Description of Bulgarian System for Operational Pollution Forecast, version 2

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INTRODUCTION

The Air Quality (AQ) is a key element for the well-being and quality of life of European citizens. According to the World Health Organization, air pollution severely affects the health of European citizens. There is increasing evidence for adverse effects of air pollution on the respiratory and the cardiovascular system as a result of both acute and chronic exposure. In particular, a significant reduction of life expectancy by a year or more is assumed to be linked to long-term exposure to high air concentrations of particulate matter (PM). There is considerable concern about impaired and detrimental air quality conditions over many areas in Europe, especially in urbanized areas, in spite of about 30 years of legislation and emission reduction. Current legislation, e.g. the Ozone daughter directive 2002/3/EC (European Parliament, 2002), requires informing the public on AQ, assessing air pollutant concentrations throughout the whole territory of Member States and indicating exceedances of limit and target values, forecasting potential exceedances and assessing possible emergency measures to abate exceedances. For the purpose, modeling tools must be used in parallel with air pollution measurements. The goals of reliable air quality forecasts are the efficient control and protection of population exposure as well as possible emission abatement measures. In last years the concept of "chemical weather" arises and in many countries respective forecast systems are being developed along with the usual meteorological weather forecasts (see, for instance, Sofiev at al., 2006, Poupkou et al., 2008a, 2008b, Monteiro et al., 2005, San Jose et al., 2006, and others).

Air pollution easily crosses national borders. It would be cost-effective and beneficial for citizens, society and decision-makers that national chemical weather forecast and information systems were networked across Europe. For the purpose several projects in the European Framework Programs (GEMS, PROMOTE, MEGAPOLI, MACC, PASODOBLE etc.) as well as the COST Action ES0602 "Towards a European Network on Chemical Weather Forecasting and Information Systems") were launched aiming at providing a forum for harmonizing, standardizing and benchmarking approaches and practices in data exchange and multi-model capabilities for air quality forecast and (near) real-time information systems in Europe. It is supposed to examine existing, and work out new solutions for integrating the development efforts at national and international levels. One can find several CW systems' (performance and descriptions) in Action web-portal (http://www.chemicalweather.eu/Domains).

Bulgaria joined the COST Action ES0602 from its very beginning. This participation invoked a project supported by the National Science Fund with the Bulgarian Ministry of Education, Youth and Science. Its main purpose was to create a Prototype of Bulgarian Chemical Weather forecast and information system (BgCWFIS v.1) intended to provide timely, informative and reliable forecasts tailored to the needs of various users (see Syrakov et al. 2009, 2012). Later on, partly in the frame of EU FP7 project PASODOBLE ("Promote Air Quality Services Integrating Observations – Development of Basic Localized Information for Europe") new versions of the

system (v.2 and v.3) were elaborated with downscaling of the service to resolution of 1 km over Sofia city. Here, the version 2 of BgCWFIS will be described and its end-user products will be presented.

MODELS USED

BgCWFIS is designed in a way to fit the real-time constraints and to deliver forecasts for the next 3 days on an hourly basis. US EPA Models-3 air quality modeling system is used, here, consisting of:

- **CMAQ v.4.6** - Community Multi-scale Air Quality model, http://www.cmaq-model.org/, Denis et al. (1996), Byun and Ching (1999), Byun and Schere (2006), the Chemical Transport Model (CTM);
- **WRF v.3.2.1** - Weather Research and Forecasting Model, http://www.wrf-model.org/, Skamarock et al. (2005), the meteorological pre-processor to CMAQ;
- **SMOKE v.2.4** - Sparse Matrix Operator Kernel Emissions Modelling System, http://www.smoke-model.org/, Coats and Houyoux (1996), Houyoux and Vukovich (1999), CEP (2003), the emission pre-processor to CMAQ.

In the System, WRF is driven by the NCEP GFS (Global Forecast System) data that can be accessed freely from http://www.ftp.ncep.noaa.gov/data/nccf/com/gfs/prod/. This data is global weather forecast in GRIB-2 format with space resolution of 1°×1° and 6-hour time resolution. The downloading of this data is invoked automatically every day at 00:00Z. 84-hour run starting at 12:00Z of the previous day is performed; the first 12 hours of this period being spinning-up followed by a 3-day weather forecast. The chemical weather forecast duration is from 00:00Z of the current day to 00:00Z of the forth day after (3-day forecast).

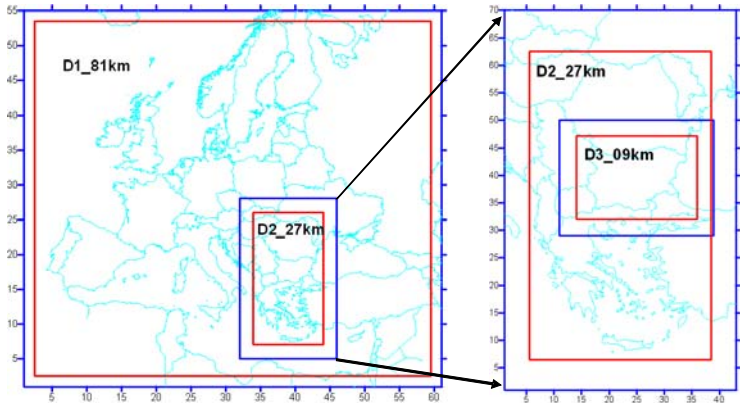

Fig 1a. *Domains of BgCWFIS, ver.2.1: **WRF** (blue) and **CMAQ** (red) domains.*

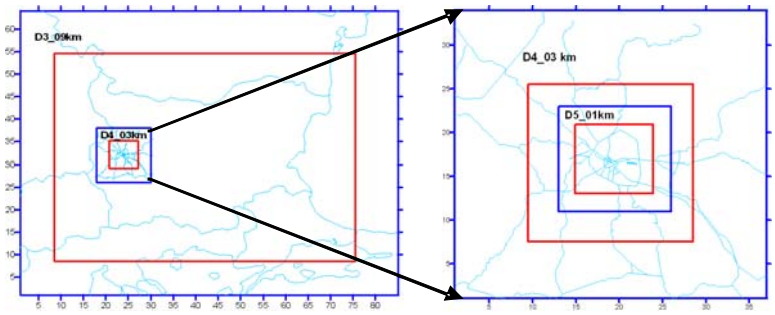

Fig 1b. *Domains of BgCWFIS, ver.2.2: **WRF** (blue) and **CMAQ** (red) domains.*

MODEL DOMAINS

The nesting capabilities of WRF and CMAQ are used to downscale the forecasts from European region to Sofia-city area. The resolution of the mother domain (Europe) is 81 km, big enough as to correspond to the GFS met-data resolution. Four other domains are nested in it and in each other – Balkan Peninsula (27 km resolution), Bulgaria (9 km), Sofia district (3 km) and Sofia city (1 km) as shown in Fig. 1a,b.

In version 2 of BgCWFIS, climatic data is used for chemical boundary conditions at the mother domain (Europe) following the presumption that the errors introduced by this assumption will decrease quickly to the center of the region due to the continuous acting of the pollution sources. All other domains receive their boundary conditions from the previous domain in the hierarchy. For the sake of convenience, the web-output of this version of the System is divided to two parts – ver.2.1 (Europe – Balkans – Bulgaria, http://info.meteo.bg/cw2.1/) and ver.2.2 (Bulgaria – Sofia_district – Sofia_city, http://info.meteo.bg/cw2.2/).

INFORMATION FLOW

The models indicated above are linked with a number of Linux scripts and interface programs in a way to be able to pre-calculate the future level of many air pollutants for every System's domain. The data flow diagram is presented in Fig.2.

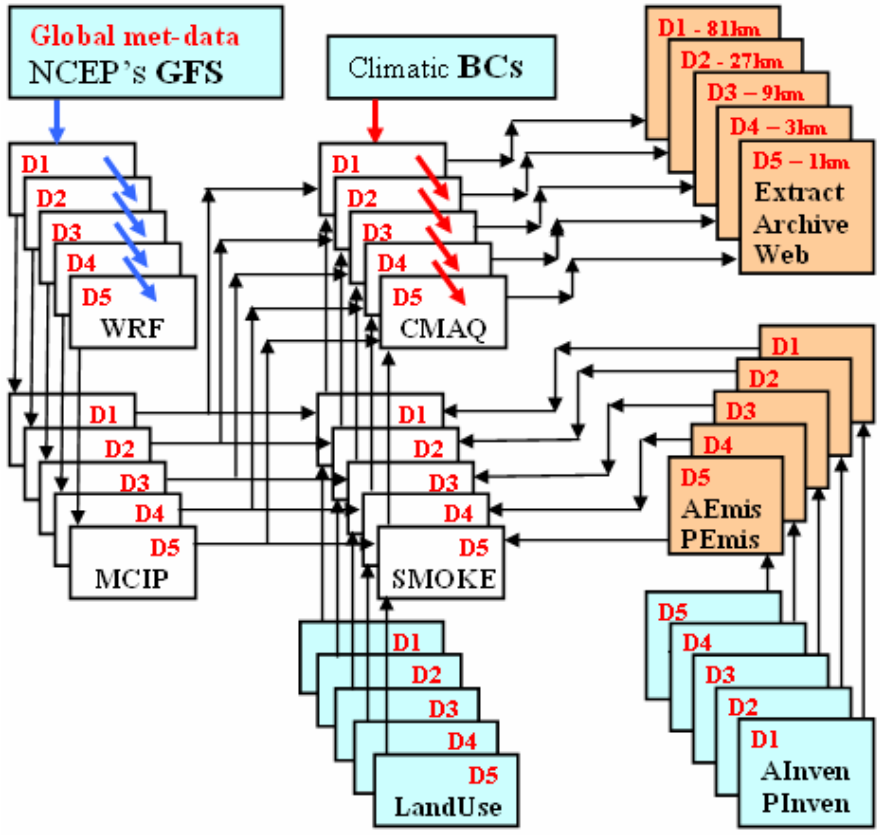

Fig 2. *BgCWFIS, ver.2, information flow diagram. The white boxes presentModels-3 elements, the blue ones – input data, and the brown ones – specific pre-and pos-processing routines. The blue arrows denote the transfer of meteorological boundary conditions between the domains and the red arrows – the chemical boundary conditions. The black arrows show the exchange of information between the System's elements in each separate domain.*

The Models-3 elements are denoted by white boxes on the diagram, the blue boxes present the different kinds of input information. Those are: the meteorological numerical forecast that drives

the meteorological pre-processor of the System (WRF) downloaded from NCEP's GFS data web-site; the climatic values of a number of air pollutants used as chemical boundary conditions for the mother domain (Europe) that do not change with time; the emission inventory data for 2005 provided by TNO, Netherlands (Denier van der Gon et al., 2010), gridded according to the System's domains, and the respective five sets of land-use data (USGS data base, http://landcover.usgs.gov/). The land use data is extracted by WRF pre-processing module. The brown boxes present FORTRAN programs aimed at emission input modeling of Area Sources (AS) and Large Point Sources (LPS), as well as data post-processing (extracting, archiving, image processing).

The data exchange in the System is denoted with arrows. The color arrows show the data exchange between computational domains, while the black arrows – the data exchange inside each one of the domains. Shortly, the WRF outputs feed MCIP (Meteorology-Chemistry Interface Processor) module of Models-3 system; MCIP prepares the meteorology input to CMAQ which is used also by SMOKE for calculating Biogenic Sources (BgS) emissions on the base of the respective LandUse data. The gridded inventory data (AInven, PInven) feeds AEmis and PEmis programs that produce the respective AS- and LPS-emission files. SMOKE is used once more to merge AS-, LPS- and BgS-data in a common emission input to CMAQ. Finally, the CMAQ output is post-processed in a way to extract the most important pollutants, to archive them, to produce hourly images with concentration distribution of 4 key pollutants (NO2, SO2, Ozone and PM10) and to upload them to the respective web-sites. These procedures are repeated for all 5 domains of the system in the next order: WRF, MCIP, AEmis, PEmis, SMOKE (BgS and merge), CMAQ, post-processing. Meanwhile, WRF and CMAQ produce boundary condition files to be used by the inferior domains. The WRF and CMAQ mother domains take boundary conditions from GFS-data and climatic chemical profiles of CMAQ, respectively.

METEOROLOGICAL MODELLING

The Weather Research and Forecasting (WRF) Model is a next-generation mesocale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. It is an evolutionary successor to the MM5 model. The creation and further development of WRF is due to the collaborative efforts of several US institutions like NCAR, NOAA, NCEP and others. The WRF is a fully compressible and non-hydrostatic model with terrain-following hydrostatic pressure coordinate. The grid staggering is the Arakawa C-grid. One can find more info on http://www.wrf-model.org/index.php. Free download can be made on http://www.mmm.ucar.edu/wrf/users/download/get_sources.htm.

In BgCWFIS, WRF-ARW (Advanced Research WRF), version 3.2.1, is exploited. The vertical structure is of 27 levels. The Analysis Nudging option (Four-Dimensional Data Assimilation, Stauffer and Seaman, 1994) is switched on for the first computational domain, only, i.e. WRF forecast is nudged to the meteorological driving data (GFS).

WRF-ARW offers multiple physics options that can be combined in any way. Here, well-tried schemes are used, namely:

Physics Options	**Parameterization**
Microphysics	WSM6 scheme (Hong and Lim, 2006)
Cumulus Parameterization	Kain-Fritsch scheme (Kain, 2004)
Planetary Boundary Layer	YSU scheme (Hong et al., 2006)
Longwave Radiation	RRTM scheme (Mlawer et al., 1997)
Shortwave Radiation	Dudhia scheme (Dudhia, 1989)
Land Surface Model	NOAH LSM scheme (Chen and Dudhia, 2001)

The coupling of a meteorological and chemical transport models is not a trivial issue. Since almost all meteorological models are not built for air quality modeling purposes, interface processing is needed. Such an element in Models-3 system is MCIP (Meteorology-Chemistry

Interface Processor). Here, MCIP v.3.6. is applied. MCIP deals with issues related to data format translation, diagnostic estimations of parameters not provided by WRF (like dry deposition velocities for various species), extraction of data for appropriate window domains, and reconstruction of meteorological data on different grid and layer structures. As far as WRF-ARW and CMAQ are concerned, both utilize the Arakawa C-grid and conformal map projections; no special horizontal interpolation is required. MCIP may modify the vertical structure by interpolation between WRF layers. The sigma-levels of CMAQ in this application are 14:

σ = 1.0, 0.993, 0.99, 0.98, 0.965, 0.945, 0.91, 0.86, 0.8, 0.74, 0.65, 0.55, 0.4, 0.2, 0.0

EMISSION MODELLING

CMAQ demands its emission input in specific format reflecting the time evolution of all pollutants accounted for by the chemical mechanism used (CB-IV in this case). Emission inventories are used as row data for anthropogenic emission processing. The inventories are made on annual basis for big territories; many pollutants are estimated as groups (VOC and PM2.5 for instance). Preparation of emission input to a Chemical Transport Model requires emission processing. Such emission processing component in EPA Models-3 system is SMOKE but it is partly used, here, because its quite strong relation to US emission sources specifics. In BgCWFIS, SMOKE is used only for calculating BgS emissions and for merging AS-, LPS- and BgS-files into a CMAQ emission input file. The area source emissions and the large point source emissions are prepared by the interface programs AEmis and PEmis.

Inputs to AEmis and to PEmis are the respective gridded AS- and LPS-inventories. For the moment, TNO inventory for 2005 (Denier van der Gon et al., 2010) is exploited for the two senior domains (Europe and Balkans). For Bulgarian domains the national inventory for 2010 as provided by Bulgarian Executive Environmental Agency is used. The TNO produced several sets of inventories for different years. The anthropogenic sources in this inventories are distributed over 10 SNAPs (Selected Nomenclature for Air Pollution) classifying them according to the processes leading to harmful material release into the atmosphere (EMEP/CORINAIR, 2002).

The 2005 TNO inventory has resolution of 0.125°?0.0625° (about 7?8 km). It is distributed as a comma- or tab-delimited text-file. Each line of the file contains data for a single source, namely the mesh coordinates, the country, the type of source (A/P), the SNAP, and the yearly emissions of 8 pollutants. The SNAP 7 (road transport) is presented as 5 sub-SNAPs. The pollutants are: methane (CH4), carbon oxide (CO), nitric oxides (NOx), sulfur oxides (SOx), non-methane volatile organic compounds (NMVOC), ammonia (NH3), Particulate Matter with $d<10\mu m$ (PM10) and Particulate Matter with $d<2.5\mu m$ (PM2.5).

As already stated, the inventory data can not be used directly as emission input to CTMs. Three operations must be applied to this data, preliminary: gridding, temporal allocation (imposing of time variations on the yearly values) and speciation (splitting of group pollutants to several simpler or lump pollutants).

The ***gridding*** is recalculation of the inventory data to the grids used (5 grids with different resolution, here). A web-based GIS system is created for the purpose. The TNO data is introduced in the system. Number of so-called custom grids can be defined on the base of the standard grid description (projection type, central point coordinates, mean meridian, distances to the grid origin, number of points, resolution). The system recalculates the inventory quantities for each cell and type of source.

Additional functionalities of the system are introduced linked to the Bulgarian inventory. A specific feature of this inventory is that the data for SNAP 1-6 is attributed to particular sources with there coordinates. For SNAP 7-10 total country amounts of the released pollutants are available. First is the possibility of the GIS-system for aggregation of SNAPs 1-6 to the custom grids. In contrast, SNAP 7-10 inventory data is disaggregated to the same grids using different geometric elements (surrogates). For instance, SNAP 7 (Road transport) is disaggregated by *HighWays* (15%), *RoadsClass1* (25%), *RoadsClass2* (20%) and *TownStreets* (40%). SNAP 8 (Non-

road transport) uses *Airports* (45%), *RoadsClass2* (20%), *RailRoads* (25%), *AgricultureAreas* (10%). For SNAP 9 (Waste disposal) the surrogates are *Population* (50%) and *WasteAreas* (50%). Finally, SNAP 10 (Agriculture) is distributed according to *AgricultureAreas* (30%) and *Pastures* (70%). It is worth to mention that new surrogates can be added to the system and used in the disaggregation. The share of each surrogate can be changed, too.

The ***temporal allocation*** is made on the base of temporal profiles, provided by TNO (Builtjes et al., 2003). They are used also in both AQMEII exercises (http://aqmeii.jrc.ec.europa.eu). According to the anthropogenic activity the profiles are divided into three groups – Monthly, Weekly, and Hourly profiles. The first two are country-, SNAP- and pollutant-specific; the hourly factors refer to the local time and are SNAP-specific only. Together with them, TNO provides a vertical profile for large point sources that is SNAP-specific.

The ***speciation*** profiles are elaborated on the base of US EPA ones (http://www.epa.gov/ttn/chief/emch/speciation/) using the expert approach. Coincidence between main US sources with European SNAPs is obtained first. The weighted averages of the respective speciation profiles are accepted as SNAP-specific splitting factors, weights being the percentage of contribution of every source type in total emission in particular SNAP. In such a way VOC, PM2.5, NOx and SOx speciation profiles are derived. It must be noticed that the choice of US source types and the weights of their contribution to the respective SNAP emissions are quite subjective. Much more work is needed to elaborate country-specific profiles.

The gridded inventories are input to the emission processing programs AEmis and PEmis, where the remaining two procedures are applied. In PEmis, vertical allocation takes place as well. Both programs produce respective emission file. The AEmis output is 2-dimensional, the PEmis one – 3-dimentional. Both outputs are in IO/API NetCDF format and contain hourly data for all forecast period.

The biogenic emissions are prepared by SMOKE by the BEIS-3.13 mechanism (Schwede et al., 2005) on the base of the gridded LandUse data. SMOKE merges the 3 emission files in a common CMAQ emission input – hourly data in NetCDF format.

OPERATIONAL PERFORMANCE OF BGCWFIS

Fourteen σ-levels with varying thickness determine the vertical structure of CMAQ. The Planetary Boundary Layer (PBL) is presented by the lowest 8 of these levels.

The CMAQ v.4.6 input consists of various files containing concentration, deposition, visibility and other variables. The concentration output is a NetCDF file with 3-D hourly data for 78 pollutants, of which: 52 gaseous, 21 aerosols (Aitken and accumulation modes), 5 aerosol distributions (3 by number, 2 by aerosol area).

The last box in Fig. 1 (upper-right) tags the post-processing that is quite important making BgCWFIS results visual. First of all the post-processing program XtrCON extracts part of the pollutants for archiving and further handling. Only surface values of the most important 17 pollutants are saved – 8 gases and 9 aerosols. Part of these pollutants is more or less monitored and they are referred in the European legislation with the respective thresholds. It must be mentioned that the sum of all aerosol compounds forms PM10 that is usually measured. The coarse particle matter (CPRM) is one of the saved aerosol compounds, so PM2.5=PM10–CPRM is also calculated and archived as separate pollutant. All this data is stored in a respective archive file.

As to make the results of BgCWIS operation public, specialized web-site was created on the NIMH server (http://www.meteo.bg/en/cw/). For the moment it presents 4 main pollutants – Ozone, NO2, SO2 and PM10. It is fed by images created using the PAVE software package (http://www.ie.unc.edu/cempd/EDSS/pave_doc/index.shtml). PAVE supports its own meta-language that allows drawing plots in an automatic way by invoking the respective scripts.

In Fig.3, an example of BgCWFIS web site is displayed. A particular pollutant is invoked by clicking in the list at the left side of the page. Note, that together with hourly ozone concentrations, two types of ozone daily maxima can be visualized.

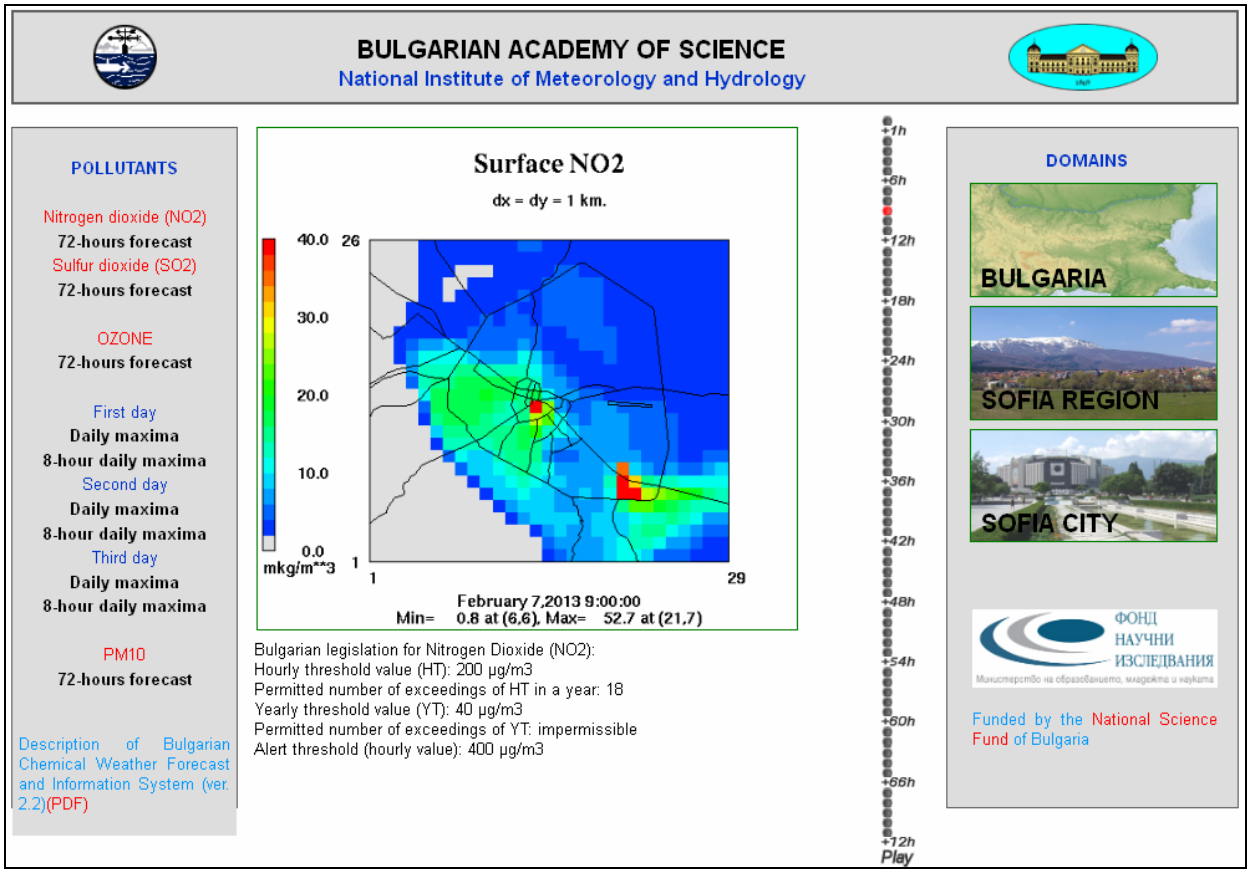

Fig 3. *Example of BgCWFIS web site.*

The region of forecast can be chosen by clicking on one of the small images on the right. In the center of the page hourly concentration field of the chosen pollutant is situated. Putting the mouse cursor on one of the points from the point column on the right side of the image invokes the forecast field for the respective hour. Putting the cursor over "Play" invokes animation of the forecast. Under each pollutant's view, respective thresholds according to Bulgarian legislation (harmonized with European one) are shown. At the bottom of pollutants list a link to a pdf-file with description of Bulgarian Chemical Weather Forecast and Information System, version 2, is placed.

CONCLUSION

The Bulgarian Chemical Weather Forecast and Information System is designed on the base of US EPA Models-3 System: MM5 (meteorological pre-processor), SMOKE (emission pre-processor) and CMAQ (Chemical Transport Model). The meteorological input to the system is the NCEP Global Forecast data. At this stage, the emission input exploits the high resolution inventory for year 2005 produced by TNO, The Netherlands. The Bulgarian national emission inventory for 2010 is used as well. The system is realized on 5 nested domains with increasing resolutions.

At the moment, the system is running automatically once a day (00Z). The forecast period is 3 days (72 hours). The results of each System's run are post-processed in a way to archive the most important pollutants. Part of these pollutants is visualized as sequences of maps giving the evolution of the air quality over Europe and Bulgaria and can be seen on the system's web-site (http://www.meteo.bg/cw/).

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