LOCAL TO REGIONAL DILUTION AND TRANSFORMATION PROCESSES OF THE EMISSIONS FROM ROAD TRANSPORT

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OUTLINE:

- INTRODUCTION
- MODEL DOMAINS, NESTING AND NUMERICAL EXPERIMENT SCENARIOS
- MODELLING TOOLS AND INPUT DATA
- NUMERICAL SIMULATIONS
- SOME EXAMPLES
- THE EFFECTS OF EMISSION RESOLUTION
- CONCLUSIONS
- ACKNOWLEDGEMENTS
- REFERENCES

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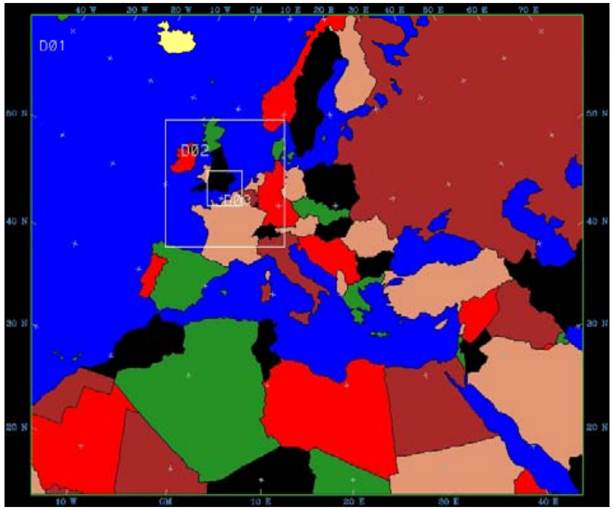
INTRODUCTION

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.

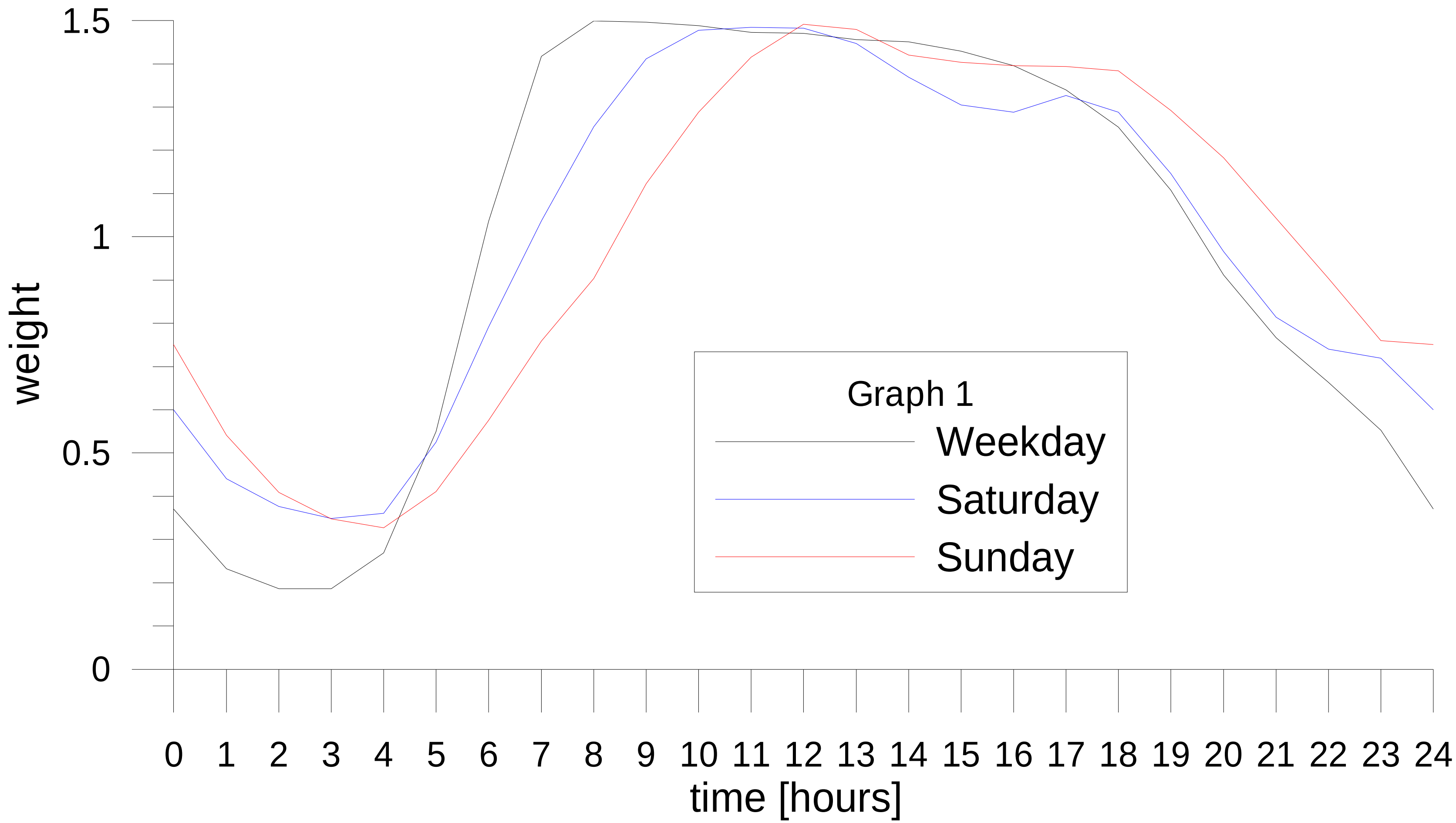


Fig. Temporal profiles of the emissions from road transport

Integrated process rate analysis

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

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

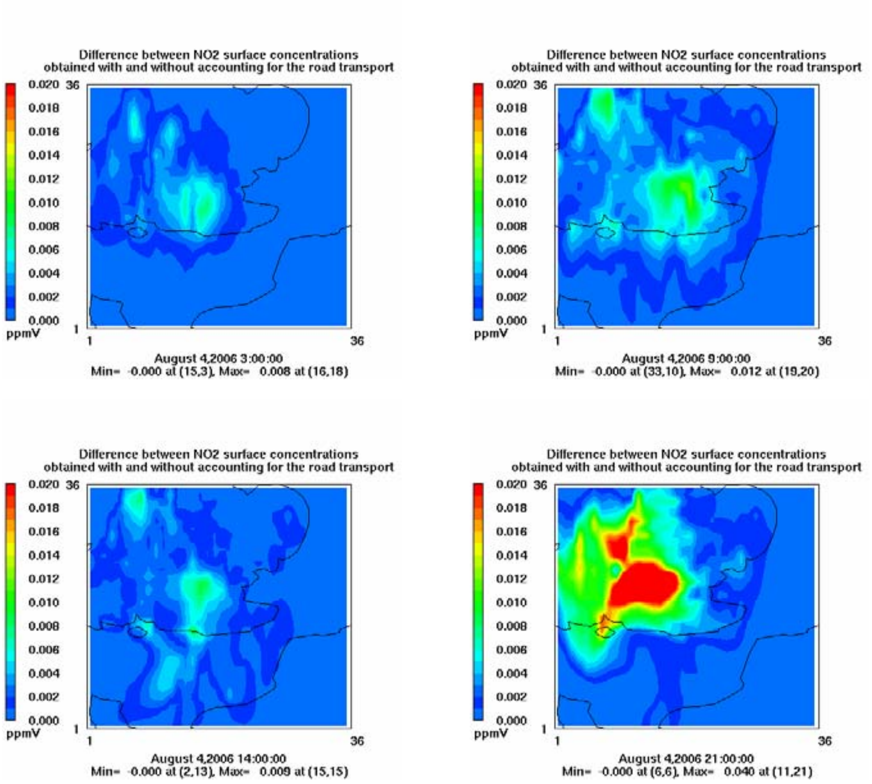
where c_i is the concentration of the respective pollutant, L_{ij}, $i = 1, \ldots, N$, $j = 1, \ldots, M$ are the operators of any kind, including emissions, which account for all the processes that lead to c_i formation.

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):

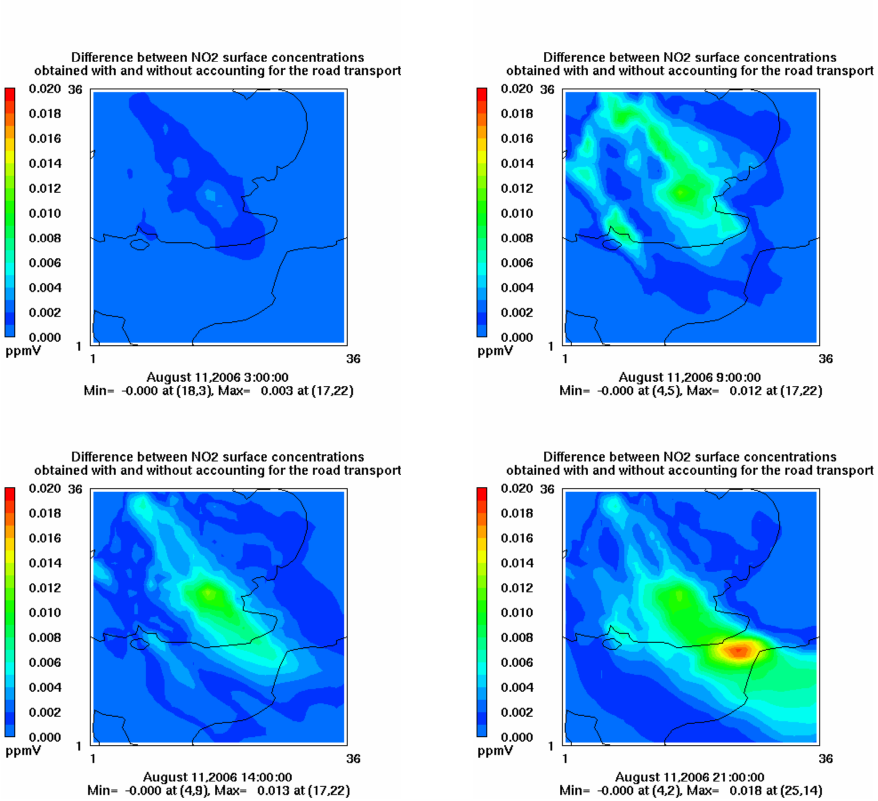
$$\Delta c_i = \sum_{j=1}^{M} \Delta c_{ij} \,, \;\; \Delta c_i = \int_{t}^{t+\tau} \frac{\partial c_i}{\partial t} dt = c_i(t+\tau) - c_i(t) \,, \;\; \Delta c_{ij} = \tau . L_{ij} \,,$$

SOME EXAMPLES

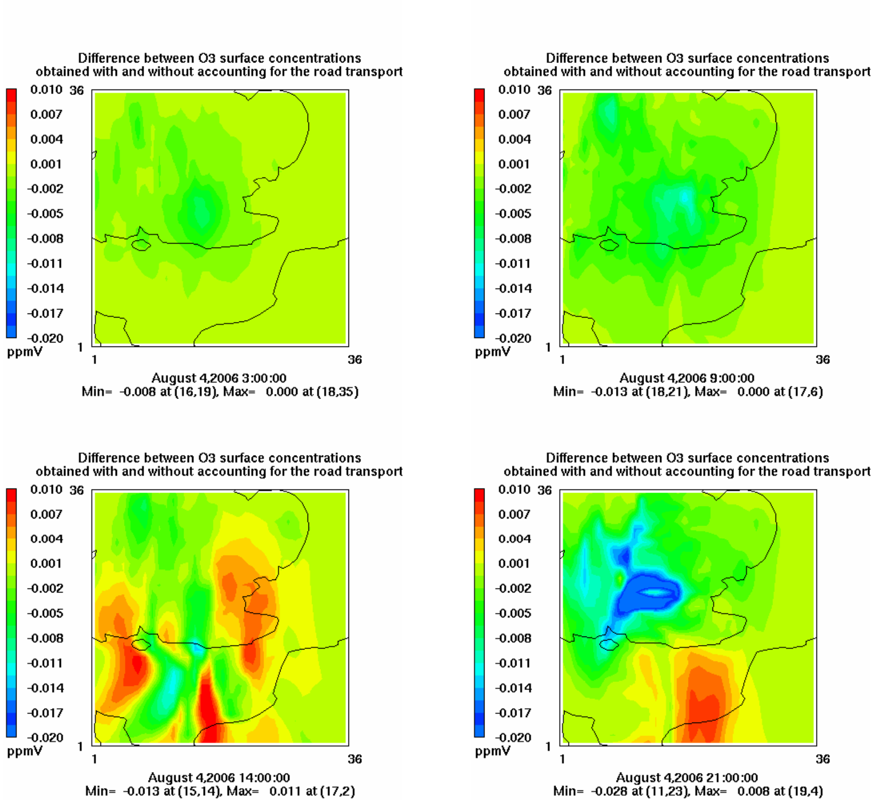
3D fields



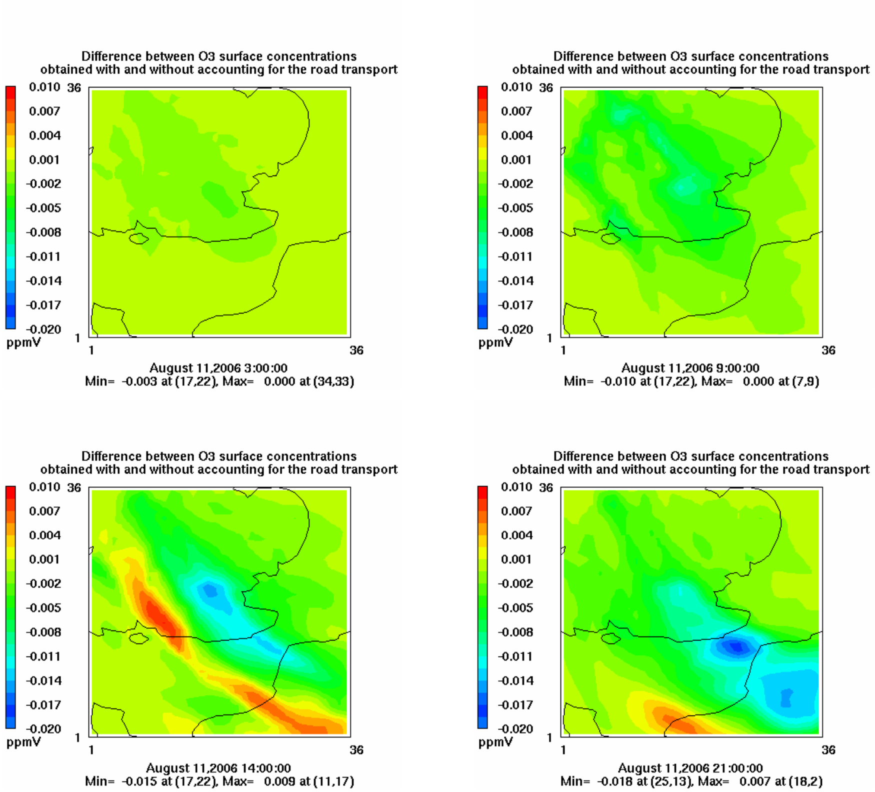
Diurnal course of NO_2 surface concentrations from road transport for August 04, 2006



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

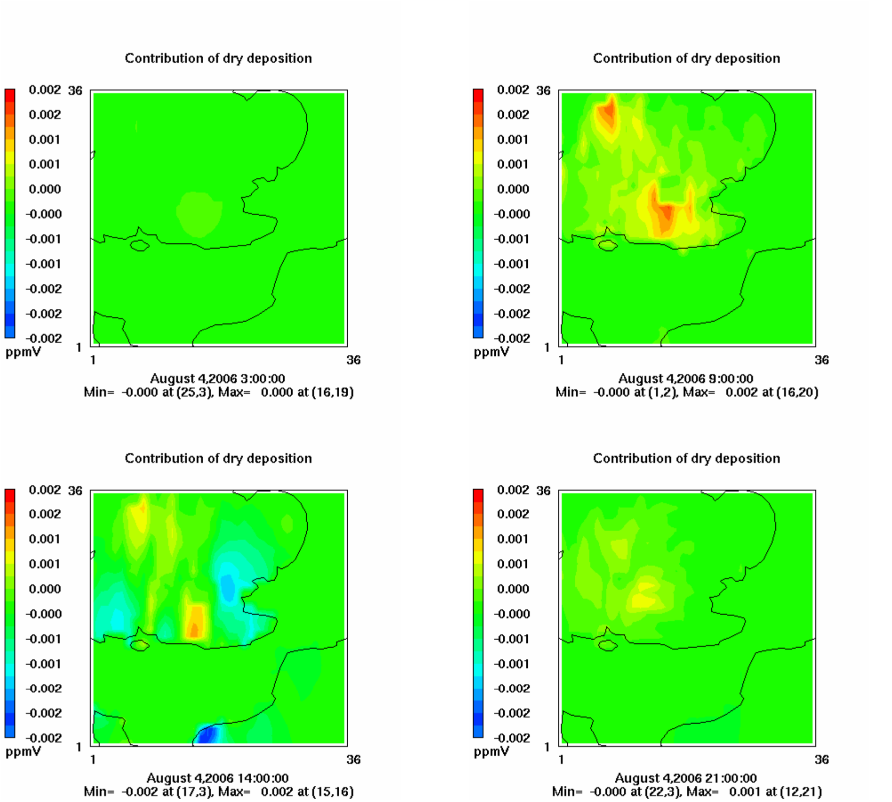


Diurnal course of O_3 surface concentrations from road transport for August 04, 2006

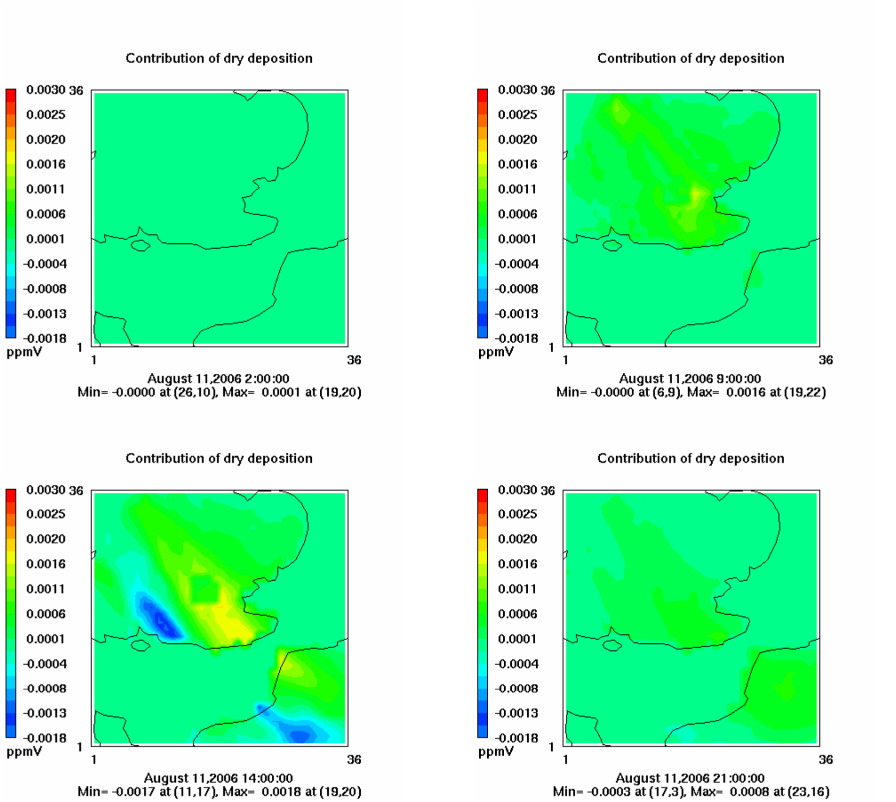


Diurnal course of O_3 surface concentrations from road transport for August 11, 2006

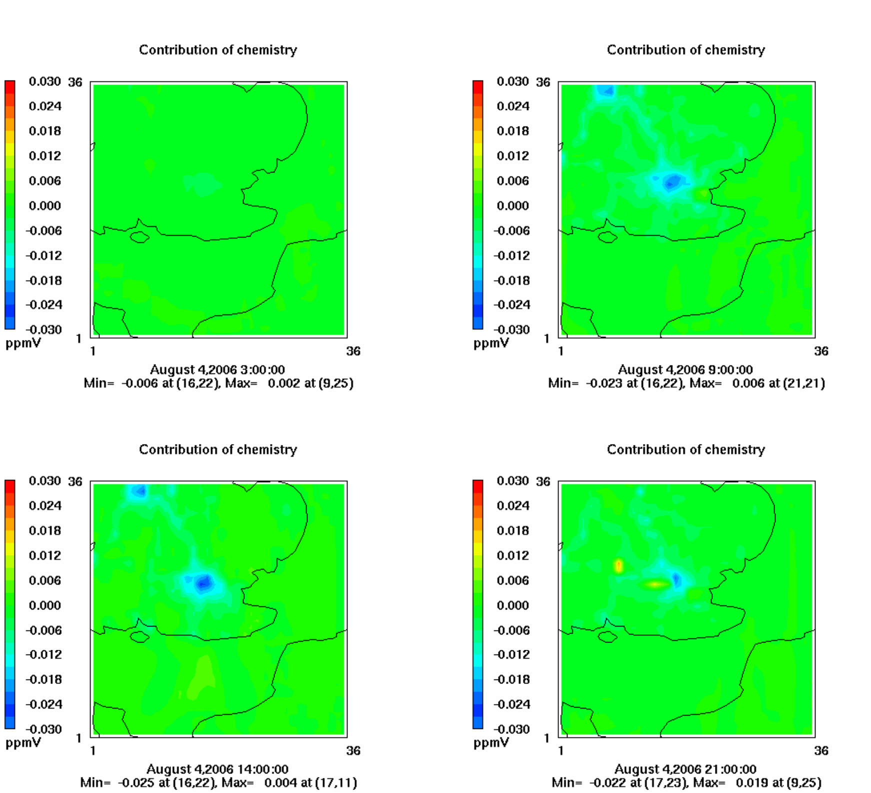
Both the effects of meteorological conditions and large city agglomerations are very well displayed – the O_3 “gaps” over the city of London and O_3 maximums to the West-Southwest of the city are formed during the day and in the evening move towards Southeast.



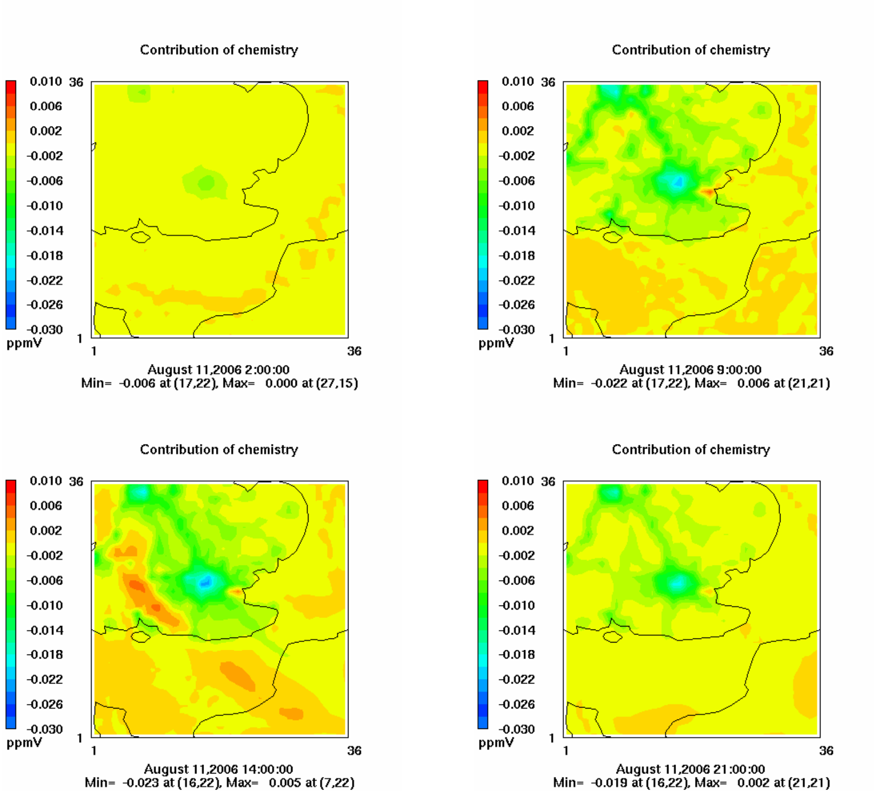
Diurnal course of the contribution of deposition processes to the formation of O_3 surface concentrations from road transport for August 04, 2006



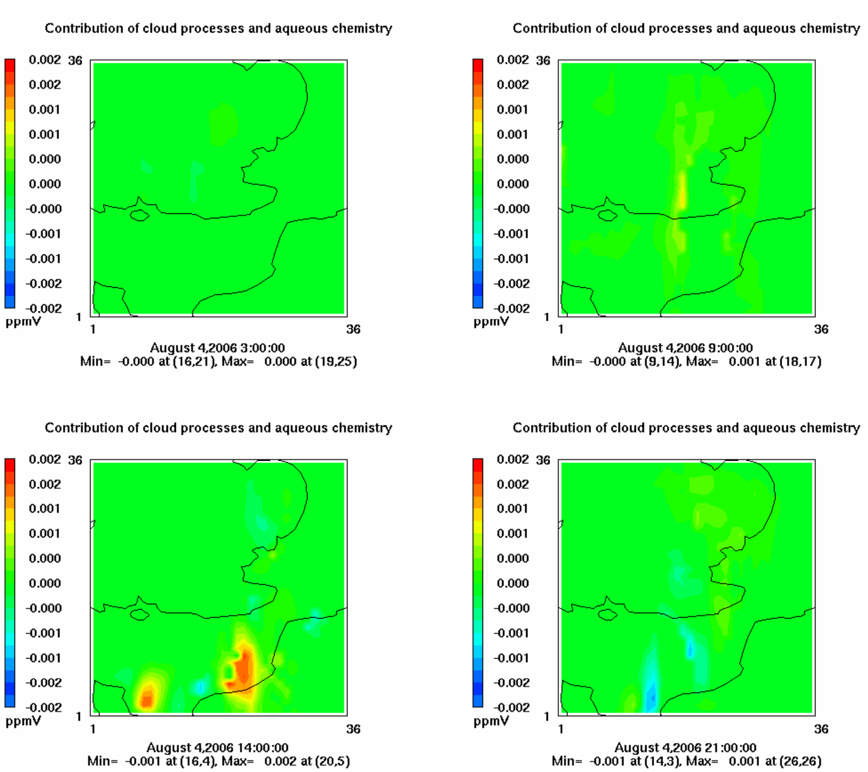
Diurnal course of the contribution of dry deposition processes to the formation of O_3 surface concentrations from road transport for August 11, 2006



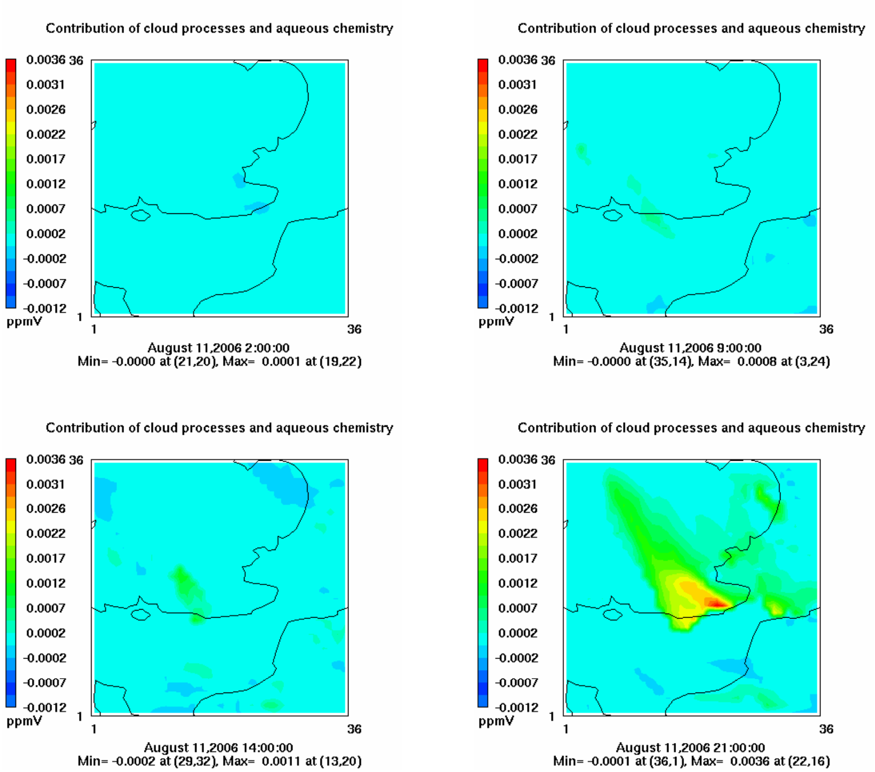
Diurnal course of the contribution of chemical transformation processes to the formation of O_3 surface concentrations from road transport for August 04, 2006



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



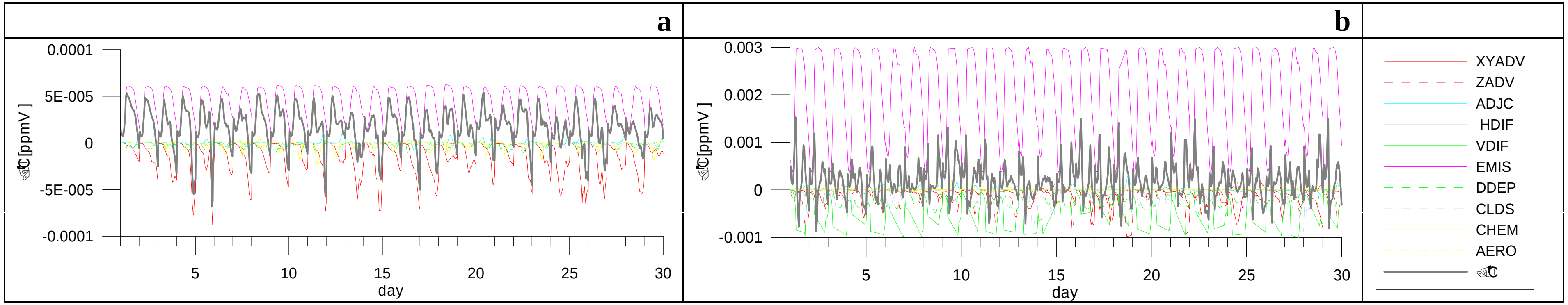
Diurnal course of the contribution of cloud processes and aqueous chemistry to the formation of O_3 surface concentrations from road transport for August 04, 2006



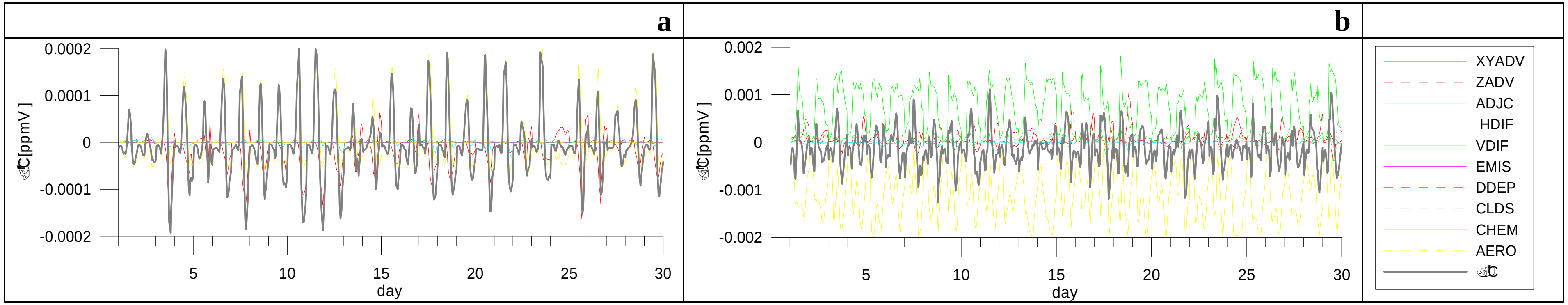
Diurnal course of the contribution of cloud processes and aqueous chemistry to the formation of O_3 surface concentrations from road transport for August 11, 2006

Time series

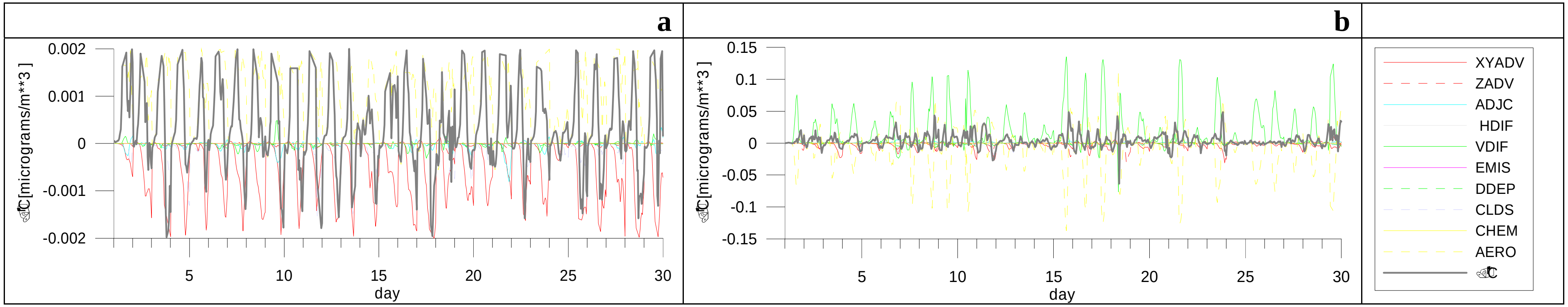
Examples for a summer month:



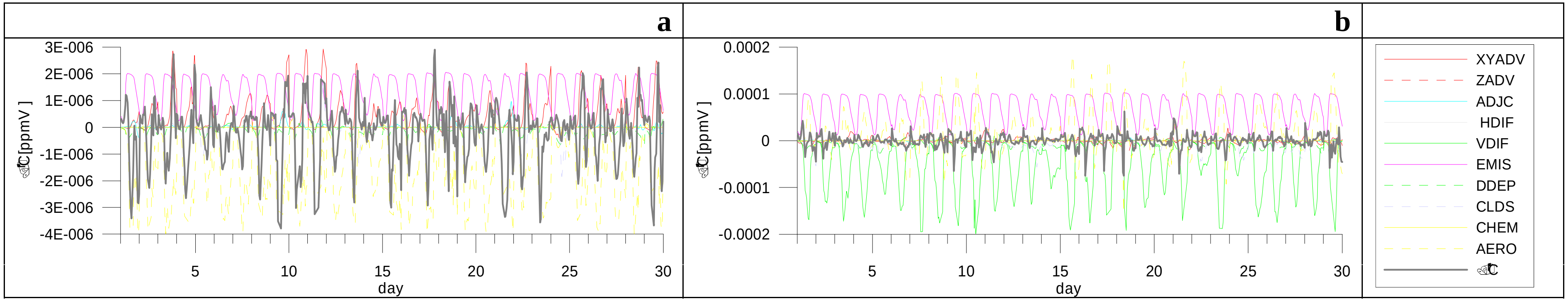
Averaged over D3 temporal change of columnar (a) and surface (b) **Nitrogen Species** concentrations and the contribution of different processes for August 2005



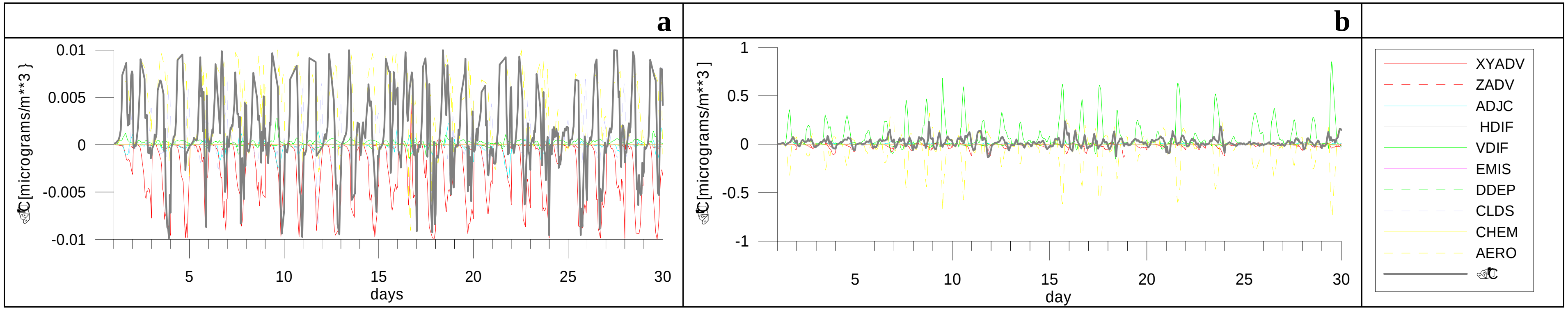
Averaged over D3 temporal change of columnar (a) and surface (b) **Ozone** concentrations and the contribution of different processes for August 2005



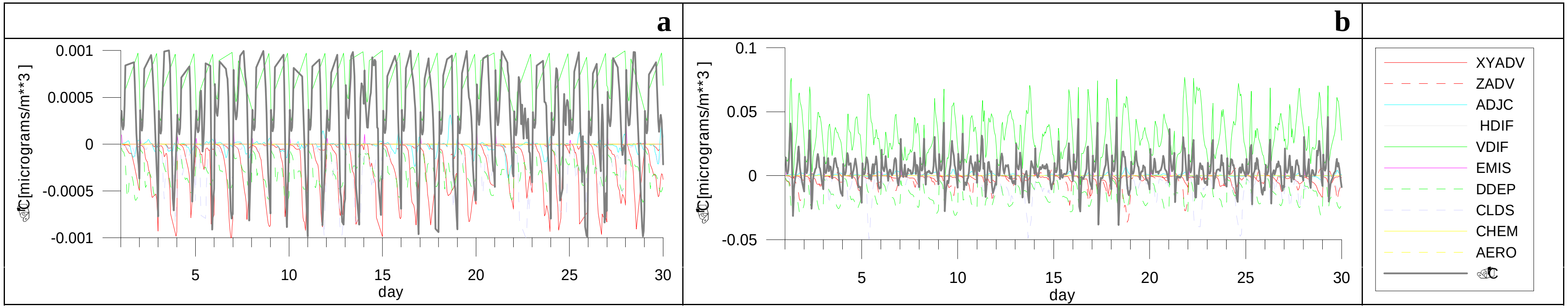
Averaged over D3 temporal change of columnar (a) and surface (b) **aerosol NH_4 (ammonium)** concentrations and the contribution of different processes for August 2005



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

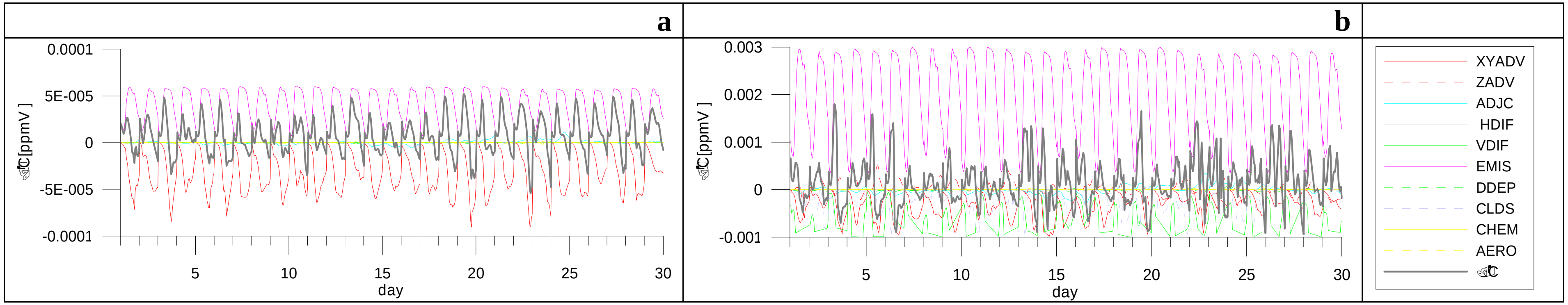


Averaged over D3 temporal change of columnar (a) and surface (b) **PM2.5** concentrations and the contribution of different processes for August 2005

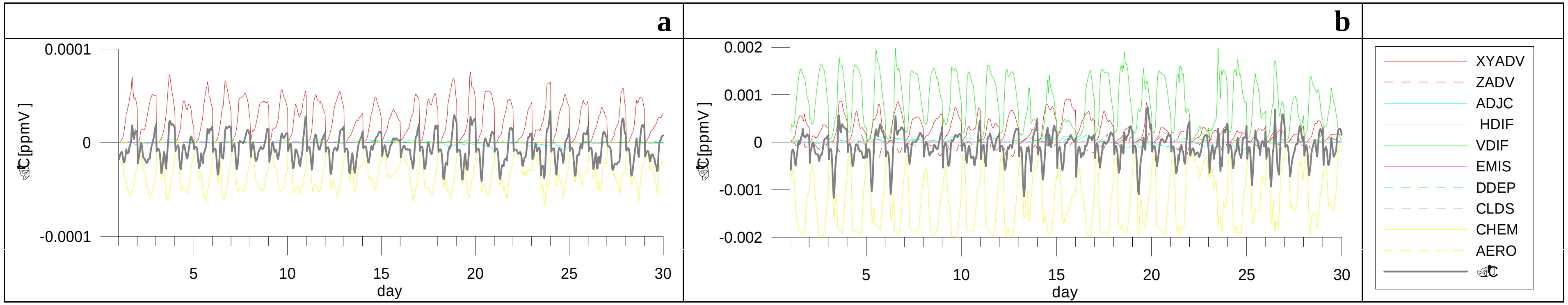


Averaged over D3 temporal change of columnar (a) and surface (b) **PM-coarse** concentrations and the contribution of different processes for August 2005

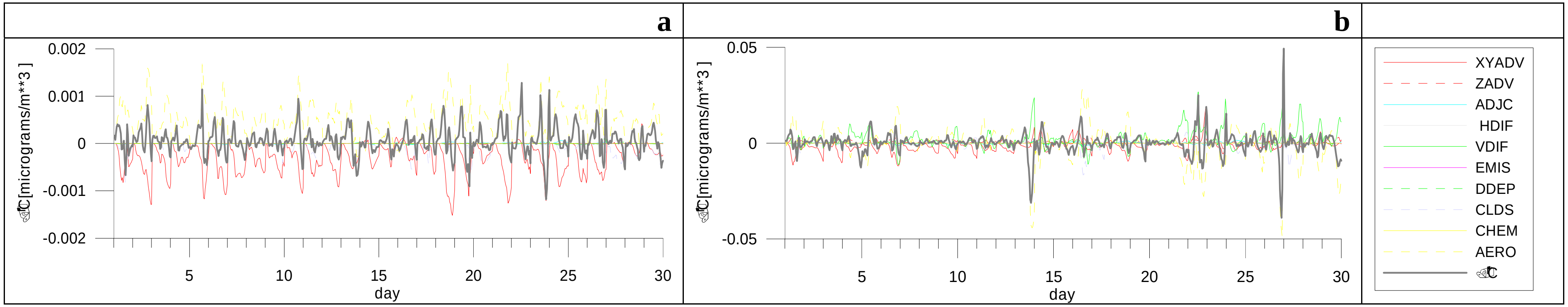
Examples for a winter month:



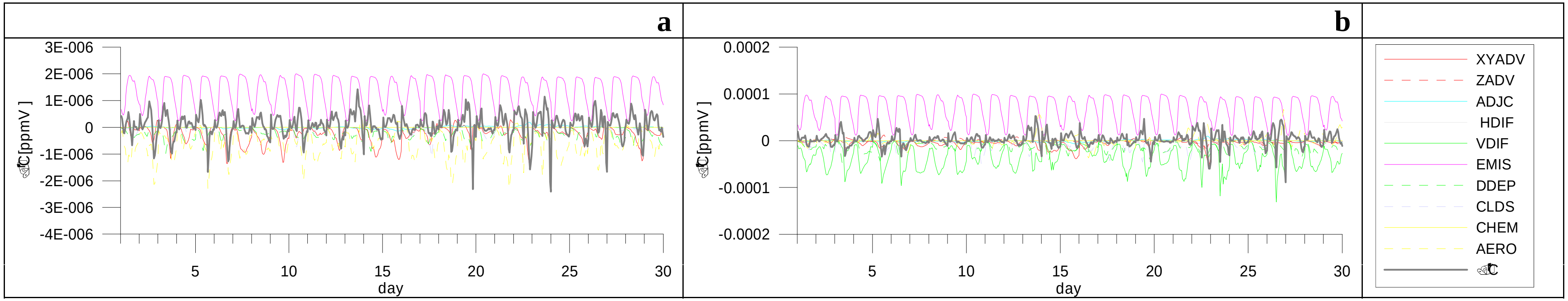
Averaged over D3 temporal change of columnar (a) and surface (b) **Nitrogen Species** concentrations and the contribution of different processes for January 2005



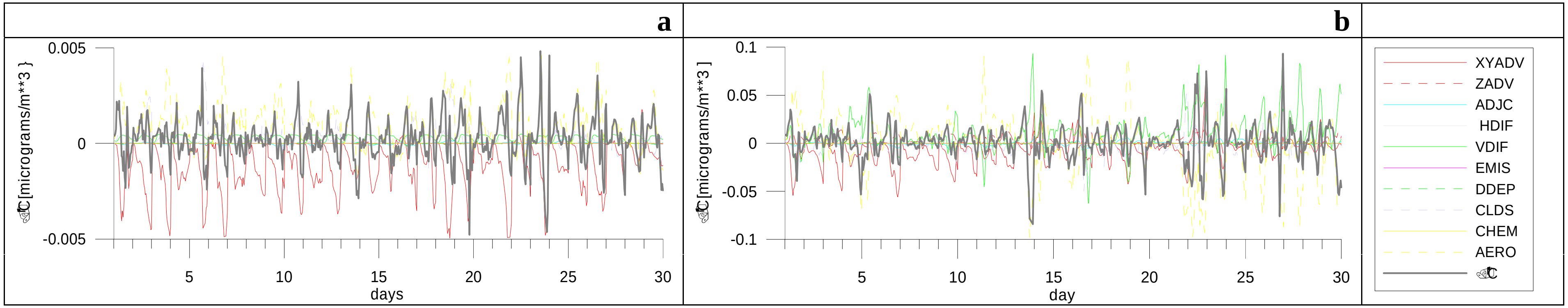
Averaged over D3 temporal change of columnar (a) and surface (b) **Ozone** concentrations and the contribution of different processes for January 2005



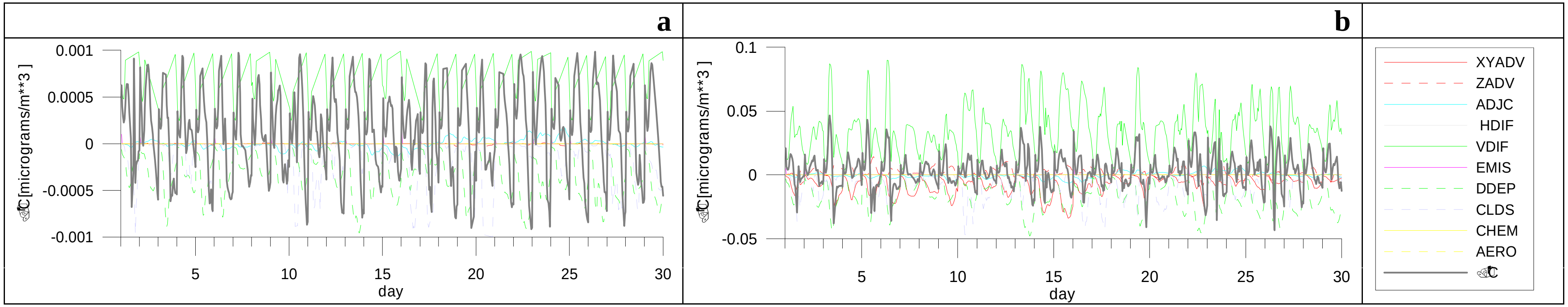
Averaged over D3 temporal change of columnar (a) and surface (b) **aerosol NH_4 (ammonium)** concentrations and the contribution of different processes for January 2005



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 interaction of the different processes is rather complex and different for different species, but still there are some common features, which can be summarized in the following way:

1.) In all the cases the diurnal course of both different processes contribution and the resulting hourly concentration change is well displayed;

2.) For most of the species the resulting hourly concentration change is a result of the interaction of a limited number of processes with different signs;

3.) In most of the cases the resulting hourly concentration change values are rather small compared to the values of the dominating processes, i.e. the concentration change is due to delicate balance between the determining processes;

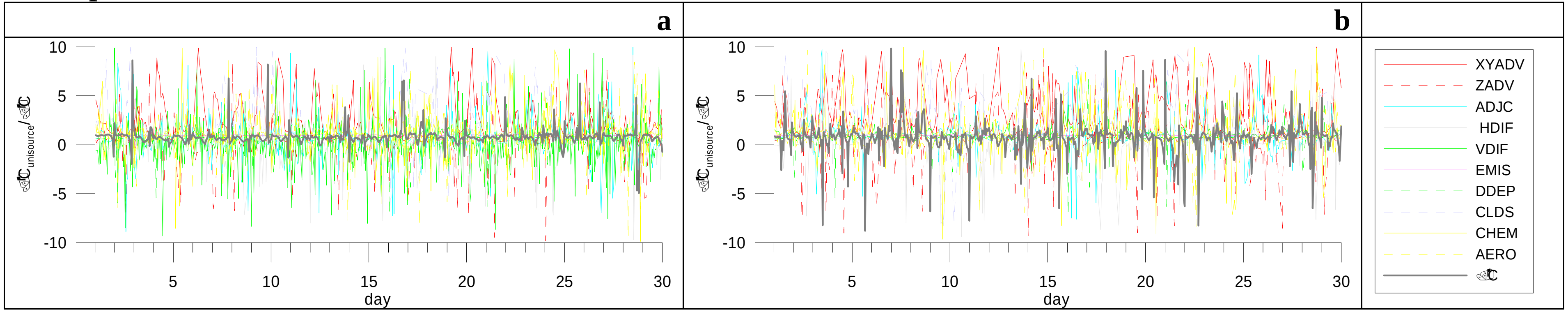
4.) As a rule during the winter months the margins within which both the process contribution and the resulting hourly concentration change are smaller compared to the summer cases;

5.) In spite of the generally periodic behaviour, the time evolution of the process contribution and the resulting hourly concentration changes are different for the different years, which demonstrates their dependence on meteorological conditions;

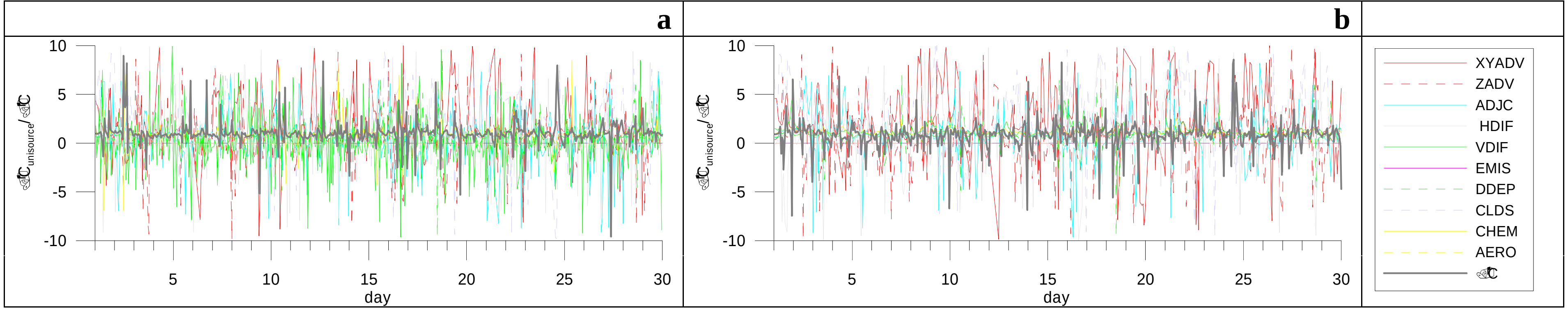
6.) The processes of vertical transport (advection/diffusion/dry deposition) are quite often among the significant ones for the surface (first model layer), while the horizontal advection is most often significant for the columnar case. For Pm-coarse, however, the vertical diffusion is an important process even for the case of analysis of the columnar values.

THE EFFECTS OF EMISSION RESOLUTION

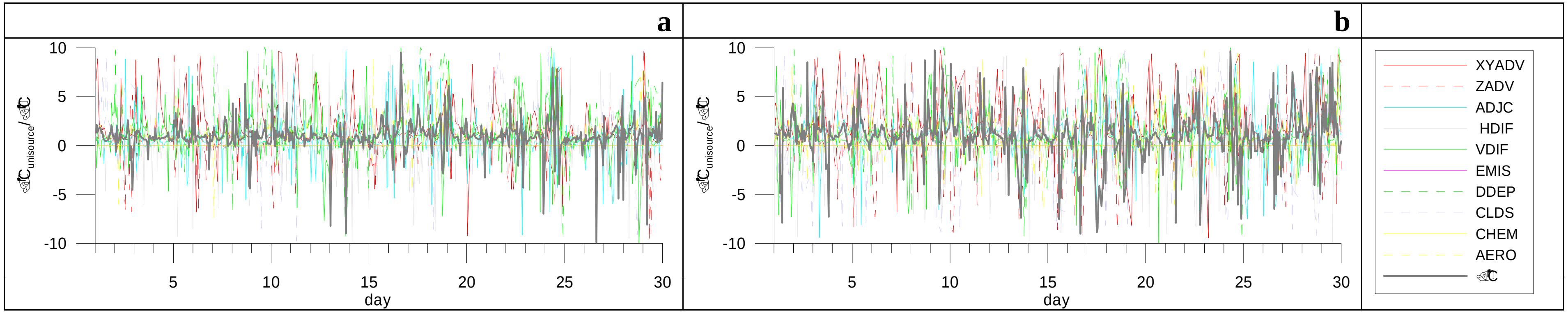
Examples for a summer month:



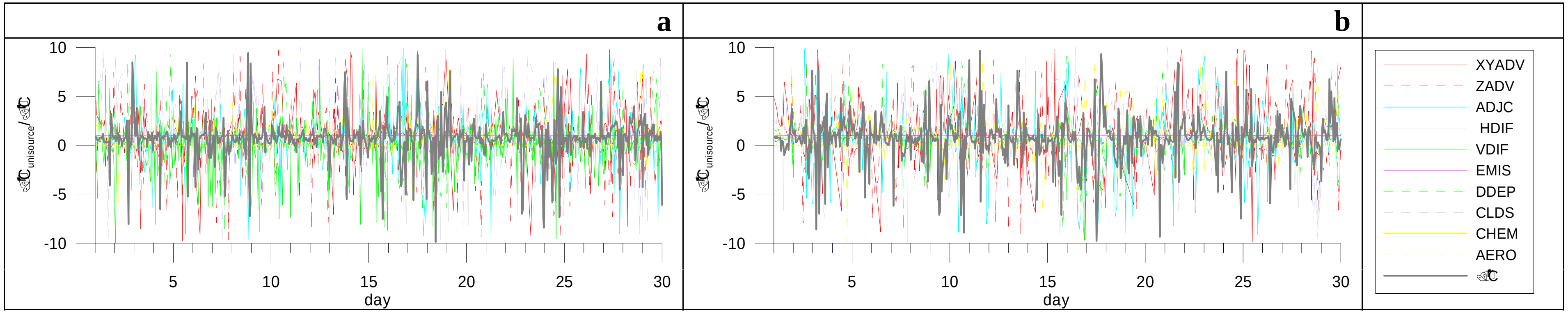
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{\det ailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **Nitrogen Species** concentrations and the ratio of contributions of different processes for August 2005



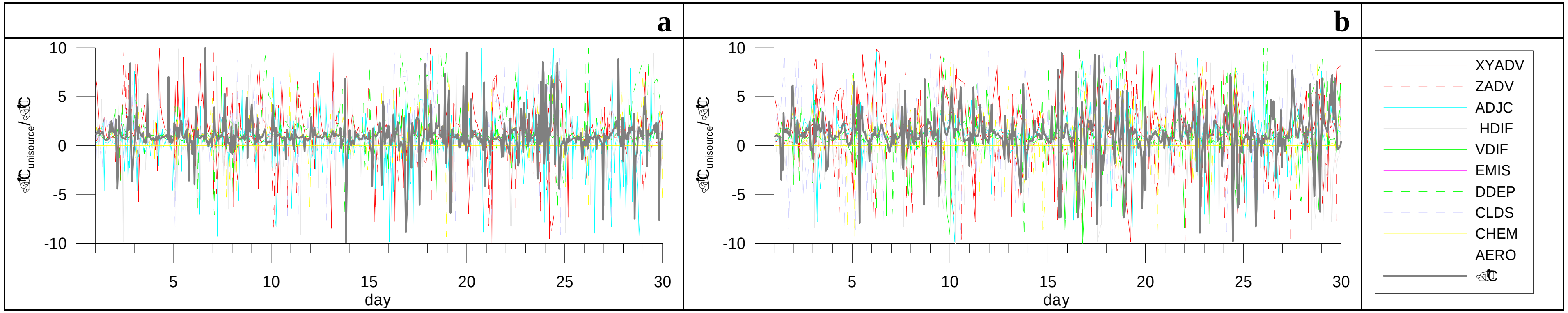
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{\det ailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **Ozone** concentrations and the ratio of contributions of different processes for August 2005



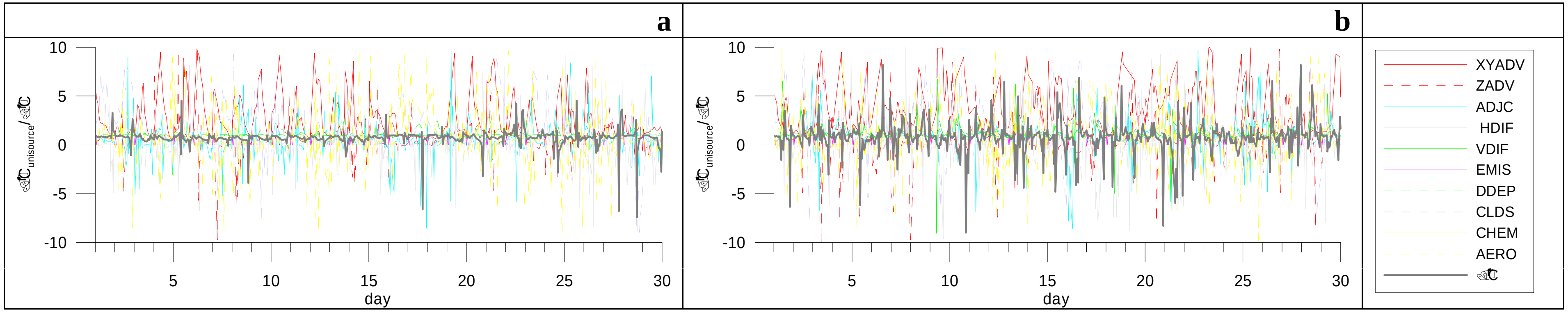
The ratio $\Delta C_{averaged\,emissions} / \Delta C_{detailed\,emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **aerosol NH_4 (ammonium)** concentrations and the ratio of contributions of different processes for August 2005



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

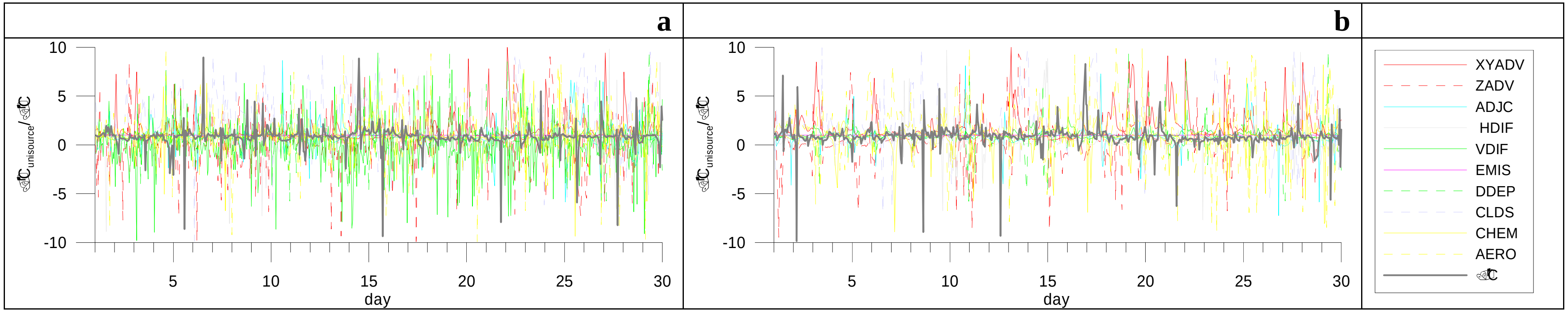


The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **PM2.5** concentrations and the ratio of contributions of different processes for August 2005

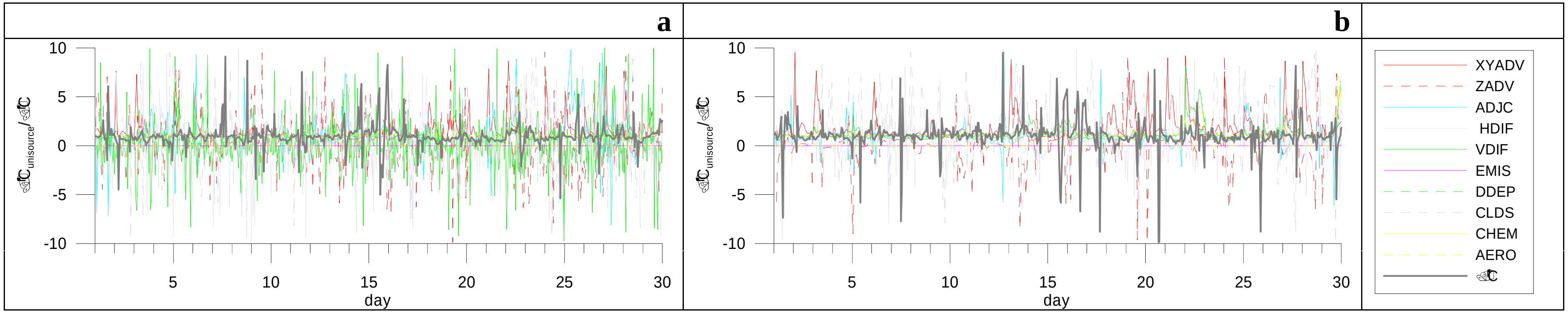


The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **PM-coarse** concentrations and the ratio of contributions of different processes for August 2005

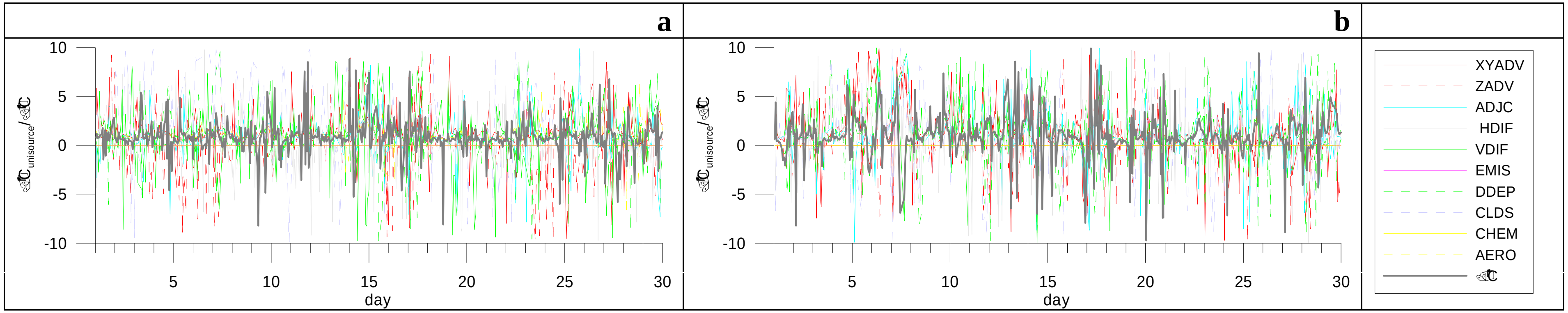
Examples for a winter month:



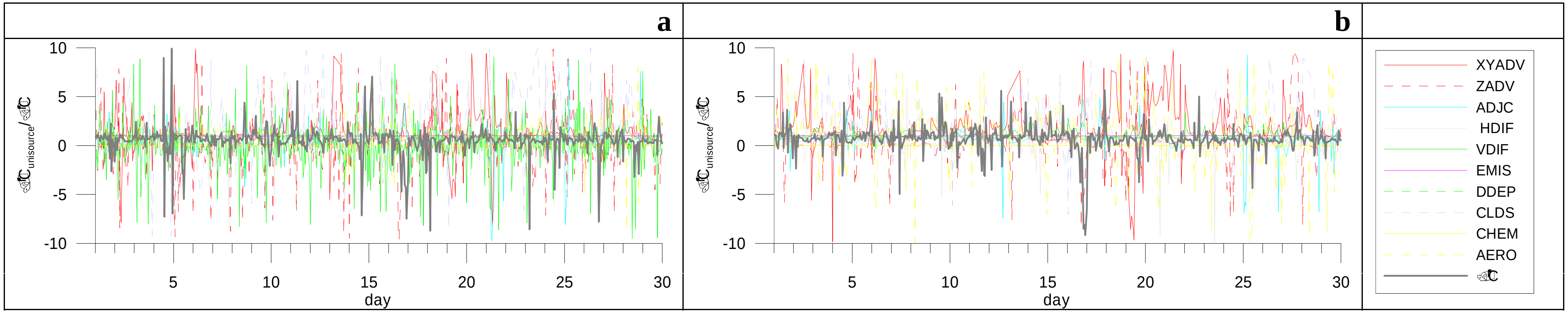
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **Nitrogen Species** concentrations and the ratio of contributions of different processes for January 2005



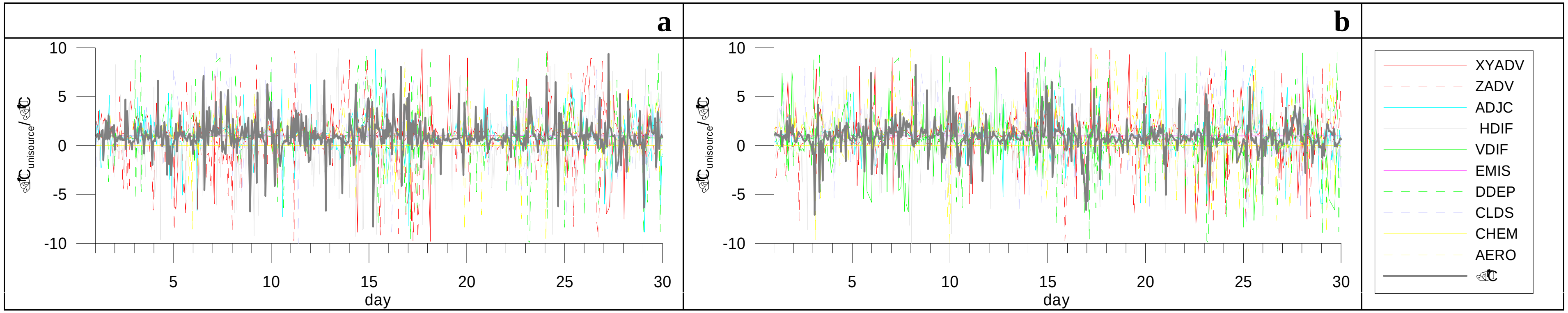
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **Ozone** concentrations and the ratio of contributions of different processes for January 2005



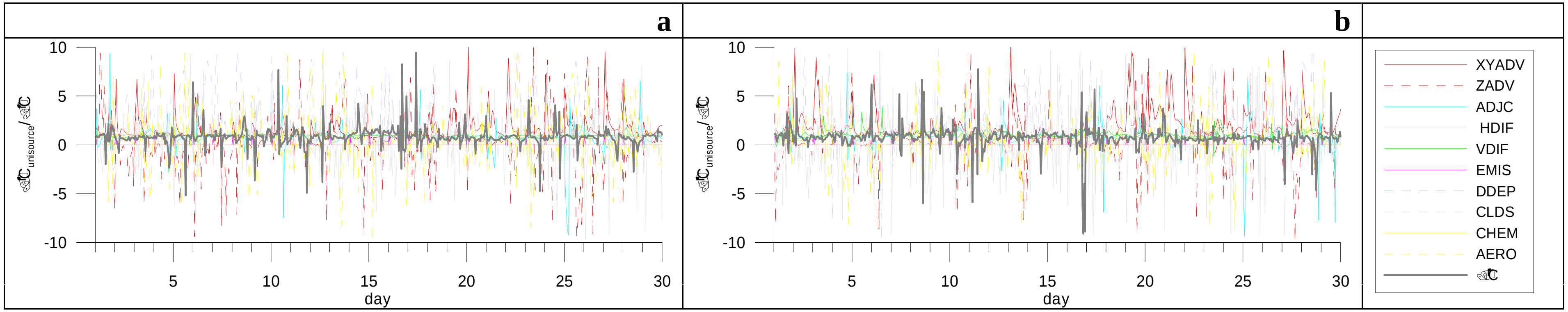
The ratio $\Delta C_{averaged\ emissions} / \Delta C_{\det ailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **aerosol NH_4 (ammonium)** concentrations and the ratio of contributions of different processes for January 2005



The ratio $\Delta C_{averaged\ emissions} / \Delta C_{\det ailed\ emissions}$ of averaged over D3 temporal changes for columnar (a) and surface (b) **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

The more general comments that can be made on these figures are the following:

1.) For practically all the processes and all the species the ratios vary within large margins way beyond 1 by absolute value.

2.) The ratios can even be negative, which means that the sign of the process contribution can be different in the cases of detailed and averaged emissions, even for these averaged over D3 characteristics. The % of occurrence of negative $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ ratios for the different processes and the resulting hourly concentration change is given in Tables 3. As it can be seen from some of the processes the percent can be higher than 40. For the resulting hourly concentration changes, however the % of negative ratios is smaller – very rarely higher than 20%.

3.) The ratios of the resulting hourly concentration changes perhaps vary within narrower margins but still they can and often are significantly different from 1.

4.) The time series are different for the different years, which demonstrates the dependence of $\Delta C_{averaged\ emissions} / \Delta C_{detailed\ emissions}$ on the meteorological conditions.

5.) The ratios tend to more or less periodic behaviour

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.

ACKNOWLEDGEMENTS

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Special Thanks to CERC, who provided realistic (hopefully) temporal profiles of the road transport emissions for the London area.

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