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AIR POLLUTION DISPERSION MODELING IN A POLLUTED INDUSTRIAL AREA OF COMPLEX TERRAIN FROM ROMANIA*

G. GRIGORAS [1], V. CUCULEANU[1], G. ENE[2], G. MOCIOACA[3], A. DENEANU[3]

[1]University of Bucharest – Faculty of Physics, P.O.Box MG-11, Bucharest, Romania,
E-mail: grigoras.georgiana@gmail.com; cuculeanu@gmail.com
[2]Politehnica University of Bucharest – Power Engineering Faculty, Bucharest, Romania,
E-mail: georgeta.ene@gmail.com
[3]WESTAGEM ltd, Bucharest, Romania, E-mail: george.mocioaca@westagem.ro
E-mail: alin.deneanu@westagem.ro

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Abstract. Air quality assessment in a polluted area with specific and complex terrain features situated in the north-western part of Romania was made using The Air Pollution Model (TAPM). This is a 3D prognostic model that solves the fundamental fluid dynamics and scalar transport equations to predict both meteorological data and air pollution concentrations. In order to properly assess the concentrations of air pollutants in the studied area, there were taken into account not only the emissions from the activities on the premises of the main industrial platform, but also the contribution from the other pollution sources from the area of interest, such as other industries, residential heating, traffic, dump heaps. The mathematical modeling results, displayed as air pollutant dispersion maps, showed the significant influence of the complex terrain features and of the other pollution sources on the concentration levels in the region, usually associated with the emissions of the main industrial platform.

Key words: The Air Pollution Model, pollutant dispersion, air quality.

1. INTRODUCTION

Dispersion modeling uses mathematical formulations to quantify the atmospheric processes that disperse a pollutant emitted by a source. Based on emissions and meteorological inputs, dispersion models can be used to predict concentrations at selected downwind receptor locations. Such models are widely used in the management of the impact of pollutant emissions on environment [1].

From the operational point of view, in air quality assessments there are used models with semi-empirical or analytical approach (ex. Gaussian plume or puff) that require as input meteorological data coming from local surface measurements.

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As an alternative to the operational applications using measured input data there are the 3D prognostic models that solve the fluid dynamics and scalar transport fundamental equations in order to predict the meteorology and pollutant concentrations. The quality of the predicted weather data is very important for the dispersion models used to assess air quality [2]. There are other studies of urban pollution in other areas of Romania [3, 4].

In this paper, an air quality assessment in a highly polluted region located in north-west of Romania has been performed by means of The Air Pollution Model (TAPM) that makes use of the second approach mentioned above.

The model has been used to calculate the pollutant concentration data series that have been measured in complex terrain conditions within the framework of the air quality monitoring stations located in the studied area.

In Section 2 of the paper The Air Pollution Model (TAPM) developed by CSIRO Atmospheric Research Australia [5, 6] is described.

Section 3 is dealing with the data and methods used for assessing the pollution source emissions as well as for modeling the air pollution dispersion in the considered area.

The intercomparison of measured and model simulated concentrations is presented in Section 4. Conclusions are shown in Section 5.

2. MODEL DESCRIPTION

The Air Pollution Model (TAPM) predicts three-dimensional meteorological data and air pollution concentrations. Technical details of the model equations, parameterizations, and numerical methods are described in the Technical Paper by Hurley, 2005 [7].

TAPM consists of coupled prognostic meteorological data and air pollution concentration components, eliminating the need to have site-specific meteorological observations. Instead, the model predicts the flows important to local-scale air pollution, such as sea breezes and terrain-induced flows, against a background of larger-scale meteorology provided by synoptic analyses.

The model solves the momentum equations for horizontal wind components, the incompressible continuity equation for the vertical velocity in a terrain-following coordinate system, and scalar equations for potential virtual temperature, specific humidity of water vapors, cloud water and rain water. Pressure is determined from the sum of hydrostatic and optional non-hydrostatic components, and a Poisson equation is solved for the non-hydrostatic component. Explicit cloud micro-physical processes are included. Wind observations can optionally be assimilated into the momentum equations as nudging terms. The turbulence closure terms in these mean equations use a gradient diffusion approach, including a counter-gradient term for the heat flux, with eddy diffusivity determined using prognostic equations for turbulence kinetic energy and eddy dissipation rate. A weighted vegetation canopy, soil and urban land-use scheme is used at the surface,

while radiative fluxes, both at the surface and at upper levels, are also included. Boundary conditions for the turbulent fluxes are determined by Monin-Obukhov surface-layer scaling variables and parameterizations for stomatal resistance.

The air pollution component of TAPM uses the predicted meteorology and turbulence from the meteorological component, and consists of an Eulerian grid-based set of prognostic equations for pollutant concentration and an optional Lagrangian particle mode [8] that can be used on the inner-most nest for pollution for selected point sources to allow a more detailed account of near-source effects, including gradual plume rise.

The model also includes gas phase photochemical reactions based on the Generic Reaction Set, gas- and aqueous-phase chemical reactions for sulfur dioxide and particles, and a dust mode for total suspended particles ($PM_{2.5}$, PM_{10}, PM_{20} and PM_{30}). Wet and dry deposition effects are also included.

3. DATA SETS AND METHODS USED

The atmospheric dispersion study of pollutants in the surveyed area was made using the pollutants emitted by non-ferrous metal industrial facilities existing in Baia Mare area and the emissions from other local anthropic activities (residential heating, traffic, dump heaps).

The air pollution modeling was made using local emissions inventories (drafted and validated for 2008 by WESTAGEM) [9] and real – time monitoring results of emissions from lead smelting from lead concentrates with high copper content and metallurgical residue with lead content [10].

The atmospheric emissions assessment was made using the chapters devoted to the following methodologies:

– EMEP/CORINAIR [11] Emission Inventory Guidebook – 2007 cod SNAP 030304 Processes with contact: Primary lead production;

– AP 42 [12];

– COPERT4 2007 [13].

In order to assess the emissions, temporal variations of the activities that lead to the time variation of emissions were considered.

Table 1

Atmospheric emission in the studied area for 2008

Sources type	Emissions		
	SO_2 [t/yr]	PM_{10} [t/yr]	Pb [t/yr]
Non – ferrous metallurgy	1023.06	20.75	1.36
Other industrial sources	30.59	43.89	0.05
Surface sources	0.94	89.56	0.05
Traffic	22.55	1715.36	0.07
Total	1077.15	1869.56	1.53

TAPM was run with four nested domains of 30 × 30 horizontal grid points at 20 km, 10 km, 3 km, 1 km spacing for the meteorology and a resolution of 500 m for pollution simulation for the inner – most grid. A number of 3481 receptors were used for calculation of the concentration fields.

The used databases contain terrain height data, type of soil and vegetation, sea surface temperature and synoptic scale meteorology supplied by the model developer CSIRO Atmospheric Research Australia. Global terrain and land use datasets have a spatial resolution of 1 km. Sea surface temperature data used are monthly averages and have a spatial resolution of 100 km. Meteorological datasets contain six-hourly synoptic scale analyses on a longitude/latitude grid at 0.75 or 1.0 degree grid spacing (approximately 75 km or 100 km).

Atmospheric pollutants concentrations assessment was performed for the specific industrial area pollutants, regulated by OM 592/2003: sulfur dioxide (SO_2), suspended particulate – PM_{10} fraction (suspended particulate with the diameter under 10 microns) and lead (Pb). The referencing to the regulations (limits for the allowable concentration of pollutants in ambient air) was made by using 1-hour and daily maximum concentration values and average concentration values for the air pollutants originated from the local sources.

Table 2

Modeling estimated concentrations

Pollutant	Modeling estimated concentrations [μg/m^3]	Averaging time	Limit Value LV [μg/m^3]	Normative
SO_2	5.79 – 601.82	1 h	350	OM 592/2002
	0.87 -316.19	24 h	125	
	0.041 – 121.27	year	20	
PM_{10}	1.26 – 89.77	24 h	50	
	0.17 – 24.33	year	40	
Pb	0.001 – 1.99	year	0.5	

The modeling results show values that exceed the legislated limits for SO_2 1-hour and daily maximum and annual averages. Also, there were legal exceeding values for PM_{10} daily maximum and for Pb annual average.

The results provided by the dispersion model for 2008 are displayed as dispersion maps in Figs. 2–7, the color range being defined after the legal thresholds (pointed as LV).

The modeling domain, the location of the air quality monitoring stations and the stack of the non – ferrous industrial platforms are shown in Fig. 1.

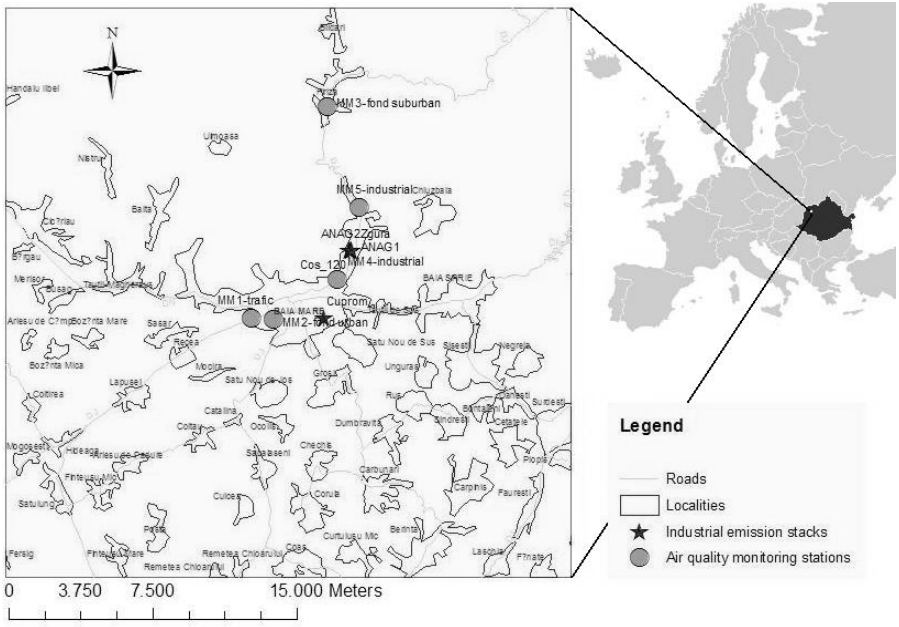

Fig. 1 – Location of the air quality monitoring stations and the stacks the non-ferrous industrial platforms.

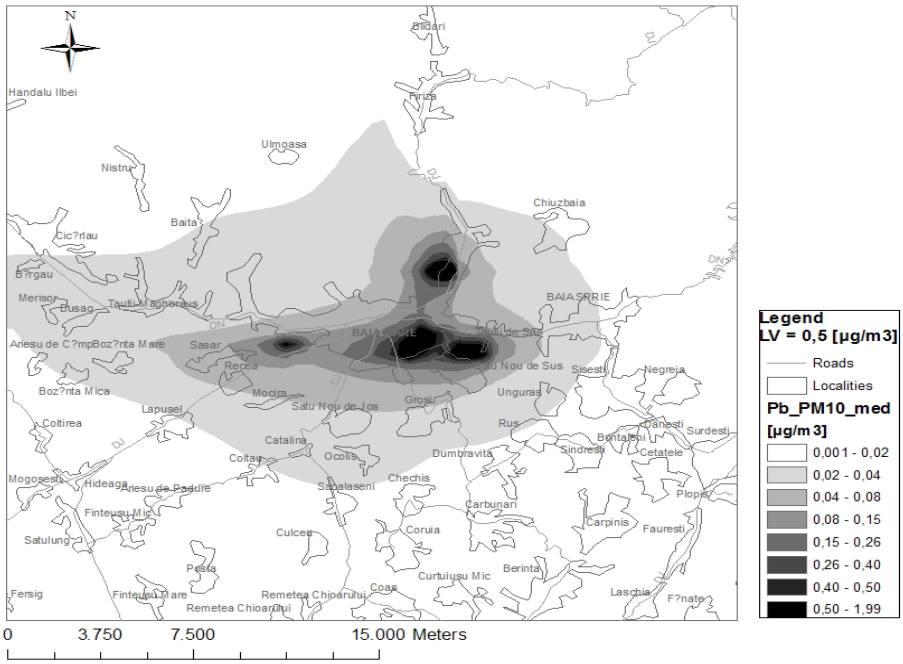

Fig. 2 – Spatial distribution of yearly average Pb in PM_{10} concentrations.

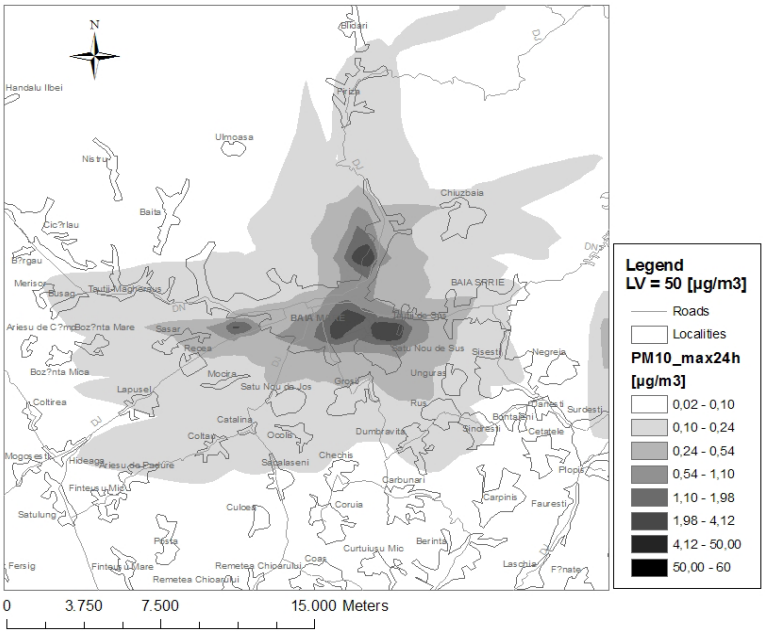

Fig. 3 – Spatial distribution of maximum daily average PM_{10} concentrations.

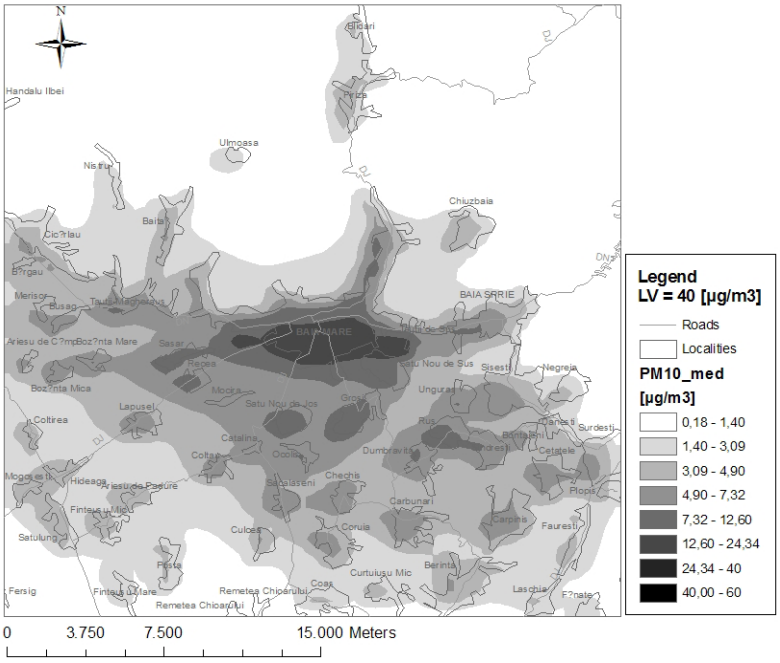

Fig. 4 – Spatial distribution of yearly average PM_{10} concentrations.

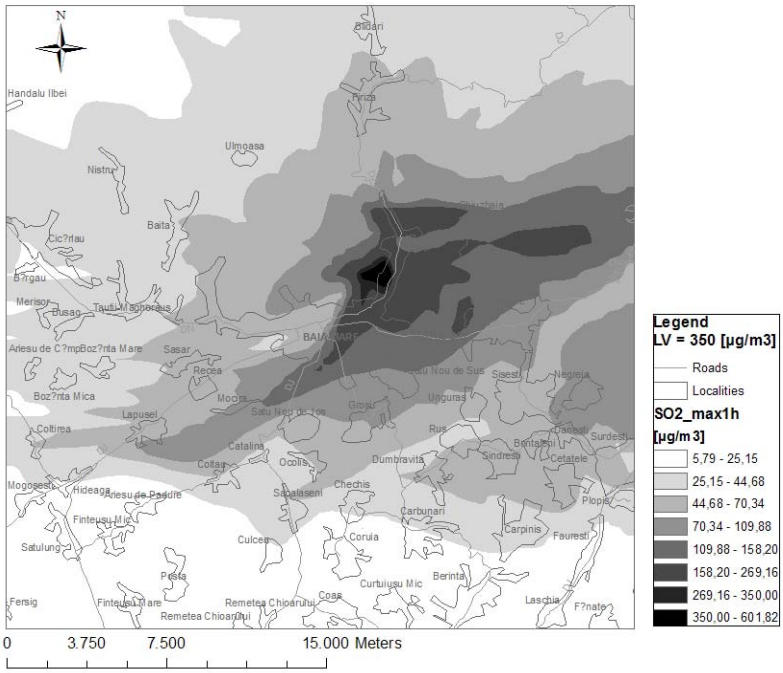

Fig. 5 –Spatial distribution of maximum 1-hour average SO_2 concentrations.

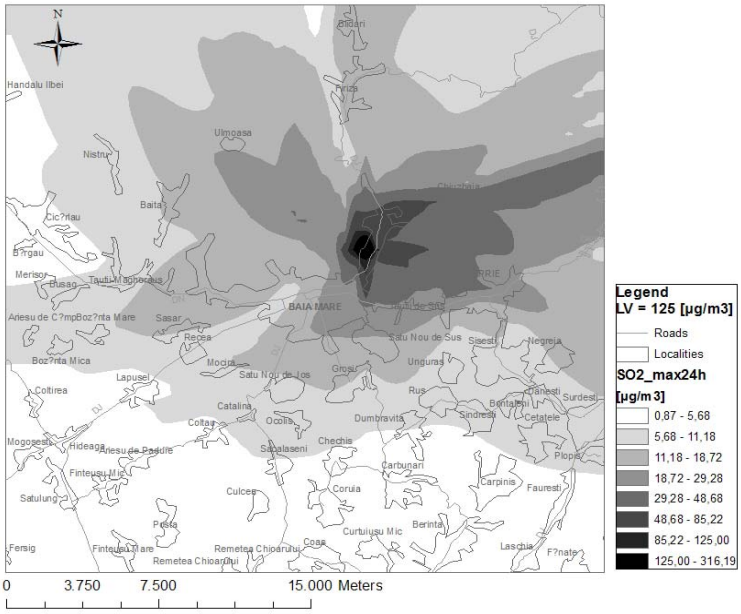

Fig. 6 – Spatial distribution of maximum daily average SO_2 concentrations.

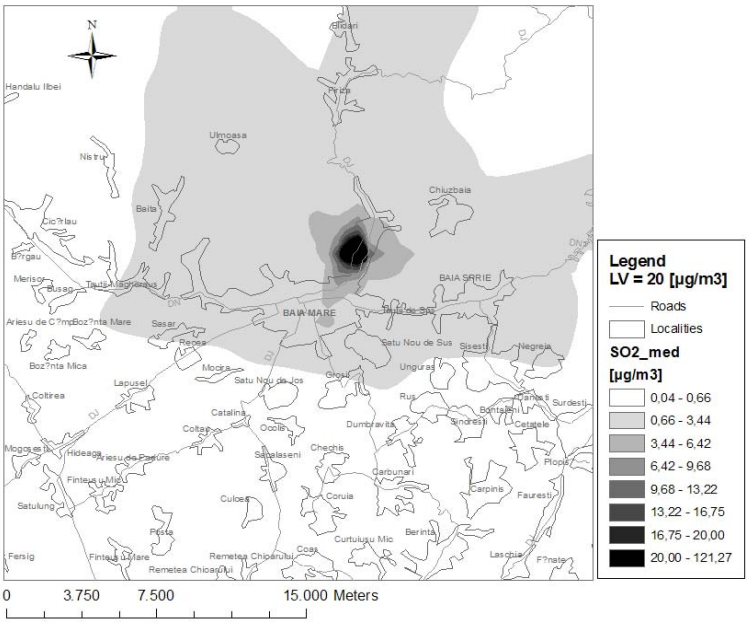

Fig. 7 – Spatial distribution of annual average SO_2 concentrations.

4. INTERCOMPARISON OF MEASURED AND CALCULATED CONCENTRATIONS

The values of Pb, SO_2 and PM_{10} daily average concentrations resulted from the modeling process in the corresponding points with the geographic coordinates for the air quality industrial monitoring stations have been set against the measured concentration values in the stations. MM4 and MM5 air quality industrial monitoring stations are located nearby the non-ferrous metallurgy industrial platforms that were the main air pollution sources in 2008.

Meanwhile, air quality improved in the region following the implementation of new technologies in some industrial units and the activity discontinuance of other units.

The intercomparison between the measured and simulated PM_{10}, Pb and SO_2 temporal series has been achieved making use of the basic statistics recommended by the Model Validation Kit for pollution predictions [14] that is used for the evaluation of the atmospheric dispersion models.

The model has been already validated by A. Luhar [15] using three field data sets, first two being part of the Model Validation Kit, the third set being used for dispersion under sea-breeze, this paper being dedicated to the model adaptability

determination to the local conditions: complex terrain of the North-Western part of Romania and the non-ferrous metallurgy specific type of air pollutants – lead and SO_2.

Thus, BOOT (Statistical Model Evaluation Software Package) [16] has been used to estimate corresponding basic statistics: mean of measured data, mean of simulated data, normalized bias as used by EPA (Environmental Protection Agency, USA), normalized mean square error, correlation coefficient with robust 95% confidence limits (t Student test).

In Figs. 8–13 the time distributions of the simulated and measured concentrations for lead, SO_2 and PM_{10} in the locations, MM4, MM5, for different time periods during the year 2008 are presented. This assessment has been done for the most relevant and reliable experimental data.

In Table 3 one presents the basic statistics calculated by means of BOOT dedicated software for the examples given in Fig. 8–Fig. 13.

Table 3 shows that the best correlation coefficient has been obtained for Pb, this means that the model better simulates the measured concentrations of lead. This could be explained by the fact that input data for Pb sources are better determined.

The intercomparison of measured and model simulated data makes evident that the modeling process is better described for stations located nearby the non – ferrous industrial platforms, the only suitable explanation being the more accurate knowledge of the emission rates of the point sources for industrial effluents.

Table 3

Basic statistics of the intercomparison between simulated and measured concentrations

Basic statistics	mmd [μg/mc]	msd [μg/mc]	nb	nmse	cc	cc robust 95% confidence limits
Pb-MM4	0.25	0.11	0.758	4.59	0.324	0.171 - 0.492
Pb-MM5	0.07	0.03	0.669	0.9	0.449	0.211 – 0.692
PM_{10}-M4	27.02	27.24	-0.008	0.22	0.418	0.058 – 0.750
PM_{10}-M5	31.82	24.62	0.255	0.21	0.424	0.061 - 0.768
SO_2-MM4	8.47	10.51	-0.212	0.98	0.355	0.229 – 0.485
SO_2-MM5	6.84	6.28	0.084	1.29	0.396	0.134 - 0.680

mmd = mean of measured data
msd = mean of simulated data
nb = normalized bias as used by EPA(Environmental Protection Agency, USA)
nmse = normalized mean square error
cc = correlation coefficient with robust 95% confidence limits (t Student test)

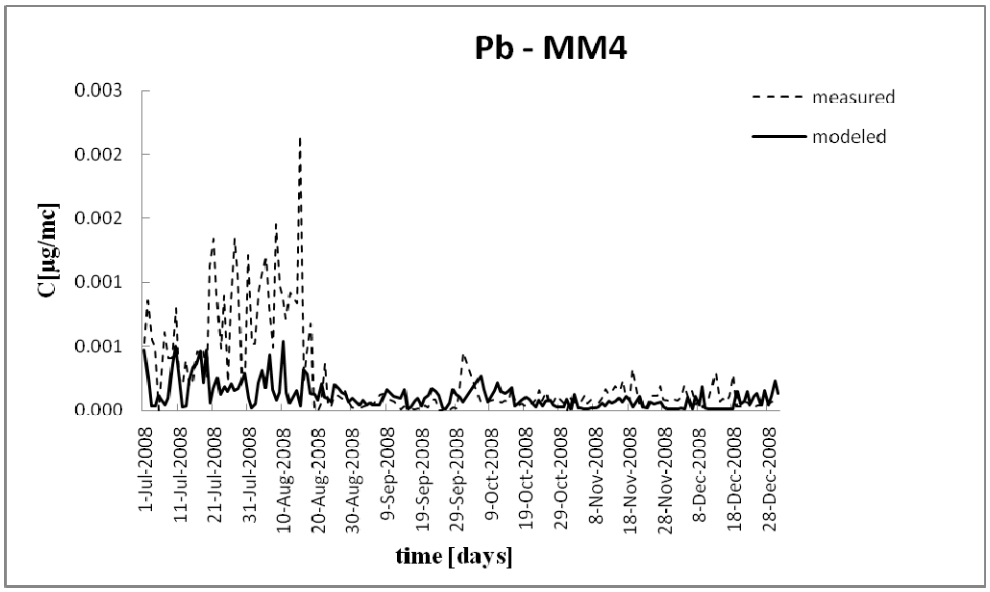

Fig. 8 – Comparison between observed and computed Pb concentrations in the industrial air monitoring station MM4.

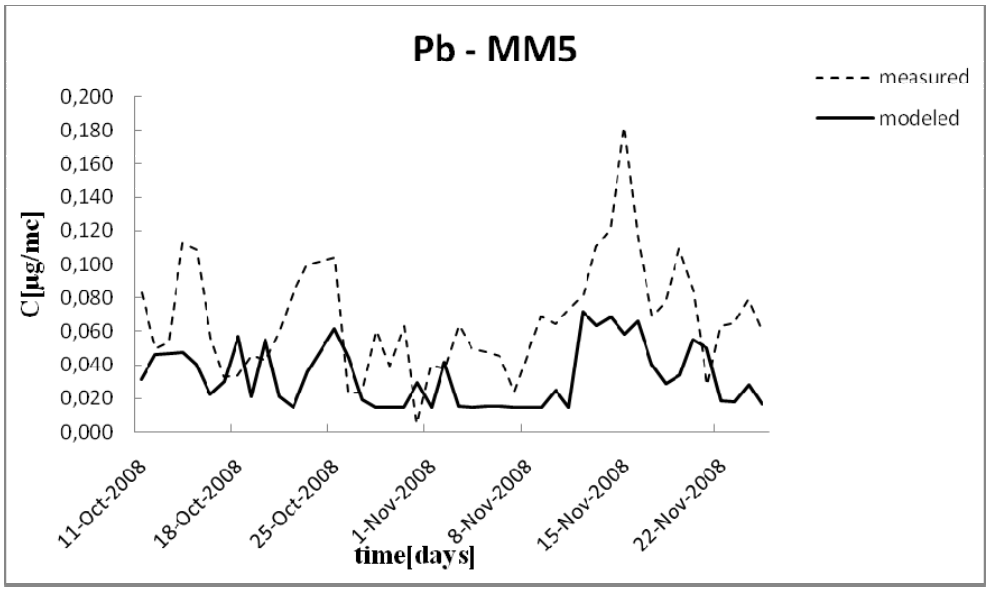

Fig. 9 – Comparison between observed and computed Pb concentrations in the industrial air monitoring station MM5

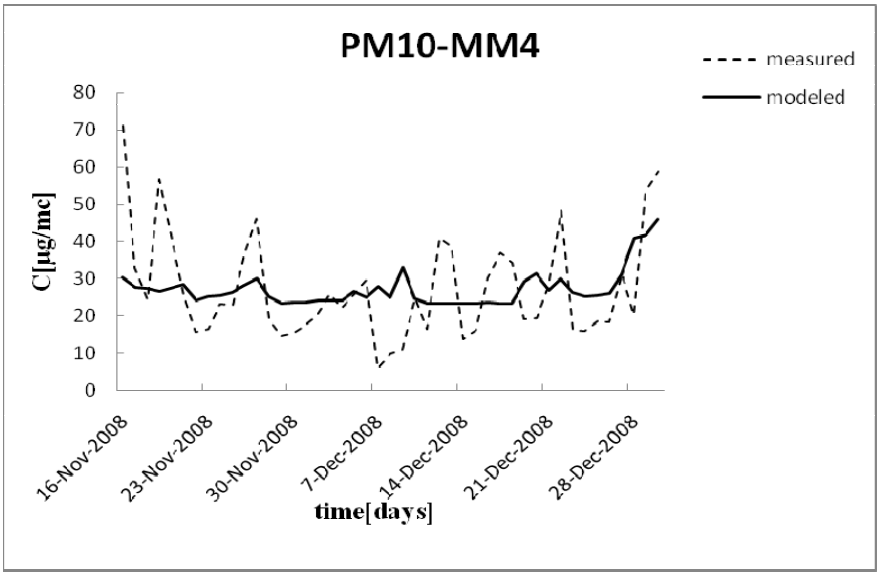

Fig. 10 – Comparison between observed and computed PM_{10} concentrations in the industrial air monitoring station MM4.

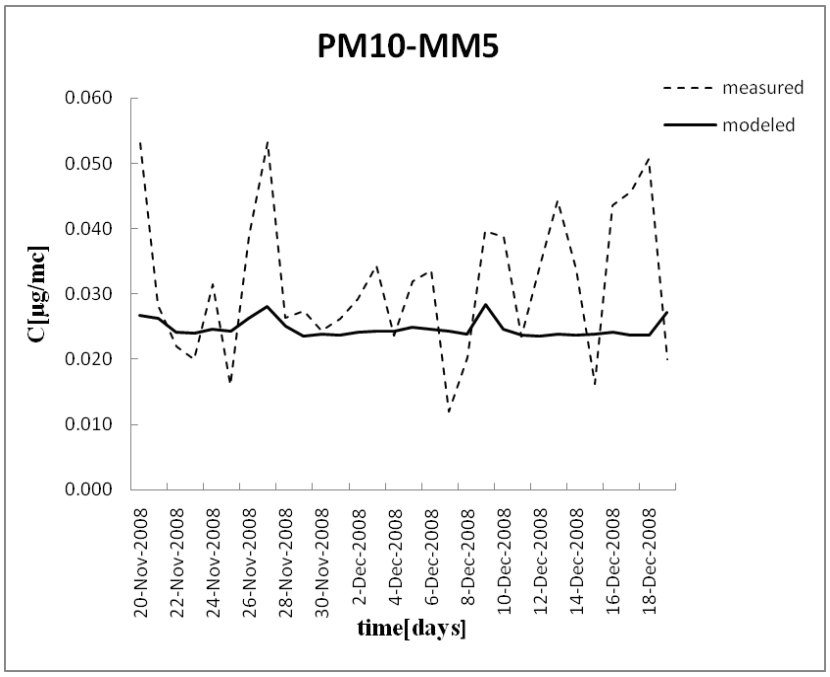

Fig. 11 – Comparison between observed and computed PM_{10} concentrations in the industrial air monitoring station MM5.

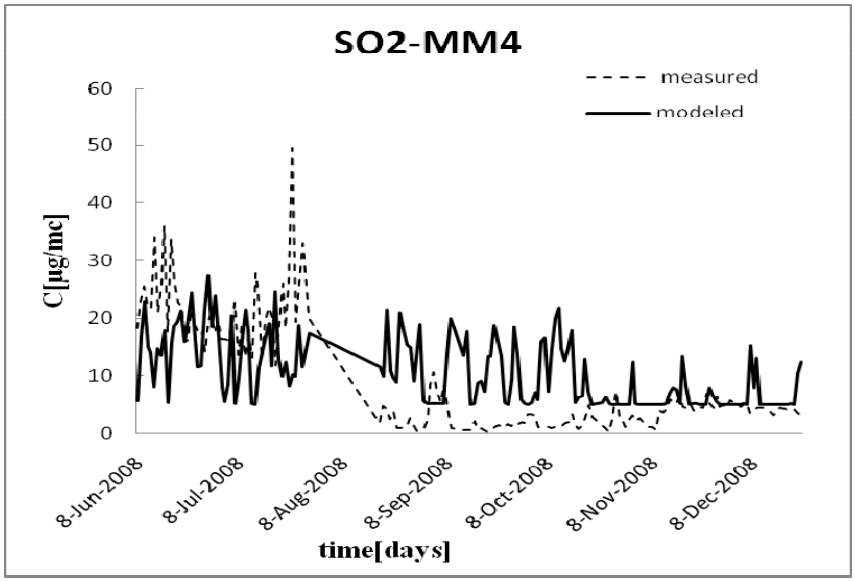

Fig. 12 – Comparison between observed and computed SO_2 concentrations in the industrial air monitoring station MM4.

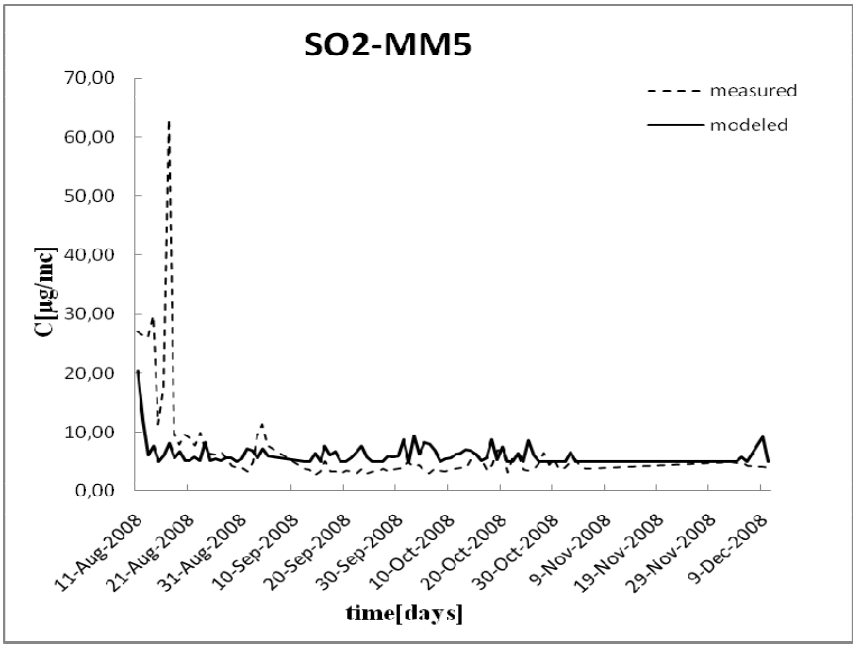

Fig. 13 – Comparison between observed and computed SO_2 concentrations in the industrial air monitoring station MM5.

5. CONCLUSIONS

The paper shows the mathematical modeling for assessment of the pollution level in a complex terrain region that favors high concentrations of noxious pollutants persistency in a high population density area that leads to severe and long lasting effects on human health.

From the dispersion maps we can see that the input from the industrial sources was a major one, the exceeding being focused around the pollution source and the impact area being on the Firiza Valley. Another impact area is located on the south side of Baia Mare City, the exceeding being concentrated around the heap dumps, showing the wind entrainment of the particulate as being the lead source of pollution.

The complex terrain conditions, with the altitude increasing from west to east and from south to north represents a blockage of the air transit towards east, promoting weak wind (speed under 2 m/s) and atmospheric calm conditions, unsuitable for pollutant dispersion.

Comparing the measured and simulated results, one can observe that the model behaves differently for Pb, SO_2 and PM_{10}, the results being consistent with the more refined emission inventory developed for Lead or SO_2 *versus* PM_{10} (the model reproduces quite well in many cases the measured concentrations). While the emission sources for lead were adequately identified and quantified, a complete emission inventory for PM_{10} is still a quite demanding task for an urban industrialized area. Although emission sources as traffic, area (residential heating, industrial heap dumps) were included into the emission inventory for modeling, there is a long list of sources and phenomenon not treated in these scenarios.

Moreover, emission sources from the industrial dumps were not completely correlated with the meteorological conditions related to high emissions during dry weather conditions. On the other hand, the model runs in the trace mode for all pollutants. This means that no chemical reactions in the atmosphere were included in the model run. It is well known that, suspended particulate with the diameter under 2.5 microns (fraction included in PM_{10}), is also generated through aerosols formation (stable non gaseous organics, stable non gaseous sulphur or nitrogen compounds). That is, not having treated these reactions that lead to these stable nongaseous compounds in an area with high emissions of them precursors (SO_2, NO_2, Volatile Organic Compounds), it is expected to underestimate the particles in the ambient air and the model confirmed that. For running the model with this photochemical scheme a more refined emission inventory should be developed. This would be the scope of future research of the authors.

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