

WRF-CMAQ REGIONAL AIR QUALITY MODELING SYSTEM RESULTS ESTIMATED VS. MEASUREMENT DATA

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Abstract

The air quality modelling system WRF-CMAQ was applied by the Bulgarian NIMH (National Institute for Meteorology and Hydrology) team to the European domain in the frame of the Air Quality Model Evaluation International Initiative, Phase 2 (AQMEII-2). The model system was set up for the European domain of 5000×5000 km size with horizontal resolution of 25 km. The emissions were available through AQMEII and further processed in a way to feed the chemistry transport model CMAQ. The meso-meteorological model WRF was driven by NCEP GFS data with 1°×1° resolution. The chemical boundary conditions were extracted from MACC global simulation data. Model performance was investigated by means of AQMEII-2 web-based evaluation platform ENSEMBLE. A preliminary model evaluation for ozone and particulate matter was conducted based on comparison between simulated and observed concentrations at different type of surface stations in the EU wide domain. Model performance was characterized by overestimation for ozone and underestimation for the other pollutants. The relative statistical indicators were also discussed in view of recently published performance criteria.

Key words: Air Quality Modeling, Regional Chemical Transport Models, AQMEII

1. INTRODUCTION

Due to the extensive worldwide development during the last three decades the chemical transport models (CTM) have been recognised to be a useful tool for air quality management and assessment at local, regional and global scales because of the increased concern regarding the impacts of atmospheric pollution on human health and sensitive ecosystems. Nowadays they are able to provide researchers, decision-makers, and the general public with more reliable information on the quality of the air, and hence, acting as valuable tools to develop and implement air quality regulations, emission control strategies, and air quality forecast for the protection of human health.

During the years air quality modelling applications at regional scale have evolved from the study of photochemical air pollution episodes to multi-pollutant and multiyear integrated analysis. Major attention has been given to ozone (O₃) and particulate matter (PM) due to their known impacts on air quality and human health and since high levels of these pollutants have been registered in monitoring stations, even overcoming the regulation limits.

AQMEII (<http://aqmeii.jrc.ec.europa.eu/>) stands for Air Quality Model Evaluation International Initiative. It aims to build a common strategy on model development and future research priorities, and establish methodologies for model evaluation to increase knowledge on processes and to support the use of models for policy development (Rao et al., 2011). Long-term air quality simulations for North America and Europe, performed by different models used worldwide, and the evaluation of results, both individually and as an ensemble approach, are the basis to achieve the objectives of this innovative initiative.

In the frame of the AQMEII exercises, all participating groups were requested to produce simulations on one year (2006 for Phase 1, and 2010 for Phase 2) for one or for two of the continents, results undergoing evaluation/inter-comparison. The input data for these calculations was partly choice of participants (such as the models, the grid, the basic meteorology) but good deal of this information was common, prepared especially for the exercises (chemical boundary conditions, anthropogenic and wild fire emissions). These exercises have produced a large set of results, in the form of 4D concentration and deposition fields of many gaseous and particulate pollutants as well as emission and meteorological parameters. A web-based platform for model inter-comparison and multi-model ensemble analysis, the ENSEMBLE system, was developed by JRC (Galmarini et al., 2004a, b, Potempski and Galmarini, 2009) and upgraded for AQMEII purposes. This tool has been used to archive and analyse, both qualitatively and quantitatively, the meteorological and air quality modelling results obtained. For the purpose, the simulation results of each participating group had to be converted to prescribed

format and uploaded to a specialized ftp-server in JRC. The performance of the AQ modelling systems was evaluated using routine AQ and meteorological surface monitoring network measurements, as well as sets of upper air measurements, obtained by ozonesondes and instrumented commercial aircrafts. All observational data were preliminary introduced in the ENSEMBLE system (<http://ensemble2.jrc.ec.europa.eu/cgi-bin/ensemble/ensemble5.cgi/>).

So far the Phase 1 of AQMEII was conducted and data analyzed, results published in many scientific papers (see AQMEII web site for list of publications), part of them gathered in special issues of the scientific journals Atmospheric Environment (v.53, June 2012) and Environmental Manager (v. 38, July 2012).

As a result of the successive completion of the Phase 1 of AQMEII, the Phase 2 was launched in 2012. It has to focus on the interactions of air quality and climate change. In this Phase, mainly coupled meteorology-atmospheric chemistry models would be applied to assess how well the current generation of coupled regional-scale air quality models can simulate not only the pollution characteristics, but also the observed space-time variability in the optical and radiative characteristics of atmospheric aerosols and associated feedbacks among aerosols, radiation, clouds, and precipitation.

The air quality modelling team with Bulgarian National Institute of Meteorology and Hydrology took part in the Phase 2 of AQMEII simulating year 2010 for Europe. Though the exercise is based on coupled models, the participation with uncoupled meteorological and chemical transport models was welcome. NIMH participated with WRF and CMAQ models, already used in constructing Bulgarian Chemical Weather Forecast Systems, version 2 (<http://www.meteo.bg/cw/> Syrakov et al, 2012) and version 3 (<http://www.niggg.bas.bg/cw3/>, Syrakov et al., 2013). The paper describes the NIMH task settings and preliminary results of verification of WRF-CMAQ modelling systems using the ENSEMBLE platform capabilities.

The study presented here makes use of the JRC ENSEMBLE model evaluation platform and the monitoring data gathered for the AQMEII-2 activity, but should not be considered as part of the current AQMEII-2 scientific program that evaluates mainly online coupled models. Thus, this work should be seen as an independent model evaluation study of the air quality model system used at NIMH.

2. THE NIMH TASK SETTINGS

Good enough time before starting the preparation for calculation, several documents prepared by AQMEII coordination team were distributed among the participants. They contained description of the exercise, recommendations for domain choice and information about the sources of necessary input information. Later on, a specialized AQMEII-2 wiki-page (<http://aqmeii-eu.wikidot.com/>) was created, intended to help mainly European participants. In this wiki-page detailed information and recommendations were posted and NIMH team intensively used this information.

2.1. Models used

As already mentioned NIMH team applied US EPA Models-3 air quality modelling system 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 of the system;
- **WRF v.3.3** - Weather Research and Forecasting Model, <http://www.wrf-model.org/>, Skamarock et al. (2005, 2008), 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.

The Community Multi-scale Air Quality model (CMAQ) is a 3D Eulerian photochemical dispersion model that allows for an integrated assessment of gaseous and particulate air pollution over many scales ranging from sub-urban to continental. CMAQ simulates the transport, dispersion, chemical reaction, and removal of pollutants in the troposphere by solving the pollutant continuity equation for each chemical species on a system of nested three-dimensional grids. In version 4.6 of CMAQ used in this study, the gas-phase photochemistry is resolved through the Carbon Bond IV (CB4) chemical mechanism. The model contains detailed algorithms for the relevant processes, including aqueous chemistry, inorganic aerosol thermodynamics/partitioning (ISORROPIA 1.7), Secondary Organic Aerosol formation/partitioning (SOAP), RADM (Regional Acid Deposition Model) cloud model scheme. The predefined mechanism configuration is set to "cb4_ae4_aq". Specific output of CMAQ is visibility data – gridded extinction coefficients and visibility haze index "deciwiew". In CMAQv4.6

this data is calculated only for the near-surface layer. As far as one of the required by AQMEII parameters is the aerosol optical depth (AOD) which is the vertically integrated extinction coefficient, CMAQ source code was remade in a way to calculate and output the visibility parameter at each model layer. Fourteen σ -levels with varying thickness determine the vertical structure of CMAQ for this exercise. The Planetary Boundary Layer (PBL) is presented by the lowest 8 of these levels.

The Weather Research and Forecasting (WRF) Model is a next-generation mesoscale 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 type. For AQMEII-2 version 3.3 of WRF is exploited. The Analysis Nudging option (Four-Dimensional Data Assimilation, Stauffer and Seaman, 1994) is switched on, i.e. WRF forecast is nudged to the meteorological driving data (NCEP GFS data). WRF-ARW offers multiple physics options that can be combined in any way. Here, the well-trying and the most frequently exploited schemes are used, namely: WSM6 scheme (Hong and Lim, 2006) for microphysics; Kain-Fritsch scheme (Kain, 2004) for cumulus parameterization; YSU scheme (Hong et al., 2006) for PBL; RRTM scheme (Mlawer et al., 1997) for longwave radiation; Dudhia scheme (Dudhia, 1989) for shortwave radiation; NOAA Land Surface Model scheme (Chen and Dudhia, 2001). The vertical structure is 27 layers with increasing thickness. The first 9 of them are in the planetary boundary layer.

The linkage of meteorological and chemical transport models is not a trivial issue. Since almost all meteorological models are not built for air quality modelling purposes, interface processing is needed. Such an element in Models-3 system is MCIP (Meteorology-Chemistry Interface Processor, Otte and al., 2005). 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 and CMAQ are concerned, both utilizing the Arakawa C-grid and conformal map projections; no special horizontal interpolation is required. MCIP modifies the vertical structure by interpolation between WRF layers (i.e. from the 27 WRF levels to the 14 CMAQ ones).

CMAQ demands its emission input in specific format reflecting the time evolution of all pollutants accounted for by the chemical mechanism used. Emission inventories are the row data for anthropogenic emission processing. The inventories are made on annual basis for big territories; many pollutants are estimated as groups (VOC and PM_{2.5}, for instance). The emission pre-processing component in EPA Models-3 system is SMOKE, but it is partly used here, because of its quite strong relation to US emission sources specification. In the current WRF-CMAQ modelling system, SMOKE is used only for calculating biogenic source (BgS) emissions, exploiting the BEIS 3.13 mechanism (Schwede et al., 2005) on the base of the current meteorology and the gridded LandUse (LU) data. The anthropogenic Area Source (AS) emissions and Large Point Source (LPS) emissions are prepared by the specially created interface programs *AEmis* and *PEmis*. SMOKE is used also for merging respective AS-, LPS- and BgS-files into a common CMAQ emission file.

2.2. Calculation domain

The Lambert conical projection is used to present the Earth surface as plane. The true latitudes are 30° and 60°. The modelling domain window has the following parameters: central point with coordinates $X_c=13^\circ$ (longitude) and $Y_c=51^\circ$ (latitude), mean meridian $X_m=13^\circ$, distances to the window origin (the first west-southern grid point) $X_{orig}=Y_{orig}= -2500$ km. The number of grid points is $N_x=N_y=201$ and the space resolution is $D_x=D_y=25$ km. In Fig.1, the NIMH modelling domain is presented (black boundary), together with ENSEMBLE domain (red boundary). This is the CMAQ area, nested in the WRF domain (not shown). WRF's pre-processing routine *geogrid.exe* produces all necessary geodetic data like gridded albedo, emissivity, vegetation type, roughness, etc, including the LU data. All this information is extracted online from the US Geological Survey (USGS) database.

2.3. Sources of emission data and emission processing

The release of harmful materials in the atmosphere is a result of many different processes, mainly the human activity. But the natural emissions as dust and sea salt production, wild fires and the release of organic gases from the soil and vegetation are linked to specific chemical and aerosol interactions and can be a dominating factor that determines the pollution status in specific regions and in particular periods of time.

2.3.1. Anthropogenic emissions

The anthropogenic emissions for AQMEII-2, are provided by TNO (Netherlands Organization for applied scientific research) and correspond to a recent update of the TNO-MACC emissions inventory (Keunen et al.,

2011, 2013, Pouliot et al., 2012). The TNO inventory consists of the anthropogenic emissions from ten SNAP (Selected Nomenclature for Air Pollution) sectors and international shipping. The ten SNAP sectors are (EMEP/CORINAIR, 2002): energy transformation, small combustion sources, industrial combustion, industrial processes, extraction of fossil fuels, solvent and product use, road transport, non road transport, waste handling, and agriculture. Subject of the inventory are 8 pollutants: methane (CH_4), carbon oxide (CO), nitric oxides (NO_x), sulfur dioxide (SO_2), non-methane volatile organic compounds (NMVOC), ammonia (NH_3), Particulate Matter with $d < 10 \mu\text{m}$ (PM_{10}) and Particulate Matter with $d < 2.5 \mu\text{m}$ ($\text{PM}_{2.5}$). The territory covered by this inventory extends well beyond the EU boundaries and encompasses 43 countries and 5 marine areas. The resolution of the gridded emission data is $1/8^\circ \times 1/16^\circ$ longitude-latitude, which is about $7 \times 8 \text{ km}^2$. The sources are specified as Area and Point ones as well.

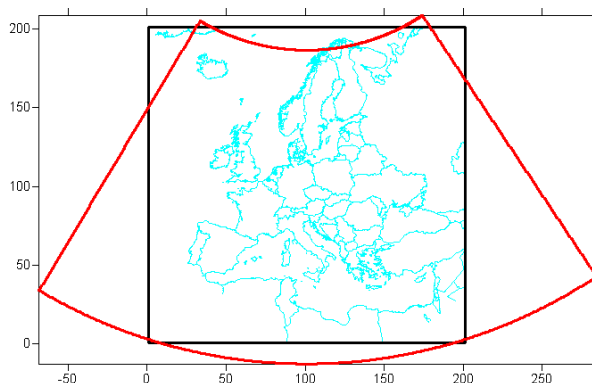


Fig. 1. NIMH's modelling domain (the black square) and ENSEMBLE domain (the red boundaries)

As far as each CTM demands its emission input in specific format reflecting the space distribution over the particular grid and time evolution of all pollutants accounted for by the chemical mechanism, the anthropogenic emission inventories are used as raw data for emission pre-processing. As already mentioned, the respective component in EPA Models-3 system, SMOKE, is not used for treating anthropogenic emissions. The *AEmis* and *PEmis* programs are exploited, instead. The processing operations are three: gridding, time/vertical allocation and speciation.

The *gridding* is recalculation (remapping) of the inventory data to the grid used. A web-based GIS system is created in NIMH for the purpose. The TNO data is uploaded in the system. Number of custom grids can be defined on the base of the standard grid description. The system recalculates the inventory quantities for each cell and type of source for a specific custom grid.

As far as the inventories are made on annual basis, *temporal allocation* is necessary consisting in over-posing of temporal profiles on the annual values. The profiles are provided by TNO (Bultjes et al., 2003). They are used also in AQMEII-1. 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 profiles for large point sources emission vertical distribution that are SNAP-specific.

In addition, some inventory pollutants are estimated as groups. The *speciation* is splitting of these groups to set of so-called lump pollutants, required by the chemical mechanism used. In NIMH, 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 the particular SNAP. In such a way VOC, $\text{PM}_{2.5}$ and NO_x speciation profiles are prepared. It must be noticed that the choice of US source types and the weights of their contribution to the respective SNAP emissions are, in a sense, subjective. More work is needed to elaborate country-specific profiles.

The gridded AS- and LPS-inventories are introduced in *AEmis* and *PEmis* programs which are the emission routines in the HIMH modelling system. They perform the two other steps of emission pre-processing. In *PEmis*, vertical allocation takes place as well. Both programs produce respective emission files. The *AEmis* output file is

2-dimensional, the *PEmis* one – 3-dimensional. Both outputs are in IO/API NetCDF format and contain hourly data for each day of the simulated period (year 2010).

2.3.2. Biomass burning emissions

The wild fire emissions are provided by the Finish Meteorological Institute (FMI), database created in the frame of IS4FIRES project (<http://is4fires.fmi.fi/>). Entering the “Fire emission data” section in the site one can access several sets of fire emission data for the last 13 years. Here, the European data has resolution of 0.1° in the native FMI *sa2* format (ASCII). The set consists of one day data files, each containing detailed description of the grid used, time period and emission intensity in all points with fire. The only pollutant is the Total Particulate Matter (TPM) in kg/s. In the web-site, recommendations how to process this data are posted as well. First, TPM must be split to coarse PM (PMC) and PM_{2.5}. A set of gase emissions (CO, NO, NH₃, SO₂ and NMVOC) is obtained by multiplying TPM by recommended coefficients. Further, PM_{2.5} and NMVOC are split to the respective compounds required by the chemical mechanism. The final procedures are the temporal and the vertical allocation. Each *sa2*-file contains the recommended temporal and vertical profiles. For vertical distribution it is recommended that one half of emitted quantities is located in the lower 200 m layer; the other half – in the layer 200-1000 m. Respective processing routine was created in NIMH and the resulting 3D emissions were added to the *PEmis* output.

2.3.3. Biogenic emissions, sea salt emissions, dust emissions

The biogenic sources are natural sources. In SMOKE, biogenic sources include VOC emissions from vegetation and nitrous oxide emissions from soil. Volcanoes and other geothermal emissions, water emissions, and other biogenic sources are not included in SMOKE. As already noted, the biogenic emissions are prepared by SMOKE on the base of the gridded LU data and the current meteorology. In addition SMOKE is used to merge the three emission files in a common CMAQ emission input – hourly data for each day of the year in IO/API NetCDF format.

The sea salt and the dust emissions are calculated by modules built in CMAQv4.6. The sea salt emission module needs additional information about sea-land distribution as well as the percentage of the surf zone (the length of the shore line multiplied by 50 m) in each cell. CMAQ requires all this data to be gathered in an OCEAN-file, specific input to the model. Additional functionality of the already mentioned web-base GIS system is the production of such OCEAN-file for a particular custom grid.

2.4. Chemical initial and boundary conditions

The chemical boundary conditions (BC) were provided by ECMWF MACC-II project (Monitoring Atmospheric Composition and Climate – Interim Implementation, <http://atmosphere.copernicus.eu>). Specifically, MACC re-analysis data from the MOZART-IFS global chemical model runs was exploited. For AQMEII-2, data for limited areas (Europe and NA) was extracted and stored on a MeteoFrance server (<ftp.cnrm-game-meteo.fr>). The European territory extends from -55.125° to 79.875° by longitude and from 16.875° to 76.5° by latitude. The spatial resolution is 1.125°. The vertical p-levels are 53. The temporal resolution is 3 hours. Three NetCDF-files are available for each day of the year – for gaseous pollutants, for aerosol ones and for the surface pressure (the pressure data is necessary to calculate vertical levels, which change in space and time).

This data is processed in a way to create BC-file for CMAQ. First, mapping of MACC pollutants to CMAQ ones took place together with units' conversion. Horizontal interpolation from MACC grid to CMAQ boundary points was performed, together with vertical and time interpolation, so as to obtain CMAQ BC-files on hourly basis for each day of the year. Following the recommendations given in the above mentioned wiki-page, the MACC sea salt fields were not used as they are considerably biased. The AQMEII simulation grid is large enough as CTMs can generate the sea salt fields internally using its sea salt parameterization. The dust data was also regrouped in the recommended way.

No specific data for chemical initial condition was provided. During the calculations initial condition for each day is the end of the previous one. The pollution fields for 1 January 2010 00:00Z were obtained by simulating all December 2009, starting with profile data, provided by CMAQ.

2.5. WRF-CMAQ calculations, data archiving, post-processing

WRF-CMAQ modelling system was run on a 32-core server (64 cores with hyper-trading). They belong to 4 Intel Xeon nodes E5530, 2.40 GHz. The RAM is 32 GB per node, 64 GB for the front-end machine. The calculation speed is 1/2 hours/day. The computational scheme is presented in Fig. 2.

One can notice that for each 3-day CMAQ calculation period a 12-hour pre-run of WRF takes place (3.5-day run of WRF). In many works (see Lo et al., 2008, for instance), it is shown that the periodical re-initialization of WRF (with nudging option switch on) gives better quality of simulation in comparison with a long run. The 12-hour spin-up at each re-initialization is recommended as well, necessary for adaptation of the interpolated initial conditions to the model's equations as well as for permeating model atmosphere with reliable amount of water vapour.

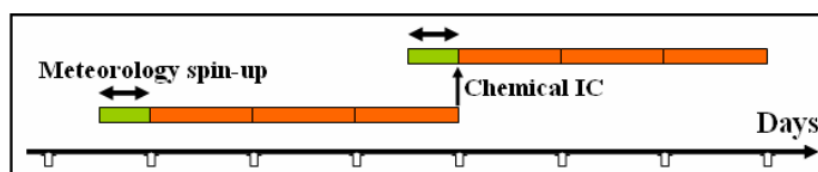


Fig. 2. Scheme of NIMH's computations for AQMEII, Phase 2.

Together with the calculations, archiving of the needed data took place. The MCIP and CMAQ outputs contain many parameters that are not of interest for AQMEII. That is why archiving scripts were created. They extract and combine in a proper way part of the output variables following the recommendations given in the overview documents distributed preliminary between AQMEII participants, as well as the different Technical Specification Documents (TSD). As a result all 1-year chemical and meteorological archive occupied about 1 TB only, while the full MCIP and CMAQ output would need 3-4 TB. All data is saved in IO/API NetCDF format.

ENSEMBLE platform requires AQMEII data in specific format. The preparation of this input required intensive post-processing performed by many post-processing programs created especially for the purpose. The exercise data was divided to different sequences (tasks, see Table 1). For each task respective TDS was prepared by AQMEII coordinating team in JRC and distributed among the participants. Each document presents the specifications for the submission of model data to the ENSEMBLE system. Each TDS is supplemented by a Metafile, containing all the information describing the case study.

Following the concept of ENSEMBLE, a number of files ought to be prepared for each task, one pollutant by file. This preparation had 3 steps:

1. Creation of so called Model Output File (MOF), an ASCII file containing interpolated values for multiple points (or vertical profiles) for each hour of the year.
2. Transformation of MOF in specific ENSEMBLE format by treating it by the special encoding programs provided by JRC.
3. Treating this file by the standard *bzip2* program and uploading the compressed file to specified JRC ftp-server.

The AQMEII team in JRC processed these data and uploaded it to ENSEMBLE storage.

Table 1. Types of TSD, number of pollutants and number of interpolation points:

# of task (TSD)	Description	Number of pollutants	Number of interpolation points
0311-001	AQMEII2 EU Grid - Concentrations and meteo	33	361×181
0311-002	AQMEII2 EU Grid - Depositions	20	361×181
0311-003	AQMEII2 EU Grid - Emissions	14	361×181
0312-001	AQMEII2 MOZAIC ¹⁾ FRANKFURT - Vertical profiles	14	53×37
0316-001	AQMEII2 EU RECEPTORS - Gas phase	15	2190

0316-002	AQMEII2 EU RECEPTORS - Aerosol	19	1837
0316-004	AQMEII2 EU RECEPTORS - Ozonesondes	6	12
0316-005	AQMEII2 EU RECEPTORS - Meteorology	11	1925
0316-006	AQMEII2 EU RECEPTORS - AERONET	4	85
0316-007	AQMEII2 EU RECEPTORS - Vertical profiles at AERONET sites	14	85
	Total	150 ²⁾	

¹⁾ MOZAIC: High quality in-flight measurements collected by instrumented commercial aircraft as part of the Measurements of **O**Zone, water vapour, carbon monoxide and nitrogen oxides by Airbus In-service airCraft (MOZAIC) programme. The evaluation is carried out for five model domains positioned around four major airports in NA (Portland, Philadelphia, Atlanta, and Dallas) and one in Europe (Frankfurt), from the surface to 8.5 km.

²⁾ The NIMH team was able to provide about 90% of the required pollutants because the remaining ones were not output by WRF(MCIP) and CMAQ models.

3. PRELIMINARY RESULTS AND DISCUSSIONS

The performance of the NIMH air quality modeling system (WRF-CMAQ) was analyzed based on comparison with surface measurements (i.e. operational model evaluation) for the whole year 2010. The tool for the evaluation was the web-based platform ENSEMBLEv5, allowing spatial and temporal analysis with different averaging periods. The ability of the model to simulate observed concentrations is discussed here on the basis of selected statistical indicators (Table 2) and graphical plots obtained mainly by the ENSEMBLE build-in tools. ENSEMBLE notification for Bulgarian WRQ-CMAQ modeling system is **BG1**.

The specific features of this preliminary estimation are as follows:

- O₃ values (daily maxima and hourly values) for the summer period August – September and for the whole year were compared;
- PM₁₀ daily mean values for the whole year were treated;
- Due to the coarse model grid resolution, only background stations were used, classified as rural;
- Since the model horizontal resolution (25 km) smoothes significantly mountainous areas, only stations situated below 1000 m a.s.l. were selected;
- Only stations with minimum data availability of 75% for O₃ and PM₁₀ were chosen for the statistical analysis

Three sub-domains were chosen for analysis (Fig. 3):

- 1st Region (Reg1) - Balkan peninsula: only 7 rural stations);
- 2nd Region (Reg2) – Central Europe: 168 stations for O₃ and 162 for PM₁₀;
- 3rd Region (Reg3) – EMEP stations (without Scandinavia): 75 stations for O₃ and 40 for PM₁₀.

Table 2. Statistical indicators used for estimation of WRF-CMAQ performance

Mean (µg/m ³)	$\bar{M} = \frac{1}{N} \sum_{i=1}^N M_i, \bar{O} = \frac{1}{N} \sum_{i=1}^N O_i, M - \text{model results}, O - \text{observations}$
Normalized Mean Bias	$NMB = \frac{\sum_{i=1}^N (M_i - O_i)}{\sum_{i=1}^N O_i}$
Normalized Mean Standard Deviation	$NMSD = \frac{\sigma_M - \sigma_O}{\sigma_O}, \sigma_M = \sqrt{\frac{1}{N} \sum_{i=1}^N (M_i - \bar{M})^2}, \sigma_O = \sqrt{\frac{1}{N} \sum_{i=1}^N (O_i - \bar{O})^2}$

Mean Fractional Bias	$MFB = \frac{1}{N} \sum_{i=1}^N \frac{M_i - O_i}{(M_i + O_i)/2}$
Root Mean Square Error ($\mu\text{g}/\text{m}^3$)	$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (M_i - O_i)^2}$
Number of modeled values within a factor of 2 of observations	$FA2 = \frac{1}{N} \sum n_i \quad \text{with} \quad n_i = \begin{cases} 1 & \text{for } 0.5 \leq M_i/O_i \leq 2 \\ 0 & \text{else} \end{cases}$
Pearson Correlation Coefficient	$PCC = \frac{\sum_{i=1}^N (M_i - \bar{M}) \cdot (O_i - \bar{O})}{\sqrt{\sum_{i=1}^N (M_i - \bar{M})^2} \cdot \sqrt{\sum_{i=1}^N (O_i - \bar{O})^2}}$



Fig.3. Three European regions used for model validation: a – Reg1, b – Reg2, c – Reg3

While Regions 2 and 3 have often been used in joint model validation exercises and studies, Region 1 is still rarely investigated in this context, provided the AQ there is not good at all as one can see from the results from EEA estimates (Fig. 4.). In addition, the measuring stations coverage density of this region is quite insufficient in comparison with most European countries. We hope that modeling results can help this

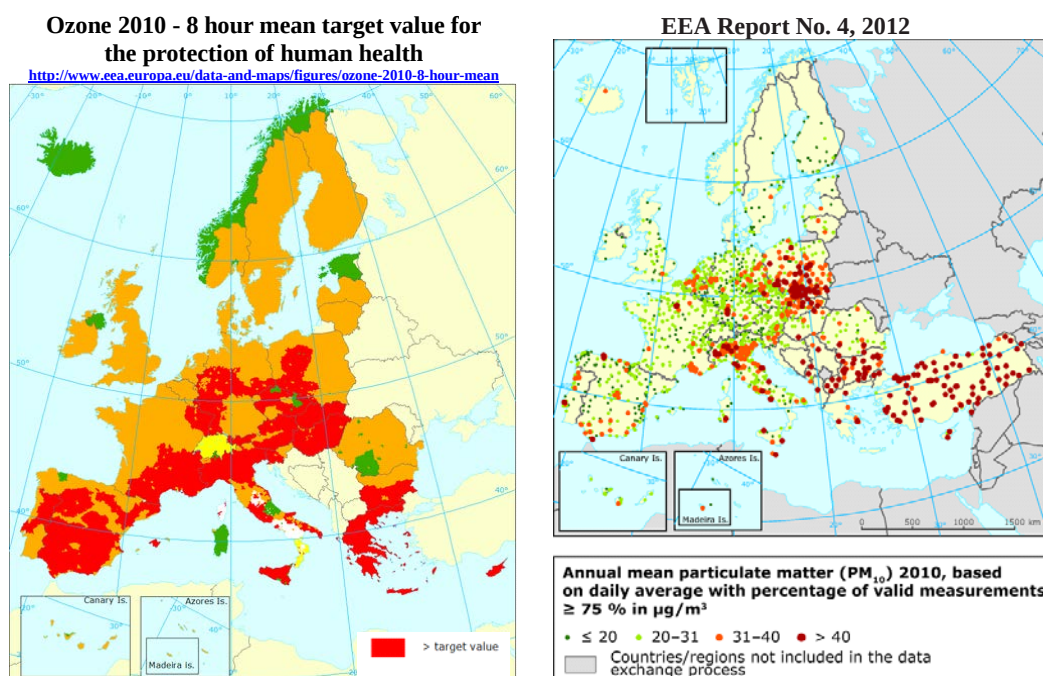


Fig.4. EEA estimates of the status of Ozone and PM_{10} pollution over Europe

3.1. Simulation quality of BG1 for Ozone pollution

Several indicators for Ozone pollution are used in this study:

3.1.1. Daily Ozone maxima (O3Dmax) for summer 2010 (April – September)

In Table 3, the values of the main statistical indicators (defined in Table 2) are shown.

The statistics definitely show that the quality of BG1 performance improve from Reg1 to Reg3: Root Means Square Error, Normalized Mean Bias and Normalized Mean Error decrease while the Person Correlation coefficient and FA2 increase. PCC is not high enough but FA2 shows that almost all points in the scatter diagram lay between lines $y=0.5x$ and $y=2x$; y being the Model-axes and x – the Observation one. For more complex analysis several combined plots, provided by ENSEMBLE, are produced.

The Taylor diagram (Taylor, 2001) provides a way of graphically summarizing how closely a model (or a set of models) result matches observations. The similarity between two patterns is quantified in terms of their correlation, their centred root-mean-square difference and the amplitude of their variations (represented by their standard deviations). These diagrams are especially useful in evaluating multiple aspects of complex models or in gauging the relative skill of many different models. In Fig. 5 the Taylor diagrams as drawn by ENSEMBLE, for the 3 regions and for a set of models including BG1 are displayed.

Table 3. Statistical indicators of BG1 for O3Dmax for the 3 regions (Aprr-Sept)

	Balkan - SEE	Central EU	EU (without Scandinavia)
Type of station	Rural (below 1000m)	Rural (below 1000m)	EMEP (all rural)
No. of station	7	186	78
RMSE	53.0427	30.9915	22.839
NMB	52.97%	31.73%	21.31%
NME	55.47%	35.36%	26.55%
PCC	0.431	0.4726	0.481
FA2	64.53%	88.48%	92.45%

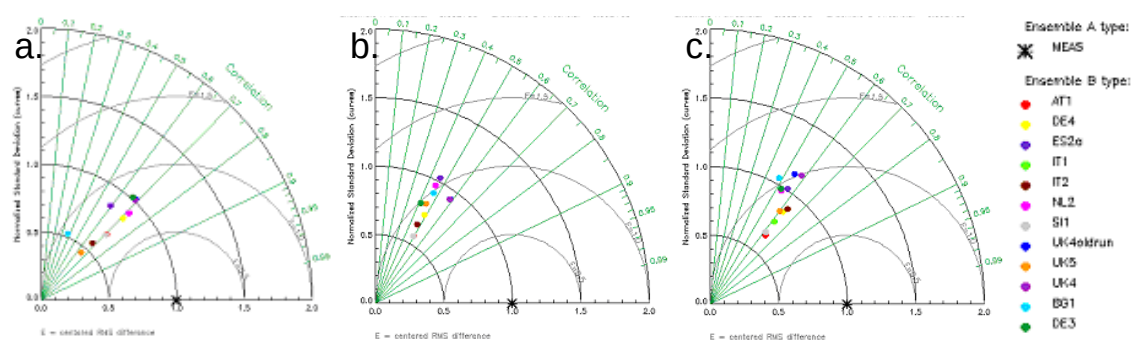


Fig. 5. Taylor diagrams of all participating models for O3Dmax: a – Reg1, b – Reg2, c – Reg3

The main features that can be seen from Fig. 5 are:

- BG1 (cyan dot) as well as the other models, do not show high simulation quality of Ozone Daily maxima – correlation coefficients around 0.5.
- BG1 improves the performance from Reg1 to Reg3, however it is quite low, especially for the Balkan region (PCC ~ 0.3).
- To note the relatively low correlation coefficient at EMEP stations (Region3) that is considered as the most representative. For all models PCC is around 0.5 - 0.6.

Another graphical tool for presenting statistical distribution of a set of numerical data is the Box-and-Whisker plot. It looks like a box with two segments at the opposite faces of the box (whiskers). It can be extended vertically or horizontally. Here, the lower base of the box presents the 25%-quartile of the distribution, the upper one – 75%-quartil. The lines in the middle show the mean and the median (50%-quartile) values. The end of the lower whisker denotes the 10%-quartile and of the upper one – 90%-quartile. The outliers (minimum and maximum values) can also be denoted by points. In one plot, several sets of data (measurements and model(s) results) can be presented, permitting an easy visual comparison. In Fig.5, the Box-and-Whisker plot of observed and BG1 data of O3Dmax for the three regions is presented.

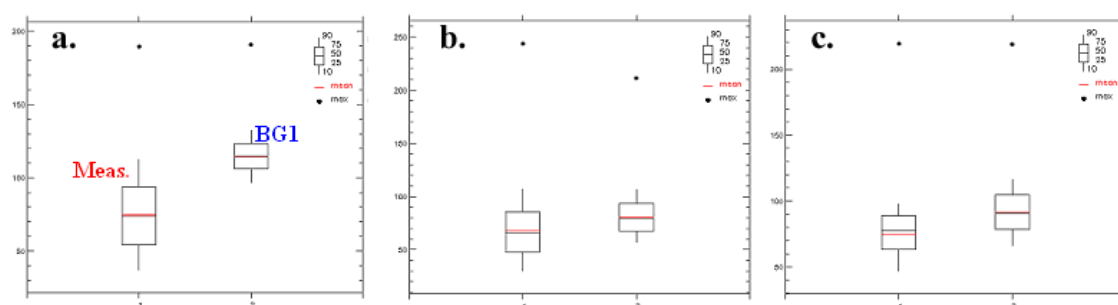


Fig. 6. Box-and-Whisker plots of BG1 for O3Dmax: a – Reg1, b – Reg2, c – Reg3

BG1 overestimates mean O3Dmax (50% for Reg1, 16% for Reg3). The standard deviation (referred by the difference between 90%- and 10%-quantiles) is twice smaller as the observed one for Reg1. For Reg2 it is smaller again but not so much, the standard deviations of modeled and measured O3Dmax for Reg3 are almost equal. The maximal values of O3Dmax are simulated well in all 3 regions.

3.1.2. Hourly Ozone values for all the year 2010.

In Fig.7, mean diurnal variation of hourly Ozone values for all the year and all observation stations is presented.

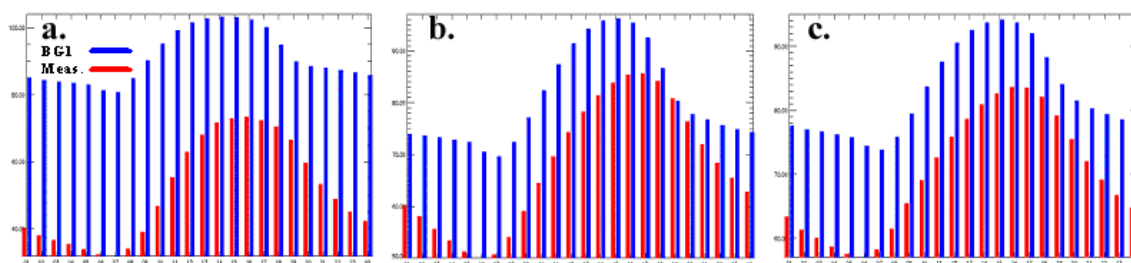


Fig. 7. Mean diurnal variation of hourly Ozone for 2010: a – Reg1, b – Reg2, c – Reg3.

It is seen that BG1 overestimates O3 values, especially during night hours. The preliminary analysis of 2m-temperature field and radiation (not shown here) does not indicate significant differences between BG1 and other models. For the moment it is not clear why BG1 has this well pronounced overestimation during night hours. Due to this smaller diurnal amplitude the standard deviation of modeled values is much smaller than of the observed ones (especially for Reg1).

3.2. Simulation quality of BG1 for PM10 daily mean values (PM10Dmean)

In Table 4, the values of the main statistical indicators (defined in Table 2) are shown.

Table 4. Statistical indicators of BG1 for PM10Dmean for the 3 regions

	Balkan - SEE	Central EU	EU (without Scandinavia)
Type of station	Rural	Rural	EMEP

	(below 1000m)	(below 1000m)	(all rural)
No. of station	7	162	40
RMSE	26.4801	29.1727	20.6939
NMB	-52.92%	-55.42%	-48.12%
NME	59.17%	58.55%	54.35%
PCC	0.3082	0.553	0.5755
FA2	47.5%	51.72%	56.79%

BG1 underestimates PM10 values, the Normalized Mean Bias being about -50%. Some improvement of the simulation from Reg1 to Reg3 can be noticed not only for NMB but for RMSE, NME, PCC and FA2 as well. The correlation coefficient for Reg1 is smaller than this of O3Dmax but for the Reg3 is higher. FA2 values are considerably smaller from these of O3Dmax.

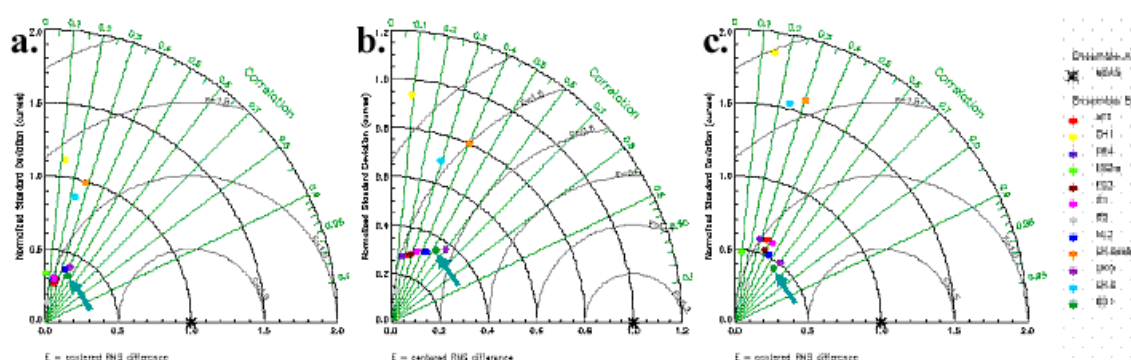


Fig. 8. Taylor diagrams of all participating models for PM10Dmean: a – Reg1, b – Reg2, c – Reg3
(BG1 dots are pointed out by green arrow)

It is clearly seen from Taylor diagrams shown on Fig. 8 that BG1 has one of the best correlation coefficient (around 0.5 – 0.6) among the participating models. The improvement of the quality of simulation from Reg1 to Reg3 is also seen. With the exception of 2 models, the others are quite grouped and BG1 dot enters the group.

From the Box-and-Whisker plot (not shown here) one can notice that BG1 simulates well the mean annual PM10 but the maxima of daily PM10 are heavily underestimated (up to 4 times). The BG1 mean daily values are lower than the observed ones. BG1 does not differ much in the mean values from other models.

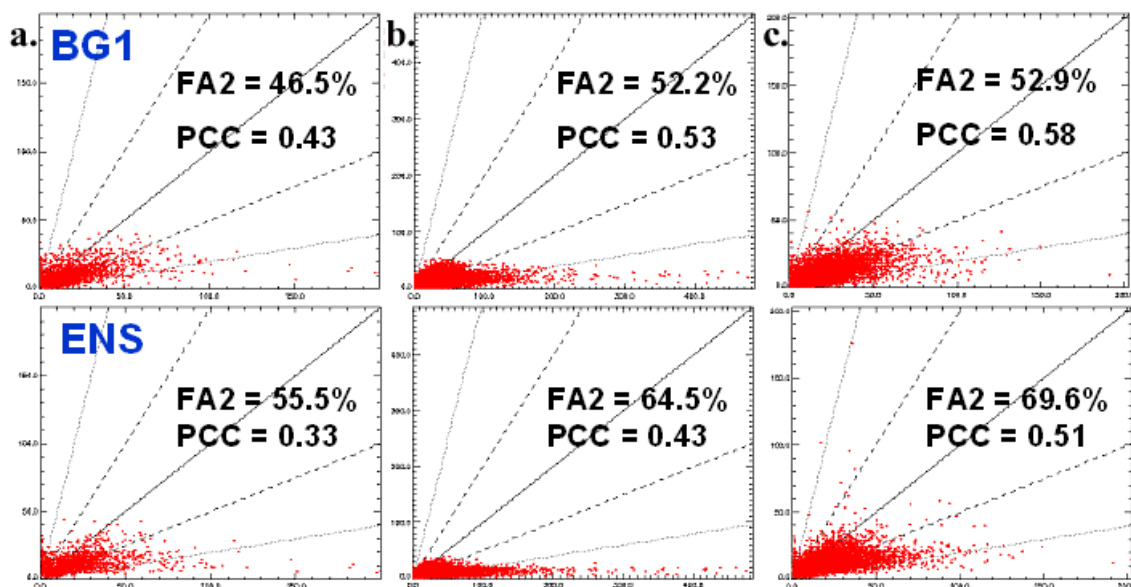


Fig. 9. Scatter plot of PM10Dmean for BG1 and for an ensemble of all participating models:

a – Reg1, b – Reg2, c – Reg3

From the scatter plots shown in Fig.9 one may conclude that BG1 and ENSEMBLE of other models both underestimate observed daily means of PM10. ENSEMBLE shows better FA2 than BG1. BG1 shows better correlation coefficients than ENSEMBLE. The improvement from Reg1 to Reg3 is not so evident as in case of O3.

4. CONCLUSIONS

The presented results can be summarized as follow:

- BG1 model results are in line with other models.
- Regarding the Ozone, BG1 model performance is a bit disappointing ($PCC_{max} \sim 0.6$ at EMEP stations and definite overestimation). Its results are quite unsatisfactory compared to the other simulations in Reg1.
- Regarding PM10, although significantly underestimated (50%) by BG1, the model is one of the best among all models ($PCC \sim 0.43 - 0.58$ for Reg1 – Reg3)).
- BG1 captures the temporal variability of both gases and aerosols better than other models.
- Although the Balkan Region (Reg1) experiences severe PM pollution problems, the observations are still limited (as number of stations and type of observations), so the use of models is quite promising.
- Exercises like AQMEII using ENSEMBLE platform capabilities are extremely useful for better estimation of Air Pollution situation.
- Much more intensive investigation of BG1 and other models results is necessary (other pollutants, profiles, integral quantities)

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