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### INVESTIGATION OF ATMOSPHERIC DISPERSION OF GAS COMPOUNDS FROM AN INDUSTRIAL INSTALLATION OVER A REALISTIC TOPOGRAPHY

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**Abstract**: The aim of the work was to compile a methodology using appropriate modelling tools for the study of the dispersion of gas pollutants from a fictitious industrial site over a realistic complex topography, treated as a point source, in a region of varying climate conditions, for regulatory purposes. To calculate the average levels and the maximum values of the pollutant concentrations in the atmosphere on an annual, daily and hourly basis, the procedure of identifying the characteristic weather types or weather days of the area of interest was followed. For the current study, meteorological files were extracted from the National Centres for Environmental Prediction (NCEP / USA) Global Forecasting System (GFS) available on a 6-hour temporal resolution from a planetary model of 1 degree horizontal resolution for a five-year period. The prevailing meteorological conditions or in other words characteristic weather types were obtained using these files and by applying a specific methodology based on Principal Components Analysis. The simulation of the 3-d meteorological fields was carried out for the characteristic weather types or days for the area of interest (computational domain extent 20x20 km<sup>2</sup>) with  $3 \times 3$  km<sup>2</sup> horizontal and 1-hour temporal resolution. The air dispersion simulations have been performed with the WRF-HYSPLIT modelling system. Modelled pollutants ground concentrations have been compared against European air quality standards (2008/50/EC), adopted by Greek legislation, considering potential receivers (residential places).

Key words: Atmospheric dispersion, air pollutants, fictitious industrial source, complex terrain

#### **INTRODUCTION**

Air dispersion and air quality modelling are unique tools for evaluating the impacts of air pollutant emission sources on the concentration fields in a region and assessing the compliance with existing air quality control legislation. Given the fact that such models incorporate the most updated progress in knowledge of atmospheric dynamics, chemical transformations and pollutant deposition, they become indispensable tools particularly in the case of investigating the impact of emission sources from future installations (Zaneti, 1990). The dispersion patterns of air pollutants can be very complex particularly over irregular topographies and where there are large number and / or different types of emission sources. Numerous studies have been carried out using Gaussian, Lagrangian, Eulerian and Computational Fluid Dynamics (CFD) dispersion models to understand and predict the concentration fields of air pollutants in various environments for impact assessment and human exposure purposes. A review of such models can be found in e.g. Holmes and Morawska (2006) and in Leelocy et al., (2014).

The integrated study presented in this paper addresses the calculation of the concentration fields of air pollutants Nitrogen Oxides ( $NO_x$ ), Non-Methane Hydrocarbons (HC), Carbon Monoxide (CO) and Particular Matter (PM10) emitted from a fictitious installation of multi stack industrial combustion source with realistic data, in a mountainous region with varying meteorological conditions through out the year. The study included the effect of varying the height of the emission stacks as well. In the following sections the methodology compiled, which includes appropriate modelling tools and data, and the results achieved are discussed in detail.

### METHODOLOGY

The aim of this work was to study the impact of the dispersion of  $NO_x$ , HC, CO and PM10 on the atmosphere from an industrial source (type of compression station of natural gas), located at a mountainous region of northwest Greece (region of Epirus), using appropriate 3-dimensional computer modelling. The work included also the investigation of varying the height of the emission stacks. The region of interest has peculiarities as regards to its topographical features and varying climatic conditions throughout the year. The climate conditions in Epirus are varying depending on the part of the region. The coastal areas experience moderate temperatures, which rarely fall below zero in winter. The summer months are typical Mediterranean and rather hot with frequent precipitation events. The inland mountainous parts of the region are characterised by heavy winters with snow and rain and rather cool summers. The computer modelling system included the Weather Research Forecasting (WRF-ARW) version 3.6.1 (Skamarock et al., 2008) and the atmospheric dispersion model Hybrid Single Particle Lagrangian Integrated Trajectory Model (HYSPLIT) (Stein et al., 2015). The position and geometry of the source as well as the necessary data on stacks, emission rates of  $NO_x$ , HC, CO and PM10 were based on construction information. The basic computational steps followed are discussed below.

#### **Topography and Meteorological Data Processing**

For the specific study, the necessary data for input to the atmospheric dispersion model included the topography and meteorological fields. The computational domain for the atmospheric modelling calculations was constructed in a way so as to include at its centre the fictitious installation. The domain size was set to  $20 \text{ km} \times 20 \text{ km}$  to include all the neighbouring urbanised areas with a minimum population of 50 residents (Figure 1). In the west, the domain included the coastline with some plains of rather limited area extent. The original topographical data used were of 100 m resolution. The topography of the area revealed a non uniform terrain with ridges (up to a height of 1000 m) alternating with valleys running in a northwest to southeast direction.



**Figure 1.** Topography map of the computational domain of size 20 ×20 km<sup>2</sup> (contour interval 200 m). The (fictitious) industrial source of emission is located in the centre of the domain denoted as IS.

The meteorological data (vertical distribution of wind speed and direction, temperature, mixing layer height, humidity, precipitation, cloud cover etc) were extracted from the National Centres for Environmental Prediction (NCEP / USA) Global Forecasting System (GFS) available on a 6-hour temporal resolution from a planetary model of 1 degree horizontal resolution. To calculate the average levels and the maximum values of the pollutant concentrations in the atmosphere on an annual, daily and hourly basis, the procedure of identifying the characteristic weather types of the area of interest was followed, addressing the varying climate over those temporal scales. The prevailing meteorological conditions or in other words characteristic weather types of the region were obtained by applying the methodology of Sfetsos et al. (2005), which is based on Principal Components Analysis (PCA). The specific methodology was applied on the GFS meteorological data of large scale, as referenced above,

covering a five year period (2006-2010). The analysis revealed the prevailing weather conditions in the defined computational domain and the corresponding frequency of their occurrence (in percentage) per year. Each weather condition was assigned a characteristic or else typical day (24-hour).

The results showed that the area of study was characterised by 7 in total weather types, WT (Table 1). The meteorological conditions from the planetary scale model, which characterise each typical weather day of the region were returned by the applied methodology in terms of WS wind speed (m/s), WD wind direction (deg.) (at 850 mbar and 10 m above sea level), T temperature (K) (at 2 m above ground level), MLH mixing layer height (m above ground level). As an example here (due to limited space), the values of the calculated variables are shown for 12:00 hrs of the typical day identified (Table 1).

Typical day &( % ) of occurrence	WS (m/s) (850 mb)	WD (deg.) (850 mb)	T (K) (2 m)	MLH (m)	WS (m/s) (10 m)	WD (deg.) 10 m)
1 (9)	17.77653	15.254	286.0511	790.3441	9.746546	16.65174
2 (11)	12.36237	28.25053	293.3918	1199.438	10.22959	7.142796
3 (23)	7.064888	16.18699	293.8235	1223.496	7.889754	18.88497
4 (10)	2.157312	278.7621	291.4452	1090.954	4.904919	19.34661
5 (13)	9.192361	218.6249	287.7477	884.8964	4.322308	60.41888
6 (13)	4.06865	26.30287	284.3701	696.6619	10.16672	43.70327
7 (21)	4.782067	356.4973	286.0512	790.3529	6.125416	15.5691

 Table 1. Characteristic weather types/typical days, frequency of their occurrence (in %) in the area of study and calculated prevailing meteorological conditions during each typical day at 12:00 hrs.

Once the typical weather days were identified, the data from the planetary model for the characteristic days were used as initial and boundary conditions to the WRF model. The model has been extensively tested, appropriately parameterised and validated in the Environmental Research Laboratory for a number of applications (e.g. Emmanouil et al., 2015, Vlachogiannis et al., 2013). The WRF model calculated the 3-d meteorological fields of the region of interest, in a horizontal and temporal resolution of  $3 \times 3 \text{ km}^2$  and 1-hour, respectively.



Figure 2. WRF calculated Mixing Layer Height above sea level (m) at 6:00 hours, during (a) WT4 and (b) WT6.

The meteorological calculations showed that the weather types 4 and 6 exhibited rather low values of the Mixing Layer Height (MLH) during early morning hours compared to the rest of the characteristic types

(Figure 2 (a) and (b)). Moreover, those days were characterised by calm conditions with very low winds between the ground surface and 50 meters height. Such stagnant atmospheric conditions favour the formulation of air pollution events, as pollutants are trapped. The meteorological data files obtained were used subsequently as input to the air dispersion model.

#### **Dispersion Model calculations**

This section presents the preparation of the input data for the dispersion model HYSPLIT and describes the results obtained, for each characteristic weather type. The installation was assumed to comprise four Compressors of 30MW each, in full annual operation (24 hours x 365 days) and one Back-up Generator (Gas turbine exhaust) of 3.5 MW, operating 350 days per year. The computational study investigated the effect of varying the height of the stacks of the compressors (19 m or 25 m) on the concentration fields of the pollutants. The data on emissions sources and the pollutant composition in the exhaust gases were realistic and those were provided by the constructor (Table 2). The modelling approach was performed without the inclusion of the photochemical reactions and background air quality concentrations. The modelled calculated concentrations of the pollutants were compared against the respective air quality limits as set by the legislation in force (Directive 2008/50/EC).

Table 2. Data on	emission s	ources from t	the fictitious	installation.
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Number of stacks	Stack Geometric characteristics		Exit gas	Exhaust gas	Exhaust gas flow	Exit gas
	Height (m)	Diameter (m)	(°C)	(kg/h)	(Nm3/h)	(m/s)
4	19 or 25	3.5	528	338400	254492	21.7
1	19 or 25	5	445	68365	51274	

The analysis of the results showed that the maximum hourly average values of NO<sub>x</sub> concentrations from the installation did not to exceed the air quality limit of 200 mg/m<sup>3</sup> for any assumed height of the stacks and during any weather type in the region even during those (WT4 and WT6) characterised by high stability in atmospheric masses and low wind speeds. The maximum hourly average NO<sub>x</sub> concentrations remained low and well below the air quality limit even in the vicinity of the stacks. In fact, the highest maximum hourly NO<sub>x</sub> concentrations values were found to be equal to 106  $\mu$ g/m<sup>3</sup> and 104  $\mu$ g/m<sup>3</sup> for stack height of 19m and 25m, respectively during WT4. Additionally, the annual average values of NO<sub>x</sub> did not exceed the respective air quality limit (40  $\mu$ g/m<sup>3</sup>) as very low values had been calculated for the two stack heights and weather types. The maximum 8-hour value of CO concentration was calculated to be equal to 4.2  $\mu$ g/m<sup>3</sup> and 4.0  $\mu$ g/m<sup>3</sup> during WT4. The CO values were calculated to remain very low compared to the legislative limit everywhere in the domain and no exceedances occurred. Similarly, no exceedances in the PM10 hourly maximum and annual concentrations of the respective air quality limits were calculated for both stack heights and weather types. The PM10 calculated concentrations were found to be very low everywhere in the area of study. Finally, an inspection of the values yielded that overall the HC concentrations were low. Even in the case of the average annual total HC concentrations, the values remained well below the level of 5 µg/m<sup>3</sup>, which was the air quality limit of Benzene. Due to the limited space of the paper, examples only of the maximum hourly NO<sub>X</sub> for the 7 weather types and the average annual PM10 near ground concentration values are shown for the 19 m and 25 m stack heights (Figure 3 (a) and (b); Figure 4 (a) and (b)).



Figure 3. Maximum average hourly concentrations of NO<sub>x</sub> for (a) 19 m and (b) 25 m stack heights near the ground for the 7 weather types (WT). Black dots indicate residential areas. (Air quality limit value for hourly concentration of NO<sub>2</sub>: 200 ( $\mu$ g/m<sup>3</sup>)).

## CONCLUSIONS

This work presented an integrated computational methodology to derive concentration values of pollutants emitted from a number of stacks of two different heights of a fictitious industrial combustion source.



Figure 4. Average annual PM10 concentration contours (in  $\mu$ g/m3) for a) 19 m and b) 25 m stack heights. (Annual Air Quality Limit for PM10: 40  $\mu$ g/m<sup>3</sup>).

The source was assumed to be located in a region of complex terrain and with varying climate through out the year. To account for the varying climate conditions, data from the Global Forecast System covering a 5 year period were analysed to obtain the characteristic weather types of the area. The meteorological model WRF-ARW and the HYSPLIT dispersion model were set up and parameterized to calculate the concentration fields of the pollutants. The investigation of the effect of varying the height of the emission stacks showed that the differences in the concentration values were found to be small. For the particular emission source, there were no exceedances found of the pollutants averaged over the time scales defined by the air quality limits of the legislation in force (Directive 2008/50/EC).

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