16th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
8-11 September 2014, Varna, Bulgaria

NUMERICAL STUDY OF THE AIR QUALITY IN THE CITY OF SOFIA – SOME PRELIMINARY RESULTS

Ivelina Georgieva[1], Georgi Gadzhev[1], Kostadin Ganev[1], Maria Prodanova[2], Dimiter Syrakov[2] and Nikolay Miloshev[1]

[1]National Institute of Geophysics, Geodesy and Geography, Bulgarian Academy of Sciences, Sofia, Bulgaria
[2]National Institute of Meteorology and Hydrology, Bulgarian Academy of Sciences, Sofia, Bulgaria[2]

Abstract: Some extensive numerical simulations of the atmospheric composition fields in the city of Sofia have been recently performed. The simulations were carried out using the following set of models: the model WRF used as meteorological pre-processor; CMAQ - the Community Multiscale Air Quality System – the chemical transport model; SMOKE - the Sparse Matrix Operator Kernel Emissions Modelling System – the emission model. As the NCEP Global Analysis Data with 1 degree resolution was used as meteorological background, the WRF and CMAQ nesting capabilities were applied for downscaling the simulations to a 1 km resolution over Sofia. The national emission inventory was used as an emission input for Bulgaria, while outside the country the emissions were taken from the TNO inventory. Special pre-processing procedures are created for introducing temporal profiles and speciation of the emissions. The biogenic emissions of VOC are estimated by the model SMOKE. Different characteristics of the numerically obtained concentration fields will be demonstrated in the present paper.

Key words: *urban scale atmospheric composition numerical modelling, ensemble of numerical simulation results*

INTRODUCTION

Recently extensive studies for long enough simulation periods and good resolution of the atmospheric composition status in Bulgaria have been carried out using up-to-date modelling tools and detailed and reliable input data (Gadzhev et al. 2011 a,b, 2012, 2013 a,b,c,d).

The next step in studying the atmospheric composition climate is performing simulations in urban scale. The simulations aim at constructing of ensemble, comprehensive enough as to provide statistically reliable assessment of the atmospheric composition climate of the city of Sofia – typical and extreme features of the special/temporal behaviour, annual means and seasonal variations, etc.

Some preliminary results from the computer simulations will be presented in the present paper.

MODELING TOOLS AND INPUT DATA

The simulations are carried out with the following set of models:

- **WRF** (Shamarock et al. 2007) used as meteorological pre-processor;
- **CMAQ** - the Community Multiscale Air Quality System (Byun et al., 1998, Byun and Ching, 1999), being the Chemical Transport Model (CTM) of the system, and
- **SMOKE** - the Sparse Matrix Operator Kernel Emissions Modelling System (CEP, 2003) – the emission pre-processor of Models-3 system.

The large scale (background) meteorological data used in the present study is the NCEP Global Analysis Data with 1º×1º resolution. WRF and CMAQ nesting capabilities are applied for downscaling the simulations to a 1 km step for the innermost domain (Sofia).

The national emission inventory was used as an emission input for Bulgaria, while outside the country the emissions were taken from the TNO inventory (A. Visschedijk et all., 2007). Special pre-processing procedures are created for introducing temporal profiles and speciation of the emissions. The biogenic emissions of VOC are estimated by the model SMOKE. A detailed description of the emission modelling is given in Gadzhev et al. (2013a).

RESULTS, COMMENTS AND DISCUSSION

The most simple and natural atmospheric composition evaluations are, of course, the surface concentrations. By averaging over the whole simulated fields ensemble the mean annual and seasonal surface concentrations can be obtained and treated as respective "typical" daily concentration patterns. Plots of some of these "typical" annual, summer and winter NO_2 and O_3 surface concentrations are shown in Figures 1, 2. The spatial, seasonal and diurnal variations in NO_2 and O_3 surface concentration fields are very well manifested.

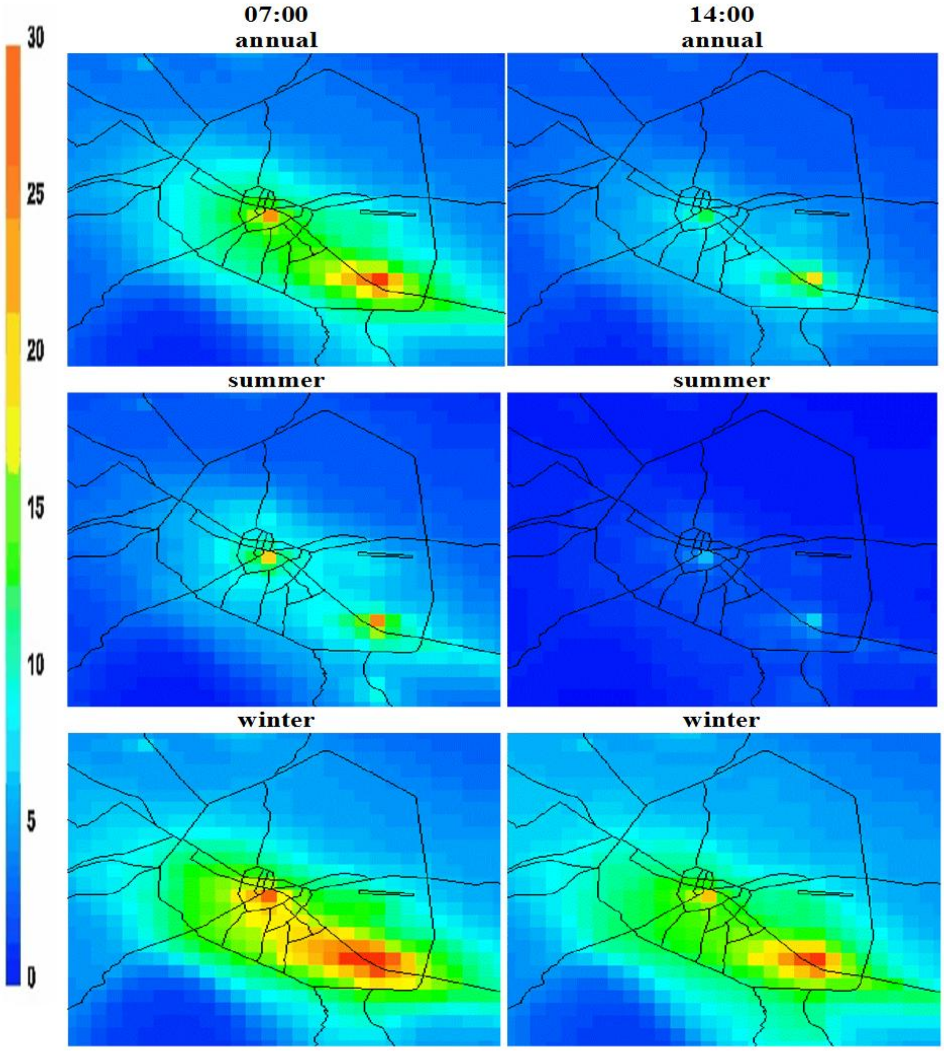

Figure 1. Surface NO_2 "typical" annual, summer and winter concentrations [$\mu g/m^3$] in 07:00 and 14:00 GMT

As it should be expected, because the major NO_2 source in the city is the road transport (surface sources) the surface NO_2 concentrations are higher early in the morning and much smaller at noon, when the atmosphere is usually unstable, and so the turbulence transports the NO_2 aloft more intensively. For the same reasons the concentrations during the winter period are bigger than those in summer, or the annually averaged. The spatial distribution is significantly heterogeneous – the maximal concentrations are formed in the city centre and along the boulevard with most busy traffic.

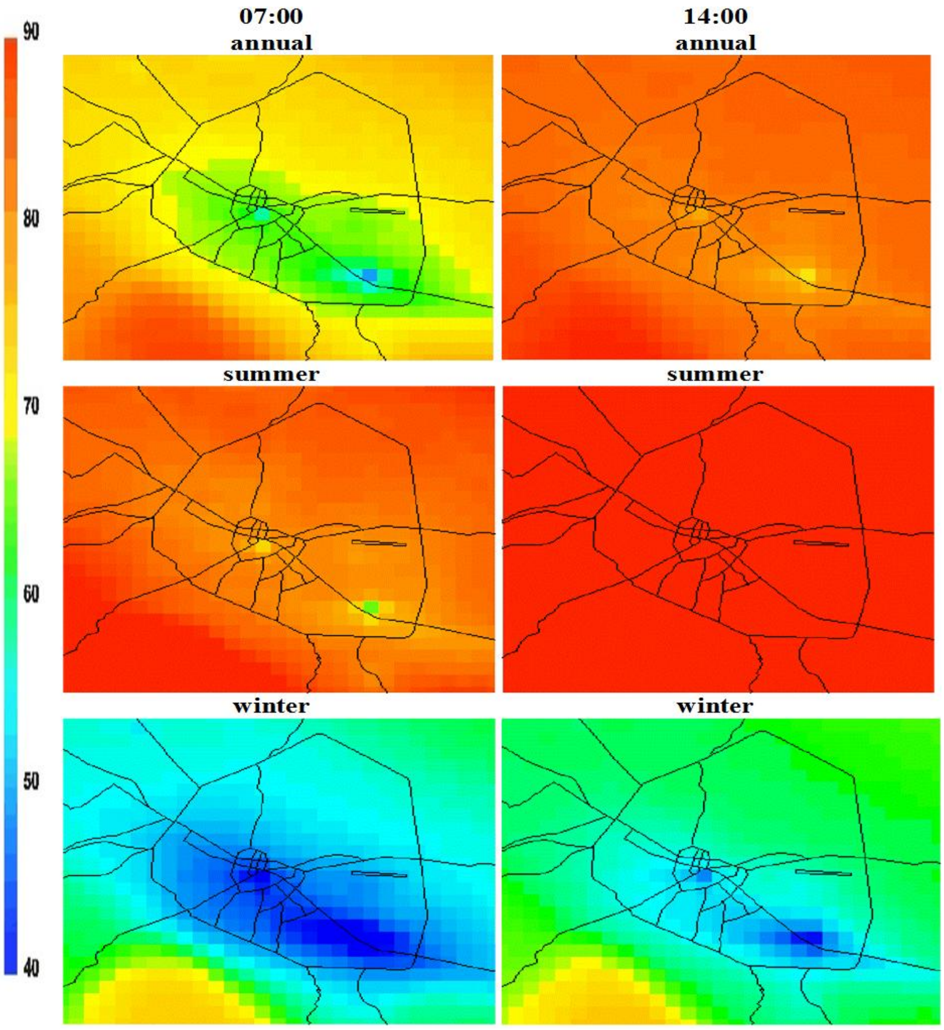

Figure 2. Surface O_3 "typical" annual, summer and winter concentrations [$\mu g/m^3$] in 07:00 and 14:00 GMT

The behaviour of the surface ozone is more complex. As shown in Gadzhev et al. (2012, 2013 a,b,c,d) the ozone in Bulgaria is to a great extend due to transport from abroad. This is one of the circumstances, because of which the ozone concentrations early in the morning are smaller than at noon (less intensive transport from higher levels). The other is, of course, the ozone photochemistry, which explains both the higher O_3 concentrations at daytime and during the summer and the O_3 gaps in the regions, where the NO_2 concentrations are large.

As already stated, the simulated fields ensemble is large enough to allow statistical treatment. In particular the probability density functions for each of the atmospheric compounds can be calculated, with the respective seasonal and diurnal variations, for each of the points of the simulation grid or averaged over the territory of the city. Knowing the probability density functions means to know everything about the ensemble.

An example of spatial and diurnal variations of the annual ensembles of surface O_3, NO_2, PM10 and PM2.5 behaviour in two points – the typically urban site "Orlov most" and the mountain site "Kopitoto" are shown in Figure 3. Together with the mean, maximal and minimal values there are also the curves denoted by 25, 75, 10 and 90%. These curves show the imaginary concentrations for which the probability of the simulated ones to be smaller is respectively 25, 75, 10 and 90%. Thus the band 25-75 contains 50% and the band 10-90 - 80% of the possible cases. The plots are self explanatory enough and demonstrate the spatial and diurnal variations of the above mentioned species. As it should be expected the NO_2, PM10 and PM2.5 concentrations at “Kopitoto” are much smaller as those at “Orlov most”, while the O_3 concentrations at both sites are of similar values. For the “Orlov most” site the O_3 concentrations reach maximum around noon, when NO_2 and PM concentrations tend towards local minimum. This is quite natural having in mind the traffic and atmospheric stability diurnal course. On the contrary for the “Kopitoto” site the NO_2 concentrations reach maximum around noon, probably due to the more intensive turbulent mixture and the slope wind effect. The PM10 and PM2.5 concentrations at “Kopitoto” do not have such a significant diurnal variations.

It could be also noticed that the NO_2, PM10 and PM2.5 ensemble behaviour is significantly asymmetric for both sites.

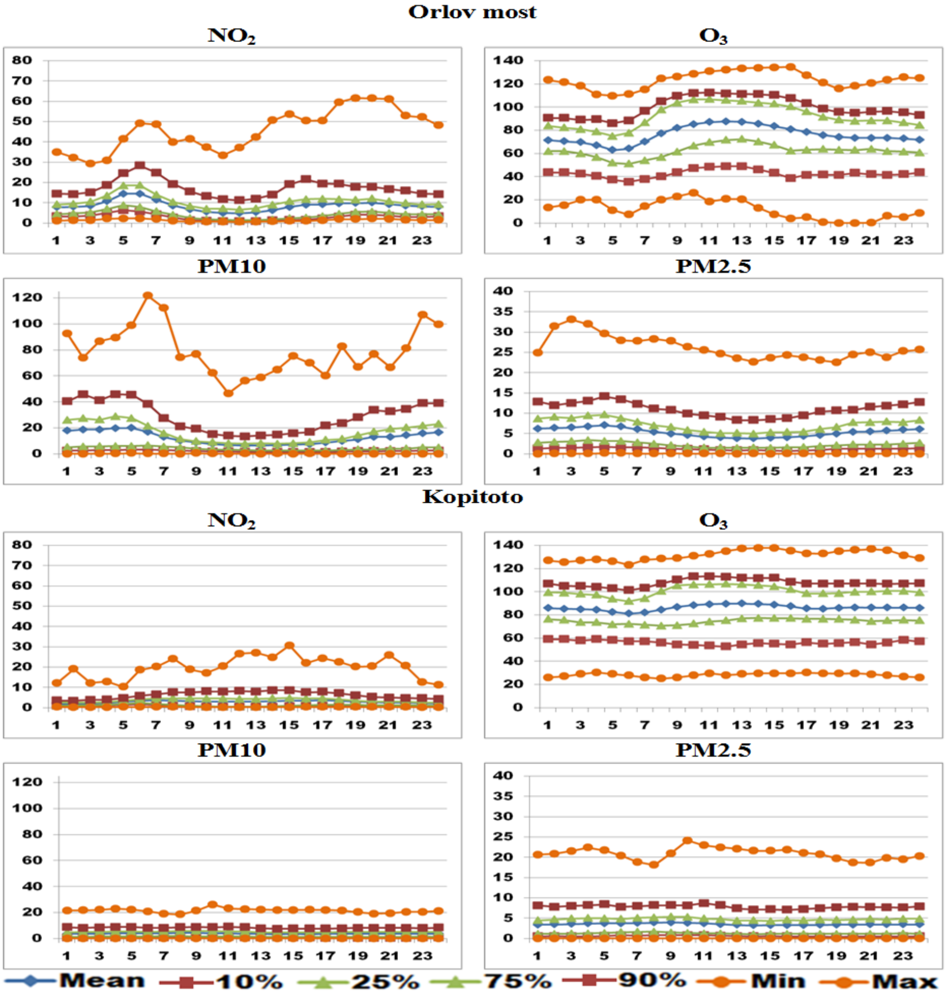

Figure 3. Diurnal variations of the annual NO_2, O_3, PM10 and PM2.3 surface concentrations [$\mu g/m^3$], for the typically urban site “Orlov most” and the mountain site “Kopitoto”: curves of mean, maximal and minimal values as well as curves show the imaginary concentrations for which the probability of the simulated ones to be smaller is respectively 25, 75, 10 and 90%.

CONCLUSIONS

The demonstrations, presented in the present paper are just a first glance on the atmospheric composition status of the city of Sofia. What can be seen so far is that the results does not defy the common sense and does not oppose the schematic concepts about how the air pollution near earth surface is formed. The numerical experiments are still going on, but when accomplished they will produce a huge volume of information, which have to be carefully analyzed and generalized so that some final conclusions can be made. It is planned computer simulations to be made for different emission scenarios, so that the contribution of different source categories to the atmospheric composition climate of Sofia can be evaluated.

The air pollution pattern is formed as a result of interaction of different processes, so knowing the contribution of each for different meteorological conditions and given emission spatial configuration and temporal behaviour could be interesting. Therefore the CMAQ "Integrated Process Rate Analysis" option was applied to discriminate the role of different dynamic and chemical processes for the air pollution formation in the city of Sofia. These results have still to be generalised and carefully analysed.

ACKNOWLEDGMENTS
The present work is supported by the Bulgarian National Science Fund (grant ДЦВП-02/1/29.12.2009) and the EC-FP7 grant 261323 (project EGI-InSPIRE).

Deep gratitude is due to US EPA, US NCEP and EMEP for providing free-of-charge data and software. Special thanks to the Netherlands Organization for Applied Scientific research (TNO) for providing us with the high-resolution European anthropogenic emission inventory.

REFERENCES

Byun, D. ,J. Young, G. Gipson, J. Godowitch, F.S. Binkowski, S. Roselle, B. Benjey, J. Pleim, J. Ching, J. Novak, C. Coats, T. Odman, A. Hanna, K. Alapaty, R. Mathur, J. McHenry, U. Shankar, S. Fine, A. Xiu, C. Jang, 1998: Description of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System, 10th Joint Conference on the Applications of Air Pollution Meteorology with the A&WMA, Phoenix, Arizona, 264-268.

Byun, D., J. Ching, 1999: Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. EPA Report 600/R-99/030, Washington DC. http://www.epa.gov/asmdnerl/models3/doc/science/science.html.

CEP Sparse Matrix Operator Kernel Emission (SMOKE) Modeling System, University of Carolina, Carolina Environmental Programs, Research Triangle Park, North Carolina 2003.

Gadzhev, G., D. Syrakov, K. Ganev, A. Brandiyska, N. Miloshev, G. Georgiev, M. Prodanova, 2011a: Atmospheric Composition of the Balkan Region and Bulgaria. Study of the Contribution of Biogenic Emissions, AIP Conf. Proc. 1404, 200, 200-209; doi: 10.1063/1.3659921

Gadzhev, G.,G. Jordanov, K. Ganev, M. Prodanova, D. Syrakov, N. Miloshev, 2011b: Atmospheric Composition Studies for the Balkan Region, Lecture Notes in Computer Sciences, Dimov, I. S. Dimova, and N. Kolkovska (Eds.): LNCS 6046, c. Springer-Verlag Berlin Heidelberg, 150-157.

Gadzhev, G., K. Ganev, D. Syrakov, N. Miloshev, M. Prodanova, 2012: Contribution of Biogenic Emissions to the Atmospheric Composition of the Balkan Region and Bulgaria, Int. J. Environment and Pollution, Vol. 50, Nos. 1/2/3/4, 2012, 130-139.

Gadzhev, G., K. Ganev, N. Miloshev, D. Syrakov, M. Prodanova, 2013a: Numerical Study of the Atmospheric Composition in Bulgaria, Computers and Mathematics with Applications 65, 402-422.

Gadzhev, G., K. Ganev, N. Miloshev, D. Syrakov, M. Prodanova, 2013b: Some Basic Facts About the Atmospheric Composition in Bulgaria – Grid Computing Simulations, 9th International Conference, LSSC, 2013, Sozopol, Bulgaria, 484-490.

Gadzhev, G.,K. Ganev, N. Miloshev, D. Syrakov, M. Prodanova, 2013c: Analysis of the Processes which Form the Air Pollution Pattern Over Bulgaria, 9th International Conference, LSSC, 2013, Sozopol, Bulgaria, 390-396 .

Gadzhev, G., K. Ganev, D. Syrakov, M. Prodanova, N. Miloshev, 2013d: Some Statistical Evaluations of Numerically Obtained Atmospheric Composition Fields in Bulgaria, Proceedings of 15th International Conference on Harmonisation within Atmospheric. Dispersion Modelling for Regulatory Purposes, Madrid, Spain.

Shamarock et al., 2007: A description of the Advanced Research WRF Version 2. http://www.mmm.ucar.edu/wrf/users/docs/arw_v2.pdf Accessed 15 June 2010.

Visschedijk, A., Zandveld P., van der Gon, H., 2007: A high resolution gridded European emission database for the EU integrated project GEMS, TNO report 2007-A-R0233/B, The Netherlands.