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IMPLEMENTATION OF COUPLED REGIONAL-TO-LOCAL SCALE MODELLING SYSTEM IN BULGARIA – AIR QUALITY STUDY FOR THE CITY OF SOFIA

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Abstract

The implemented and adapted to Bulgarian conditions Multi-Model Air Quality System was applied to study air pollution in the city of Sofia. Combining the advantages of complex chemical mechanisms from regional numerical modelling with a better representation of the concentration field of harmful substances from well-defined sources from local models, overcomes the deficiencies and provides a more reliable approach for studying pollution at urban scales. Applying best practices and sophisticated techniques on sparce incomplete datasets, detailed "bottom-up" emission inventory was developed for the city of Sofia. The spatial distribution of the main transport-related pollutants is significantly improved by taking into account explicitly resolved emissions from the main road network.

Key words: air pollution in urban areas, multi-scale modelling approach, development of a detailed bottom-up local emissions inventory

Introduction. Air pollution ranked 2nd among the leading risk factors for premature mortality on a global scale (8.1 million cases) in 2021, and it is also

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one of the main contributors to the global disease burden [1]. Urban areas are particularly vulnerable to the formation of smog, causing adverse effects on human health. Unfortunately, the lack in observations of the major pollutants is a big problem in Bulgaria.

Air quality modelling is an important tool for simulation of the combined effects of emissions, dispersion, physical and chemical processes in the atmosphere and for the quantification of air pollution concentrations at a variety of spatial and temporal scales. Numerical simulations can alleviate some of the deficiencies arising from the lack of official measurement and communication campaigns, but it requires careful consideration of underlying assumptions and pre-set parameters in computational models. The scientific community in Bulgaria has decades of experience with the regional modelling system that consists of three models:

- The Weather Research and Forecasting model (WRF) – mesoscale numerical weather prediction system is used for modelling the thermo-hydrodynamics in the atmosphere `http://www.mmm.ucar.edu/wrf/users`.
- The Sparse Matrix Operator Kernel Emissions (SMOKE) system is applied for emissions processing, designed to produce hourly values disaggregated by pollutants in a selected calculation grid to be used as input to various air quality models `https://www.cmascenter.org/smoke`. It should be noted that only individual SMOKE modules are used in this study, due to the difference between the Selected Nomenclature for Air Pollution categories in the USA and the EU, which necessitated the development of own emission processing codes.
- The Community Multiscale Air Quality (CMAQ) modelling system `https://www.epa.gov/cmaq/cmaq-models-0` is a chemical transport model for modelling the concentration of gases and particles in the air and the deposition of these pollutants on the Earth's surface.

The Bulgarian Chemical Weather Forecast System (BCWFS), based on the described above models, has been running operationally since 2012 [2,3]. BCWFS was used in numerous research studies [4,5]. Local scale numerical models (such as Gaussian or Lagrangian type) are applied in the operational system for air quality management in the city of Plovdiv [6] and in the preparation of Comprehensive Programme for Improvement of Ambient Air Quality of Sofia Municipality for the Period 2021–2026 `https://www.sofia.bg/en/components-environment-air`.

Despite decades of study in Bulgaria on air quality in different scales, the contribution of physical environment on pollution in urban areas was not specifically investigated. A few recent studies on air quality, including a detailed description of the urban structures (buildings, streets, etc.), were published for assessment of the particulate matter (PM) air pollution in Sofia [7], pollution distribution around a block of buildings located near a road with heavy traffic [8], adjustment of emission factors for PM and the relationship between the fractions of NOx from road transport [9]. Both PM fractions related to human health (with diameter less than 10 µm – PM_{10} and less than 2.5 µm – $PM_{2.5}$) are used in this study.

Recently the Air Quality Management & Assessment System (ADMS-Urban) `https://www.cerc.co.uk/environmental-software/ADMS-Urban-model.html`, developed and maintained by the Cambridge Environmental Research Consultants (CERC) Ltd., was implemented and set up for Bulgarian conditions. ADMS-Urban is a comprehensive software suited for modelling air quality in urban areas. The model integrates with geographical information system (GIS) tools and emissions databases and supports calculation of concentrations based on a range of averaging periods, including percentiles. The GIS interface is an important visualization tool and provides a means of manipulating the spatial element of the model input data. The Comprehensive Emissions Inventory Toolkit EMIT `https://www.cerc.co.uk/environmental-software/EMIT-tool.html` provides the emission input and allows calculation of reliable emissions from all sources in an urban area.

The Multi-Model Air Quality System (MAQS) `https://cerc.co.uk/environmental-software/MAQS.html` is an automated system for coupling the high-resolution ADMS-Urban model to a regional air quality model with hourly concentration output such as CMAQ. The aim of the MAQS is to combine the complementary advantages of regional and local models to improve the prediction of concentration values. Regional (usually Eulerian) models contain complex chemistry mechanisms, which act over long spatial and temporal scales, and can model the accumulation of concentrations in very low wind speed conditions. Local (usually Gaussian-type plume) models can represent the fine-scale concentration gradients from explicitly defined sources in detail, but generally only account for simplified chemical mechanisms and spatially homogeneous meteorological data, limiting their applicability for receptors far from the source (e.g. more than 50 km). Coupling local and regional models allows both the resolution of high concentration gradients close to a source, and the accurate representation of transport and chemistry over large spatial and temporal scales. MAQS combines regional and local inputs in such a way as to minimize double counting of emissions, while remaining computationally efficient and user-friendly. Meteorological data from the WRF meso-scale model is used for both the regional modelling and the local modelling.

The aim of this work is to present newly implemented and adapted to Bulgarian conditions MAQS and applied it to study air pollution in the city of Sofia. Sofia was selected for this pilot study as it is the biggest urban area in the country and despite the efforts made during the last decades, the citizens in the capital are still exposed to high levels of PM as well as other pollutants, especially nitrogen dioxide NO_2. The latter is mostly related to transport, but the evidence has stayed somehow hidden due to gaps in the monitoring of areas with more intensive traffic.

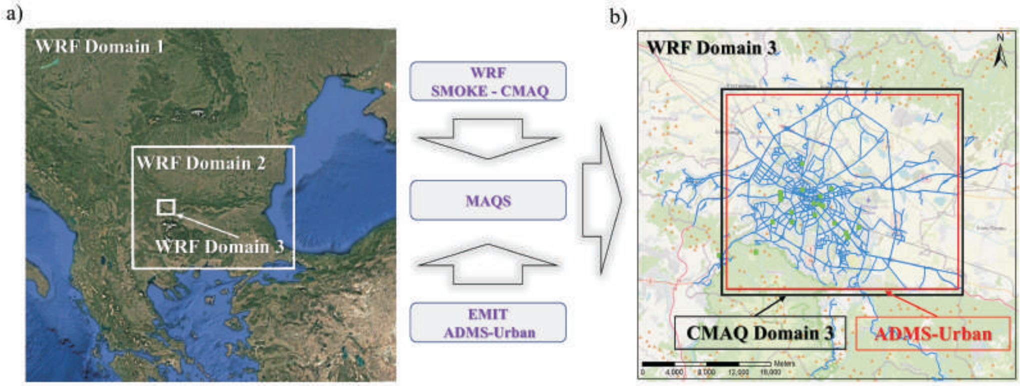

Fig. 1. a) Domain setting in regional WRF and CMAQ models (with 1 km resolution) and b) nested inside ADMS-Urban model domain (with 100 m resolution) for modelling with MAQS. Emission sources (the main roads) in the ADMS-Urban mode are shown (blue lines) together with the locations of measurements for model validation (green symbols)

Methodology. CMAQ model v5.0.1 has been coupled with the meteorological WRF model v3.9.1 for atmospheric chemistry simulations focused on the region of Sofia municipality, Bulgaria. A system of 3 nested domains (Fig. 1a) has been set up to allow both models to simulate meteorological fields and air pollutant concentrations at spatial resolutions of 9, 3 and 1 km. All domains account for 51 vertical levels above ground, with 26 levels below 1 km height. Anthropogenic emissions for CMAQ simulations were processed from the Bulgarian National Atmospheric Emissions Inventory for 2019 `https://unfccc.int/documents/194772` and from the CAMS-TNO emission inventory 2019 for south-east continental Europe `https://airqualitymodeling.tno.nl/emissions/2019`. Both inventories' annual totals have been temporally distributed according to monthly, weekly, and hourly variations using time varying profiles [10]. The vertical distribution of anthropogenic emissions follows CAMS-TNO profiles. Biogenic emissions were obtained with the SMOKE system, and the same system was used to merge different types of emission sources. The baseline year of the simulation is 2018.

The MAQS coupled system nested the local ADMS-Urban model within the regional CMAQ model over the city of Sofia in this study (Fig. 1b). This coupled system combines both regional and local scale dispersion and chemical processes without double-counting local emissions, passing regional meteorology and background concentrations into local modelling for each regional model grid cell. This modelling system was installed and run on Nestum cluster `https://hpc-lab.sofiatech.bg` at the HPC laboratory, Sofia Tech Park.

Own local emission inventory for the transport from the main roads with intensive traffic was developed for Sofia municipality. The quality of the underlying traffic and fleet data was a challenge due to sources with poor access to the more complete sets, low interoperability and many mismatches in the data gathering approaches in terms of spatial and temporal representation among others.

We processed and integrated data for key boulevards and junctions, various types of streets in Sofia from several sources at our disposal: measurements provided by the Road Infrastructure Agency, the Directorate "Traffic Management and Analysis", of the municipality via its planning enterprise Sofiaplan from single days in 2017 and 2018 for almost 40 junctions, car count geolocation sample along the street network for the entire 2018 and 2019, as well as traffic count campaigns from consultancies and the Open Transport Model.

For the processing, analysis, visualization, and traffic modelling of the available data we used both QGIS tools and Python modules. The approach we proposed resorts on the advantages of ensemble learning using a large number of related features such as road and street categories, population density, functional analysis, space syntax calculations, the described traffic measurements and models, etc. We used advanced regression models such as Random Forest, XGBoost, CatBoost etc., ranked according to the chosen evaluation metrics and stacked in a

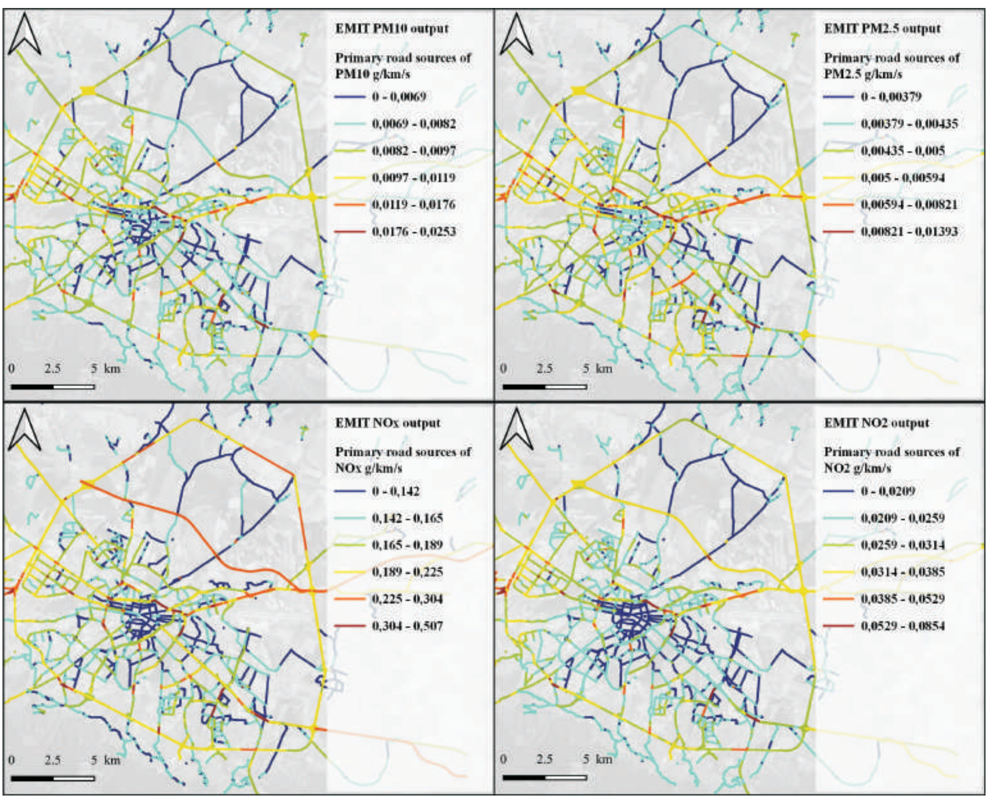

Fig. 2. Estimated pollutant emissions with EMIT. Clockwise from top left: PM_{10}, $PM_{2.5}$, NO_2, NO_x

weighted ensemble for optimal fitting. More details are available in [11] and [12]. These activity data describe vehicle types (motorcycles, light and heavy vehicles), traffic intensity and speed input, together with additional data such as surface types, gradients and morphology of the street canyons. The latter were calculated with the help of the CERC Urban Canyon Tool as an extension to ArcGIS 10.6.1. Consequently, the data was used as an input to the EMIT module to calculate emissions from transport for the main roads (Fig. 2). The output from EMIT as a spatially determined emission inventory of street and road segments was then used as an input for ADMS-Urban.

Results and discussion. Comparison of the results obtained by MAQS with observations of official air quality stations (AQS) is shown in Table 1. Statistical measures such as mean biases (MB), mean error (ME), root-mean-squared error (RMSE), Pearson correlation coefficient (r) and the index of agreement (IA) are used. The IA parameter [13] is a standard method to determine the degree of the model prediction error, and IA ranges between 0 and 1, with 1 indicating a perfect match, 0 – no agreement. In addition, maximum (Max) values from measurements and modelling are presented, as well as the percentage of missing data from observations. Concentrations are underestimated at AQS sites, but this is expected, as other sources such as secondary road network and domestic heating, which have significant contributions [7], are not explicitly included in this study. The concentrations produced by all additional sources are taken as background concentrations from the CMAQ model. The inclusion of explicitly resolved additional sources in the municipality is forthcoming, which we expect to lead to an even more significant improvement in the results. The largest ME and RMSE are found for PM_{10} at AQSs Hipodruma, Pavlovo and Nadezhda, r is in the range 0.41 to 0.71 with the worst correlation at AQS Mladost for NO_2, and IA – in the range 0.23 to 0.74 with the worst agreement at AQSs Nadezhda and Mladost for PM_{10}. High agreement IA corresponds to low correlation r due to different meaning of both measures. The correlation is positive (correspondence between high and low concentrations from measurements and modelling), the IA value detects additive and proportional differences in the observed and simulated means and variances, however, it is sensitive to extreme values due to squared differences.

Maps with annual mean concentration of the main transport-related pollutants in the city of Sofia are shown in Fig. 3, for MAQS with 100 m resolution (Fig. 3a) and CMAQ with 1 km resolution (Fig. 3b). The increase in maximum values is approximately 3 times for NO_2 when using MAQS compared to CMAQ results, with the highest concentration values being most often at intersections between boulevards with heavy traffic. The differences in maximum PM values are not substantial, but spatial distribution improved significantly, showing an increase in concentrations near main roads and intersections, which are expected

Table 1

MAQS validation for NO_2, PM_{10} and $PM_{2.5}$ at AQSs in city of Sofia for 2018

Nitrogen dioxide (NO_2)							
AQS	MB μg/m^3	ME μg/m^3	RMSE μg/m^3	IA	r	Missing data %	Max obs/mod μg/m^3
Druzhba	−16.95	17.10	23.28	0.55	0.61	1.97	131.68/101.82
Hipodruma	−22.19	22.73	28.29	0.58	0.61	1.19	155.08/127.84
Mladost	−5.76	10.45	22.94	0.74	0.41	26.37	160.96/192.18
Nadezhda	−15.26	16.44	22.36	0.57	0.50	11.84	122.40/107.71
Pavlovo	−20.78	21.32	29.74	0.58	0.61	14.44	176.14/122.46
Particulate matter with diameter less than 10 μm (PM_{10})							
AQS	MB μg/m^3	ME μg/m^3	RMSE μg/m^3	IA	r	Missing data %	Max obs/mod μg/m^3
Druzhba	−16.93	17.37	23.54	0.57	0.56	4.20	180.62/138.03
Hipodruma	−29.02	29.25	44.93	0.43	0.64	1.24	386.76/132.11
Mladost	−24.84	25.02	37.21	0.37	0.61	4.67	301.36/129.62
Nadezhda	−33.86	34.01	45.82	0.23	0.57	1.58	326.91/128.38
Pavlovo	−30.75	30.87	43.63	0.40	0.71	9.09	331.79/117.32
Particulate matter with diameter less than 2.5 μm ($PM_{2.5}$)							
AQS	MB μg/m^3	ME μg/m^3	RMSE μg/m^3	IA	r	Missing data %	Max obs/mod μg/m^3
Hipodruma	−22.19	22.73	28.29	0.58	0.61	1.19	253.04/126.92

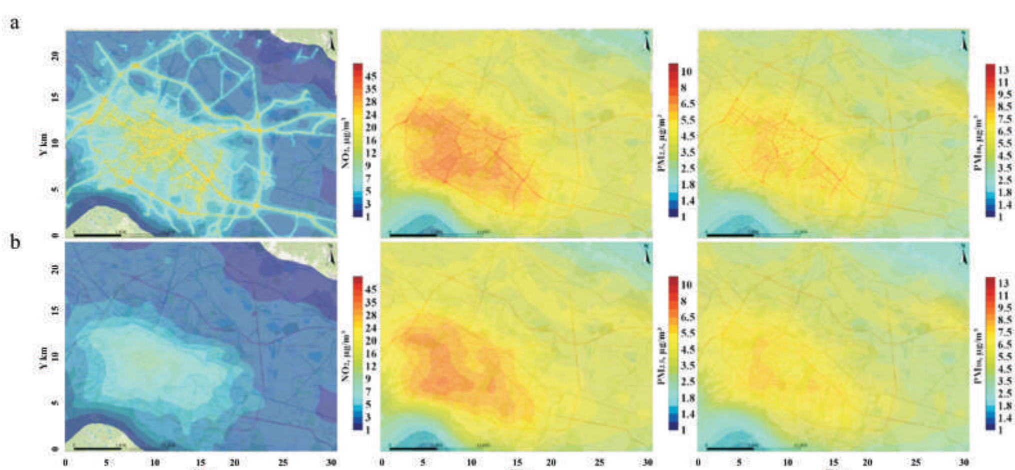

Fig. 3. Annual mean concentration for the main transport-related pollutants – NO_2, $PM_{2.5}$ and PM_{10} obtained by using models (a) MAQS with 100 m resolution, and (b) CMAQ with 1 km resolution

results, taking into account the explicitly resolved emissions only from the main roads.

Conclusions. Healthy urban environments, health prevention, well-being, are particularly important topics. Combining the advantages of complex chemical mechanisms from regional numerical modelling over coarse spatial and long temporal scales, with a better representation of the concentration field of harmful substances from well-defined sources from local models, will overcome the deficiencies and provide a more reliable approach and methodology for studying pollution at urban scales.

The implementation and adaptation of MAQS to Bulgarian conditions is part of our efforts to improve the modelling of atmospheric pollution, and air quality assessment. The short-term goal is to conduct novel interdisciplinary research on monitoring and modelling of meteorological conditions and air quality. The long-term goal is to develop a new methodology for modelling and forecasting of atmospheric pollution with a special focus on the needs of urban planning decisions and human health. The new techniques applied will provide tools to address specific urban planning needs by developing numerical scenarios in the process of selecting potential pollution reduction and health prevention measures and preparing recommendations for decision-making institutions.

REFERENCES

[1] Health Effects Institute (2024) State of Global Air 2024, Special Report, Boston, MA: Health Effects Institute.

[2] Syrakov D., M. Prodanova, K. Slavov et al. (2013) Bulgarian System for Air Pollution Forecast, J. Intern. Sci. Publ. Ecol. Saf., **7**, 325–334, ISSN: 1313-2563.

[3] Georgieva E., D. Syrakov, M. Prodanova et al. (2015) Evaluating the Performance of WRF-CMAQ Air Quality Modelling System in Bulgaria by Means of the DELTA tool, Int. J. Environ. Pollut., **57**(3–4), 272–284.

[4] Syrakov D., V. Spiridonov, M. Prodanova et al. (2011) A system for assessment of climatic air pollution levels in Bulgaria: description and first steps towards validation, Int. J. Environ. Pollut., **46**(1/2), 8–42.

[5] Georgieva E., D. Syrakov, D. Atanassov et al. (2021) Use of Satellite Data for Air Pollution Modeling in Bulgaria, Earth, **2**(3), 586–604.

[6] Atanassov D., S. Spassova, D. Grancharova et al. (2006) Air Pollution Monitoring and Modelling System of the Town of Plovdiv (phase I), J. Environ. Prot. Ecol., **7**(2), 260–268.

[7] Dimitrova R., M. Velizarova (2021) Assessment of the Contribution of Different Particulate Matter Sources on Pollution in Sofia City, Atmosphere, **12**(4), 423, `https://doi.org/10.3390/atmos12040423`.

[8] Petrov A., E. Georgieva, E. Hristova (2024) Sensitivity Analysis of Modelled Air Pollutant Distribution around Buildings under Different Meteorological Conditions, Atmosphere, **15**(6), 638, `https://doi.org/10.3390/atmos15060638`.

[9] Velizarova M., R. Dimitrova, P. O. Hristov et al. (2024) Evaluation of Emission Factors for Particulate Matter and NO_2 from Road Transport in Sofia, Bulgaria, Atmosphere, **15**(7), 773, `https://doi.org/10.3390/atmos15070773`.

[10] Simpson D., A. Benedictow, H. Berge et al. (2012) The EMEP MSC-W chemical transport model – technical description, ACP 2012, **12**(6), 7825–7865.

[11] Burov A., D. Brezov (2023) Transport Emissions from Sofia's Streets – Inventory, Scenarios, and Exposure Setting. In: EnviroRISKs 2022, LNNS 638 (Eds N. Dobrinkova and O. Nikolov), 223–233.

[12] Brezov D., A. Burov (2023) Ensemble Learning Traffic Model for Sofia: A Case Study, Appl. Sci., **13**(8), 4678, https://doi.org/10.3390/app13084678.

[13] Willmott C. J. (1981) On the validation of models, Physical Geography, **2**(2), 184–194.

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