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CALCULATION OF SOME OZONE POLLUTION INDECES FOR BULGARIA

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Abstract

As an active photo-oxidant the atmospheric ozone can cause serious damages to human health and vegetation – forests, crops. That is why the ozone studies are of primary importance for adequate formulation of the environmental policy of the country.

A set of integral ozone characteristics (ozone indices) has been developed, which make it possible the ozone pollution impact on human health and ecosystems to be quantitatively evaluated.

Calculation and analysis of these ozone indices for Bulgaria are the overall goals of the present work.

The US EPA Models-3 system is chosen as a modelling tool. As the NCEP Global Analysis Data with 1 degree resolution is used as meteorological background, the MM5 and CMAQ nesting capabilities are applied for downscaling the simulations to a 9 km resolution over Balkans and 3 km over Bulgaria. The TNO emission inventory is used as emission input. Special pre-processing procedures are created for introducing temporal profiles and speciation of the emissions.

The study is based on a large number of numerical simulations carried out day by day for years 2000-2007.

Key words: *ozone levels, air pollution modelling, US EPA models-3 system, AOT40C, AOT40F, NOD60*

1. INTRODUCTION

As an active photo-oxidant the atmospheric ozone can cause serious damages to human health and vegetation – forests, crops. That is why the ozone studies are of primary importance for adequate formulation of the environmental policy of the country.

A set of integral ozone characteristics (ozone indices) has been developed, which make it possible the ozone pollution impact on human health and ecosystems to be quantitatively evaluated.

Calculation and analysis of these ozone indices for Bulgaria are the overall goals of the present work.

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, 2012, 2013 a,b,c,d).

The simulations aimed at constructing of ensemble, comprehensive enough as to provide statistically reliable assessment of the atmospheric composition climate of Bulgaria – typical and extreme features of the special/temporal behaviour, annual means and seasonal variations, etc. This ensemble was used for calculating the ozone indices, demonstrated in the paper.

The present paper will focus on some important characteristics of the atmospheric composition climate of Bulgaria – the concentrations of different compounds and the evaluation of the contribution of different emission categories to the overall air pollution in the country.

2. BASIC APPROACHES AND MODELLING TOOLS

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, 2012, 2013 a,b,c,d). This experience have been fully utilised in the present study.

All the simulations are based on the US EPA Model-3 system. The system consists of three components: MM5 (Dudhia, 1993, Grell et al., 1994), used as meteorological pre-processor, CMAQ (Byun et al., 1998, Byun and Ching, 1999), the Chemical Transport Model of the system and SMOKE (CEP, 2003) – the emission pre-processor of Models-3 system.

The large scale (background) meteorological data used by the study is the NCEP Global Analysis Data with $1^o \times 1^o$ resolution. The MM5 and CMAQ nesting capabilities are used to downscale the problem to a 3 km horizontal resolution for the innermost domain (Bulgaria).

The TNO high resolution emission inventory (A. Visschedijk et all., 2007) is exploited. A detailed description of the emission modeling is given in Gadzhev et al. (2013a).

3. OZONE INDICES

High ozone concentrations can cause damages on plants, animals and human health. In fact, when the effects from high ozone levels are studied, one should look not at the ozone concentrations but on some related quantities. The following four quantities are important (see Amann et al., European Parliament, 2002):

AOT40C - Accumulated over threshold of 40 ppb in the day-time hours during the period from May 1 to July 31 concentrations), which are damaging crops when they exceed 3000 ppb.hours.

AOT40F - Accumulated over threshold of 40 ppb in the day-time hours during the period from April 1 to September 31 concentrations), which are damaging crops when they exceed 10000 ppb.hours.

NOD60 - Number of days in which the running 8-hour average of ozone concentrations exceeds at least once the critical value of 60 ppb. If the limit of 60 ppb is exceeded in at least one 8-hour period during a given day, then the day must be classified as “bad”. People with asthmatic diseases have difficulties in “bad” days. Therefore, it is desirable not to have “bad” days at all. Removing all “bad” days is a too ambitious task. The requirement is often relaxed to the following: the number of “bad” days should not exceed 20. It turns out that in many European regions it is difficult to satisfy even this relaxed requirement.

4. BRIEF DESCRIPTION OF THE NUMERICAL EXPERIMENTS

As far as the background meteorological data is the NCEP Global Analysis Data with $1^o \times 1^o$ resolution, it is necessary to use MM5 and CMAQ nesting capabilities to downscale the simulations to a 3 km step for the innermost domain. The MM5 pre-processing program TERRAIN was used to define four domains with 81 (D1), 27 (D2), 9 (D3) and 3 (D4) km horizontal resolution. These four nested domains were chosen in such a way that the finest resolution domain contains the whole territory of Bulgaria and the domain with a horizontal resolution of 9 km contains the whole Balkan Peninsula.

The meteorological pre-processor MM5 was forced by the NCEP global scale data. In the D1 domain the model was set to relax toward observed temperature, wind and humidity through four dimensional data assimilation (FDDA) (Stauffer and Seaman, 1990). FDDA amounts to adding an additional term to the prognostic equations that serves to “nudge” the model solution toward the individual observations. This significantly reduces the drift in the solution for simulations of several days or more. The NCEP data set does not include observations, but analyzed data every 6 hours in all its grid points. MM5 is configured with FDDA option on as to nudge the model toward analyzed data in D1 only. For all the domains (D1, D2, D3, D4) MM5 was run simultaneously with “two-way” nesting mode on. All simulations were made with 23 σ-levels going up to 100 hPa height. The MM5 simulations were made on portions of 3 days. Every portion has additional 12 hours that are an initial spin-up period that overlaps the last 12 hours of the preceding run.

CMAQ meteorological input was created from the MM5 output exploiting the CMAQ meteorology-chemistry interface - MCIP, v2.3. CMAQ simulations were performed in D2, D3 and D4 domains. The CMAQ pre-defined (default) concentration profiles were used as boundary conditions for D2. The boundary conditions for the inner domains were determined through the nesting capabilities of CMAQ. The CB-4 chemical mechanism with Aqueous-Phase Chemistry and MEBI solver has been exploited for all the domains. The CMAQ simulations were made with 15 σ-levels vertical resolution.

The CMAQ simulations for domains D2 and D3 and those for D4 were organized in separate jobs, which again makes the jobs run time for 3 days real time fairly reasonable.

The MM5/CMAQ simulations were performed day by day for a period of 8 years - from 2000 to 2007.

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Table 1 Description of stations from the Bulgarian National Network for Air Quality Control, for which the scatter diagrams of simulated and measured ozone levels are demonstrated in Figs. 1, 2

code	Station	Latitude	Longitude	Height [m]	Location
BG0012A	Yan Palah-Varna	27.897791	43.227222	60	Varna
BG0044A	D.Ezerovo	27.366947	42.518055	17	Burgas
BG0051A	Evmolpia-AMS	24.778345	42.147781	166	Plovdiv
BG0053R	Rojen peak	24.738615	41.695835	1750	Rojen
BG0054A	AMS Orlov most-Sofia	23.338058	42.690834	500	Sofia
BG0056A	AIS Meden rudnik	27.389729	42.466946	28	Burgas

5. VALIDATION OF THE COMPUTER SIMULATION RESULTS

The ozone computer simulations were validated by comparison with data of the ozone levels, measured by the Bulgarian National Network for Air Quality Control.

Scatter diagrams of simulated and measured ozone levels for some of the stations, described in Table 1 are given in Fig. 1. It can be seen, that almost all the points are within the FA2 margins, which means that the condition for no more than 50% uncertainty of the hourly ozone values, defined in the respective European directive (European Parliament, 2002) is fulfilled.

The running 8-hour average values for simulated and measured ozone concentrations have been also calculated. The respective scatter diagrams are shown in Fig.2.

It can be immediately seen that the agreement between the simulated and measured running 8-hour average ozone values is much better in comparison to the hourly values. The less dispersion around the ideal correspondence line and the better correlation is obvious.

The above quoted requirement for less than 50% uncertainty is strictly fulfilled.

The results from only 6 stations are demonstrated here, but the results for all the other stations of the Bulgarian National Network for Air Quality Control are qualitatively similar.

The comparison of simulated and measured data ensure that the simulated surface ozone concentrations are reliable enough and can be used for calculating the ozone indices.

6. SOME COMMENTS ON THE OZONE INDICES

Maps of the simulated AOT40C, AOT40F and NOD60 fields for years 2000-2007 are shown in Figs. 3-5. The common feature of all the maps is the great difference of the configuration of the fields for different years, which obviously reflects the influence of meteorological conditions.

The AOT40C fields show, that for all the years the highest values are mostly in mountain regions. The areas, where the 3000 ppb.hour threshold values are exceeded are relatively small, except for years 2000 and to some extend 2003.

The areas where the 10000 ppb.hour threshold AOT40F values are exceeded are small for all the years.

The NOD60 fields show, that for most of the years in the major part of the countries the number of bad days is no more than 10. Significant exceeding of NOD60 values above 20-25 days in the year happen in 2000, 2003 and particularly in 2007, when the regions of exceeding above 20 days are quite large.

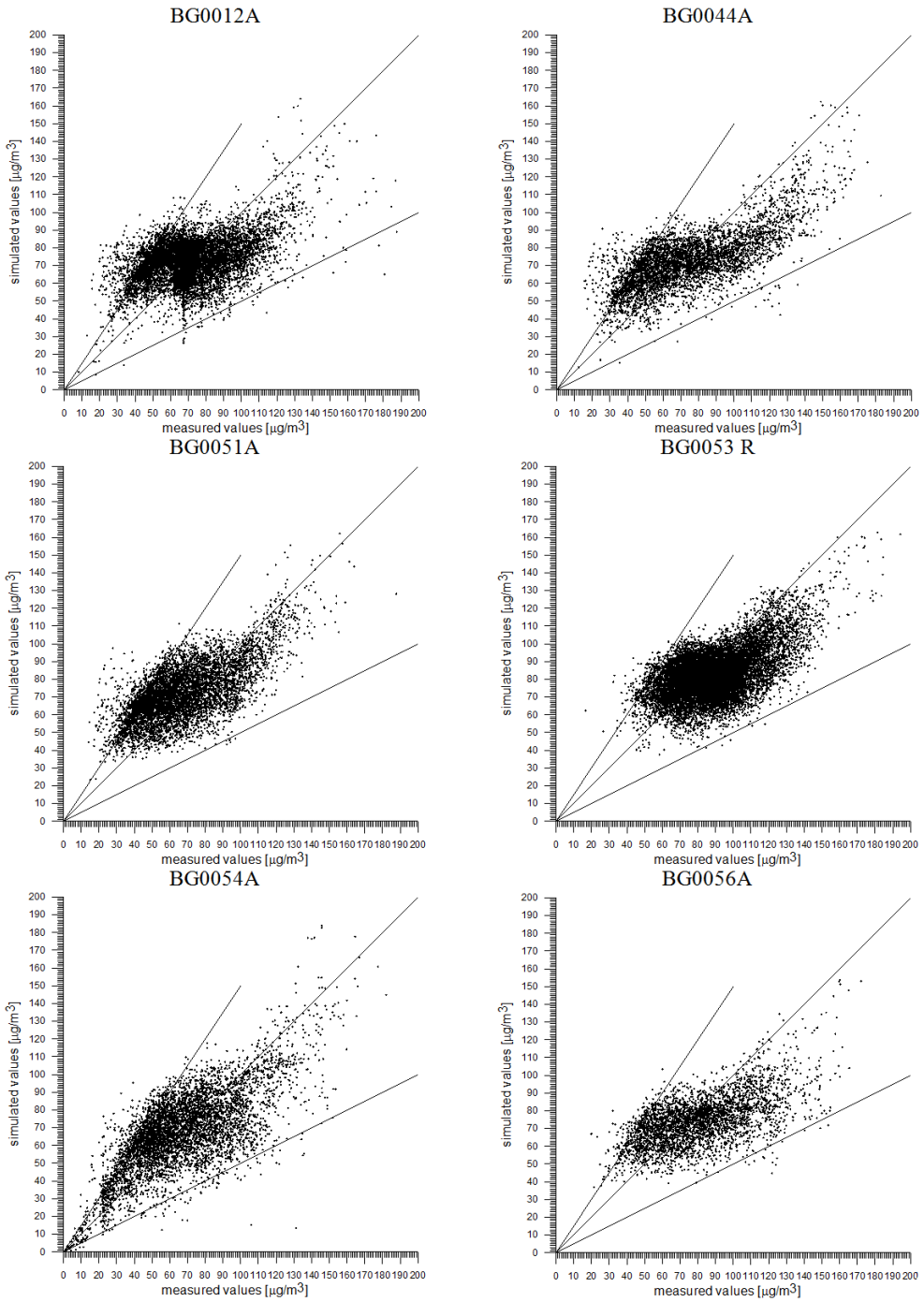

Fig. 1. Scatter diagrams of simulated and measured ozone levels for some of the stations of the Bulgarian National Network for Air Quality Control.

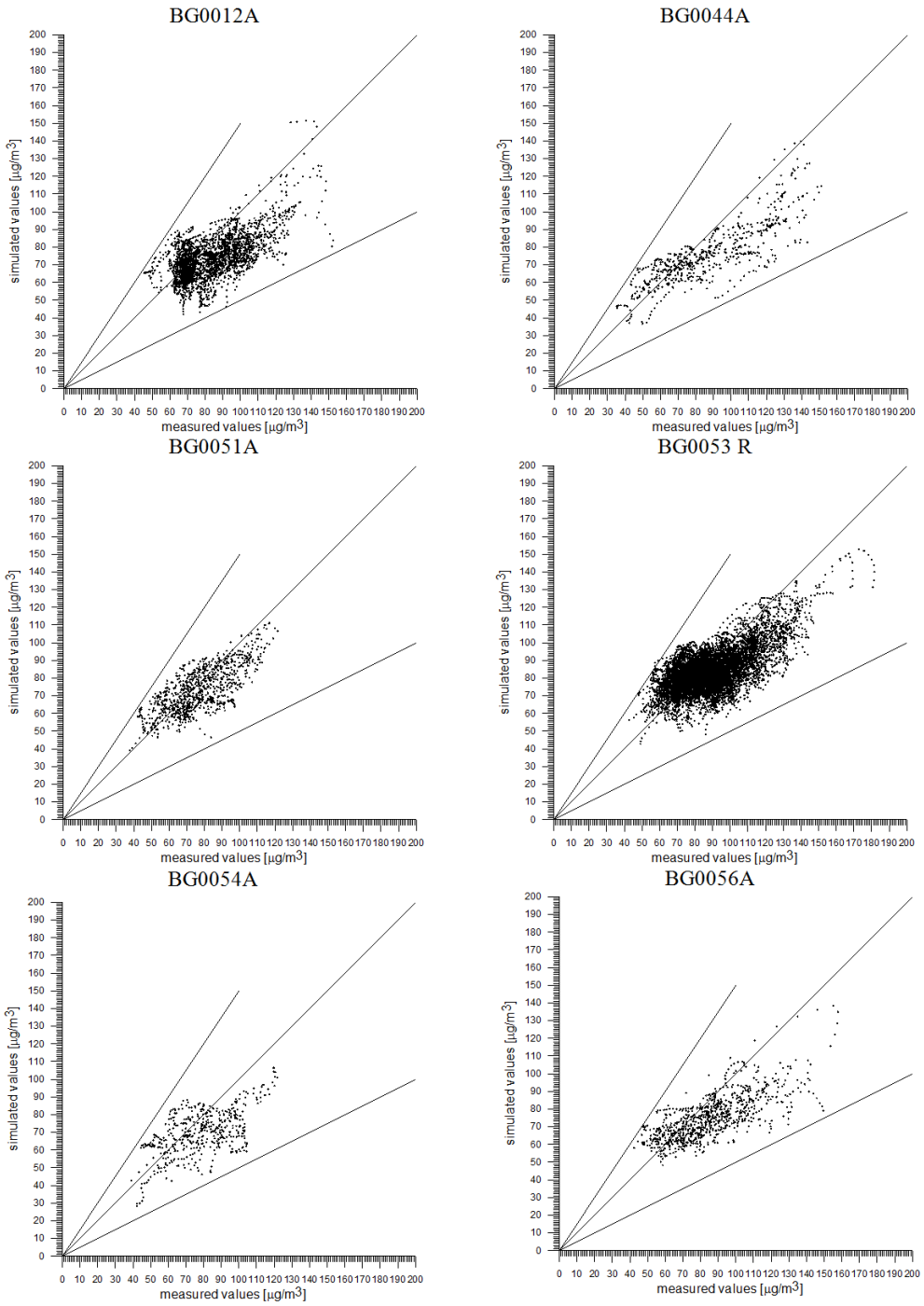

Fig. 2. Scatter diagrams of running 8-hour average values for simulated and measured ozone levels for some of the stations of the Bulgarian National Network for Air Quality Control.

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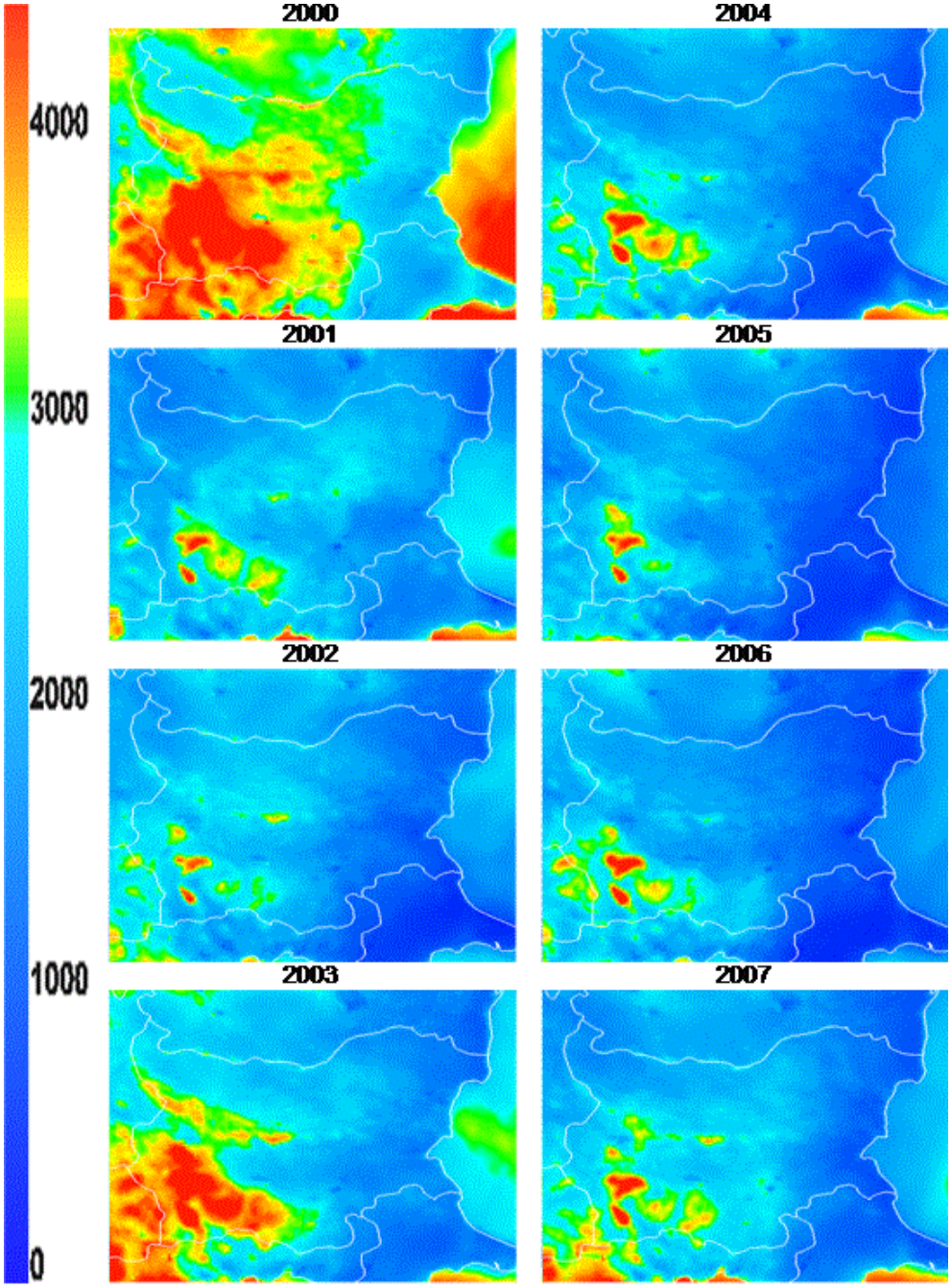

Fig. 3. Simulated AOT40C [ppb.hour] fields for years 2000-2007

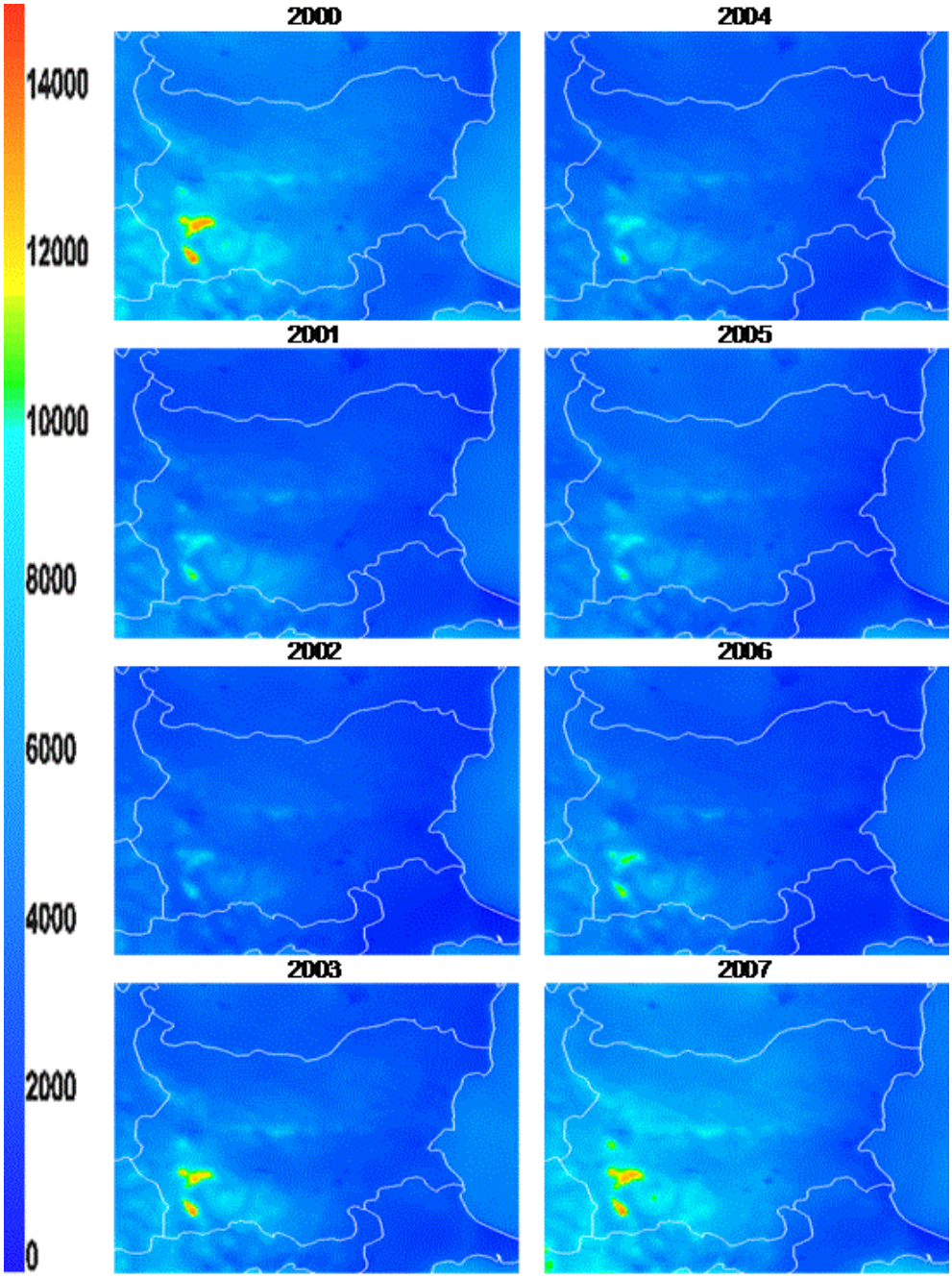

Fig. 4. Simulated AOT40F [ppb.hour] fields for years 2000-2007

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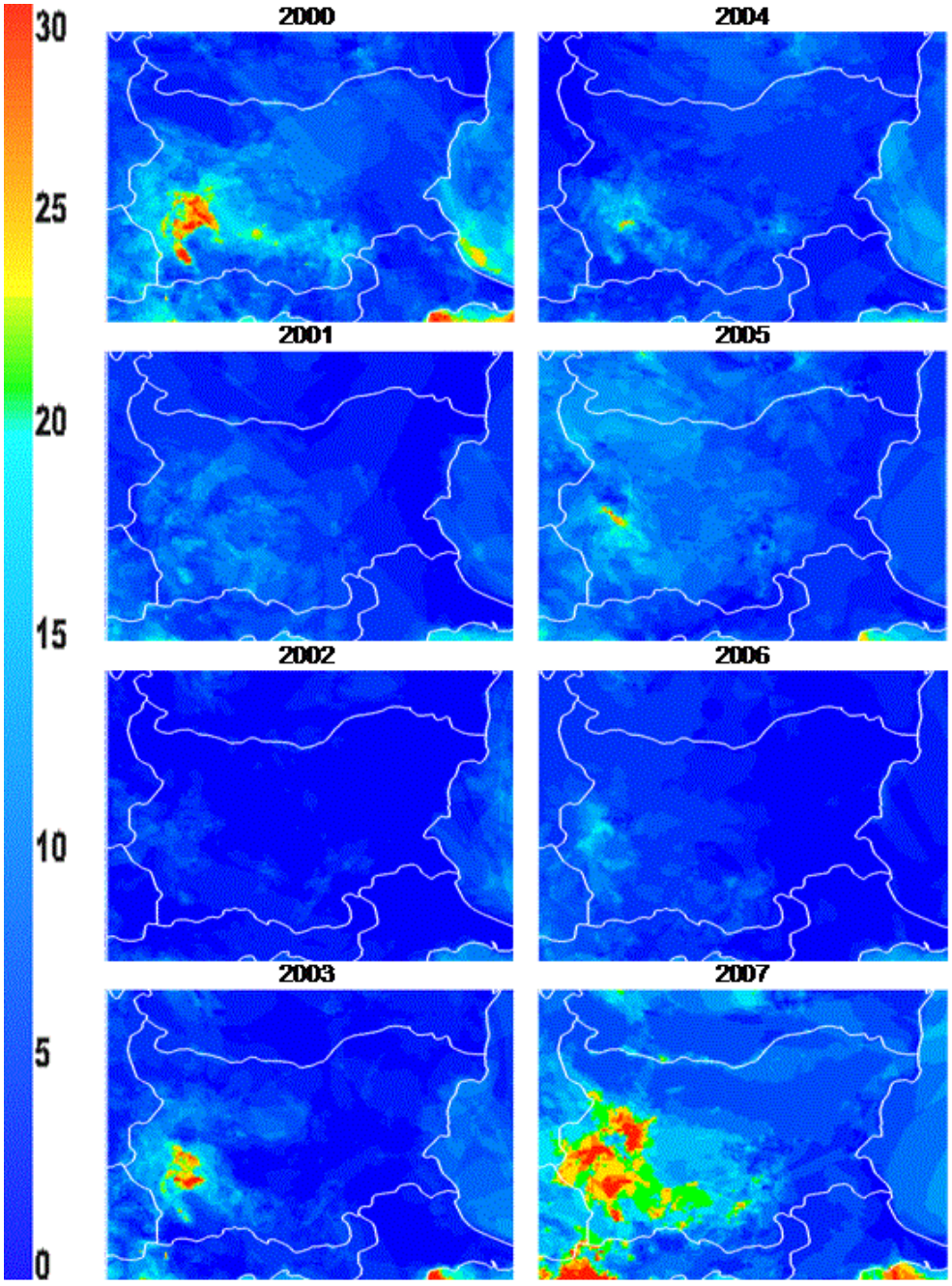

Fig. 5. Simulated NOD60 [number of days] fields for years 2000-2007

7. CONCLUSIONS

The ozone indices demonstrated above show that the environmental status of the country, at least evaluated with a resolution of 3 km, is not so bad from a point of view of ozone pollution.

The generated ensemble of meteorological/air quality computer simulations is rather extensive and can be used for constructing other quantities, which give comprehensive and reliable enough evaluations of the impact of the atmospheric status on environment and human health, for example of some more general air quality indices (Georgieva, 2014), discomfort indices, etc.

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REFERENCES

Amann, M., Bertok, I., Cofala, J., Gyarfas, F., Heyes, C., Klimont, Z., Makowski, M., Schöpp, W., and Syri, S. (1999): Cost-effective control of acidification and ground-level ozone. Seventh Interim Report, International Institute for Applied System Analysis (IIASA), A-2361 Laxenburg, Austria.

Byun, D., Ching, J. (1999) Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. EPA Report 600/R-99/030, Washington DC.

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, and 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, 11-16 January 1998, Phoenix, Arizona, 264-268.

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

Dudhia, J. (1993) A non-hydrostatic version of the Penn State/NCAR Mesoscale Model: validation tests and simulation of an Atlantic cyclone and cold front. Mon. Wea. Rev. 121, 1493-1513.

European Parliament (2002): DIRECTIVE 2002/3/EC of 12 February 2002 relating to ozone in ambient air, *Official Journal of the European Communities* (9.3.2002), **L67**, pp. 14-30.

Gadzhev G., G. Jordanov, K. Ganev, M. Prodanova, D. Syrakov, N. Miloshev (2011) 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**,** in the Proceedings of 9th International Conference on "Large-Scale Scientific Computations". June 3-7, 2013, Sozopol (accepted for publishing).

Gadzhev G., K. Ganev, N. Miloshev, D. Syrakov, M. Prodanova (2013c) Analysis of the Processes which Form the Air Pollution Pattern Over Bulgaria**,** in the Proceedings of 9th International Conference on "Large-Scale Scientific Computations". June 3-7, 2013, Sozopol (accepted for publishing).

Gadzhev G., K. Ganev, D. Syrakov, M. Prodanova and N. Miloshev (2013d) Some Statistical Evaluations of Numerically Obtained Atmospheric Composition Fields in Bulgaria, in the Proceedings of 15th International Conference on Harmonisation within Atmospheric. Dispersion Modelling for Regulatory Purposes. 6-9 May 2013, Madrid, Spain, 373-377.

Georgieva I. (2014) Air Quality Index Evaluations for Bulgaria, in the Proceedings of International Conference on "Numerical Methods for Scientific Computations and Advanced Applications", May 19-22, 2014, Bansko (accepted for publishing).

Grell, G.A., Dudhia J., and Stauffer D.R. (1994) A description of the Fifth Generation Penn State/NCAR Mesoscale Model (MM5). NCAR Technical Note, NCAR TN-398-STR, 138 pp.

Stauffer D.R. and N.L. Seaman (1990) Use of four-dimensional data assimilation in a limited area mesoscale model. Part I: experiments with synoptic data, Mon. Wea. Rev. 118, pp.1250-1277.

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