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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OUTLINE:

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MODEL DOMAINS, NESTING AND NUMERICAL EXPERIMENT SCENARIOS
MODELLING TOOLS AND INPUT DATA
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SOME EXAMPLES
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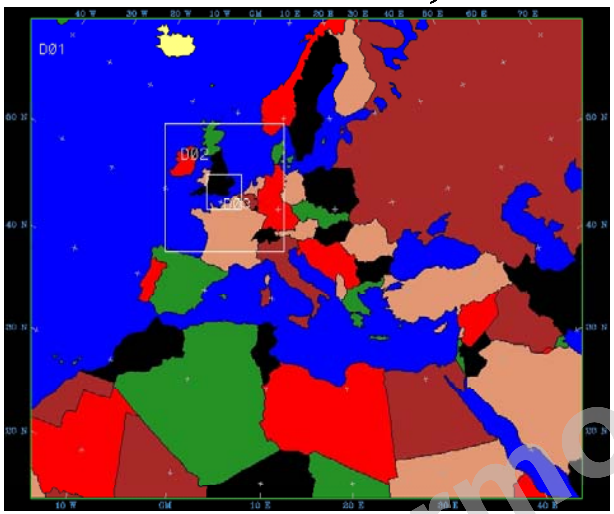
INTRODUCTION

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



The three computational domains produced by TERRAIN

The three model domains are shown on Fig.1, the innermost domain (D3) including 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 in D3 were used for the numerical experiments:

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:

$$\mathbf{C_{road} = C_{all\ emissions} - C_{all\ emissions\text{-}road\ emissions}}$$

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 Analysis" (IPA) 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 σ-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 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.

Integrated process rate analysis

The CMAQ "**Integrated Process Analysis**" (IPR) utility is used to differentiate the contribution of different dynamic and chemical processes

$$\frac{\partial c_i}{\partial t} = \sum_{j=1}^{M} L_{ij} , \qquad i=1,\dots,N ,$$

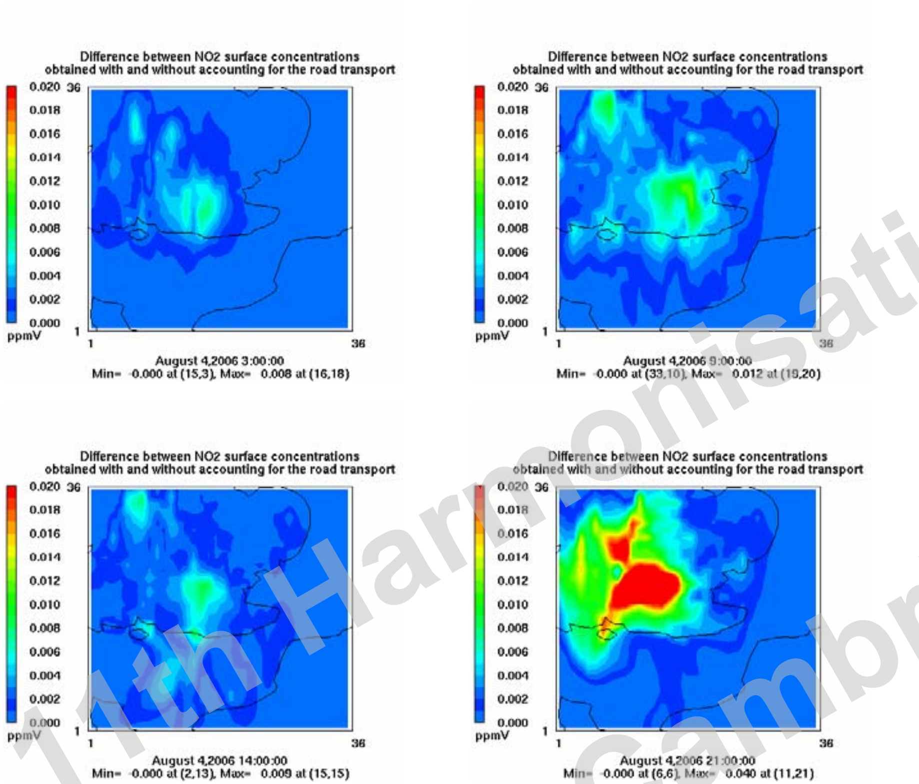
where c_i is the concentration of the respective pollutant, L_{ij}, $i=1,\dots,N$, $j=1,\dots,M$ are the operators of any kind, including emissions, which account for all the processes that lead to c_i formation.

The CMAQ "Integrated Process Rate Analysis" (IPR) utility, which is used to differentiate the contribution of different dynamic and chemical processes, is actually just another way to write (1):

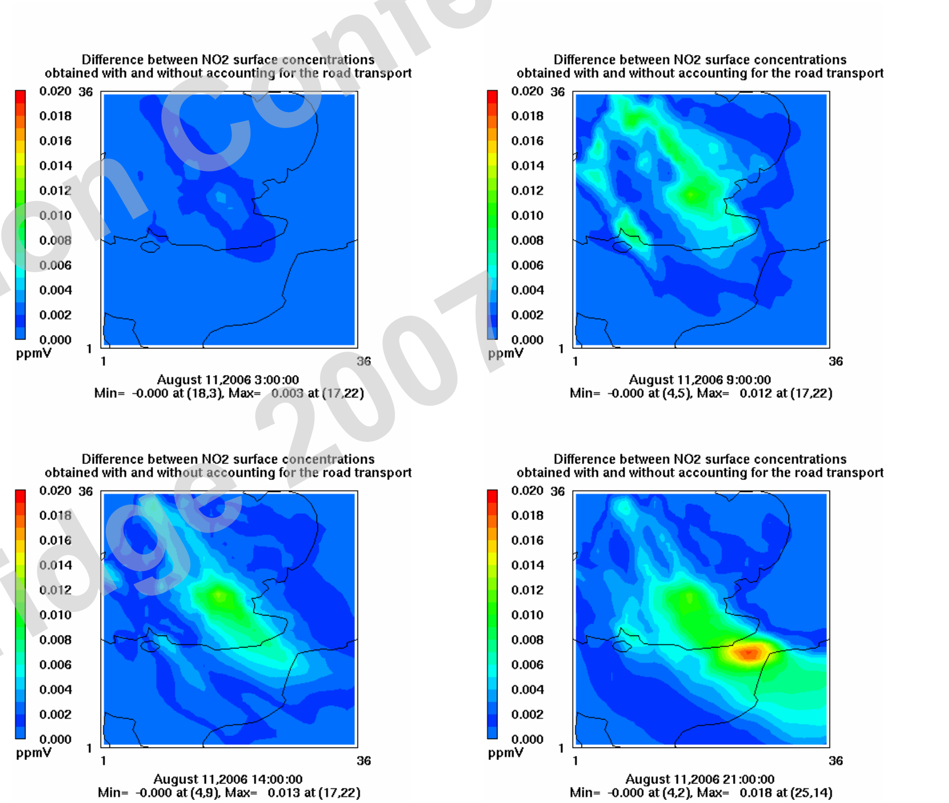
$$\Delta c_i = \sum_{j=1}^{M} \Delta c_{ij} , \quad \Delta c_i = \int_{t}^{t+\tau} \frac{\partial c_i}{\partial t} dt = c_i(t+\tau) - c_i(t), \quad \Delta c_{ij} = \tau . L_{ij} ,$$

SOME EXAMPLES

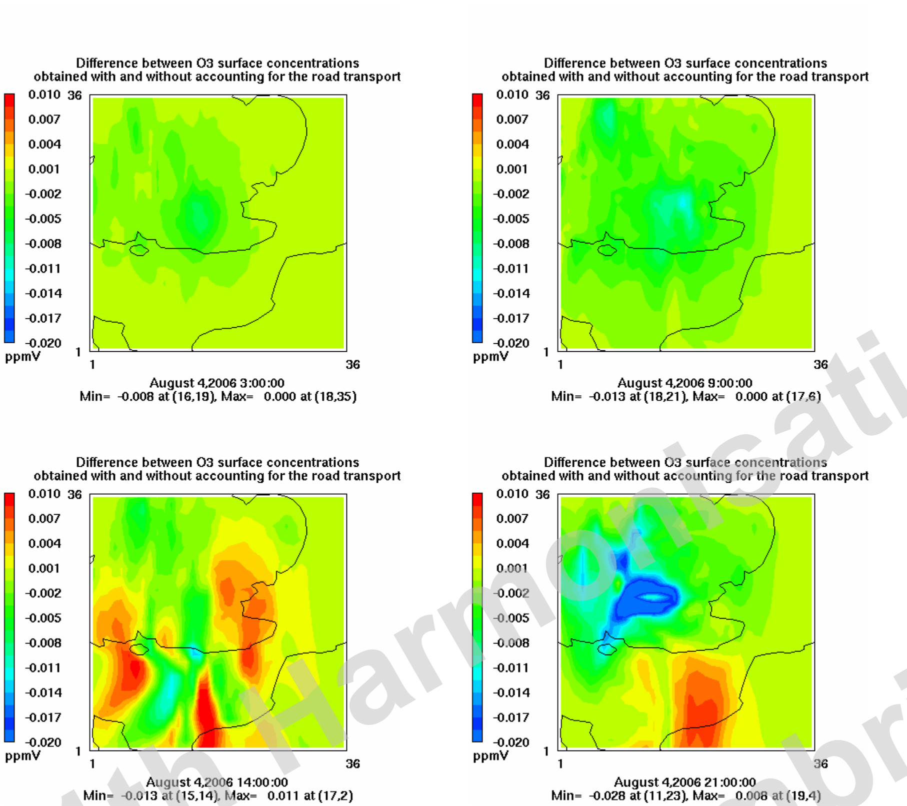
3D fields



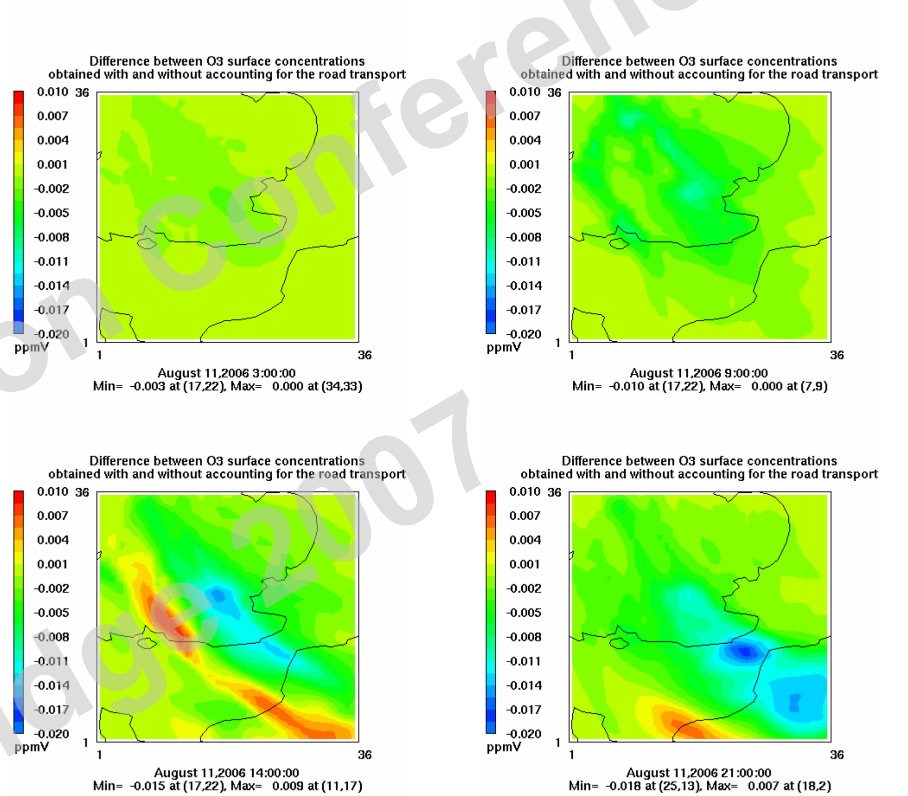
Diurnal course of NO_2 surface concentrations from road transport for August 04, 2006



Diurnal course of NO_2 surface concentrations from road transport for August 11, 2006

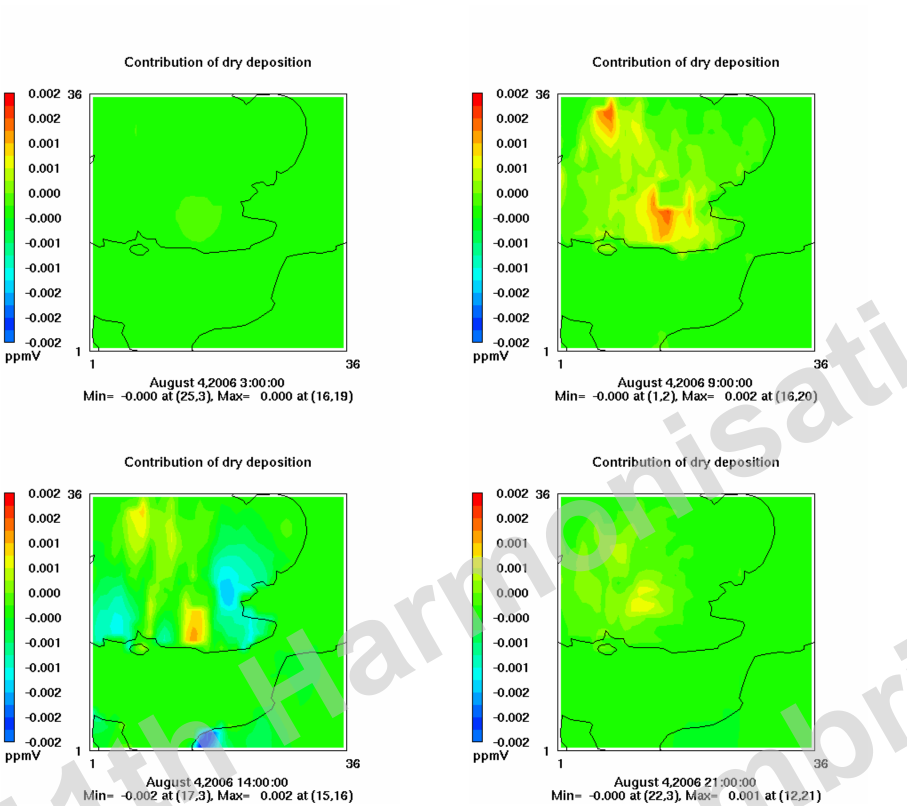


Diurnal course of O_3 surface concentrations from road transport for August 04, 2006

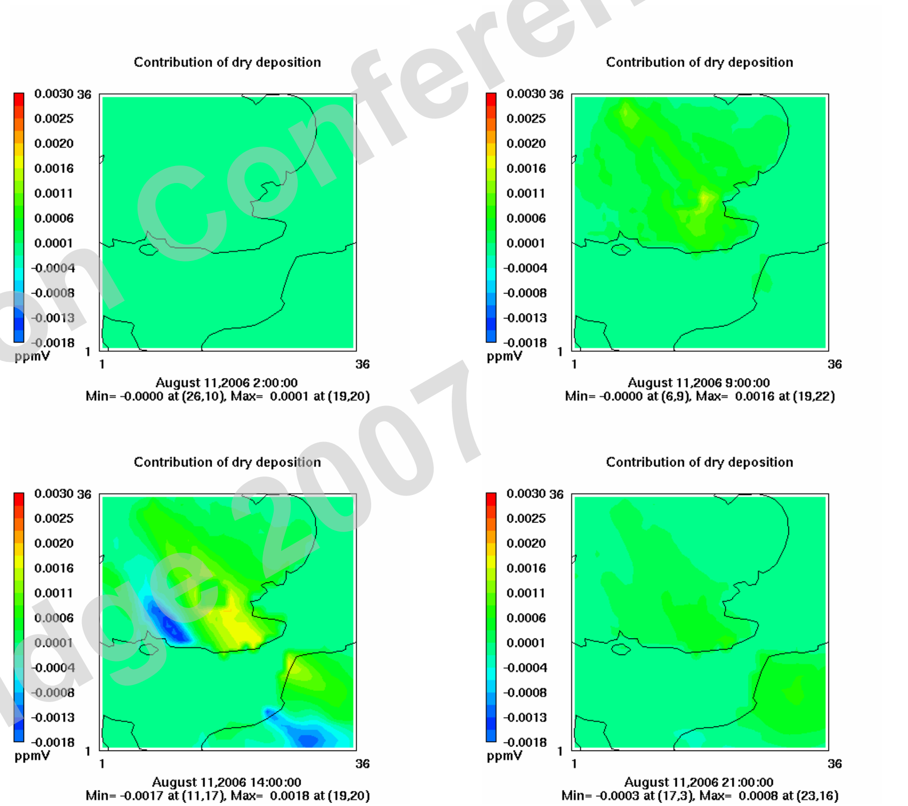


Diurnal course of O_3 surface concentrations from road transport for August 11, 2006

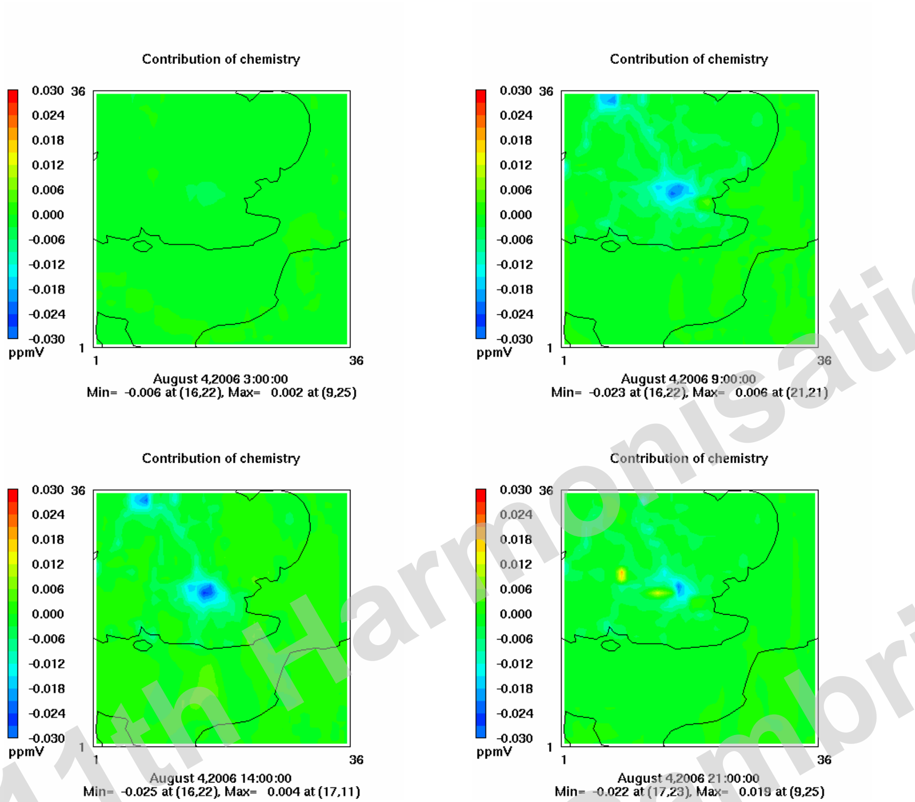
Both the effects of meteorological conditions and large city agglomerations are very well displayed – the O_3 "gaps" over the city of London and O_3 maximums to the West-Southwest of the city are formed during the day and in the evening move towards Southeast.



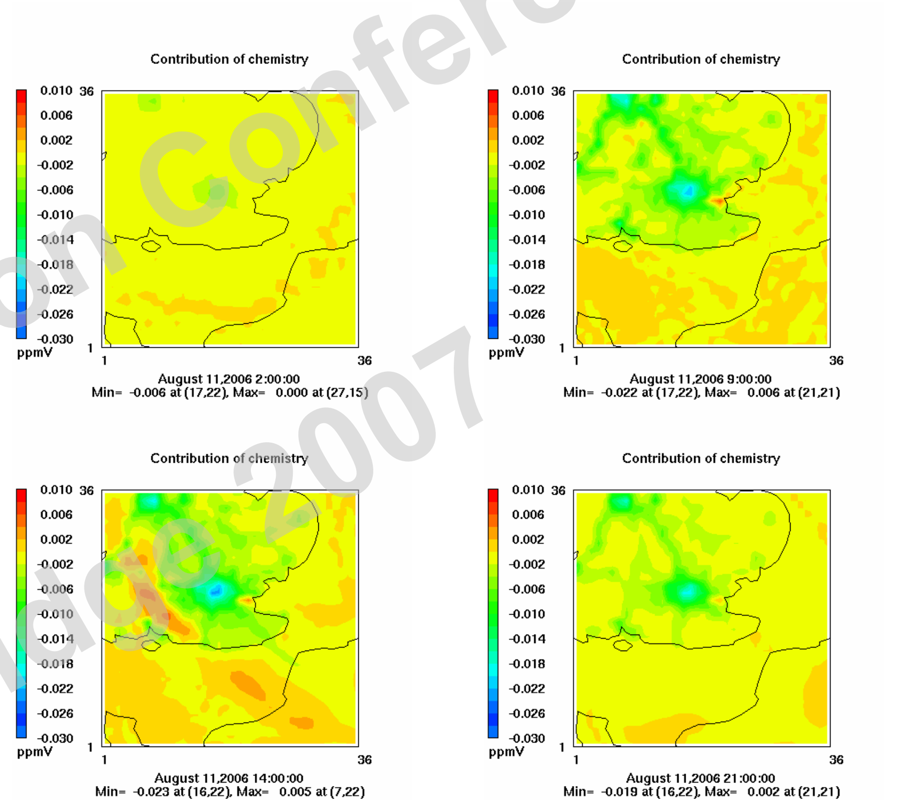
Diurnal course of the contribution of deposition processes to the formation of O_3 surface concentrations from road transport for August 04, 2006



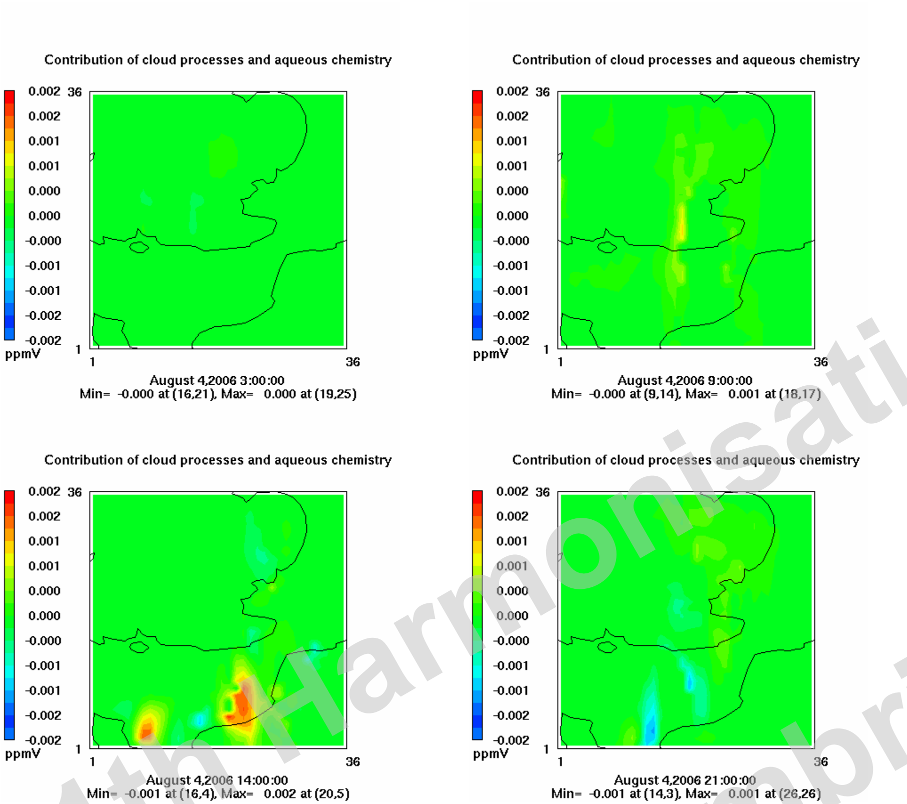
Diurnal course of the contribution of dry deposition processes to the formation of O_3 surface concentrations from road transport for August 11, 2006



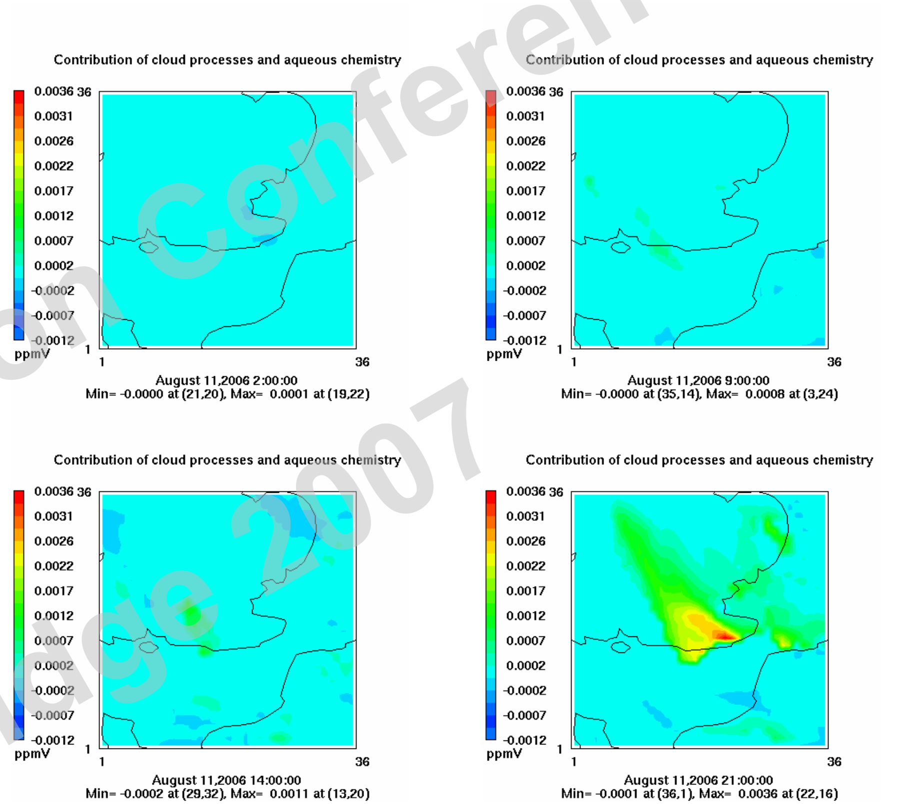
Diurnal course of the contribution of chemical transformation processes to the formation of O_3 surface concentrations from road transport for August 04, 2006



Diurnal course of the contribution of chemical transformation processes to the formation of O_3 surface concentrations from road transport for August 11, 2006



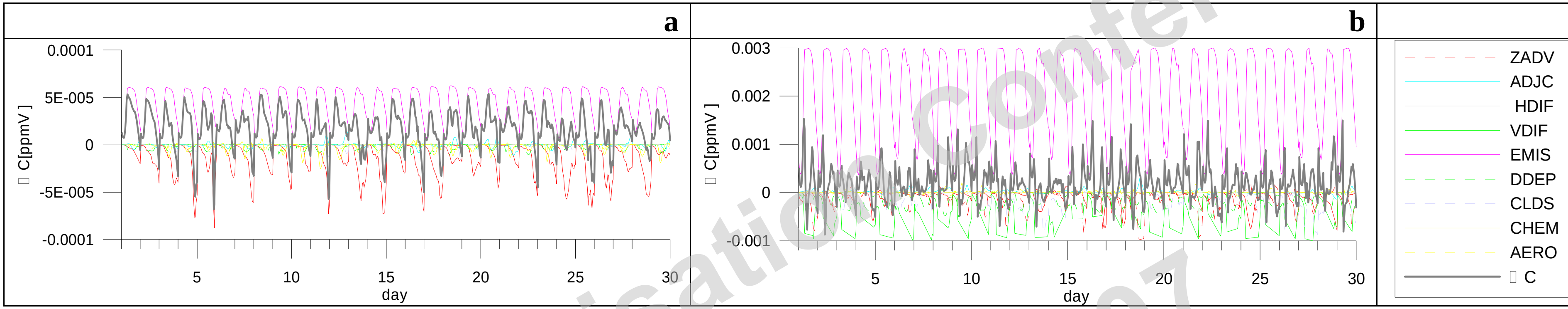
Diurnal course of the contribution of cloud processes and aqueous chemistry to the formation of O_3 surface concentrations from road transport for August 04, 2006



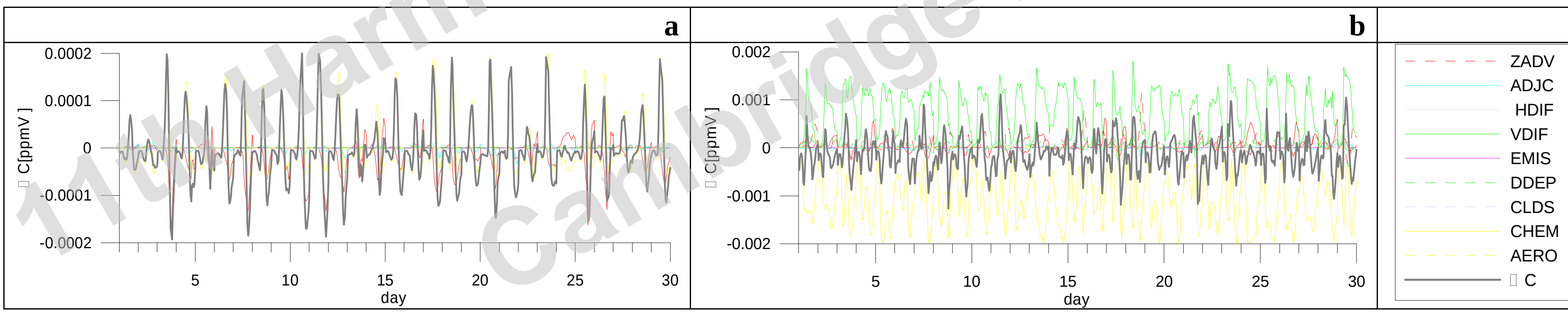
Diurnal course of the contribution of cloud processes and aqueous chemistry to the formation of O_3 surface concentrations from road transport for August 11, 2006

Time series

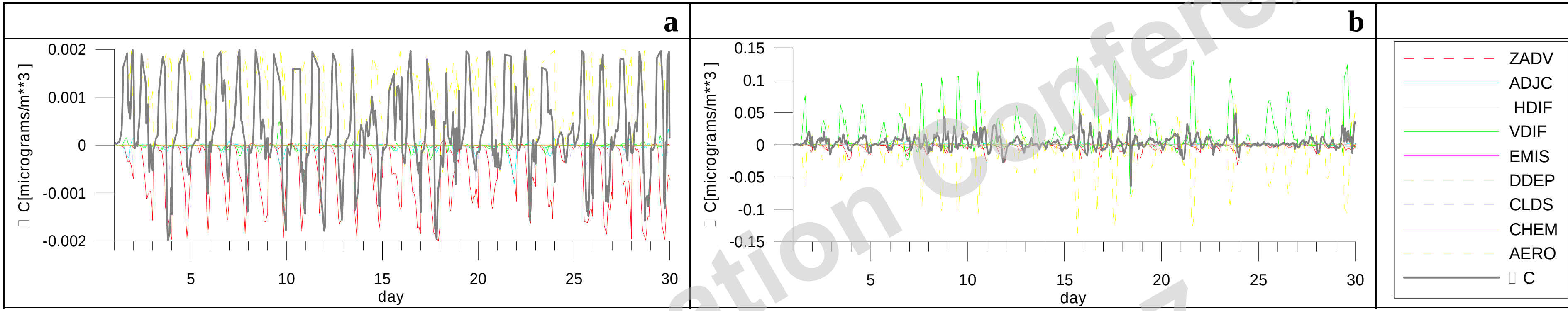
Examples for a summer month:



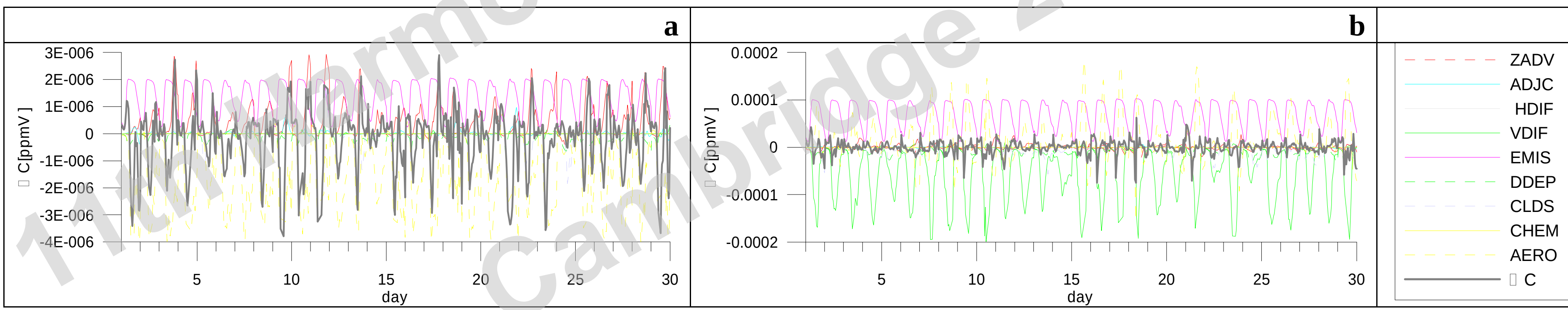
Averaged over D3 temporal change of columnar (a) and surface (b) **Nitrogen Species** concentrations and the contribution of different processes for August 2005



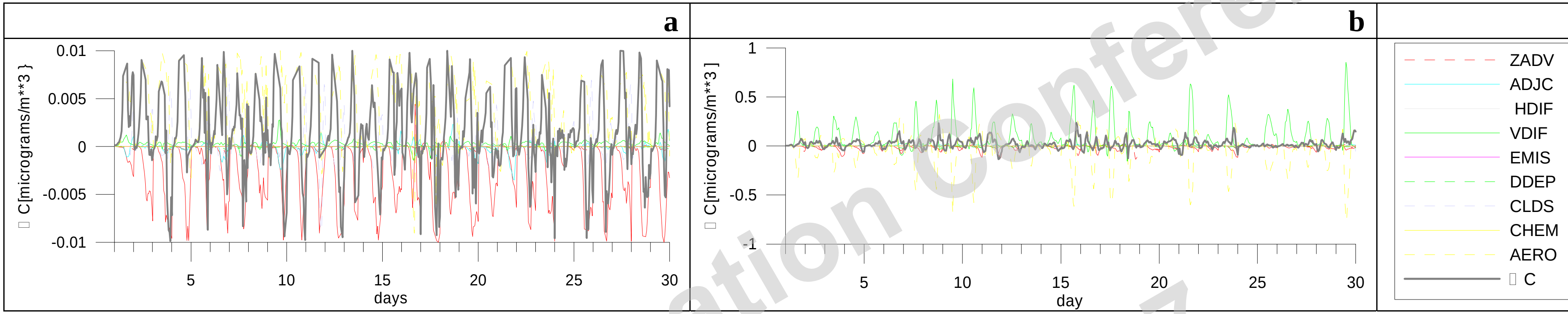
Averaged over D3 temporal change of columnar (a) and surface (b) **Ozone** concentrations and the contribution of different processes for August 2005



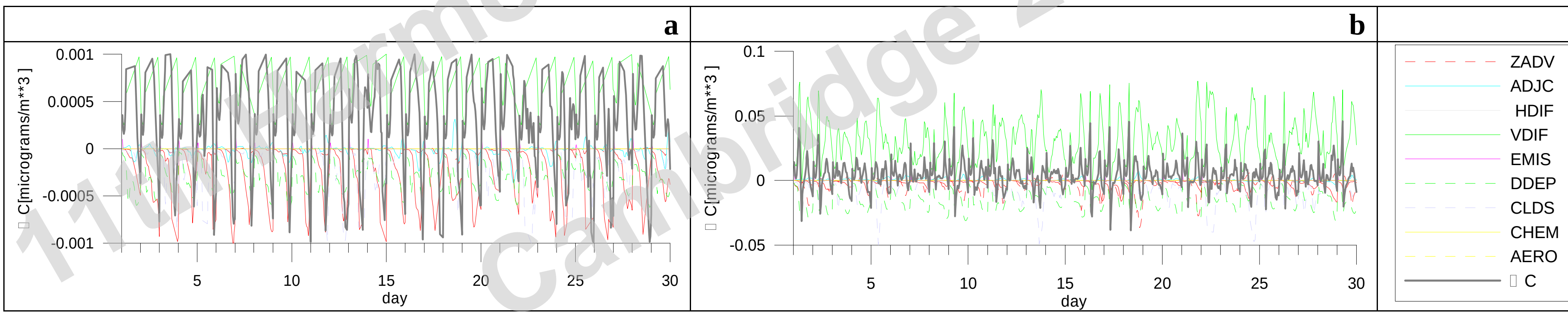
Averaged over D3 temporal change of columnar (a) and surface (b) **aerosol NH_4 (ammonium)** concentrations and the contribution of different processes for August 2005



Averaged over D3 temporal change of columnar (a) and surface (b) **NH_3 (ammonia)** concentrations and the contribution of different processes for August 2005

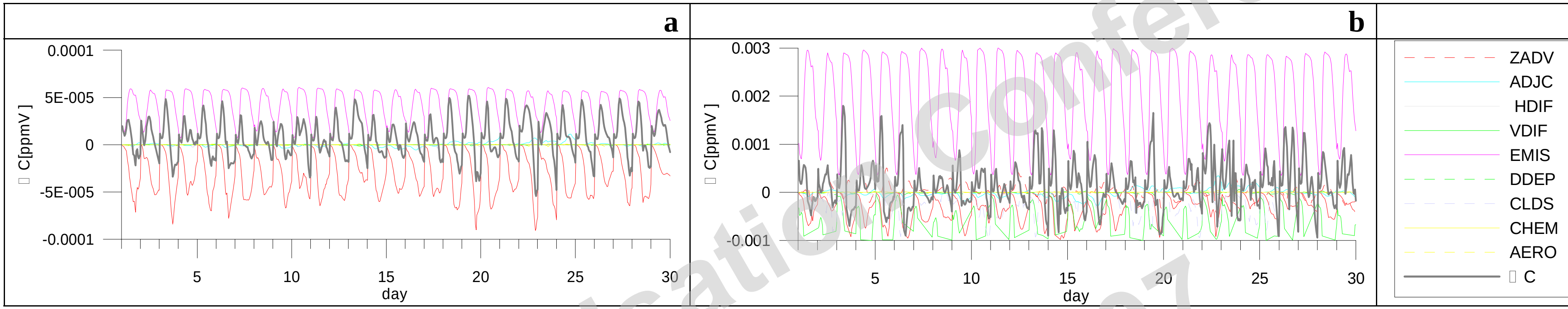


Averaged over D3 temporal change of columnar (a) and surface (b) **PM2.5** concentrations and the contribution of different processes for August 2005

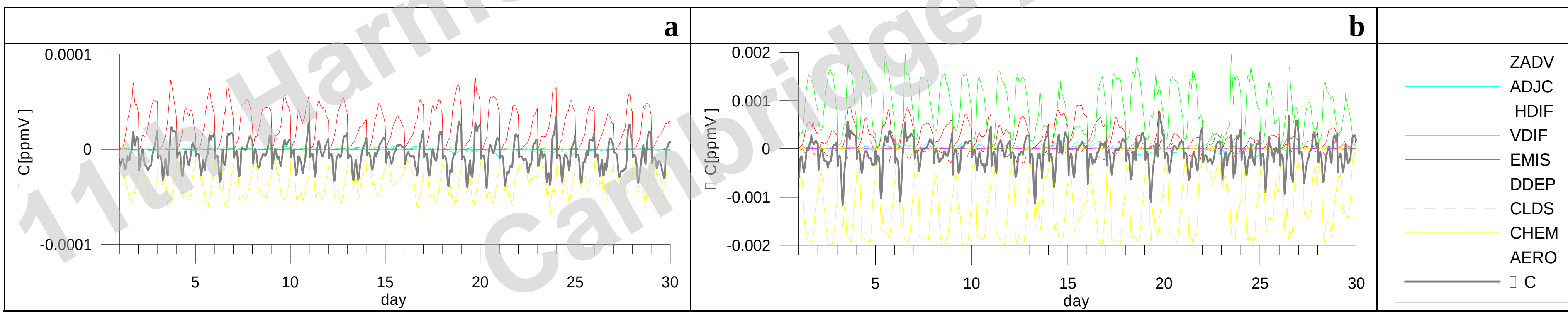


Averaged over D3 temporal change of columnar (a) and surface (b) **PM-coarse** concentrations and the contribution of different processes for August 2005

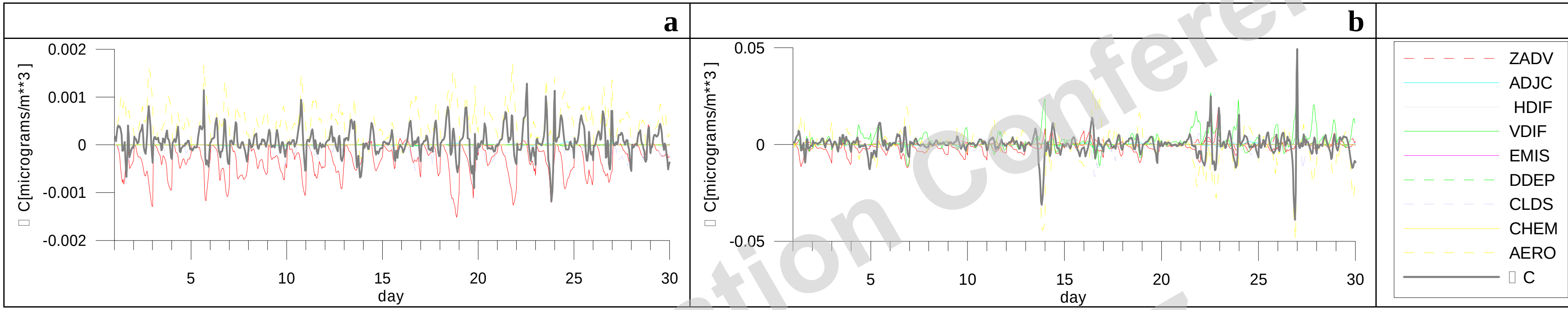
Examples for a winter month:



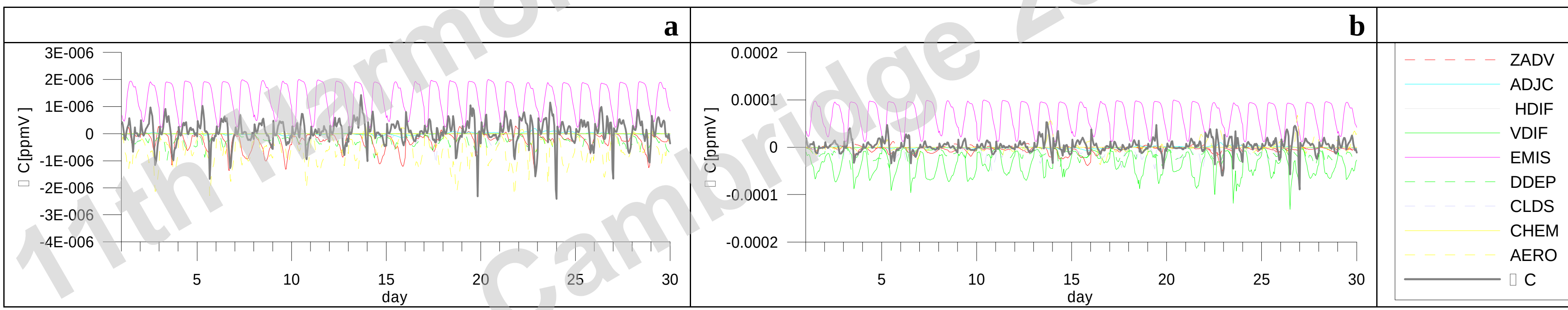
Averaged over D3 temporal change of columnar (a) and surface (b) **Nitrogen Species** concentrations and the contribution of different processes for January 2005



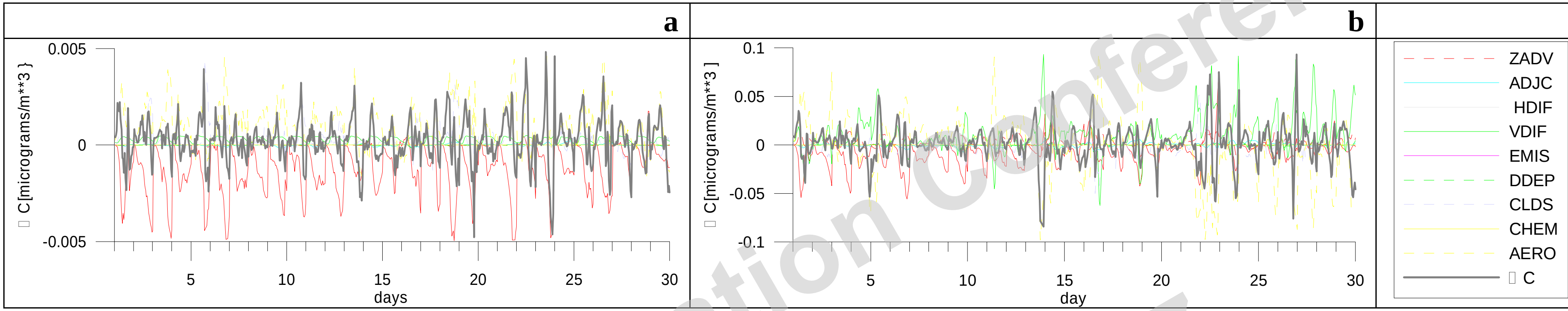
Averaged over D3 temporal change of columnar (a) and surface (b) **Ozone** concentrations and the contribution of different processes for January 2005



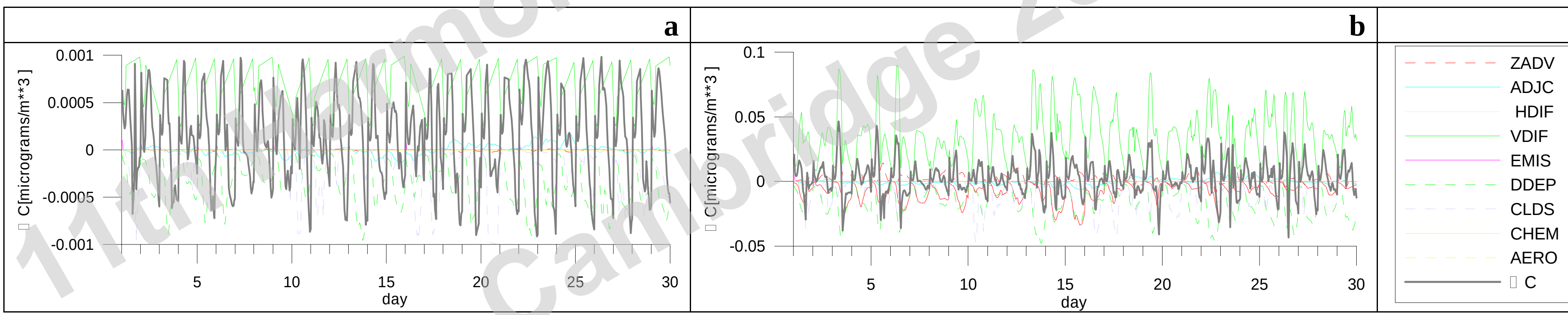
Averaged over D3 temporal change of columnar (a) and surface (b) **aerosol NH_4 (ammonium)** concentrations and the contribution of different processes for January 2005



Averaged over D3 temporal change of columnar (a) and surface (b) **NH_3 (ammonia)** concentrations and the contribution of different processes for January 2005



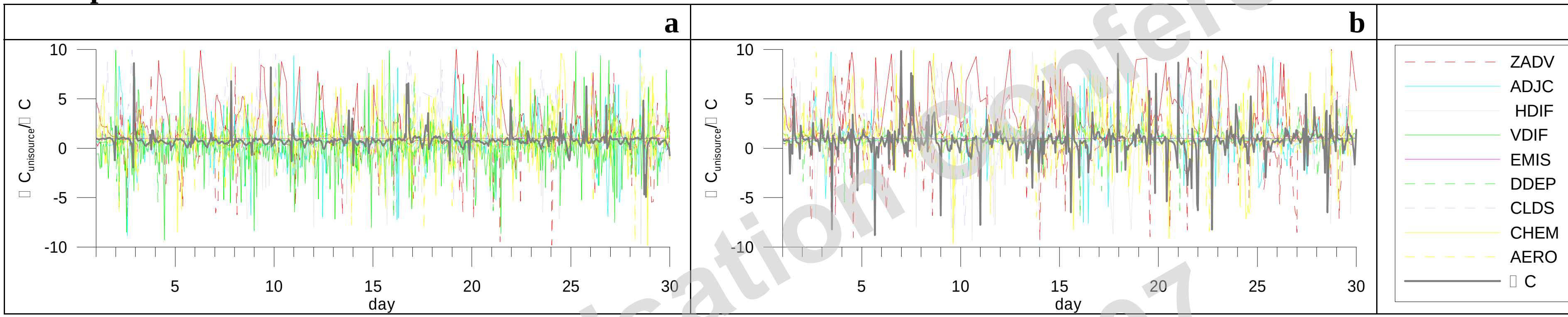
Averaged over D3 temporal change of columnar (a) and surface (b) **PM2.5** concentrations and the contribution of different processes for January 2005



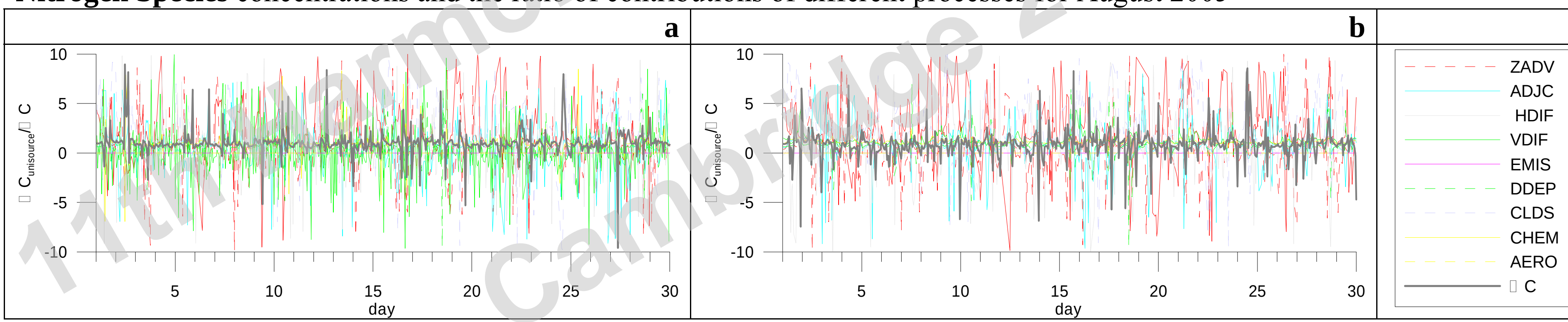
Averaged over D3 temporal change of columnar (a) and surface (b) **PM-coarse** concentrations and the contribution of different processes for January 2005

THE EFFECTS OF EMISSION RESOLUTION

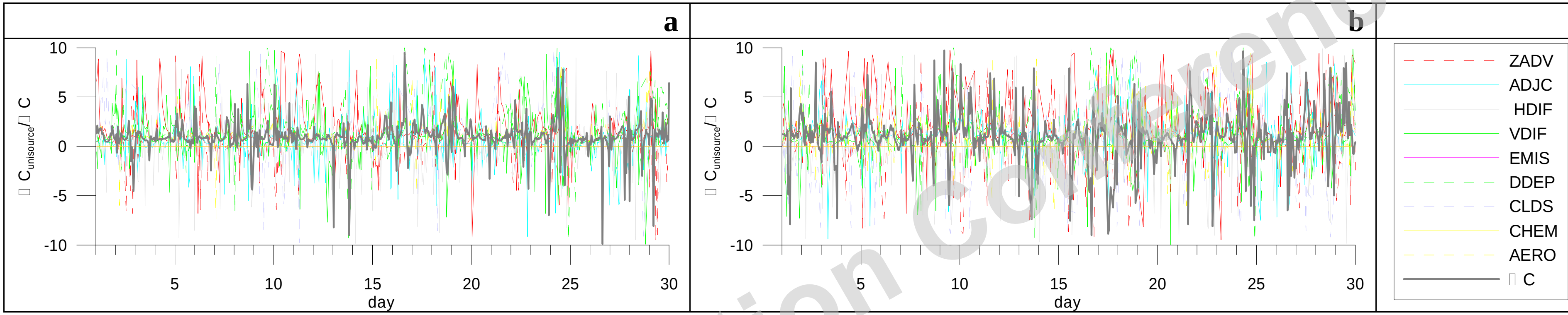
Examples for a summer month:



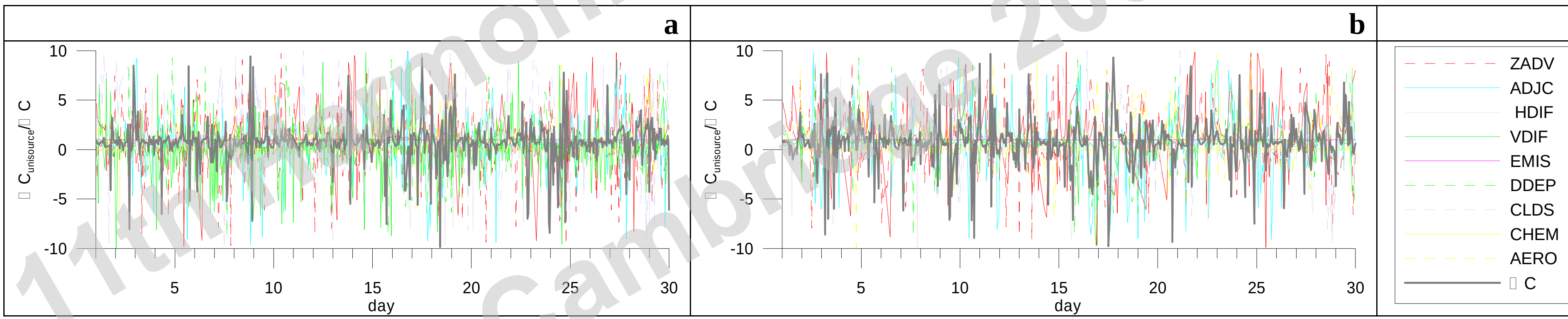
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **Nitrogen Species** concentrations and the ratio of contributions of different processes for August 2005



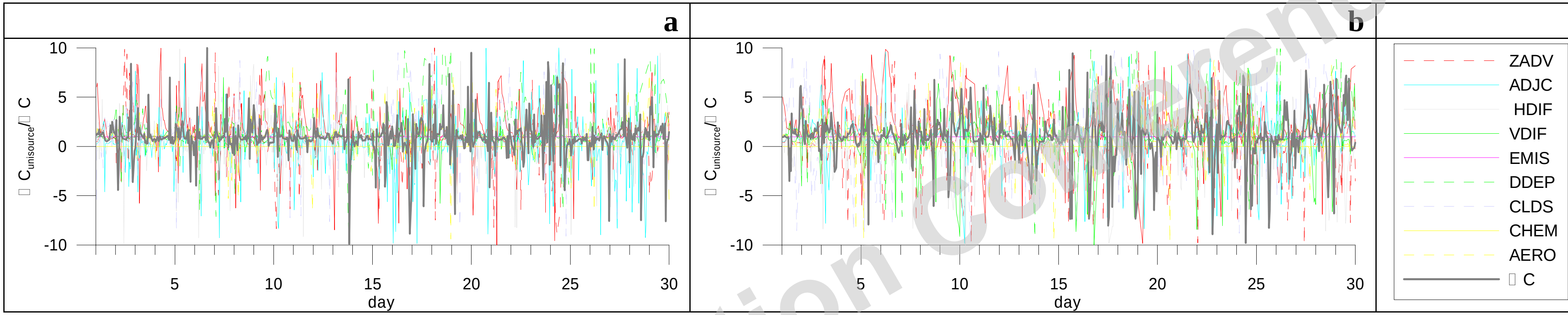
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **Ozone** concentrations and the ratio of contributions of different processes for August 2005



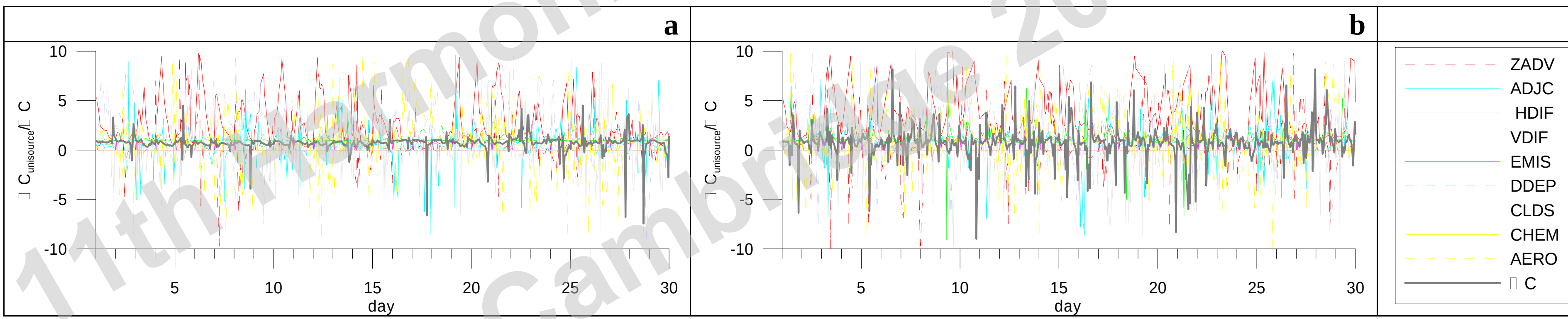
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **aerosol NH_4 (ammonium)** concentrations and the ratio of contributions of different processes for August 2005



The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **NH_3 (ammonia)** concentrations and the ratio of contributions of different processes for August 2005

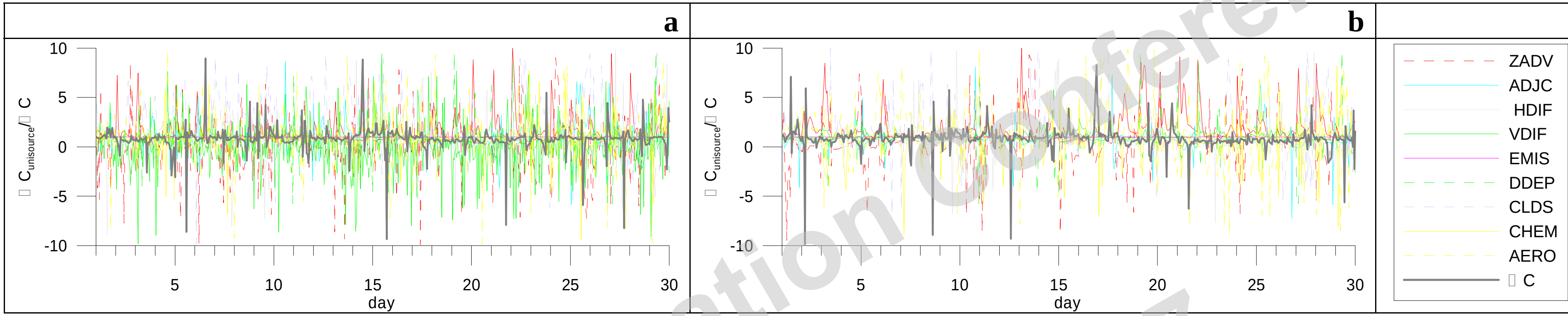


The ratio $\Delta C_{averaged\ emissions} / \Delta C_{det\,ailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **PM2.5** concentrations and the ratio of contributions of different processes for August 2005

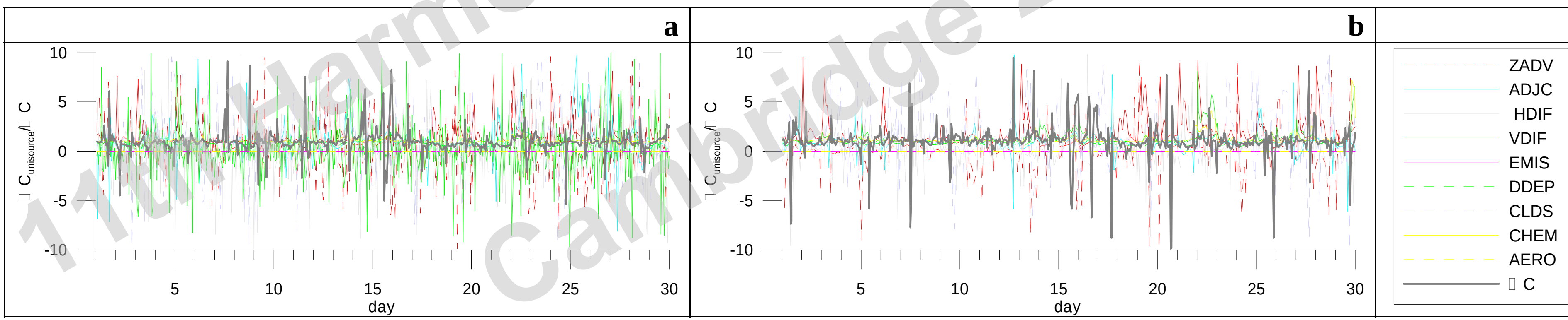


The ratio $\Delta C_{averaged\ emissions} / \Delta C_{det\,ailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **PM-coarse** concentrations and the ratio of contributions of different processes for August 2005

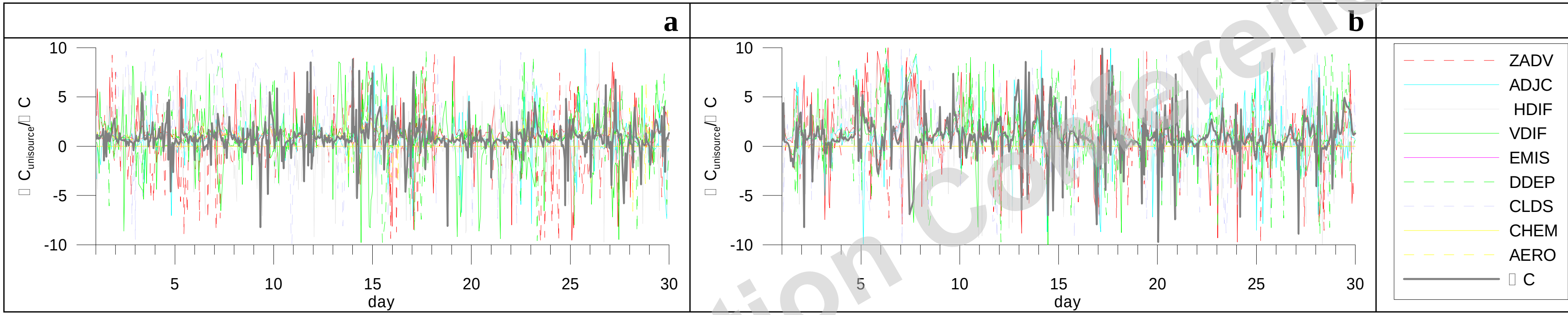
Examples for a winter month:



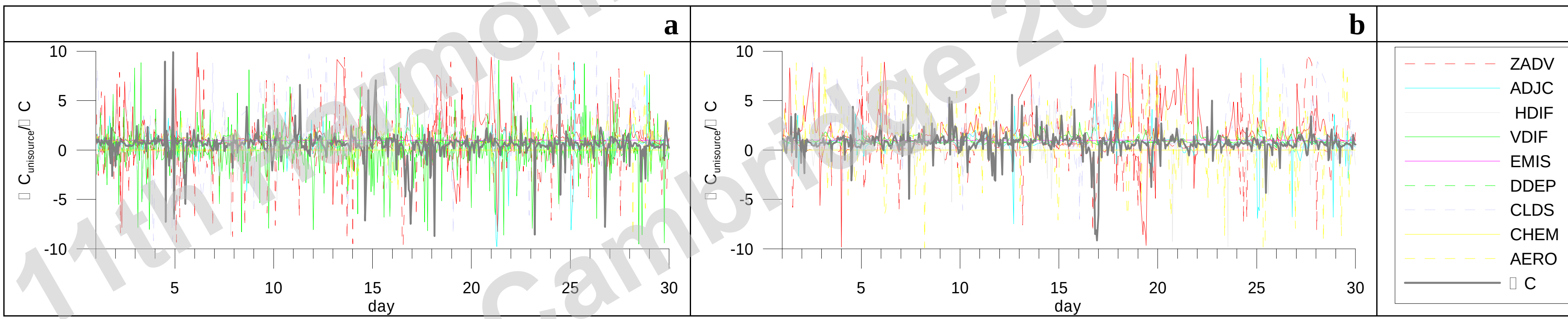
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{\det ailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **Nitrogen Species** concentrations and the ratio of contributions of different processes for January 2005



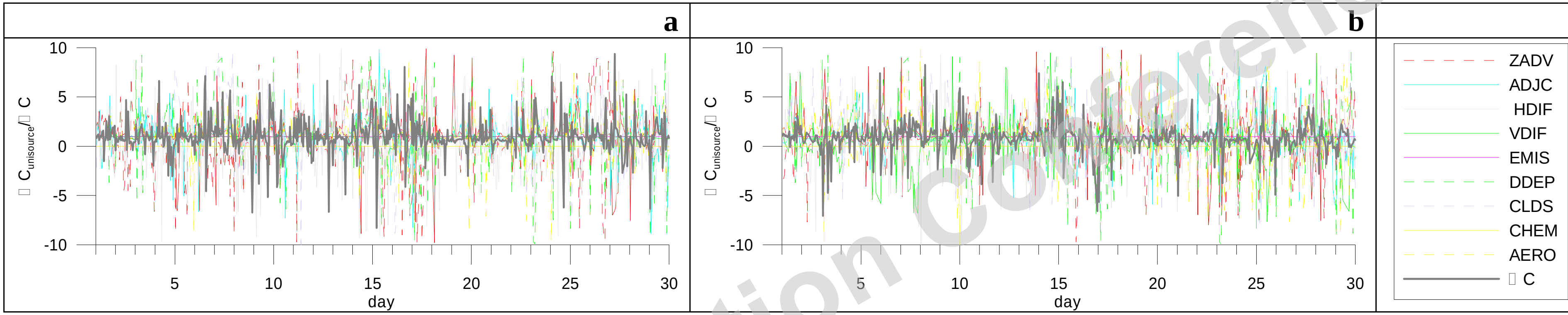
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{\det ailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **Ozone** concentrations and the ratio of contributions of different processes for January 2005



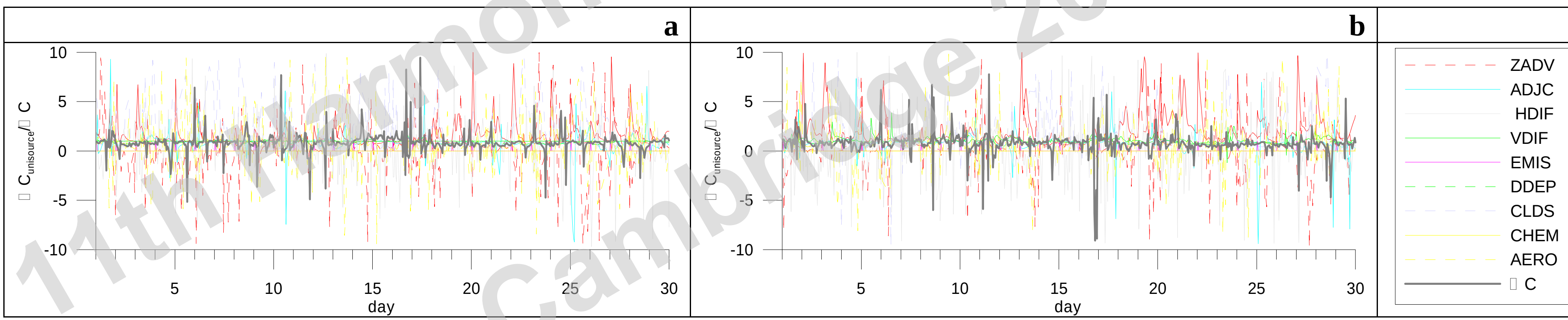
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **aerosol NH_4 (ammonium)** concentrations and the ratio of contributions of different processes for January 2005



The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **NH_3 (ammonia)** concentrations and the ratio of contributions of different processes for January 2005



The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **PM2.5** concentrations and the ratio of contributions of different processes for January 2005



The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **PM-coarse** concentrations and the ratio of contributions of different processes for January 2005

Columnar values-summer

	Process:	XYAD	ZADV	ADJC	HDIF	VDIF	EMIS	DDEP	CLDS	CHEM	AERO	DeltC
GNOY	averaged	4.23E+00	3.53E-01	1.89E-01	4.27E-01	1.61E-01	9.88E-01	6.01E-01	7.83E+01	1.95E+00	1.32E+00	7.35E-01
	maximal	1.74E+03	6.75E+03	7.69E+02	6.56E+03	2.48E+03	1.01E+00	2.18E+02	1.39E+05	9.81E+02	3.17E+03	6.57E+01
	minimal	-5.78E+00	-3.57E+03	-1.83E+03	-5.56E+03	-1.78E+03	0.00E+00	-7.10E+02	-3.15E+04	-4.27E+02	-1.96E+03	-5.45E+01
ORG_N	averaged	-1.07E+00	-2.98E+00	-7.26E-01	1.41E+00	4.87E+00	0.00E+00	2.07E+00	-5.69E+01	3.24E+00	0.00E+00	2.08E+00
	maximal	1.30E+03	1.97E+03	1.55E+03	5.00E+03	2.28E+04	0.00E+00	5.89E+03	2.85E+04	3.47E+03	0.00E+00	2.31E+03
	minimal	-9.21E+03	-1.18E+04	-3.93E+03	-1.23E+03	-2.50E+03	0.00E+00	-1.22E+03	-1.45E+05	-3.57E+02	0.00E+00	-7.64E+02
NO2	averaged	3.95E+00	-1.55E+00	-5.54E-02	-3.33E-01	-1.22E+00	9.88E-01	7.45E-01	2.88E+03	5.09E-01	0.00E+00	1.10E+00
	maximal	1.63E+02	4.17E+02	6.75E+02	1.39E+03	7.26E+02	1.01E+00	1.73E+00	9.50E+06	5.78E+01	0.00E+00	1.09E+03
	minimal	0.00E+00	-6.54E+03	-2.01E+03	-1.38E+03	-3.38E+03	0.00E+00	0.00E+00	-3.30E+05	-9.87E+02	0.00E+00	-9.88E+01
O3	averaged	4.06E+00	-1.37E-01	2.06E+00	-1.67E+00	-6.92E-01	0.00E+00	6.88E-01	8.51E+00	1.82E+00	0.00E+00	1.87E+00
	maximal	7.97E+02	7.71E+03	4.27E+03	1.40E+03	8.95E+02	0.00E+00	2.07E+02	1.01E+04	2.21E+03	0.00E+00	1.84E+03
	minimal	-3.53E+02	-1.45E+04	-3.63E+02	-4.42E+03	-9.61E+02	0.00E+00	-3.29E+02	-1.63E+04	-3.45E+02	0.00E+00	-2.92E+02
CO	averaged	2.85E+00	4.07E-01	3.87E-01	2.63E-01	-9.53E-01	9.89E-01	7.49E-01	2.08E+02	9.59E+00	0.00E+00	7.49E-01
	maximal	3.83E+02	6.92E+02	4.58E+02	2.66E+03	5.82E+02	1.01E+00	1.57E+00	7.54E+05	2.32E+04	0.00E+00	5.18E+01
	minimal	-3.70E+03	-7.91E+02	-4.46E+02	-2.28E+03	-2.03E+03	0.00E+00	0.00E+00	-8.82E+04	-1.15E+03	0.00E+00	-7.76E+01
HYDC	averaged	3.36E+00	3.63E-01	1.62E-01	2.00E-01	-2.68E+00	9.89E-01	0.00E+00	-3.96E+01	1.63E+00	0.00E+00	3.46E+00
	maximal	5.15E+02	6.38E+02	5.05E+02	2.11E+02	4.40E+02	1.01E+00	0.00E+00	1.71E+04	3.25E+03	0.00E+00	6.33E+03
	minimal	-5.83E+02	-7.02E+02	-7.05E+02	-1.90E+02	-9.90E+03	0.00E+00	0.00E+00	-5.73E+04	-3.00E+03	0.00E+00	-1.89E+02
CAR_PHE	averaged	1.30E+00	1.07E+01	1.65E+00	3.20E-01	-8.20E-01	9.88E-01	8.82E-01	1.06E+04	2.45E+00	0.00E+00	1.54E+00
	maximal	1.14E+03	4.05E+04	2.45E+03	2.14E+03	4.32E+03	1.01E+00	1.46E+02	3.57E+07	3.42E+03	0.00E+00	1.44E+03
	minimal	-3.32E+03	-1.01E+04	-5.01E+02	-1.52E+03	-3.72E+03	0.00E+00	-1.70E+02	-1.62E+05	-2.68E+03	0.00E+00	-9.57E+02
NH3	averaged	4.50E+00	-7.72E-02	4.94E-01	4.12E+00	-3.24E+00	9.89E-01	1.14E+00	2.75E+01	0.00E+00	1.32E+00	1.39E+01
	maximal	1.05E+03	4.90E+02	1.08E+03	1.49E+04	1.07E+03	1.01E+00	2.06E+03	1.59E+05	0.00E+00	2.07E+02	4.55E+04
	minimal	-4.90E+02	-7.57E+02	-8.60E+02	-9.18E+02	-1.04E+04	0.00E+00	-2.42E+02	-9.33E+04	0.00E+00	-4.23E+02	-1.22E+03
ANH4	averaged	4.03E+00	4.33E-01	6.01E-01	1.39E+00	-2.01E+01	0.00E+00	1.65E+00	9.41E+00	0.00E+00	1.45E+00	-5.93E-02
	maximal	1.61E+03	2.73E+02	3.51E+02	2.86E+03	1.38E+03	0.00E+00	1.17E+03	5.96E+04	0.00E+00	2.06E+02	3.25E+02
	minimal	-1.35E+03	-5.13E+02	-6.99E+02	-1.01E+03	-5.21E+04	0.00E+00	-9.48E+03	-2.09E+04	0.00E+00	-9.50E+01	-3.31E+03
AH2O	averaged	-1.18E+00	1.63E+00	-6.96E-01	9.61E-01	3.95E+00	0.00E+00	1.29E+00	-3.57E+01	0.00E+00	0.00E+00	7.29E-01
	maximal	2.30E+03	1.74E+03	1.57E+03	9.39E+02	4.35E+03	0.00E+00	3.81E+03	2.52E+04	0.00E+00	0.00E+00	3.97E+02
	minimal	-7.26E+03	-6.64E+02	-2.54E+03	-3.27E+02	-1.09E+03	0.00E+00	-2.65E+04	-1.46E+05	0.00E+00	0.00E+00	-4.61E+03
A2_5	averaged	-7.09E-01	1.17E+00	2.94E-01	-8.34E-01	9.06E-01	9.84E-01	4.50E+00	-1.78E+01	0.00E+00	1.03E+00	5.51E+00
	maximal	5.25E+03	7.60E+02	4.37E+02	1.81E+03	3.99E+01	1.00E+00	2.62E+03	1.73E+04	0.00E+00	2.33E+02	1.11E+04
	minimal	-8.19E+03	-5.21E+02	-4.89E+02	-8.22E+03	-4.06E+01	0.00E+00	-1.41E+03	-6.79E+04	0.00E+00	-4.06E+02	-1.04E+03
ACOARSE	averaged	5.42E+00	5.11E-01	-1.32E+00	4.09E-01	9.97E-01	4.13E-02	1.07E+00	2.31E+01	0.00E+00	-2.53E+25	8.39E-01
	maximal	1.21E+03	2.79E+02	7.58E+02	2.38E+03	1.10E+00	1.00E+00	3.23E+00	2.91E+04	0.00E+00	3.45E+28	1.00E+02
	minimal	0.00E+00	-6.83E+02	-6.32E+03	-1.06E+03	0.00E+00	0.00E+00	0.00E+00	-8.42E+03	0.00E+00	-1.09E+29	-1.77E+02

First Layer values-summer

	Process:	XYAD	ZADV	ADJC	HDIF	VDIF	EMIS	DDEP	CLDS	CHEM	AERO	DeltC
GNOY	averaged	6.32E+00	2.17E+00	-1.57E+01	3.85E+00	9.87E-01	9.88E-01	6.01E-01	1.03E+03	1.34E+00	7.12E-01	1.00E-02
	maximal	2.93E+03	3.82E+03	3.75E+02	7.89E+03	4.49E+00	1.01E+00	2.18E+02	3.96E+06	5.62E+02	1.24E+03	3.40E+02
	minimal	-2.73E+03	-6.58E+02	-4.24E+04	-1.57E+03	0.00E+00	0.00E+00	-7.11E+02	-1.42E+06	-7.07E+02	-2.35E+03	-2.34E+03
ORG_N	averaged	4.93E+00	-1.91E+00	2.64E+00	-3.82E-01	2.01E+00	0.00E+00	2.08E+00	-6.43E+01	3.46E-01	0.00E+00	3.32E-01
	maximal	4.02E+03	5.68E+02	3.79E+03	3.73E+03	3.01E+02	0.00E+00	5.90E+03	3.59E+05	7.16E+02	0.00E+00	1.14E+03
	minimal	-1.24E+03	-7.42E+03	-5.68E+02	-6.33E+03	-9.69E+01	0.00E+00	-1.22E+03	-6.51E+05	-3.60E+03	0.00E+00	-3.35E+03
NO2	averaged	7.52E+00	1.20E+00	1.51E+00	-8.04E-01	1.11E+00	9.88E-01	7.45E-01	9.42E+01	1.12E+00	0.00E+00	4.53E-01
	maximal	1.65E+04	1.36E+03	8.79E+02	1.08E+03	5.19E+00	1.01E+00	1.73E+00	7.90E+05	2.67E+00	0.00E+00	1.44E+02
	minimal	-5.88E+03	-8.08E+02	-3.06E+02	-3.59E+03	0.00E+00	0.00E+00	0.00E+00	-1.09E+06	0.00E+00	0.00E+00	-3.25E+02
O3	averaged	-1.84E+00	6.08E+00	1.27E+00	3.36E+00	1.18E+00	0.00E+00	6.88E-01	3.50E+02	1.07E+00	0.00E+00	1.06E+00
	maximal	1.52E+04	1.10E+04	2.78E+03	4.55E+03	4.83E+00	0.00E+00	2.07E+02	1.17E+06	2.77E+01	0.00E+00	3.47E+02
	minimal	-3.70E+04	-6.71E+02	-1.24E+03	-5.22E+02	-6.14E+00	0.00E+00	-3.28E+02	-4.35E+04	-9.69E+01	0.00E+00	-3.04E+02
CO	averaged	5.00E+00	4.02E-01	1.87E+01	-1.97E+00	1.00E+00	9.89E-01	7.49E-01	1.58E+02	6.38E-01	0.00E+00	5.51E-01
	maximal	7.54E+02	3.47E+02	5.77E+04	1.80E+03	4.23E+00	1.01E+00	1.57E+00	2.16E+05	5.55E+02	0.00E+00	5.36E+02
	minimal	-3.25E+03	-1.03E+03	-1.58E+02	-3.90E+03	0.00E+00	0.00E+00	0.00E+00	-1.16E+05	-1.73E+03	0.00E+00	-1.05E+03
HYDC	averaged	6.92E+00	-2.84E+00	8.61E-01	6.97E-01	9.91E-01	9.89E-01	0.00E+00	2.39E+02	-2.20E-01	0.00E+00	6.36E-01
	maximal	5.82E+03	6.56E+02	1.21E+02	8.18E+02	4.33E+00	1.01E+00	0.00E+00	6.60E+05	5.24E+02	0.00E+00	2.22E+03
	minimal	-1.22E+03	-8.43E+03	-2.20E+02	-4.13E+02	0.00E+00	0.00E+00	0.00E+00	-3.14E+05	-5.99E+03	0.00E+00	-3.02E+03
CAR_PHE	averaged	4.87E+00	-8.59E-02	4.82E-01	-4.35E+01	1.04E+00	9.88E-01	8.82E-01	5.09E+01	6.75E+00	0.00E+00	5.35E-01
	maximal	9.45E+03	9.50E+02	2.34E+03	2.11E+03	5.19E+01	1.01E+00	1.47E+02	1.38E+05	9.82E+03	0.00E+00	1.06E+03
	minimal	-1.92E+03	-2.03E+03	-3.54E+03	-1.35E+05	-2.15E+01	0.00E+00	-1.70E+02	-4.84E+04	-8.22E+02	0.00E+00	-3.34E+03
NH3	averaged	5.37E+00	2.40E+00	1.42E-01	1.65E+00	6.38E-01	9.89E-01	1.14E+00	-3.11E+01	0.00E+00	4.05E-01	5.45E+00
	maximal	2.53E+03	3.75E+03	7.89E+02	7.06E+03	6.18E+01	1.01E+00	2.06E+03	8.01E+03	0.00E+00	2.65E+02	2.04E+04
	minimal	-2.53E+03	-3.19E+02	-6.69E+02	-1.83E+04	-5.06E+02	0.00E+00	-2.42E+02	-4.69E+04	0.00E+00	-3.51E+02	-7.55E+03
ANH4	averaged	7.37E+00	2.54E+00	3.01E+00	-1.99E+00	1.55E+00	0.00E+00	1.64E+00	-7.45E+01	0.00E+00	6.48E-01	2.39E+00
	maximal	3.38E+03	5.23E+03	9.69E+03	3.69E+02	2.63E+03	0.00E+00	1.17E+03	1.52E+04	0.00E+00	6.18E+02	1.14E+03
	minimal	-3.80E+03	-1.32E+03	-6.54E+03	-1.11E+03	-2.99E+03	0.00E+00	-9.48E+03	-2.08E+05	0.00E+00	-3.51E+02	-1.16E+03
AH2O	averaged	6.40E+00	3.31E+00	4.36E+00	1.15E+00	1.22E+00	0.00E+00	1.26E+00	1.10E+02	0.00E+00	0.00E+00	-9.98E-01
	maximal	1.60E+04	1.08E+04	1.48E+04	2.93E+03	2.08E+03	0.00E+00	3.81E+03	3.97E+05	0.00E+00	0.00E+00	8.38E+02
	minimal	-1.88E+04	-1.62E+03	-1.10E+04	-1.43E+03	-5.31E+03	0.00E+00	-2.66E+04	-2.21E+04	0.00E+00	0.00E+00	-8.84E+03
A2_5	averaged	1.01E+01	2.28E+00	2.69E+00	3.79E+00	-8.52E+00	9.84E-01	4.50E+00	3.76E+01	0.00E+00	2.23E+00	1.46E+00
	maximal	5.22E+03	4.47E+03	3.43E+03	9.71E+03	3.92E+02	1.00E+00	2.62E+03	1.19E+05	0.00E+00	3.07E+03	1.10E+03
	minimal	-4.18E+03	-2.82E+02	-9.51E+02	-2.58E+03	-3.06E+04	0.00E+00	-1.41E+03	-4.40E+04	0.00E+00	-3.55E+02	-8.70E+02
ACOARSE	averaged	8.13E+00	-3.78E+00	2.43E+00	-8.54E+00	1.25E+00	4.13E-02	1.07E+00	3.64E+00	0.00E+00	2.83E+24	6.49E-01
	maximal	2.58E+02	3.37E+03	4.30E+03	2.03E+02	1.71E+02	1.00E+00	3.23E+00	3.62E+04	0.00E+00	6.29E+27	5.02E+02
	minimal	-1.41E+03	-1.28E+04	-1.50E+03	-2.47E+04	-5.99E+01	0.00E+00	0.00E+00	-4.46E+04	0.00E+00	-1.64E+26	-7.77E+02

Species	$\frac{\Delta C_{averaged\ emissions}}{\Delta C_{det\,ailed\ emissions}}$	Summer		Winter	
		Columnar Values	First Layer Values	Columnar Values	First Layer Values
GNOY	averaged	7.35E-01	1.00E-02	6.87E-01	8.43E-01
	maximal	6.57E+01	3.40E+02	1.08E+02	4.76E+02
	minimal	-5.45E+01	-2.34E+03	-3.74E+02	-2.69E+02
ORG_N	averaged	2.08E+00	3.32E-01	1.86E+00	1.28E+00
	maximal	2.31E+03	1.14E+03	5.09E+03	1.25E+03
	minimal	-7.64E+02	-3.35E+03	-5.28E+03	-6.56E+02
NO2	averaged	1.10E+00	4.53E-01	6.20E-01	3.19E+00
	maximal	1.09E+03	1.44E+02	4.27E+01	5.90E+03
	minimal	-9.88E+01	-3.25E+02	-6.93E+02	-2.27E+02
O3	averaged	1.87E+00	1.06E+00	4.32E-01	8.54E-02
	maximal	1.84E+03	3.47E+02	1.00E+02	1.28E+02
	minimal	-2.92E+02	-3.04E+02	-1.14E+03	-3.27E+03
CO	averaged	7.49E-01	5.51E-01	1.09E+00	6.39E+00
	maximal	5.18E+01	5.36E+02	1.26E+03	1.05E+04
	minimal	-7.76E+01	-1.05E+03	-2.34E+02	-7.05E+01
H2O2	averaged	-5.57E+00	2.71E+00	3.59E+00	7.24E+00
	maximal	1.31E+03	1.74E+03	5.16E+03	2.02E+04
	minimal	-2.27E+04	-2.97E+02	-1.51E+03	-1.21E+03
HYDC	averaged	3.46E+00	6.36E-01	3.84E-01	-3.95E-01
	maximal	6.33E+03	2.22E+03	1.12E+02	2.98E+02
	minimal	-1.89E+02	-3.02E+03	-1.34E+03	-4.16E+03
CAR_PHE	averaged	1.54E+00	5.35E-01	1.33E+00	5.97E-01
	maximal	1.44E+03	1.06E+03	1.09E+03	9.47E+02
	minimal	-9.57E+02	-3.34E+03	-5.44E+02	-1.13E+03
NH3	averaged	1.39E+01	5.45E+00	9.20E-01	5.27E-01
	maximal	4.55E+04	2.04E+04	3.13E+02	1.51E+02
	minimal	-1.22E+03	-7.55E+03	-3.86E+02	-1.68E+02
ANH4	averaged	-5.93E-02	2.39E+00	6.83E-01	1.17E+00
	maximal	3.25E+02	1.14E+03	8.69E+02	9.97E+02
	minimal	-3.31E+03	-1.16E+03	-5.84E+02	-4.80E+02
AH2O	averaged	7.29E-01	-9.98E-01	1.44E+00	1.10E+00
	maximal	3.97E+02	8.38E+02	7.30E+02	7.57E+02
	minimal	-4.61E+03	-8.84E+03	-2.42E+02	-8.46E+02
A2_5	averaged	5.51E+00	1.46E+00	6.79E-01	-3.68E+00
	maximal	1.11E+04	1.10E+03	2.02E+03	3.95E+02
	minimal	-1.04E+03	-8.70E+02	-1.09E+03	-1.34E+04
ACOARSE	averaged	8.39E-01	6.49E-01	5.88E-01	7.76E-01
	maximal	1.00E+02	5.02E+02	2.43E+02	3.20E+02
	minimal	-1.77E+02	-7.77E+02	-1.28E+03	-1.73E+02

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.

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 quite sensitive to emission resolution.

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