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ANALYZIS OF THE PROCESSES WHICH FORM THE AIR POLLUTION PATTERN OVER THE BALKAN PENINSULA

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Abstract: The air pollution transport is subject to different scale phenomena, each characterized by specific atmospheric dynamics mechanisms, chemical transformations, typical time scales etc. The specifics of each transport scale define a set of requirements for appropriate treatment of the pollutants transport and transformation processes, respectively for suitable modelling tools, data bases, scenarios and time scales for air pollution evaluation. The air pollution pattern is formed as a result of interaction of different processes, so knowing the contribution of each for different meteorological conditions and given emission spatial configuration and temporal behaviour. The present study attempts to make some evaluations of the contribution of different processes of the local to regional pollution over the Balkans.

***Key words**: Regional scale modelling, US EPA Model-3 system, Integrated Process Rate Analysis*

INTRODUCTION

The main scientific challenge of local to regional atmospheric composition pattern modelling probably is the accounting for the strong dependence of concentrations on fluctuations of local and regional meteorological conditions, the complex interaction of transport scales (different life times of the pollutants make it even more complex), uncertainties and responses to emission forcing and boundary conditions, both introducing information noise.

The air pollution transport is subject to different scale phenomena, each characterized by specific atmospheric dynamics mechanisms, chemical transformations, typical time scales etc. The specifics of each transport scale define a set of requirements for appropriate treatment of the pollutants transport and transformation processes, respectively for suitable modelling tools, data bases, scenarios and time scales for air pollution evaluation. The air pollution pattern is formed as a result of interaction of different processes, so knowing the contribution of each for different meteorological conditions and given emission spatial configuration and temporal behaviour. The present study attempts to make some evaluations of the contribution of different processes of the local to regional pollution over the Balkans.

Modelling tools

The US EPA Model-3 system was chosen as a modelling tool because it appears to be one of the most widely used models with proven simulation abilities. Important advantages of this software are that it is free downloadable and it can be run on contemporary PCs. In the same time, this is a modelling tool of large flexibility with a range of options and possibilities to be used for different applications/purposes. Many research groups in Europe already use the Model-3 system or some of its elements and this number is going to increase rapidly.

The system consists of three components:

MM5 - the 5th generation PSU/NCAR Meso-meteorological Model MM5 - Dudhia (1993), Grell *et al.* (1994), used as meteorological pre-processor;
CMAQ - the Community Multiscale Air Quality System CMAQ - Byun *et al.* (1998), Byun and Ching (1999);
SMOKE - the Sparse Matrix Operator Kernel Emissions Modelling System - CEP (2003).

Input data

The large scale (background) meteorological database used by the application is the NCEP Global Analysis Data with 1º×1º resolution. At the moment the created database contains all the necessary information since year 2000.

The TNO high resolution inventory (A. Visschedijk *et al.* ,2007) is exploited. The inventory is produced by proper disaggregation of the EMEP 50-km inventory data base. The TNO inventory resolution is 0.125°×0.0625° longitude-latitude, that is on average about 14×7 km. GIS technology is applied as to produce area and large point source input from this database. It must be mentioned that the TNO emissions are distributed over 10 SNAPs (Selected Nomenclature for Air Pollution) classifying pollution sources according the processes leading to harmful material release to the atmosphere. The inventory contains 8 pollutants: CH4, CO, NH3, NMVOC (VOC), NOx, SOx, PM10 and PM2.5.

CMAQ demands its emission input in specific format reflecting the time evolution of all polluters accounted for the used chemical mechanism. A specific approach for obtaining speciation profiles is used here. The USA EPA data base is intensively exploited. A Bulgarian emission expert has found coincidence between main Bulgarian sources for every SNAP with similar source types from US EPA nomenclature. 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 Bulgarian emission in particular SNAP. In such a way VOC and PM2.5 speciation profiles are derived. It must be noticed that the choice of source types and their contribution to the respective SNAP emissions are country specific, i.e. the obtained speciation profiles are applicable for Bulgarian territory, mainly.

Domains and nesting

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

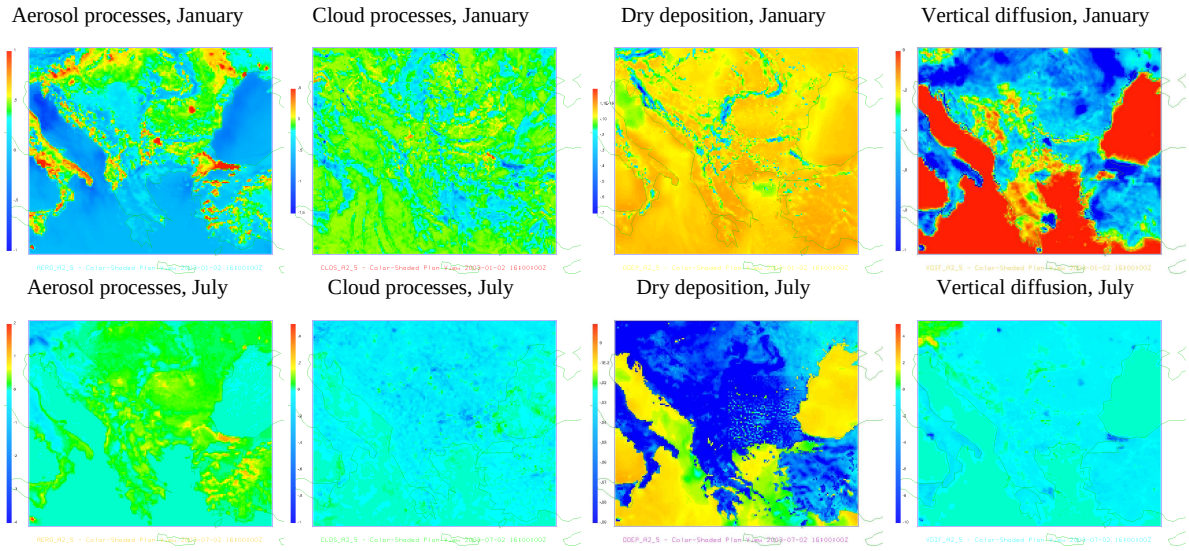

Figure 1. Plots of the contribution [μg/m^3] of aerosol, cloud, dry deposition and vertical diffusion processes to the formation of PM2.5 at 16.00 on a "typical" day in January and July.

Integrated process rate analysis

The Models-3 "Integrated Process Rate Analysis" option is applied to discriminate the role of different dynamic and chemical processes for the air pollution pattern formation. The procedure allows the concentration change for each compound for an hour Δc to be presented as a sum of the contribution of the processes, which determine the concentration:

$$\Delta c = \sum_{i=1}^{N} \Delta c_i \qquad (1)$$

The processes that are considered are: advection, diffusion, mass adjustment, emissions, dry deposition, chemistry, aerosol processes and cloud processes/aqueous chemistry.

Grid computing

Multi-scale numerical experiments have to be carried out, which are to clarify to some extend different scale processes interaction, but also to further specify requirements for input data (emissions, boundary conditions, large scale forcing). Model interfaces from synoptic trough meso- to local scale have to be tailored (two-way nesting effects have to be checked). Simply speaking, extensive sensitivity studies have to be carried out, tailoring the model set-up and parameters. Performing extensive simulations of this kind with up to date highly sophisticated numerical models obviously requires computer resources of the order of magnitude of those provided by the so-called supercomputers. Using supercomputers, however, is rather expensive and far beyond what most of the research groups can afford. Luckily an alternative technology – the grid computing (Atanassov *et al.*, 2006, Foster and Kesselmann, 1998, Ganev *et al.*, 2009), is recently developing very intensively, which makes formulating and solving problems absolutely unthinkable several years ago already quite relevant.

SOME EXAMPLES OF PROCESS ANALYZIS SIMULATIONS

The modelling infrastructure (models and input data, Grid simulation practices) has been well validated (see for example Ganev, 2009) which allows applying it for air pollution studies for the Balkan region with some trust in the obtained results.
Following the methodology described above, MM5 and CMAQ simulations were simulations which were carried out for the years 2003- 2009 and the respective process contributions for each day for all the period were calculated. Averaging the process contribution fields over the whole ensemble of results for the respective month produces a diurnal behaviour of given pollution characteristic, which can be interpreted as "typical" for the month (respectively season). The characteristic, which will be demonstrated and discussed as an example further in this paper are the surface process contributions Δc_i and the resulting hourly concentration changes Δc for months January and July.

Plots of the horizontal fields of some of the processes which determine the concentration change of O_3 and PM2.5 for January and July are shown in Figs. 1, 2. The pattern is indeed very complex. Some typical effects can be followed however. For example the roads, big cities and agglomerations appear as big sinks in the O_3 chemical transformation plot and as big sources in the PM2.5 aerosol processes plot.

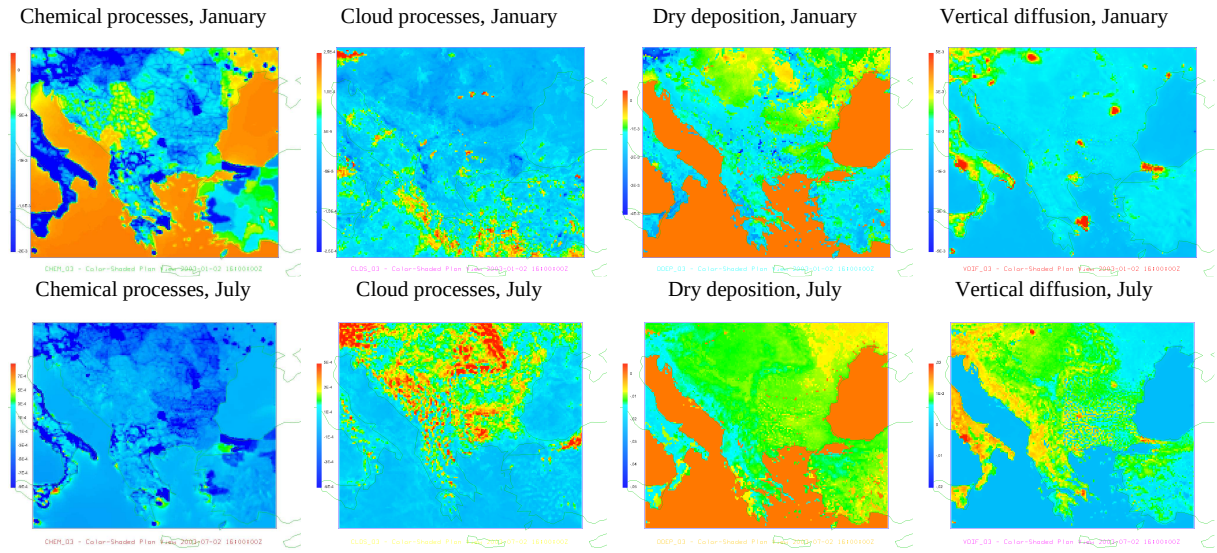

Figure 2. Plots of the contribution [μg/m^3] of chemical, cloud, dry deposition and vertical diffusion processes to the formation of O_3 at 16.00 on a "typical" day in January and July.

Plots of this kind are rather spectacular and can give a good qualitative impression of the spatial complexity of the different processes contribution. In order to demonstrate the process contribution behaviour and the process interaction in a more simple and easy to comprehend way, the respective fields can be averaged over some domain (in this case the territory of Bulgaria), which makes it possible to jointly follow and compare the diurnal behaviour of the different processes contribution and their resultant hourly surface concentration Δc .

Such plots for NOx, SO_2, PM2.5 and PM10 are given in Figures 2-3 for January and July respectively. A detailed description even of these much simpler images will take a lot of space and probably is not necessary. Some more general features could be mentioned, however:

- First of all the hourly surface concentration Δc is determined mainly by a small number of most important processes (which could be different for different compounds), while the role of the others is minor;

- The temporal behaviour of the processes is also complex;

- For some processes the contribution sign is obvious (like emissions or dry deposition), but some can change their sign during the day;

- For all of the compounds some of the advection/diffusion processes have a major role.

CONCLUSIONS

The numerical experiments performed produced a huge volume of information, which have to be carefully analyzed and generalized so that some final conclusions can be made. The conclusions that can be made at this stage of the studies are that the processes interactions are indeed very complex.

The results produced by the CMAQ "Integrated Process Rate Analysis" demonstrate the very complex behaviour and interaction of the different processes – process contributions change very quickly with time and these changes for the different points on the plane hardly correlate at all. The analysis of the behaviour of different processes does not give a simple answer to the question of how the air pollution in a given point or region is formed.

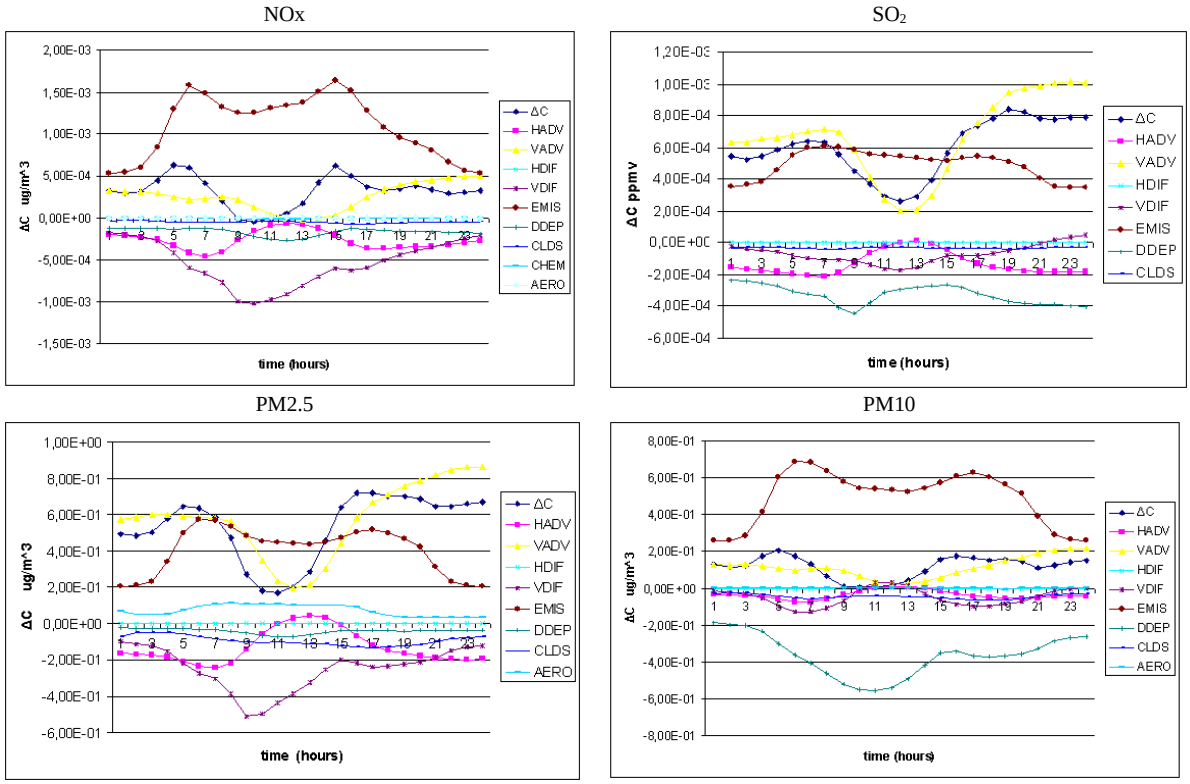

Figure 3. Plots of the diurnal course of the contributions [µg/m^3 and ppmV] of the different processes to the formation of NOx, SO_2, PM2.5 and PM10 and the resulting hourly concentration change Δc for a "typical" day in January.

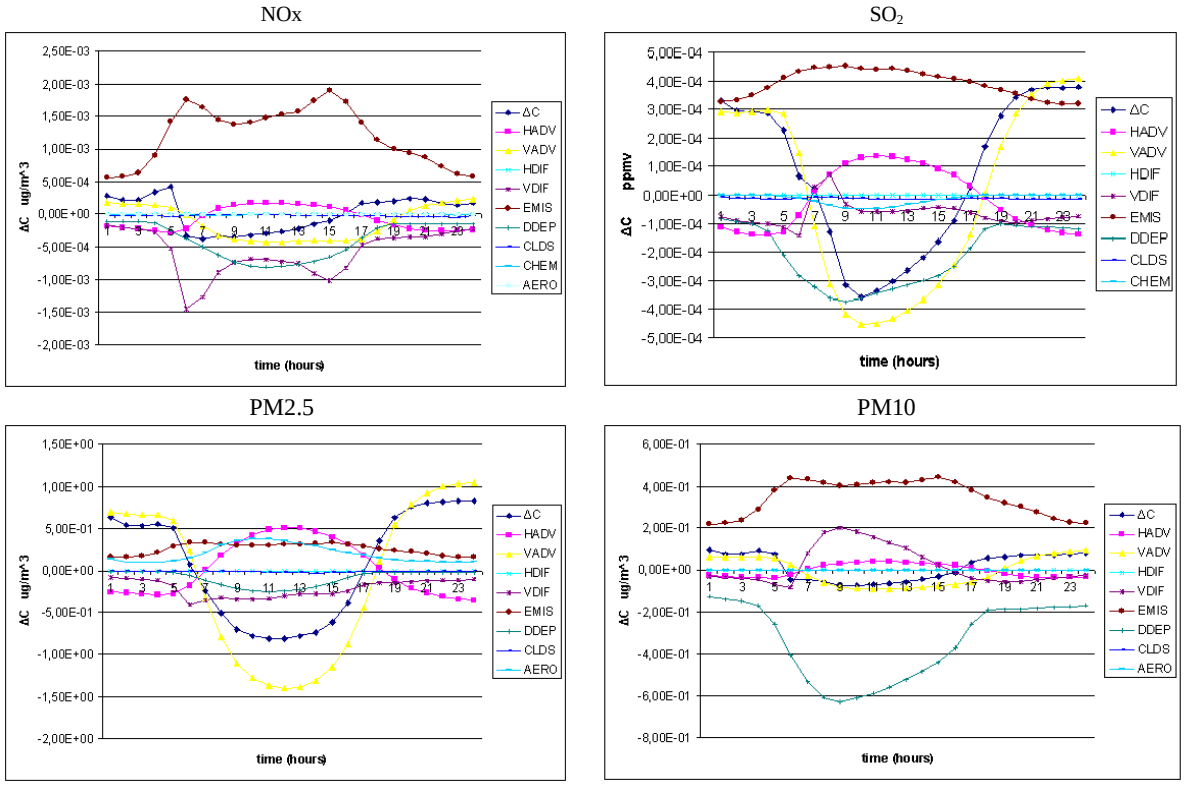

Figure 4. Plots of the diurnal course of the contributions [µg/m^3] of the different processes to the formation of NOx, SO_2, PM2.5 and PM10 and the resulting hourly concentration change Δc for a "typical" day in July.

The "Integrated Process Rate Analysis" is a fruitful approach, however, so an attempt should be made for the evaluation and analysis of the processes to be presented in a more general way. The characteristics demonstrated above are averaged over a

large ensemble of simulations. A more extensive statistical treatment – calculating not only the mean process contributions fields, but also standard deviations, skewness, etc. with their dominant temporal modes (seasonal and/or diurnal variations).

The "Integrated Process Rate Analysis" could be also applied in combination with emission sensitivity tests (see for example Jordanov *et al.*, 2010)) which can outline the impact of different emission categories on the processes by which the air pollution is formed.

Studying the impact of the numerical special resolution to "Integrated Process Rate Analysis" results seems to be a promising task as well.

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