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Study on the Applicability of BREEZE AERMOD Software for Nitrous Oxide Emission Modeling

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Abstract: *BREEZE AERMOD software is used worldwide for dispersion modeling of main atmospheric air pollutants – particulate matter, sulphur dioxide, nitrogen dioxide, carbon monoxide, ozone, etc. Within the present research the applicability of BREEZE AERMOD software product is studied in regards with modeling the dispersion of the greenhouse gas nitrous oxide* N_2O *in the ground atmospheric layer. A computer simulation is done studying the dispersion of* N_2O *emissions from an industrial source at a nitric acid production plant in Devnya, Bulgaria. The dispersion models are done by using validated meteorological data and by considering the topography of the source region. The hourly average* N_2O *concentration is computed in a grid of preliminary defined receptors. In order to check model adequacy, measurements of the hourly average* N_2O *concentration are done in a point that corresponds to the grid receptor with the highest hourly average* N_2O *concentration. A comparison is made between the computed and the measured highest hourly average* N_2O *concentrations in the atmospheric air. The failure rate is within the legally permissible range. Based on the comparison made between prognosis and experimental data, the adequacy of the software model is proven. BREEZE AERMOD software is applicable regarding dispersion modeling of* N_2O *emissions. The software product can be used for the purposes of quantitative assessment of atmospheric air pollution regarding emissions of the greenhouse gas* N_2O *from industrial sources.*

Keywords: *dispersion modeling, Breeze Aermod, software applicability, nitrous oxide emissions, industrial source*

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I. Introduction

Mathematical modeling is practically approbated approach for gathering reliable information on the dispersion of pollutants in the environment. The main purpose in mathematical modeling of ambient air quality is to define the effect of various pollution sources and to estimate their cumulative effect including at a long distance and in the higher layers of the atmosphere. Modeling is the only approach that can be used for predicting the concentrations of air pollutants in the ground atmospheric layers based on emission parameters and environment characteristics and for this reason it is an approved tool for ambient air quality assessment worldwide [1-9].

There are multiple software products in modeling practice that are designed for air quality assessment. These products have various options for simulating the dispersion of the main atmospheric pollutants: particulate matter, sulphur dioxide, nitrogen dioxide, carbon monoxide, ozone, benzene, lead, ammonia, etc. [5, 10-14]. BREEZE AERMOD software is widely used product for assessing the level of atmospheric air pollution and for simulating the dispersion of air pollutants in a certain atmospheric area [15, 16].

Nitrous oxide N_2O is a greenhouse gas with a significant adverse effect upon the climate system. Although it is proved to have a considerable global warming potential, N_2O is not assigned a pollutant that defines ambient air quality [17,-20]. For that reason, there are not any specific software products designed for modeling the dispersion of N_2O emissions in the ground atmospheric layer.

The present research aim is to study the applicability of BREEZE AERMOD software for dispersion modeling of N_2O emissions from an organized industrial source and to estimate the emission dispersion in the ground atmospheric layer considering the specific environmental parameters.

II. Material And Method

A dispersion modeling is done for simulating the dispersion of N_2O emissions from a single industrial point source by using BREEZE AERMOD software. The N_2O emission source P1 is a 130 m high stack affiliated to a nitric acid production plant with a capacity of 363000 tons per year, situated in the industrial region of Devnya, Bulgaria. For the purpose of dispersion modeling detailed information on the source geometrical dimensions and N_2O emission parameters has been input. The software simulation is done over a topographic map of the source region so that the effect of the terrain upon the emission dispersion is considered.

Validated meteorological data is used in the form of an hourly meteo file containing information on 6 meteorological parameters at the source region – wind speed and direction, air temperature, relative air humidity, atmospheric pressure, solar radiation. The following dimensions of the research area have been set: 20000 m on the east-west direction and 10000 m on the north-south direction. A receptor grid of total 861 receptors is formed with 41 receptors on the **x** (east) and 21 receptors on the **y** (north) at 500 m spacing or a total of 861 receptors. An hourly average N_2O concentration is computed in each receptor of the defined grid [21, 22].

To check the adequacy of the simulated dispersion models a comparison is made between computed N_2O concentration and measured hourly average N_2O concentration in the ambient air. The N_2O concentration has been measured by using a portable gas analyzer G200-PACK (produced by Bedfont Scientific Ltd., Great Britain). Meteorological parameters have also been registered – air temperature, wind speed and direction.

A comparison is made between the computed and the measured maximum hourly average N_2O concentration. The calculated uncertainty of the model is compared to the legislative requirements [23].

III. Results And Discussions

By using BREEZE AERMOD software a mathematical modeling of the dispersion of N_2O emissions from an organized industrial source P1 is done [22]. The hourly average N_2O concentration in the ambient air is computed in every receptor of the defined grid. The computed maximum hourly average N_2O concentration and the geographic coordinates of the receptor, where it is calculated are indicated on Table 1. Fig. 1 presents contours of the hourly average N_2O concentration in the ambient air.

Table 1: Maximum hourly average N_2O concentration in the ambient air

Parameter		Value
Maximum hourly average N_2O concentration	μg/m^3	1244.23
UTM	X, m	553791.95
	Y, m	4784610.56
Altitude	m	155.40
Date	YYYY/MM/DD/HH	2013/07/02/06
Wind Speed	m/s	2.82
Wind Direction	deg	180
Air Temperature	^{0}C	17
Tail Gas Temperature	^{0}C	18.4
Tail Gas Flow rate	m/s	26.1

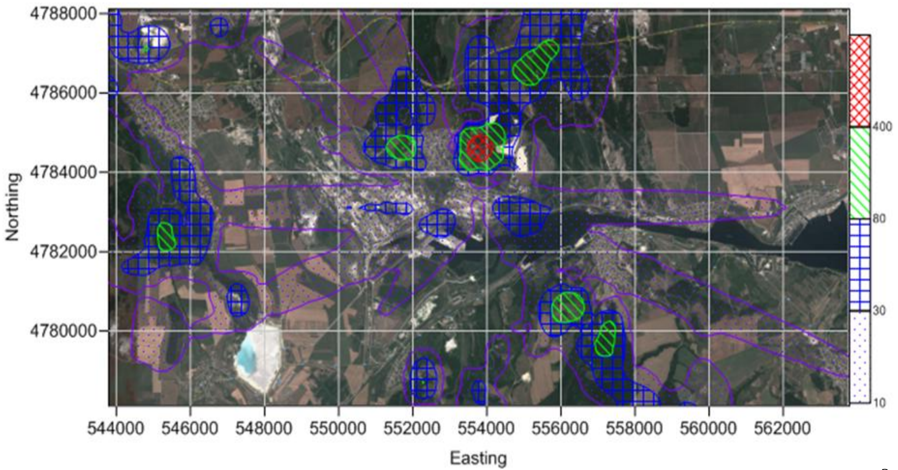

Fig. 1: Contours of the hourly average N_2O concentration in the ambient air (μg/m^3)

As indicated on Fig. 1, the maximum hourly average N_2O concentration is registered at a receptor that is located at a hilly area, 760 m away on the east form the nearest settlement. This is to prove that specific characteristics of the terrain (such as rising ground and lowlands) have considerable effect upon the dispersion of air pollutants even at flat country [24, 25].

Considering the fact that there are no approved methods for measuring N_2O concentration in the ambient air [26-29], the present research is done in accordance with the general criteria and legal requirements for ambient air quality assessment and positioning of monitoring stations [23]. The monitoring point for measuring the atmospheric N_2O concentration is located at a spot that corresponds to the grid receptor with the highest hourly average N_2O concentration (Fig. 2). All the requirements for positioning of monitoring stations in micro scale are complied.

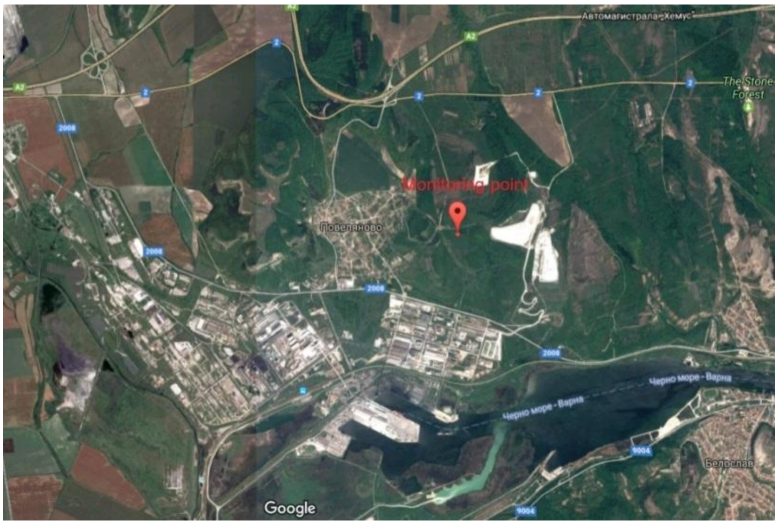

Fig. 2: Location of the monitoring point for measuring N_2O concentration in the ambient air

To ensure the measurement data quality, all the requirements regarding indicative measurements of ambient air quality are completely met (see Table 2).

Table 2: Requirements towards data quality

Parameter		Value
Uncertainty	%	25
Minimum data capture	%	90
Minimum time coverage	%	14

Within the present research measurements are done during 8 weeks period, equally distributed along the year so that representative data is collected during cold and warm seasons. Measurement periods are chosen so that data is collected during different parts of the day (day, evening, night). When conducting the indicative measurements of the average hourly concentration of N_2O in the ambient air, the main meteorological parameters in the defined observation point were also taken into account.

The measurement results indicate that maximum hourly average N_2O concentration in the ambient air is 1033.17 $\mu g/m^3$. It is measured on 20 November 2015 at 22.00. The wind direction is south-southeast and the wind speed is 2.7 m/s [30]. These meteorological conditions are almost identical to the weather conditions at which the maximum hourly average N_2O concentration in the ambient air is simulated in the dispersion modeling. Table 3 gives a summary of the meteorological conditions at which maximum hourly average N_2O concentration is computed and measured.

A comparison is made between the computed and the measured hourly average N_2O concentration in the ambient air. The following Table 4 gives a summary of the uncertainty of the model.

Table 3: Conditions at which maximum N_2O concentration is computed and measured

Parameter	Computed value	Measured value
Maximum N_2O concentration, $\mu g/m^3$	1244.23	1033.17
X, m	553791.95	553791.95
Y, m	4784610.56	4784610.56
Altitude, m	155.40	155.40
Date YYYY/MM/DD/HH	2013/07/02/06	2015/11/20/22
Wind Speed, m/s	2.82	2.70

Wind Direction	S	SSW
Air Temperature, ^{0}C	17	17.8

Table 4: Uncertainty of the model

Parameter	Computed value	Measured value	Failure rate
Maximum N_2O concentration	1244.23 μg/m^3	1033.17 μg/m^3	20.43 %

Result analysis indicates that the failure rate is within the permissible range [23]. Based on the analysis results a reasonable conclusion can be made that the dispersion modeling is applicable for air quality assessment in regards with N_2O pollution.

IV. Conclusion

The effect of N_2O emissions from an industrial source upon ambient air quality depends on the specific topographic and meteorological conditions at the source region that define the dispersion of the pollutants in the ground atmospheric layer. Although a variety of mathematical modeling products is developed worldwide, there isn't specific software for dispersion modeling of N_2O emissions. A study is done upon the applicability of a practically approbated software product BREEZE AERMOD for dispersion modeling of N_2O emissions from an industrial source and assessment of dispersion processes in various by duration periods.

Research results indicate that the failure rate between the computed and measured maximum hourly average N_2O concentration is within the legally permissible range. BREEZE AERMOD software can be used for dispersion modeling of N_2O emissions and air quality assessment regarding N_2O emissions from industrial sources. The software product is applicable in investment project engineering of new industrial plants with N_2O emission sources for the purposes of assessing the effect of N_2O emissions upon human's health and ambient air quality. The assessment should be done considering the specific topography of the region and a possible cumulative effect with other pollution sources in the region.

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