DILUTION AND TRANSFORMATION PROCESSES OF THE AIR POLLUTION FROM THE ROAD TRANSPORT – STUDY OF THE MODELS-3 SYSTEM SENSITIVITY TO TRANSPORT SCALES AND GRID RESOLUTION

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INTRODUCTION

The objective of the present work is to study in detail the dilution processes of the plumes and the chemical transformations of pollutants generated by road transport from the local scale to the scale of the global models. More precisely the study aims at clarifying the US EPA air quality modelling system MODELS-3 sensitivity to transport scales and emission resolution and deriving some conclusions about the key parameters, which quantify the local dilution and transformation processes impact on larger scale pollution characteristics.

It is expected the results of the current work to give some clues for specification of the "effective emission indices" linking emission inventories to the emissions to be used as input in large scale models.

MODEL DOMAINS, NESTING AND NUMERICAL EXPERIMENT SCENARIOS

Applying the MODELS-3 downscaling abilities the simulations are consecutively carried out in 3 nested domains – D1, D2 and D3 with horizontal resolutions of 90, 30 and 10 km respectively. The innermost domain (D3) includes a region with very intensive road transport – the city of London and its "footprint". The horizontal dimensions of D3 are of the typical order of the size of a grid of a large scale CTM.

For the bigger domains the simulations are carried out with all the emissions included in order to obtain boundary conditions for the innermost (D3) domain. The following emission scenarios are envisaged for D3:
1.) Simulations with all the emissions (detailed inventory) in the domain;
2.) Simulations with the emissions from the road transport excluded (detailed inventory);
3.) Simulations with all the emissions (averaged over D3) in the domain;
4.) Simulations with the emissions averaged over D3, but emissions (averaged) from the road transport excluded.

Each pollution characteristic (concentration, deposition, process contribution, etc.) $C_{roadtransport}$, referring to the road transport emissions is obtained in the following way:

$$C_{roadtransport} = C_{allemissions} - C_{allemissions-roademissions}, \quad (1)$$

where $C_{allemissions}$ and $C_{allemissions-roademissions}$ are the characteristics obtained from scenario 1 and 2 (detailed emissions) or from scenario 3 and 4 (averaged over D3 emissions) respectively.

The combined analysis of these scenarios will make it possible (hopefully) to clarify the role of different dynamic and chemical processes which determine the pollution from road transport pattern and time evolution. Some conclusions about the role of the road traffic

emission inventories spatial resolution on the simulated fields and the local to regional scale interaction can also be made.

MODELLING TOOLS AND INPUT DATA

Modelling tools

The US EPA Models-3 system (*Dudhia J.*, 1993, *Grell G.A. et al.*, 1994, *Byun D. et al.*, 1998, *Byun D. and J. Ching*, 1999)) was chosen as a modelling tool because it appears to be one of the most widely used models with proved simulation abilities.

The CMAQ Integrated Process Rate Analysis utility is used to differentiate the contribution of different dynamic and chemical processes which form the pollution characteristics in the region of interest.

Input data

Meteorological background input: US NCEP Global Analyses data. The data has 1×1 degree grid resolution covering the entire globe, the time resolution is 6 hours. The data is available since year 2000.

Emission data: This appears to be a major problem. Two sets of emission data are used in the present study:

1.) EMEP data with a resolution of 50 *km*, divided to sectors, including road transport – this data is used for all the countries except the UK. Using bi-linear interpolation the data was interpolated in the grid cells of domains D2 and D3;

2.) For the UK data from the National Atmospheric Emissions Inventory (NAEI) is used. The data is with resolution of 1km – high enough for the present study needs.

NUMERICAL SIMULATIONS

MM5 simulations

First, MM5 was run on both outer grids (D1 and D2) simultaneously with "two-way" nesting mode on. Then, after extracting the initial and boundary conditions from the resulting fields for the 10 km domain, MM5 was run on the finer 10 km grid as a completely separate simulation with "one-way" nesting mode on. In this approach, information from the 30 km grid was transferred to the 10-km domain through boundary conditions during the simulation, but there is no feedback from the 10 km field up-scale to the 30 km domain. All simulations were made with 23 s-levels going up to 10 hPa height.

Emission input to CMAQ

Two inventory files (for D2 and D3 domains) were prepared exploiting the EMEP 50×50 km girded inventory and the UK NAEI 1×1 km girded inventory. These inventory files contain the annual emission rates of 5 generalized pollutants – SO_x, NO_x, VOC, ammonia (NH_3), CO, PM10 and PM25 for every grid cell of both domains.

As to prepare the CMAQ emission input file, these inventory files were handled by a specially prepared computer code E_CMAQ. Two main procedures were performed in E_CMAQ. First, the pollutant groups were speciated following the way recommended in *Zlatev Z.* (1995. The next procedure in E_CMAQ is the over-posing of proper time variation profiles (monthly, weekly and hourly). The methodology developed in USA EPA Technology Transfer Network) was applied. As far as in the used gridded inventory the type of sources is not specified, some common enough area sources were chosen from the EPA SCC (Source Category Code) classification and their profiles were averaged. The resulting profiles were

implemented. For the UK road transport emissions weekly and daily temporal profiles, provided by CERC were applied.

The biogenic VOC emissions were estimated, using a simple scheme recommended by *Lübkert B. and W. Schöp* (1989).

CMAQ simulations

The CMAQ model requires inputs of three-dimensional gridded wind, temperature, humidity, cloud/precipitation, and boundary layer parameters. From the MM5 output CMAQ meteorological input was created exploiting the CMAQ meteorology-chemistry interface - MCIP, v2.3. CMAQ v4.4 was run using an open-source, portable implementation of the Message-Passing Interface Standard (MPICH), version 1.2.5. The CB-4 chemical mechanism with Aqueous-Phase Chemistry and EBI solver (Eulerian iterative method) was used.

The CMAQ pre-defined (default) concentration profiles were used for initial conditions over both domains at the beginning of the simulation. The concentration fields obtained at the end of a day's run were used as initial condition for the next day. Default profiles were used as boundary conditions of the 30-km domain (D2) during all period. The boundary conditions for the 10-km domain (D3) were determined through the nesting capabilities of CMAQ.

The simulations for D2 were carried out only for scenario 1 (all the emissions). The simulations for D3 were carried out for scenarios 1 - 4 (emissions from the road transport excluded). The CMAQ simulations were carried out for January and August 2002 - 2006.

SOME RESULTS

The numerical experiments performed produced a huge volume of information. Due to the limited volume of the extended abstracts only some examples can be given here.

The diurnal course of surface O_3 from road transport is demonstrated in Fig. 1. Both the effects of meteorological conditions and large city agglomerations are very well displayed – the O_3 "gaps" over the city of London and O_3 maximums to the West-Southwest of the city are formed during the day and in the evening move towards Southeast.

Plots of the contribution of dry deposition, chemical transformations, cloud processes and aqueous chemistry and the summary advection/diffusion effects for August 11, 14 h are shown in Fig. 2. Comments on each individual figure will take a lot of space. Shortly it could be stated that the figure demonstrates in details the processes of plumes dilution and chemical transformations of pollutants generated by road transport. The negative contribution of the chemical processes and the positive one of advection/diffusion outlines very well the city of London and the surrounding road network.

An example of the time evolution of the different processes contribution and the resulting O_3 surface concentrations change per hour are shown in Fig. 3. It can be seen that advection/diffusion and chemistry are the processes with major contribution. The mean, maximal and minimal values for the same characteristics, obtained from all the 5 summer months simulations for the cases of detailed and averaged over D3 emissions. It can be seen that the mean contribution of different processes can differ by orders of magnitude, that the contribution of each process itself may vary within a wide range and that some of the processes are quite sensitive to emission resolution.

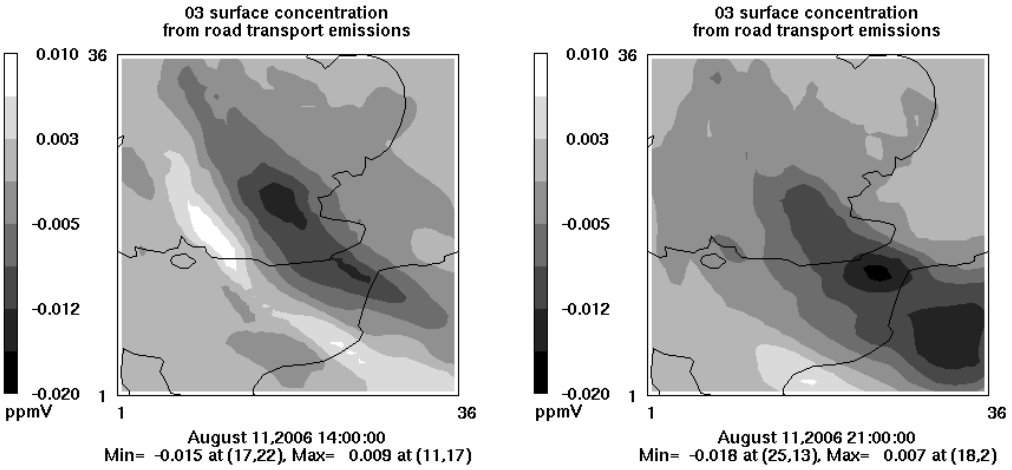

Fig.1. Diurnal course of O_3 surface concentrations from road transport for August 11, 2006

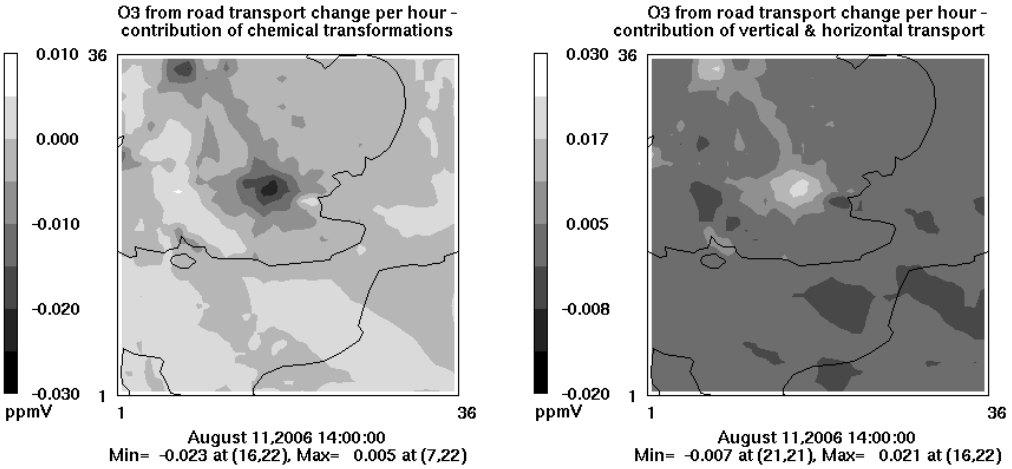

Fig.2. The contribution of some processes to the one hour evolution of O_3 surface concentrations from road transport for August 11, 2006, 14 h.

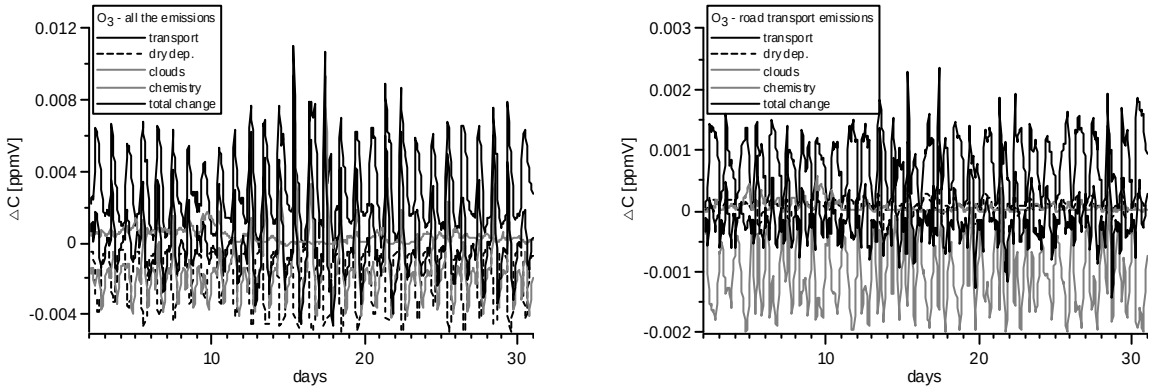

Fig.3. Averaged over D3 temporal change of surface ozone concentrations and the contribution of different processes for August 2002

CONCLUSIONS

The numerical experiments performed produced a huge volume of information, which have to be carefully analysed and generalized so that some final conclusions, concerning not only clarification of local scale processes of dilution and chemical transformation but also how to

account for them in large scale CTMs could be made. Comprehensive survey of the output from all the numerical experiments will be possible only if some integral quantities, characterising the dilution and transformation processes within D3 domain are introduced.

Table 1. Horizontally/temporally averaged process contribution to surface Ozone change per hour [ppmV]; emissions from road transport

Characteristics:	Emission resolution:	Advection & diffusion	Dray deposition	Clouds and aerosol	Chemical transformations	Total change per hour
Mean values	detailed	8.48E-04	7.23E-05	6.06E-05	-1.11E-03	-1.28E-04
	averaged	1.03E-03	1.79E-05	1.02E-04	-1.26E-03	-1.15E-04
Maximal values	detailed	2.36E-03	4.46E-04	9.42E-04	1.40E-03	1.75E-03
	averaged	2.42E-03	3.48E-04	9.91E-04	3.39E-03	3.10E-03
Minimal values	detailed	-4.50E-04	-8.81E-04	-7.01E-05	-2.19E-03	-1.42E-03
	averaged	-1.28E-03	-9.72E-04	-6.44E-05	-2.59E-03	-1.89E-03

The conclusions that can be made at this stage of the studies are:
1.) The effect of the road transport emissions is well displayed in both the concentration and process analysis fields;
2.) The contributions of different processes have very complex spatial/temporal behavior and variability;
3.) Even horizontally/temporally averaged process contributions may be sensitive to emission resolution.

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