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# Comparative Analysis of the Results from Frequently Applied Methodologies and Approaches for Dispersion Modeling

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## ABSTRACT

*Accurate air quality assessment through dispersion modeling is crucial for regulatory compliance and environmental management, particularly in complex industrial areas. In Bulgaria, the software package PLUME is frequently used, often employing an unofficial instruction from the Ministry of Environment and Water (MEW) to merge multiple emission sources into a single "Virtual Emission Device" (VED) when their number exceeds ten. This study performs a critical comparative analysis of this approach.*

*The annual average concentrations of NOx (nitrogen oxides) and* $PM_{10}$ *(particulate matter) from sources in the industrial zone of Devnya, Bulgaria, were modeled using three distinct methods: PLUME with the MEW's VED instruction; PLUME applying the methodologically sound superposition principle; and the advanced regulatory model Breeze AERMOD as a benchmark.*

*The results reveal significant discrepancies. The VED approach was found to severely underestimate both the maximum concentration values and the spatial extent of pollution impacts. For* $PM_{10}$*, the maximum annual concentration calculated using VEDs was* $2.36\ \mu g\ m^{-3}$*, whereas the superposition method yielded a value of* $13.09\ \mu g\ m^{-3}$*. Furthermore, the analysis shows that the PLUME model's inherent limitations, such as its inability to process hourly meteorological data or account for terrain, lead to unrealistic "feather-like" pollutant distributions, in contrast to the more precise results from Breeze AERMOD.*

*The study concludes that the VED method is flawed, introduces substantial errors, and contradicts established dispersion principles. For accurate and reliable air quality assessments required for regulatory purposes such as Environmental Impact Assessments and Integrated Permits, the use of advanced models like Breeze AERMOD is essential.*

*Keywords: air quality modelling, pollutant dispersion, PLUME, Breeze AERMOD, Virtual Emission Device (VED), industrial pollution, comparative analysis,* $PM_{10}$*, NOx.*

## INTRODUCTION

Air quality is an important condition for a healthy environment. The atmosphere is the gaseous envelope of the Earth, which represents a mechanical mixture of gases, water vapor, and

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**Correspondence to: Nina Ilieva, University of Chemical Technology and Metallurgy, 8 Kliment Ohridski Blvd., Sofia 1797, Bulgaria, e-mail: nilieva@uctm.edu* tiny solid or liquid impurities (aerosols). The constant composition of atmospheric air includes nitrogen, oxygen, argon, inert gases, and others.

Any change in the percentage content of the listed elements, as well as the introduction of new ones, leads to air pollution.

The sources of air pollution are both anthropogenic and natural in origin. The most significant anthropogenic sources can result from human activity in the following sectors: burning of fossil fuels in electricity production, transportation industry, and households, industrial processes and use of solvents, for example in the chemical and mining industries, agriculture and livestock farming, and waste treatment.

Generally, pollutants can be divided into solid, liquid, and gaseous. Their harmful effects can be both direct and subsequent to chemical transformation or because of combined action with other substances.

Atmospheric air quality is assessed by measuring the content of harmful substances over a different period. Their levels must be such that they do not exert either direct or indirect harmful effects on the environment and the human body, which is why limits for ambient air quality have been adopted for several pollutants. Furthermore, there are regulations defining the control of generated and emitted pollutants.

Dispersion modelling is a simulation of the real air pollution in a given territory and is performed using globally recognized modelling software. It is applied in a comprehensive overall assessment of ambient air quality for the purposes of developing Air Quality Management Programs (AQMP) and their associated plans, environmental impact assessments, where cases in which air quality is assessed only with modelling are regulated in Ordinance No. 12 of July 15, 2010, on the limits for sulfur dioxide, nitrogen dioxide, fine particulate matter, lead, benzene, carbon monoxide, and ozone in ambient air, Art. 10 (1).

Other cases in which dispersion modelling is used are in the design and construction of new installations and facilities or discharge devices, by preparing a forecast to assess the contribution to air pollution from the pollutants generated by these sources. Such procedures in our country include, for example, the issuance of Integrated Permits and their modification, Environmental Impact Assessment (EIA) reports, and others. The choice of modeling software, as well as its correct application, are essential for preparing an accurate assessment.

That is why the present thesis is dedicated to the analysis of the results obtained with some of the most frequently applied software packages and approaches for dispersion modeling.

## Physicogeographical characteristics of the area

### *Terrain and climate*

According to the physiogeographical division of the Republic of Bulgaria, Devnya Municipality falls within the eastern sub-region of the Danubian Hilly Plain. The western and eastern parts of the municipality's territory are characterized by a different type of flat relief.The valley, thus surrounded, predisposes the occurrence of frequent inversions and radiation fogs due to the presence of polluting sources. The altitude varies from 0 to 352 meters, with the highest areas located in the northeastern and southwestern parts of the municipality's territory [1].

### *Climate*

Northwest winds prevail in the municipality, but east winds also appear very often. Cases of calm (stillness) and the formation of radiation fogs are noted, for which atmospheric pollution also plays a role. Compared to the neighboring cities of Varna and Provadia, the foggy days are twice as many. The relatively more frequent droughts, especially during the summer and autumn, along with light winds, create conditions for ground-level inversion and an increase in the concentration of atmospheric pollution. Precipitation is relatively low, with its seasonal distribution having a winter-autumn maximum [2].

### *Wind rose*

For the wind rose, data from the "Climatic Handbook of Bulgaria," Volume 4, Wind, were used. The data relate to MS Suvorovo (Meteorological Station Suvorovo). The type of underlying surface is set as a rural area. The wind rose by frequency is presented in Fig. 1, and the data upon which it was constructed is in Table 1.

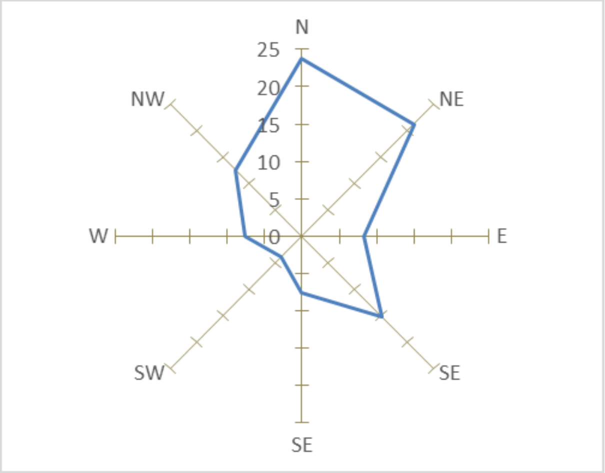

Fig. 1. Frequency wind rose, %, MS Suvorovo.

### Regulatory framework

The principal legislative act governing environmental protection in Bulgaria is the Environmental Protection Act. The quality of ambient air is regulated by the Clean Ambient Air Act (CAAA), which is harmonized with the relevant European Union directives. In accordance with this act, the legislator has adopted several ordinances, decrees, and administrative orders that establish:

- Limit values for pollutants in ambient air and emissions from stationary sources;
- Methods for sampling and measurement of air pollutants both in ambient air and in waste gases;
- Procedures for monitoring and reporting, in line with EU requirements for air quality assessment and management;
- Measures to ensure compliance with air quality standards and to safeguard public health and the environment.

These legal instruments collectively aim to ensure the effective implementation of air quality policies, consistent with the principles of sustainable development and the precautionary approach enshrined in EU environmental law.

The content of nitrogen dioxide and particulate matter in the ambient air is regulated by Ordinance No. 12 of 15 July 2010 on the norms for sulfur dioxide, nitrogen dioxide, particulate matter, lead, benzene, carbon monoxide, and ozone in the ambient air. In Annex No. 1, Table 2 of the Ordinance, the annual limit values (ALVs) are stipulated as 40 µg $m^{-3}$ for $NO_2$ and $PM_{10}$, and 20 µg $m^{-3}$for $PM_{2.5}$. An hourly limit value (HLV) of 200 µg $m^{-3}$is also set for nitrogen dioxide, while the short-term norm for particles with a diameter up to 10 µm is a 24 h limit value (24hLV) of 50 µg $m^{-3}$. It is important to note that the short-term limits are subject to the requirement that they must not be exceeded more than a specified number of times in a calendar year (the permitted number of exceedances for the $NO_2$ HLV is 18, and for $PM_{10}$, the exceedances of the 24 h LV can be up to 35). Assessing ambient air quality also requires the analysis of an additional criterion, specifically, percentile values.

### Methods and models for assessing the dispersion of pollutants in ambient air

#### *Types of mathematical models*

Air quality assessment models use mathematical and numerical techniques to simulate the physical and chemical processes that affect air pollutants as they disperse and react in the atmosphere [3].

Based on input meteorological data and output data such as the pollutant emission and stack height, these models are designed to characterize primary pollutants, which are released directly into the atmosphere, and in some cases, secondary pollutants, which are formed because of complex chemical reactions in the atmosphere. These models are important for air quality management systems because they are widely used by regulatory bodies, both to identify the source's contribution to air quality problems and to assist in developing effective strategies for reducing air pollutants [3].

Air quality assessment (AQA) models play a crucial role in Air Quality Management (AQA), aiding in planning, permitting new emission sources, and evaluating regulatory programs. These models are validated and controlled against monitoring data [3].

Models are categorized into three main groups:

### ***Dispersion models***

Dispersion models are the most frequently used, especially for applications like IPPC permits and EIAs, to assess pollutant concentrations in the surface atmospheric layer near a source.

#### *Gaussian Plume Model (GPM)*

This is the most widespread dispersion model. It's based on the assumption that pollutant concentration follows a normal (Gaussian) distribution perpendicular to the wind direction [4].

The ground-level concentration C(x,y) from a point source is given by Eq. (1):

$$C(x,y) = \frac{Q}{\pi U \sigma_y \sigma_z}\left(e^{-\frac{y^2}{2\sigma_y^2}} e^{-\frac{H^2}{2\sigma_z^2}}\right) \tag{1}$$

where Q is the emission rate, H is the effective stack height (the actual height plus plume rise Delta), U is the wind speed and $\sigma_y$ and $\sigma_z$ are dispersion coefficients.

GPMs are primarily used for Local Scale problems (scope < 1 km) and Open Roads (or Open areas), often in combination with a parameterized meteorological model [4].

#### *Lagrangian Particle Models*

Lagrangian models, or Particle Tracking models, track the movement of individual pollutant particles. They account for advection, diffusive transport, and radioactive decay [5].

- Advection (Transport): The particle's new spatial location $r(t+\Delta t)$ is determined using the flow's velocity vector $q(t)$.
- Diffusion Transport: The horizontal ($D_h$) and vertical ($D_v$) steps are calculated using the horizontal ($K_h$) and vertical ($K_v$) diffusion coefficients and a random number (RAN).
- Radioactive Decay: The change in concentration over time is proportional to the concentration itself, defined by the decay constant λ, Eq. (2):

$$\frac{\partial C}{\partial t} = -\lambda C \tag{2}$$

where λ is the radioactive decay constant.

These models are applicable to Open Roads and Street Canyons [5].

#### *Eulerian Models*

Eulerian models (or Grid Models) solve fluid motion equations over a fixed spatial grid. They are based on Euler's Equations for the Motion of an Ideal Fluid, Eq. (3) [6]:

$$\rho \frac{du}{dt} = \rho \cdot X - \frac{\partial p}{\partial x} \tag{3}$$

where ρ is density, $\frac{du}{dt}$ is acceleration, $\rho \cdot X$ is the mass force, $\frac{\partial p}{\partial x}$ is the pressure gradient.

Applicability and Comparison:

Models accounting for obstacles are applicable for Street Canyons but involve expensive calculations. They are generally computationally infeasible for the Urban Scale and Regional Scale.

Models accounting for terrain have low resolution and require prolonged calculation for Open Roads.

There are some other model types such as

Photochemical Models and Receptor Models.

Photochemical Models are used in environmental policy development to simulate the impact of all sources, assessing concentrations and deposition of both inert and chemically reactive pollutants over large spatial scales.

Receptor Models use observation techniques that quantify source contributions to pollutant concentrations at receptors by analysing the chemical and physical characteristics of pollutants measured at both the source and the receptor [7].

### Software packages for modelling the dispersion of pollutants in ambient air

The PLUME package is based on the Gaussian equation and adheres to the established methodology in Bulgaria for calculating pollutant dispersion from stationary sources. It is used to calculate surface layer concentrations, determine the necessary effective stack height to meet air quality standards, and ascertain maximum pollution from existing sources. However, its application, like the Gaussian model itself, is associated with limitations such as the assumption of constant emission parameters, constant wind speed, no pollutant decay or deposition, and flat, open terrain [8, 9].

Traffic ORACLE is designed to model emissions and dispersion from motor vehicles (approximated as line or area sources) moving on roads and street networks. It has two main modules: EMISSIONS, which calculates emissions using simplified or detailed (EMEP/CORINAIR-based) approaches, and DIFFUSION, which is based on a Gaussian plume model. The DIFFUSION module calculates expected instantaneous, climatologically averaged, period-averaged, and maximum single-event concentrations. Its limitations are like those of the base Gaussian model, assuming constant emissions, constant wind speed, no decay/reactions, and flat terrain [10].

The Breeze AERMOD/ISC system is the preferred dispersion model of the US EPA and is also a Gaussian model. It uses a variety of modifications to account for complex sources, terrain relief, and wind flow around buildings. The package can model pollution from an unlimited number of sources, including point, area, volume, open flare, and a specialized Roadway source type for traffic. It requires detailed input on source load non-uniformity (hourly, weekly, monthly, etc.) and, for particle deposition assessment, requires data on average particle diameter, mass fraction, density, precipitation, and air humidity. Due to its rich capabilities and user interface, it is suitable for Air Quality Assessment tasks, including EIA Reports and Integrated Permits [11 - 14].

Table 1 compares the capabilities of the software packages PLUME and Breeze AERMOD.

## EXPERIMENTAL

### Comparative analysis of the results from modelling the dispersion of pollutants from multiple sources using different approaches and various software

The experiment involves the sequential calculation of average annual pollutant concentrations generated by all sources located in the Industrial Zone in the town of Devnya. This is done using different approaches with the PLUME model, as well as through modelling with Breeze AERMOD.

Since the computer package PLUME, among its other drawbacks (a 16-bit program), can only operate with up to 10 sources, an instruction (unofficial) from the Ministry of Environment and Water (MEW), titled Creation of Virtual Devices (VD) for the purpose of mathematical modelling with the software product PLUME in cases of more than 10 emission sources at a given site, which must be included in the model, recommends that all sources be merged into virtual sources according to the following

Table 1.Summary of model capabilities.

| Software | Plume | Breeze AERMOD |
|---|---|---|
| Meteorology | Wind in one direction, a discrete 8-rhumb wind rose, and an hourly meteorological file containing date, wind speed and direction, temperature, and cloud cover; it works with the Pasquill atmospheric stability classification | Hourly meteorological data containing 26 columns, including temperature, air humidity, wind speed and direction, precipitation, and others; instead of the Pasquill classification, it works with the mixing layer height |
| Terrain | It assumes the area is flat and open; it does not work with terrain data | It works with terrain data in .NED and .DEM formats in all resolutions |
| Source types | Works with only point souces | It works with point sources (including capped and horizontal); area sources (including polygonal); open pit; volume; flare; roadway; line, and buoyant line sources |
| Averaging periods | Depending on the selected meteorology - hourly average and annual average | 1h, 2h, 3h, 4h, 6h, 8h, 12h, 24h, month and annual |
| Results and data export | Only records the results and input parameters in a text file (.DAT) | Plot files, post or percentile files, tabular data with maximum values, sensitive receptor summary, as well as a complete list of all input and output files |
| Coordinate systems | It only works with relative coordinates | Geographical, UTM, WGS84 |

algorithm:

The Virtual Emission device (VED) in question includes all existing emission sources on the site that emit a specific pollutant into the ambient air (e.g., sulfur dioxide, nitrogen oxides, etc.) and must be included in the modeling. The parameters of the VES are determined using the following formulas:

1. Height of the VED that is created for the purposes of the modelling, Eq. (4) - h [m]:

$$h = \frac{h_1V_1 + h_2V_2 + \ldots + h_nV_n}{\sum_{i=1}^{n} Vi} \quad (4)$$

where $h_1$, $h_2$ … $h_n$ - height of the respective existing emission sources (ES) [m];

V1, V2 … Vn - flow rate of the discharged gases from the respective existing ES [Nm $s^{-1}$].

2. Physical velocity of the discharged gases from each existing, ES Eq. (5), Si [m $s^{-1}$]:

$$S_I = \frac{V_i}{F_i} \quad (5)$$

where $V_i$ - Flow rate of the discharged gases from the respective existing ES [$Nm^3$ $s^{-1}$]; $F_i$ - area of the cross-sections of the respective existing ES [$m^2$].

3. Average velocity of the discharged gases from the VES, Eq. (6), S [m $s^{-1}$]:

$$S = \frac{S_1V_1 + S_2V_2 + \cdots + S_nV_n}{\sum_{i=1}^{n} Vi} \quad (6)$$

4. Cross-section area of the VED, Eq. (7) - F [m$^2$]:

$$F = \frac{V_1 + V_2 + \cdots + V_n}{S} \tag{7}$$

5. Average temperature of the discharged gases from the VED, Eq. (8) - T [°C]:

$$T = \frac{T_1 V_1 + T_2 V_2 + \cdots + T_n V_n}{\sum_{i=1}^{n} Vi} \tag{8}$$

where $T_1$, $T_2$ ... $Tn$ - temperature of the discharged gases from the respective existing ES [°C]; Vi - flow rate of the discharged gases from the respective existing ES [Nm$^3$ s$^{-1}$];

6. Flow rate of the discharged gases from the VED, Eq. (9) - V [Nm$^3$ s$^{-1}$]:

$$V = V_1 + V_2 + \cdots + V_n \tag{9}$$

where $V_1$, $V_2$ ... $Vn$ - flow rate of the discharged gases from the respective existing ES [Nm$^3$ s$^{-1}$].

To facilitate the modelling process, the center of gravity of the site, based on the flow rate and height of the existing ES (Emission Sources), is not sought. Instead, the VED (Virtual Emission Device) is placed at the location of the existing emission source with the largest flow rate.

As can be seen from the instruction proposed by the MEW (Ministry of Environment and Water), some guidelines contradict the "Methodology for calculating the height of emission sources, dispersion, and expected concentrations of polluting substances in the ground layer," with the most significant contradictions being:

- First, it must be noted that it is permissible for groups of sources with identical or similar characteristics, located immediately next to each other (such as groups of ventilation pipes often are), to be represented without loss of information or computational accuracy in the form of a single common (virtual) source. Here, however, the issue is the merging of all sources on a single site, which in most cases would lead to a severe distortion of the results, if only because of the loss of their mutual spatial arrangement;
- The algorithm, based on the Gaussian model for calculating ground-level pollutant concentrations, works by using the exit velocity of the exhaust gases, which is, however, obtained by dividing the user-provided flow rate by the cross-section of the ES (Emission Source). This is an internal procedure in PLUME and means that if the flow rates are specified at normal conditions, the gas velocity used for the calculations will only be correct at a gas temperature of 0°C. Obviously, if not impossible, this is an extremely unlikely event.
- The calculation of the equivalent diameter of the VED (Virtual Emission Device) should be done in a way that ensures an equivalent exit velocity of the discharged gases. A formula for this could be: $d_e = \sqrt{4 \sum S_i / 3.14}$, However, the proposed method results in smaller equivalent diameters, which leads to higher exit velocities.

In addition to everything said so far, it should be noted that the representation of source groups as a single one (VED - Virtual Emission Device) is only necessary when the third branch of the program is used, since there is no recording of intermediate information in that branch and it is impossible to apply the superposition principle. In the assessment of pollutant concentrations in the ground layer of the atmosphere (the first branch of the program), this is not necessary, as the product records the calculated concentration value at every point of the computational grid in the form of an x, y, z record in a file with the DAT extension. This way, the user has the opportunity, by running the procedure multiple times, to calculate the concentrations in the study area from separate groups of sources (up to 10 sources), and then to sum them up into a total text record using the SUPERPOSITION concentration summator, which is a module of the Traffic ORACLE package. Given that the internal procedure of PLUME is practically the same action, it can undoubtedly be concluded that this method will yield identical results to the original methodology without introducing additional error.

As mentioned above, the use of the PLUME package is associated with several approximations and limitations. However, it is essentially a screening model, and its application for certain procedures (such as the issuance of Integrated Pollution Prevention and Control (IPPC) permits, some preliminary assessments) is not without purpose due to its simplicity and accessibility.

The study used data for all sources of $PM_{10}$ and NOx located on the territory of the Industrial Zone of the town of Devnya. The total number of sources is 176 for $PM_{10}$ and 13 for NOx, distributed across a total of 7 industrial enterprises with Integrated Pollution Prevention and Control (IPPC) permit. The initial data contain the following for each point source: geographic coordinates, stack height from ground level (m), diameter of the clear opening of the emission source (m), temperature of the exhaust gases (°C), flow rate of the outgoing gases ($m^3$ $s^{-1}$), and Limits for Permissible Emissions of the studied pollutants ($Nm^3$ $s^{-1}$).The flow rates are standardized at normal conditions (273K and 101.325 kPa).

The large number of sources necessitates the use of one of the possible procedures for assessing ground-level pollutant concentrations for sites with over 10 sources using PLUME. Because of this fact, the question here is to what extent the proposed procedure by the Ministry of Environment and Water (MEW) for the creation of Virtual Emission Devices (VEDs) is adequate and to what extent it deviates from the approved methodology of the same ministry.

For this purpose, an approach was chosen using a comparative analysis of the modeling results obtained with VEDs (Virtual Emission Devices) and by the principle of superposition, using the same input parameters. Additionally, these results will be compared with the results from modelling the pollutant dispersion, generated by the same sources, using Breeze AERMOD.

## Dispersion modelling of pollutants from sources on the territory of the Devnya Industrial Zone with PLUME, using the VEDs (Virtual Emission Devices) according to the MEW's instructions

### *Model input parameters*

An area was created with a discretization of NX=50, NY=50 and a step size of 200 m (length of each grid cell) in both directions, thus resulting in area dimensions of 10x10 km. The underlying surface is a rural area, and the ambient air temperature, when using the Wind Rose, is 15°C. The Wind Rose was constructed using data from MS Suvorovo (Fig. 1), the Climatic Reference Book of Bulgaria, Volume 4, Wind.

The parameters of the emission sources for the purposes of modelling, calculated according to the MEW's instructions, are presented in Tables No. 2 and No. 3. One VED (Virtual Emission Device) was created for each industrial operator for each of the pollutants, and it is located at the site of the source with the highest flow rate within the industrial site.

### *Results from the model*

*Annual mean concentration for NOx and $PM_{10}$*

The maximum value of the annual average concentration of NOx when using VEDs is 5.84 $\mu g\ m^{-3}$ and is obtained at 3630 m from the last source. Fig. 2 presents the distribution of the NOx Annual mean concentration values in this case, with isolines drawn in the range of 0.1 to 4.5 $\mu g\ m^{-3}$. The value is indicated on each isoline, and where this is not possible, it is determined from the colour legend. Additionally, they are combined with a map of the area.

As can be seen from the graph presented in Fig. 2, the more significant values of NOx concentration are obtained to the south and southwest of the site of KOMPLEX GALENIKA SUPER OIL KOMERS, even though this activity has no nitrogen oxide emissions and no sources included in the study. This effect of the

Table 2. Parameters of the VEDs (Virtual Emission Devices) for the purpose of modelling with PLUME for $PM_{10}$.

| Industrial site | X, m | Y, m | H, m | D, m | T, °C | Wg, m s$^{-1}$ | Flow rate, m$^3$ s$^{-1}$ | Emission, mg s$^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| Devnya Ciment JSC | 1728 | 9367 | 89.5 | 11.4 | 114.0 | 0.01 | 1767.9 | 19356.4 |
| Solvei Sodi AD | 4920 | 5077 | 146.7 | 4.9 | 112.2 | 0.01 | 864.5 | 30669.4 |
| Agropolichim AD | 6977 | 5213 | 67.2 | 4.8 | 48.7 | 0.01 | 494.0 | 9486.1 |
| Agro Plant Invest LTD | 3284 | 6607 | 16.6 | 0.9 | 183.9 | 0.01 | 10.5 | 937.4 |
| Aliphos Bulgaria EAD | 7119 | 5164 | 18.9 | 1.3 | 71.7 | 0.01 | 13.4 | 820.2 |
| EcoSafe LTD | 2987 | 7037 | 12.0 | 0.2 | 281.0 | 0.01 | 0.9 | 4.3 |

Table 3. Parameters of the VEDs for the purpose of modelling with PLUME for NOx.

| Industrial site | X, m | Y, m | H, m | D, m | T, °C | Wg, m s$^{-1}$ | Flow rate, m$^{-3}$ s$^{-1}$ | Emission, mg s$^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| Agropolichim AD | 7031 | 5336 | 80.3 | 3.5 | 90 | 0 | 209.0 | 58229.2 |
| Solvei Sodi AD | 4920 | 5077 | 182.5 | 3.9 | 135 | 0 | 685.0 | 314583.3 |
| Agro Plant Invest LTD | 3284 | 6607 | 18.0 | 0.7 | 207 | 0 | 9.6 | 3553.0 |
| EcoSafe LTD | 2987 | 7037 | 12.0 | 0.2 | 281 | 0 | 0.88 | 86.7 |
| Plastchim-T AD | 3808 | 5526 | 14.0 | 0.7 | 204 | 0 | 1.5 | 213.8 |
| Devnya Ciment JSC | 1728 | 9367 | 148.2 | 8.9 | 170 | 0 | 988.8 | 422541.7 |

displacement of the isolines is due to the mutual arrangement of the virtual emission devices and the loss of the mutual spatial arrangement of the individual sources of the pollutants. The areas enclosed by the red isoline will be with a concentration of 4.5 to 5.84 µg m$^{-3}$ and are located entirely outside residential areas. With this approach, even the maximum calculated concentration represents only 14.6 % of the average annual limit.

Fig. 3 presents the distribution of the values for the Annual mean concentration of $PM_{10}$, with the graph constructed analogously to the one in Fig. 2. Here, the formation of two groups of isolines is observed, which suggests a predominant contribution from Devnya Cement AD's VED (the northwestern group of isolines) and the VED of the Agropolychim JSC site. The areas enclosed by the red isoline will be with a concentration of 1.5 to 2.37 µg m$^{-3}$ and are located entirely outside residential areas. The isolines formed by Agropolychim AD's VED occur with a northeastern wind and are located at Port Varna . With this approach, even the maximum calculated concentration represents only 5.925 % of the average annual limit.

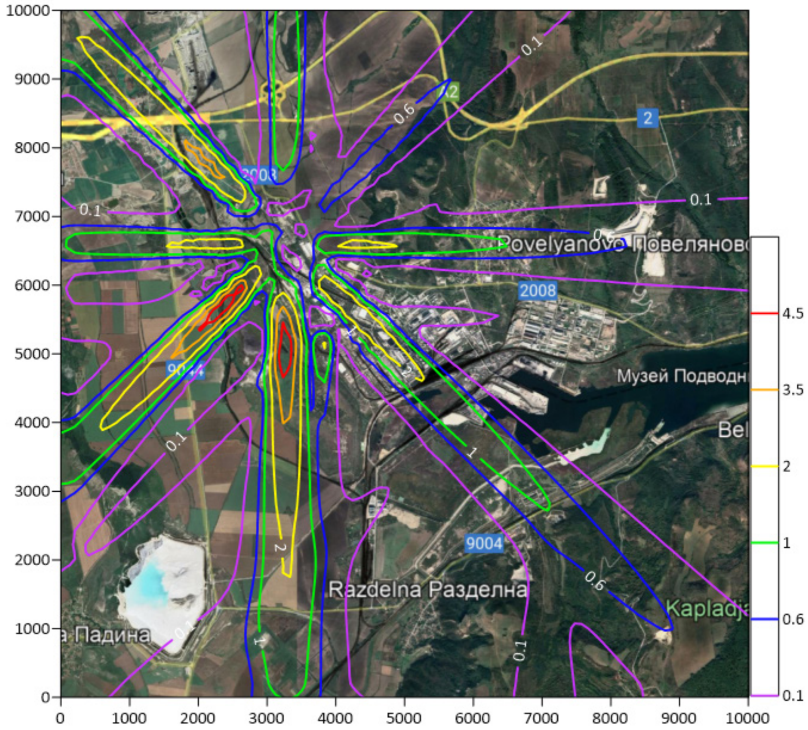

Fig. 2. Isolines of the Annual mean concentration of Nox in the surface layer of the atmosphere when using VED, μg m$^{-3}$.

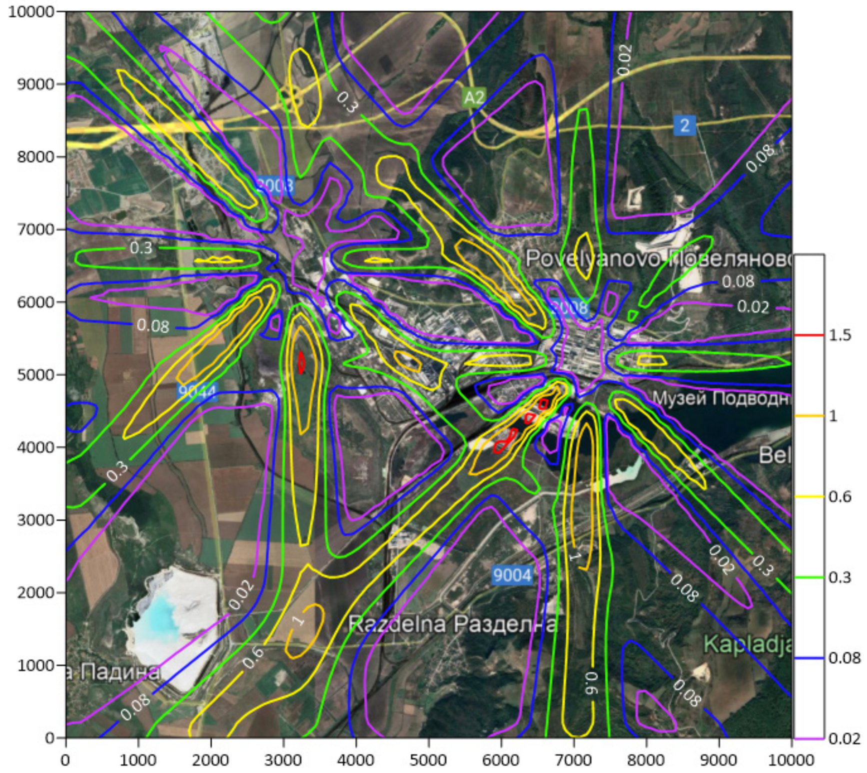

Fig. 3. Isolines of the Annual mean concentration of $PM_{10}$ in the surface level of the atmosphere when using VED, μg m$^{-3}$.

### Dispersion modeling of pollutants from Sources within the Devnya Industrial Zone using the PLUME software, based on the Principle of Superposition

Here are presented the results of simulating the dispersion of pollutants with the same software product-PLUME-but using the SUPERPOSITION module from the TrafficORACLE package, as a summing function of the concentrations obtained from the sequential execution of the procedure "Expected concentrations of harmful substances in the surface layer" for series of groups with up to 10 sources of $PM_{10}$ and NOx.

This is not necessary for the emission sources of the other pollutants covered in the study, since their number is less than 10.

It must be noted that with this approach, the mutual arrangement of the sources is preserved, and the algorithm of the "Methodology for calculating the height of emission devices, dispersion, and expected concentrations of polluting substances in the surface layer" is also not violated. In other words, PLUME uses an internal procedure where the surface concentrations of the pollutant emitted by the first source are calculated, a temporary concentration field is saved, and then the procedure is repeated for the second source, its concentration field is summed with the previous one, and the cycle concludes with the last source entered. Since the number of sources is limited to 10, it is obvious that if intermediate .DAT files with the results from the first, second, etc., groups of sources are saved, and then summed based on the principle of superposition, this practically repeats the product's internal procedure and does not introduce an additional error in the calculations. It is sufficient to comply with the requirement for an identical size and discretization of the area.

18 groups for $PM_{10}$ and two groups of sources for NOx were created, with each source preserving its relative coordinates, therefore not violating the principle of superposition, along with all its other parameters.

The results of the modelling using the described approach for $PM_{10}$ and NOx are presented in Figs. 4 and 5, where, for the purposes of comparative analysis, the study area and the meteorological conditions are the same as those in the previous approach.

#### *Annual mean concentration of the pollutants*

For these two pollutants, an annual standard has been established for the protection of human health, which is the same for both pollutants (40 $\mu g\ m^{-3}$), which is why the distribution of the Annual mean concentration of the pollutants in the surface layer of the atmosphere has been assessed. The results of this calculation are presented in Fig. 4 and Fig. 5.

The maximum value of the Annual Mean Concentration of NOx is 9.601 $\mu g\ m^{-3}$ at 4612 meters, which is well below the Annual Standard, but as can be seen from the results presented above, it is 3.761 $\mu g\ m^{-3}$ greater. At first glance, this does not represent a particularly large difference, but considering that it represents about a 40 % increase, the error when using virtual sources becomes significant, since this is not an error inherent to the model, but an additional one to its other deficiencies.

What has been stated so far refers to the maximum value of the Annual Mean Concentration, its location and the distribution of the remaining concentration values within the study area are a separate issue. Upon comparing the graphs presented in Fig. 2 and 4, the maximum calculated concentration value occurs at a fundamentally different location, and the areas under the influence of the pollutant at a significant concentration are also quite different in size. For instance, those areas using Virtual Sources, which are enclosed by the isoline with a value of 4.5 $\mu g\ m^{-3}$ are situated over an area of no more than 0.06 $km^2$. In contrast, when using the Superposition Method, the total area of the study domain impacted by Nitrogen Oxides at a concentration of 4.5 $\mu g\ m^{-3}$ amounts to 4.76

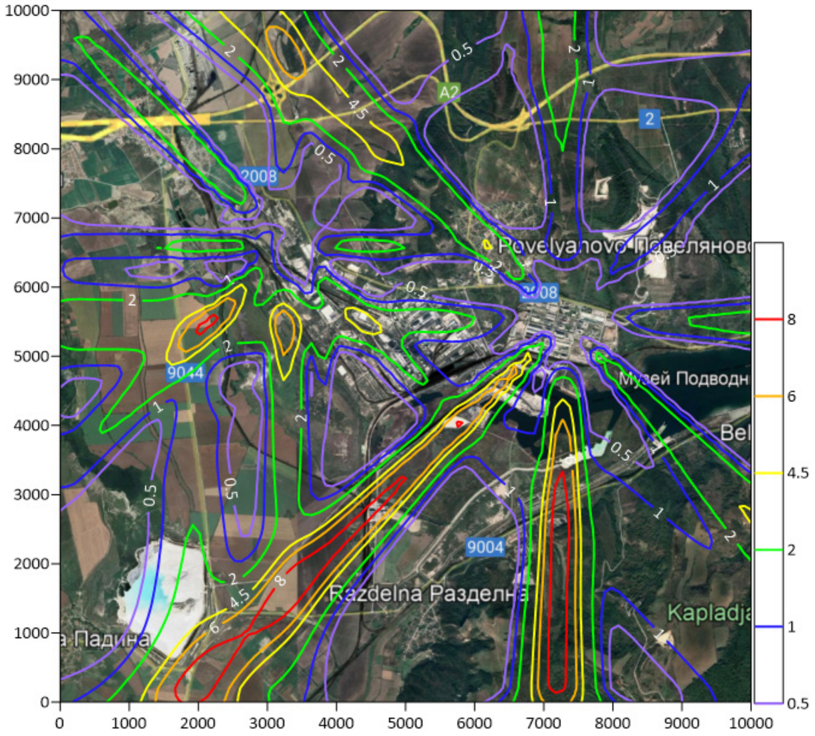

Fig. 4. Isolines of the annual mean concentration of NOx in the ground layer of the atmosphere using the Superposition principle, µg m$^{-3}$.

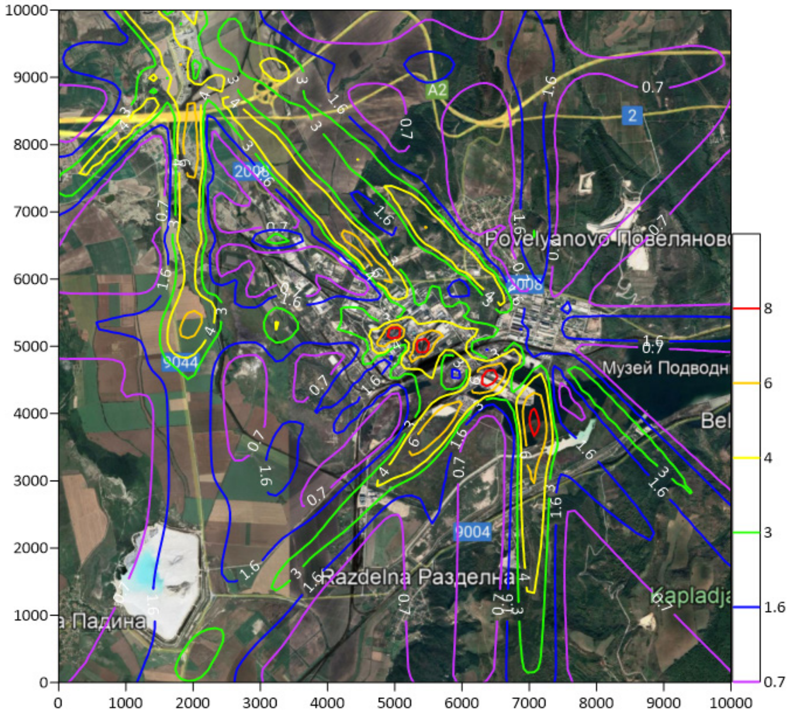

Fig. 5. Isolines of the annual mean concentration of PM$_{10}$ in the ground layer of the atmosphere using the Superposition principle, µg m$^{-3}$.

km$^2$, and this includes residential areas. It is undeniably clear that the use of Virtual Sources according to the Ministry of Environment and Water instruction leads to the underestimation of both the maximum concentration value of the pollutant and impact area of the sources, with the error in the latter being truly enormous.

The other pollutant whose sources exceed 10 in number within the study area is $PM_{10}$, for which the differences when using the two approaches are even greater. This is due, on the one hand, to the much larger number of individual pollutant sources, and on the other, to the type of pollutant - namely, its rate of gravitational deposition.

From the analysis of the results presented in Fig. 3 and Fig. 5, it is clearly visible that:

- When using Virtual Sources (Fig. 3), two distinct groups of isolines are formed, characterized by the location of the two VEDs with the largest emission and flow rate, meaning the cumulative effect is severely underestimated.
- When comparing the areas enclosed by isolines with values of 1.5 µg m$^{-3}$ (the red isoline in Fig. 3) and 1.6 µg m$^{-3}$ (the blue isopleth in Fig. 5), it's clearly seen that the scope of impact area of the sources represented as VEDs is severely underestimated. For example, the village of Razdelna falls under the influence of $PM_{10}$ at a concentration ranging from 0.4 µg m$^{-3}$ up to 1.2 µg m$^{-3}$, as assessed by the Superposition Method, while when using the VED approach, this influence is estimated to be below 0.02 µg m$^{-3}$ (the purple isoline).
- Over the Poveliyanovo Quarter, the influence of $PM_{10}$ is estimated to be below 0.3 µg m$^{-3}$ when using VEDs, whereas with the Superposition Method, the concentration variation range will be up to 1.6 µg m$^{-3}$.
- The maximum value of the calculated Annual Mean Concentration is 2.36 µg m$^{-3}$ when using VEDs, and 13.09 µg m$^{-3}$when using the Superposition Method.

The use of Virtual Sources according to the MEW instruction significantly underestimates not only the maximum value of the calculated Annual Mean Concentration, but also the size of the areas under the influence of the pollutants at a given concentration. The cumulative effect is also heavily underestimated when using VEDs. It must be noted here that the flow rates under real conditions were used for the VEDs, and despite this, there is a substantial increase in the model error.

## Dispersion modelling of pollutants from sources within the Devnya Industrial Zone using Breeze AERMOD

### *Model input parameters*

An area of the same size as in the previous sections has been defined, along with a computational grid of 51 × 51 receptors in the X and Y directions, respectively, distributed in a uniform Cartesian coordinate system. The distances between them are 200 meters, totalling 2 601 receptors at a height of 2 m above ground level. Breeze AERMOD works with both relative and geographic coordinates; for the purposes of the study, the Universal Transverse Mercator (UTM) coordinate system, specifically WGS84 UTM Zone 35, was used

Since the system has the capability to include various procedures for evaluating the conversion of NOx to $NO_2$, the Ozone Limiting Method (OLM) was chosen in this case for the assessment of the Ground-Level Concentrations of $NO_2$. This method uses the average annual background concentration of ozone, measured at the KFS Rozhen monitoring station for 2017, which was 48 µg m$^{-3}$.

The capabilities of the system were used to simultaneously (with a single product run) record files containing the calculated values for the maximum 1 h Average, the 24 h Average, as well as the values for the Annual Mean Concentration for each receptor. These are the so-called "Plot Files." In addition to these, the results of the calculations for every point in the computational grid for every h (or 24 h period) of the year were also saved in the form of "Post Files."

### *Meteorological conditions*

In addition, terrain data for the domain were also used, in the form of a .DEM file, even though it is relatively flat. It must be noted here that the terrain is one of the main climate-forming factors, having the least influence on the obtained results when modelling flat areas like the current one.

### *Source parameters*

As mentioned above, since the product operates with UTM coordinates, the geographic coordinates of the sources in the same system were used, and instead of flow rate, the velocity of the exhaust gases calculated according to:

$$v_s = \frac{4V}{\pi d^2} \qquad (10)$$

Additionally, the sources are grouped to determine the contribution of the individual industrial facilities to both the maximum annual average or hourly average concentration and the concentration (annual average or hourly average) at selected points within the studied area.

Fig. 7 and Fig. 8 present the isolines of the Annual Average Concentration of NOx and $PM_{10}$ obtained with Breeze AERMOD

## RESULTS AND DISCUSSION

The comparison of the modelling results will be performed only between the two models, as the air quality indicators are measured only at the "Devnya - Izvorite" station, which is located in proximity to the Hemus Highway (AM Hemus) and about 4 km from the Devnya Industrial Zone.

At this monitoring point, the concentration of $NO_2$ is mainly formed by the influence of traffic on the highway. Its classification is an urban background station, which means its range is 2 km.

From what has been stated, it follows that a direct comparison of the concentrations at the measurement point would not be correct without considering the other sources that contribute to the concentration of $NO_2$ and $PM_{10}$.

The measured annual mean concentration of $NO_2$ at the station in 2017 was 13.04 µg m$^{-3}$ and the maximum for the period 2015 - 2019 was measured in 2016 and was 22.11 µg m$^{-3}$.

The maximum calculated annual average

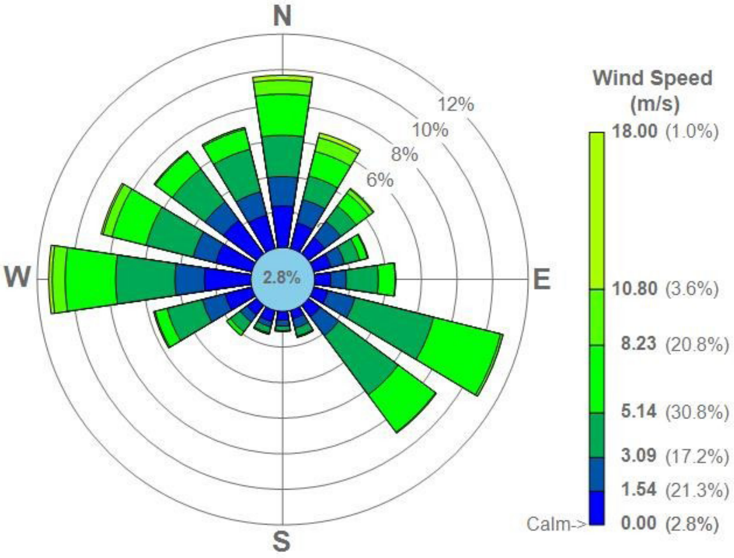

Fig. 6. Wind rose, MS Varna 2017.

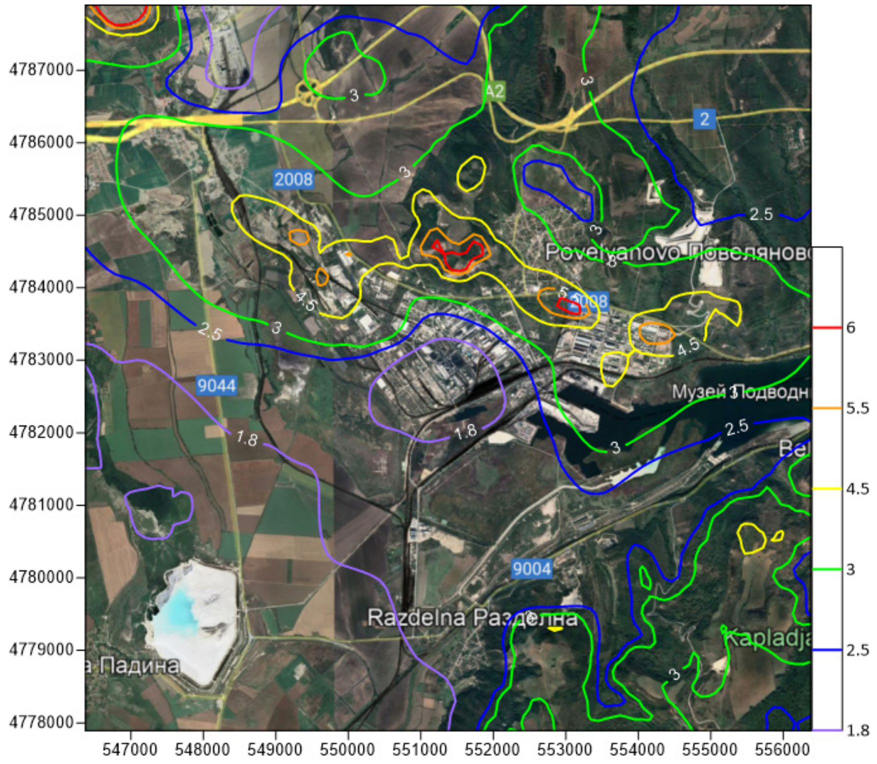

Fig. 7. Isolines of the annual average concentration of NOx obtained using Breeze AERMOD, µg m$^{-3}$.

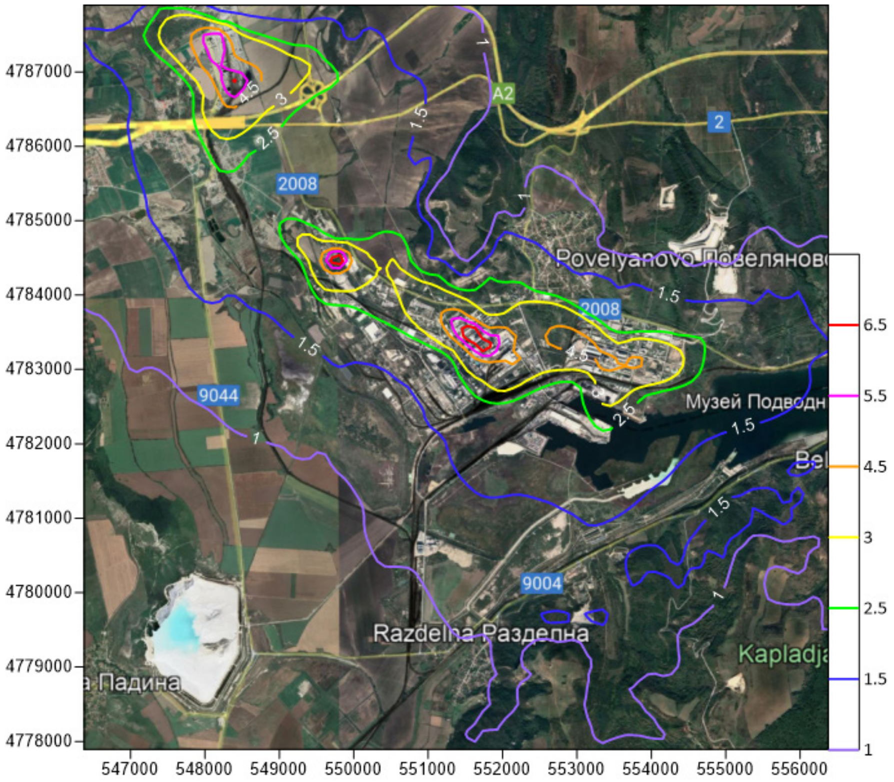

Fig. 8. Isolines of the annual average concentration of $PM_{10}$ obtained by using Breeze AERMOD, µg m$^{-3}$.

concentration $NO_2$ from all sources amounts to 8.01 µg $m^{-3}$ and occurs on the northern boundary of the area, at a distance of 1.3 km northwest of the industrial site of Devnya Cement JSC. Although the maximum Annual Average Concentration values calculated by PLUME (based on the superposition principle) and Breeze AERMOD are very close, a comparison of Fig. 4 and Fig. 7 shows that the distributions of the remaining values of the annual average concentration obtained by the two software packages are quite different.

It should be noted here that this is partly since a discrete wind rose was used for the annual average concentration assessment with PLUME, and the Breeze AERMOD package has the capability to input hourly meteorological data via a pre-prepared .MET file. The characteristic "feather-like" distribution of the isolines is due to the type of meteorological data used in PLUME. For the same reason, the highly simplified algorithm for distributing the pollutant emission in a specific direction causes the overestimation effect of the concentration in certain areas compared to Breeze AERMOD.

For example, the village of Razdelna is under the influence of $NO_2$ at a concentration in the range of 1.8 µg $m^{-3}$ to 2.5 µg $m^{-3}$, as assessed with Breeze AERMOD, whereas for the same assessment using PLUME, the NOx concentration above the village of Razdelna will not exceed 0.05 µg $m^{-3}$. This effect is consistently observed when using a discrete wind rose in PLUME (the most common use case for the product), or in other words, there are areas with overestimated concentration inside the "feathers" and areas with a severely underestimated, nearly zero concentration between them. This is especially important when assessing the contributions of a given industrial facility or sector of human activity, since the results obtained with PLUME overestimate the extent of the impact of the sources.

For example, again comparing the two figures, it is clearly visible that in the Hemus Motorway interchange (the so-called "cloverleaf"), the industrial contribution to air pollution by NOx calculated with PLUME will amount to 6 to 8 µg $m^{-3}$, over an area of about 0.5 km. This contribution calculated with Breeze AERMOD is between 3 to 4.5 µg $m^{-3}$, over an area of about 1 $km^2$. This comparison is important because the other main NOx source is transportation.

The other main difference is due to PLUME's inability to account for the influence of terrain. When comparing the two graphics, this characteristic is most pronounced in Povelyanovo neighborhood, as this neighborhood is situated on a hill. As seen in Fig. 4, the group of isolines originating from the industrial site of Agropolychim JSC in the direction northwest of the facility passes over Povelyanovo neighborhood, which could not correspond to reality, as it has a higher elevation - around 90 m and in this situation, only the highest NOx sources at the Agropolychim JSC industrial site could provide any contribution to that location. Accounting for the influence of terrain is clearly visible in the results obtained with Breeze AERMOD around the same neighborhood.

Analogous conclusions regarding the distribution of the Annual Average Concentration ($PM_{10}$) values obtained through PLUME and Breeze AERMOD can be drawn from the comparison of the results presented in Fig. 5 and Fig. 8.

**Short-term concentration assessment**

The case with the assessments of short-term values of pollutant concentrations calculated with the two software packages is more interesting. Firstly, it should be noted that PLUME cannot be used to calculate 24 h average pollutant concentrations. The procedure for assessing the maximum hourly average concentration values is labor-intensive and severely limited, introducing additional error. It consists of the following steps:

1. The "Maximum Background Pollution"

module is launched with the purpose of assessing the most unfavourable meteorological conditions. This module does not save intermediate or other types of results in file format, which is why, for a larger number of sources (more than 10), the use of Visual Sources is required, which introduces inaccuracies.

2. The "Expected Concentrations in the Atmospheric Surface Layer" module is launched (by selecting the "Single Wind Direction" option from the Meteorology menu). This module is executed as many times as there are superposition groups for a single wind direction. The entire procedure is repeated for the next selected wind direction to assess the distribution of the Hourly Average Concentration (HAC) values with wind blowing toward every settlement (residential area) in the area.
3. The resulting superposition.DAT files for each settlement are merged into one overall grid using Golden Software Surfer, while adhering to the maximum principle. Only then can the isolines of the pollutant's HAC be plotted.

As can be seen from the description of the procedure, in addition to the fact that the Gaussian model in PLUME uses discrete stability classes when assessing the Hourly Average Concentration (HAC) of pollutants, there is a probability of introducing additional user error.

Breeze AERMOD maintains complete documentation of the input data entered by the user, as well as all model settings, and a numerical record of all results obtained. Furthermore, all types of averaging periods are generated with a single calculation, and the initial input file becomes editable for subsequent additions, revisions, and analyses. This means that pollutant dispersion modelling, as well as air quality assessment through such modelling, are easily traceable, which is essential for regulatory agencies.

**Contribution assessment**

The ability of the software package (Breeze AERMOD) to group the sources offers the researcher the opportunity to perform additional assessments, the most useful of which is the determination of contributions to the pollutant concentration at a given receptor location. For example, Fig. 9 and Fig. 10 present the contributions of the individual industrial facilities to the maximum Annual Average Concentration (AAC) values of NOx and $PM_{10}$ respectively.

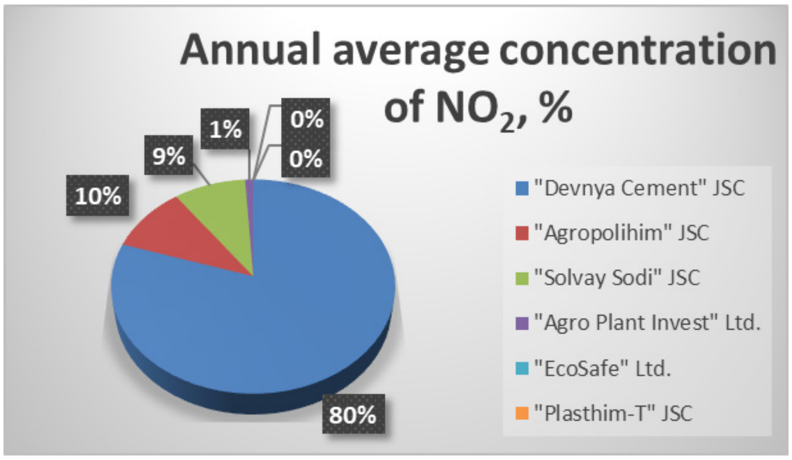

Fig. 9. Contributions of individual industrial facilities to the maximum annual average concentration of $NO_2$, %.

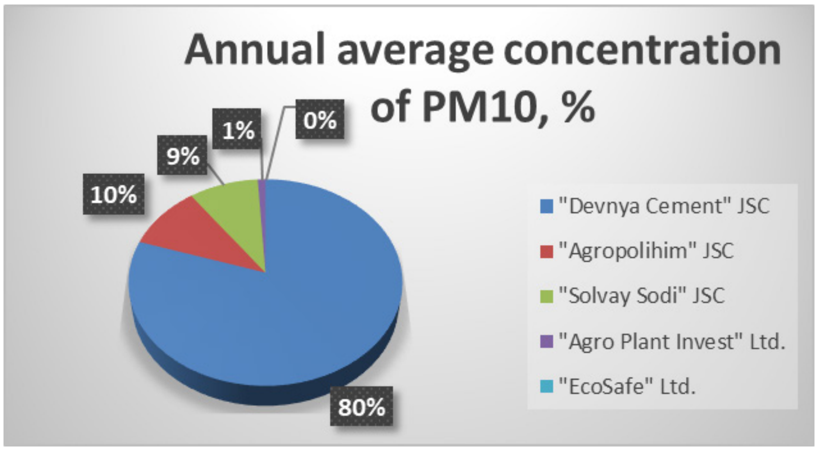

Fig. 10. Contribution of the individual industrial facilities to the maximum annual average concentration of $PM_{10}$, %.

### Flawed methodology for multiple sources (VED)

The study found that it is often necessary to assess pollutant dispersion generated by more than 10 sources using the PLUME software package. In such cases, based on the recommendation of the Ministry of Environment and Water (MEW), an unofficial instruction for creating so-called VED (Virtual emission devices) is used. Since this instruction constitutes a list of formulas and actions for merging (grouping) an undefined number of sources, and not a complete methodology, the frequent application of the "all-in-one" principle inevitably leads to the introduction of additional errors into the already inaccurate assessment resulting from the limitations of the model upon which the PLUME software is based. A comparative analysis was made of the results from applying the methodology for multiple sources using two approaches with the PLUME software package and those obtained with the significantly more precise Breeze AERMOD software.

## CONCLUSIONS

As a result of the analysis, it can be concluded that:

Certain directives in the MEW (Ministry of Environment and Water) instruction contradict the "Methodology for Calculating the Height of Emission Devices, Dispersion, and Expected Concentrations of Pollutants in the Surface Layer," with the most significant contradictions being:

- Merging all sources on a single industrial site would lead to a severe distortion of results, if only due to the loss of their spatial arrangement relative to one another.
- According to the MEW instruction, the flow rate of the VED (Virtual emission devices) is defined under Normal Conditions ($Nm^3 s^{-1}$) which is a gross error, since PLUME operates using the flue gas velocity without temperature conversion.
- The calculation of the equivalent diameter of the VED should ideally be performed in a way that ensures equivalent exhaust gas velocity. The proposed method yields smaller equivalent diameters, which leads to higher exhaust velocities.

The instruction does not define in which cases or for which types of assessments the VED should be used. Consequently, users employ it for both types of concentration assessment - annual average and hourly average as well as in the third program module - Maximum Background

Pollution - even though the use of the VED is only necessary for the program's third module.

The analysis of the results obtained using the VED and the superposition principle leads to the conclusion that the use of the VED according to the MEW instruction significantly underestimates not only the maximum calculated Annual Average Concentration (AAC) value but also the magnitude of the areas influenced by the pollutants at a given concentration.

The cumulative effect is also heavily underestimated when using the VED. It should be noted here that the flow rates under actual conditions were used for the VED, and despite this, there is a significant increase in the model error.

Although the selected area has flat terrain, and the "Methodology for Calculating the Height of Emission Devices, Dispersion, and Expected Concentrations of Pollutants in the Surface Layer" is applicable, the pollutant concentration results calculated with Breeze AERMOD are significantly influenced by terrain. All input parameters and the area size are identical where permissible for the PLUME and Breeze AERMOD packages.

Although PLUME and Breeze AERMOD calculate comparatively close maximum Annual Average Concentration (AAC) values for the two studied pollutants, the receptor locations where they occur are different. The areas influenced by a pollutant with a given concentration differ in both size and location, and furthermore, PLUME provides no capability for assessing the contributions of individual industrial facilities to the concentration at a given calculation point.

In conclusion, although PLUME and Breeze AERMOD calculate comparatively close maximum Annual Average Concentration (AAC) values for the two investigated pollutants, the receptor locations where they occur are different. The areas influenced by a pollutant with a given concentration differ in both magnitude and location.

Given that the PLUME software is a development from 1998, the most logical approach would be to develop a new software tool based on the same methodology, which would allow input data to be submitted via files. This would solve the issue with the limit on the number of sources. Working with the UTM coordinate system would improve data export and their analysis on mapping materials. Recording data in text files would make the entire procedure transparent and easily verifiable. On the other hand, Breeze AERMOD does not have any of the above-mentioned drawbacks, but it is a paid version. This is why both software tools would find application in different types of assessments, but the need for an update to PLUME remains undisputed.

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