildings - top view
 Source: Author's findings.

After entering the source and pollutant emission data, as well as the necessary meteorological data, a terrain roughness map was entered. Next, simulation calculations were then performed using the program, and the results obtained were rounded to the nearest values from Table 1. The area surrounding the power plant and its various terrain roughness values are shown in Fig. 12.

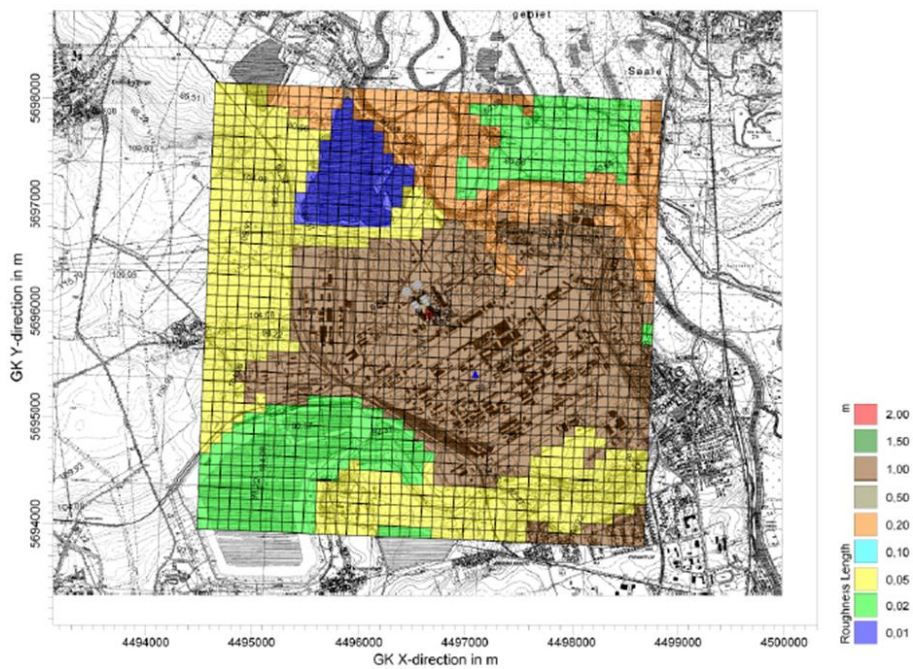


Fig. 12. Graphical interpretation of terrain roughness in the area of the Schkopau power plant in Germany
 Source: Author's findings.

In Fig. 12, blue areas are water reservoirs, buildings and industrial sites are brown, and green marks pastures and scarcely overgrown areas, while yellow is arable land and mineral mining sites. Due to the number of the defined buildings, calculations were made for quality level 1 and for pollutants such as SO_2 and NO_x , as these compounds are some of the most harmful and most often emitted in combustion processes (the results are shown in Figures 13 and 14).

The orange points shown in Figure 14 represent the locations with the highest concentrations of the contaminants analyzed. It should be noted that these are concentrations of pollutants coming directly from the power plant, not considering the concentrations of local pollutants originating, for example, from domestic furnaces occurring in this area.

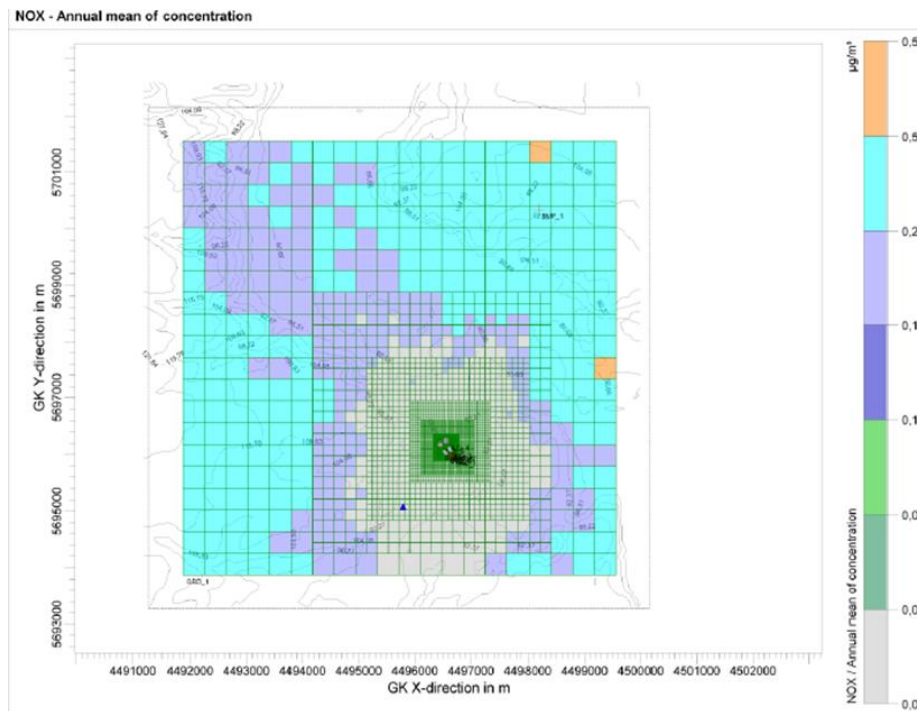


Fig. 13. The simulation of annual mean concentrations for NO_x - Schkopau, Germany
Source: Author's findings.

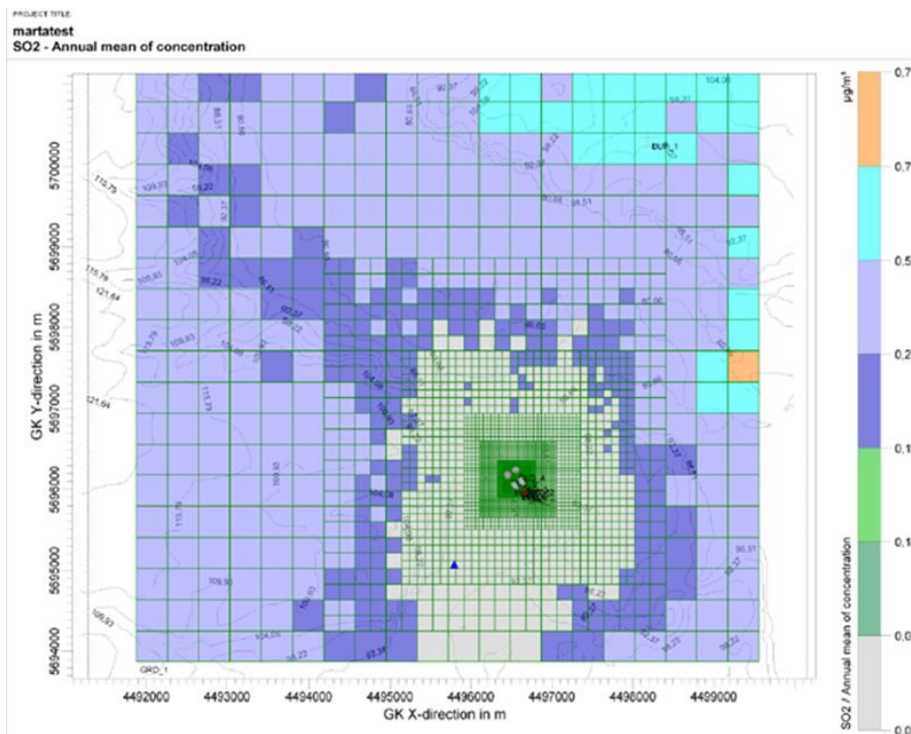


Fig. 14. The simulation of annual mean concentrations for SO₂ - Schkopau, Germany
Source: Author's findings.

Fig. 15 and 16 illustrate the exemplary results of calculations of the amount of pollutants spread in the given cardinal directions. The calculation was made summing concentrations depending on the distance from the

source of the emission. The values concern the dispersion of SO₂ and NO_x for the average annual concentration from the Schkopau power plant in Germany.

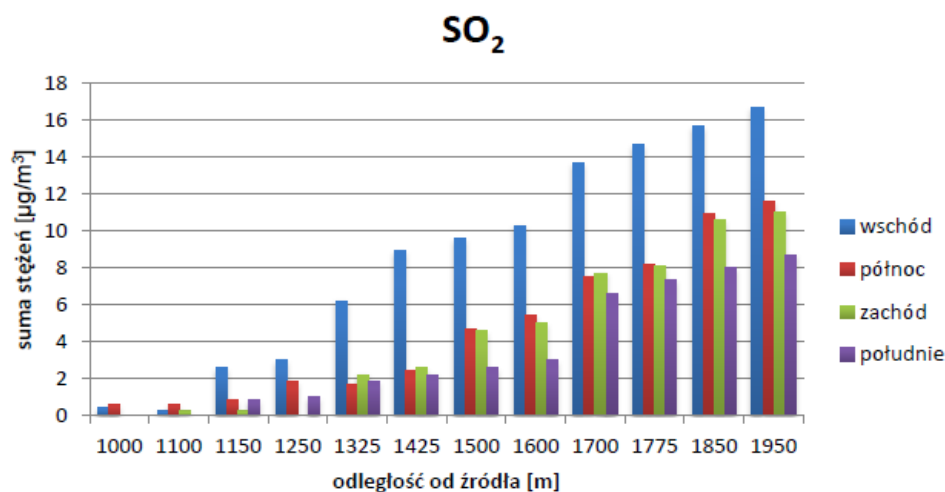
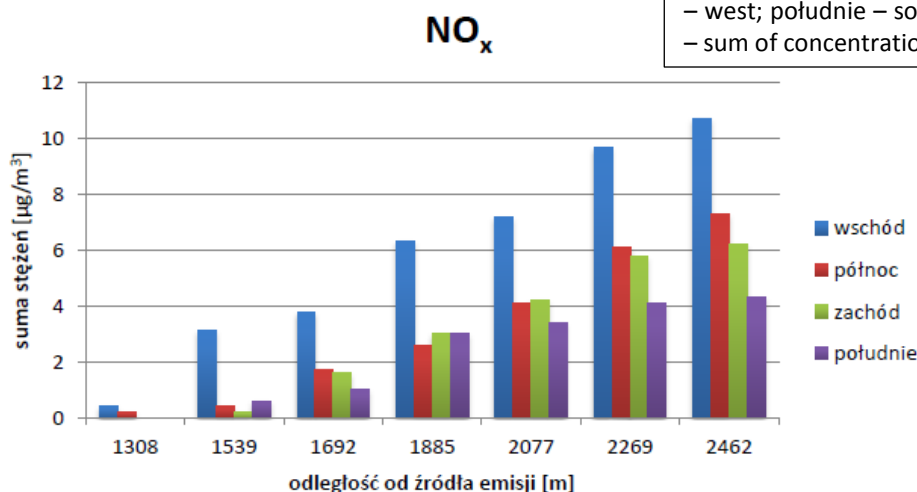


Fig. 15. The sum of concentrations depending on the distance from the SO₂ emission source - Schkopau, Germany (annual average)

Source: Author's findings.



Wschód – east; północ – north; zachód – west; południe – south; suma stężeń – sum of concentrations

Fig. 16. The sum of concentrations depending on the distance from the NO_x emission source - Schkopau, Germany (annual average)

Source: Author's findings.

The values presented in Fig. 15 and 16 refer to the case where only one chimney was assumed in the calculation, such as a single emission source. By analyzing the values obtained, it can be observed that the concentrations of pollutants increase along with the distance from the emitter, and that their dispersion for both SO₂ and NO_x is most evident in the eastern direction.

Conclusion

Pollution dispersion is determined not only by meteorological conditions, but also by the influence of the terrain shape and the buildings near the source of the emission. The wind stream is capable of transferring pollutants over long distances, often up to a few kilometers further, with pollutants reaching their maximum concentrations. Gathering meteorological information helps in performing an effective simulation using the Lagrange method, predicting the places where the pollutants will occur in the largest concentrations. The discussed software allows for designing or planning industrial plants in appropriate areas, reducing human exposure to the emitted harmful substances. In addition, simulation calculations can be very helpful in conducting air monitoring as they allow for predicting the concentration of pollution on a given surface in different states of the atmosphere and dispersion classes, depending on the source parameters and the amount of pollutants produced.

Acknowledgments

We would like to thank Prof. Dietmar Heinz of the Hochschule Merseburg (Germany) for organizing access to the Austal 2000 and AustalView software and for the possibility of carrying out the studies related to the air monitoring system in Sachsen-Anhalt (LÜSA), which is operated by the State Office for Environmental Protection (LAU).

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