Eberhard Schaller, Peter Builtjes, Annette Münzenberg (Editors)

Proceedings

4th GLOREAM Workshop

20 - 22 September 2000
Cottbus, Germany

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20 to 22 September 2000
Cottbus, Germany

Workshop Program

20-09-2000

09:00 - 09:40 Opening Session

09:00 - 09:15 Welcome
              Prof. Ernst Siegmund, President, BTU Cottbus

09:15 - 09:30 GLOREAM Coordinator

09:30 - 09:40 Local Organizer

09:40 - 10:30   **Session 1: Global modelling**
Chairperson: Adolf Ebel, University of Cologne

09:40 - 10:05 Savage, N.H., Law, K., Plantevin, P., O'Connor, F., Arnold, S., Cobb, M., Pyle, J., Green, T., Brough, N., Penkett, S.A., Mills,G., Bandy, B., Schmitgen, S., Kley, D., Richer, H., Kent, J., Dewey, K., Hawke, I.D., Foot, J., Edwards, G.D., Monks, P.S., Davies, J., McQuaid, J. and Lewis, A.:
Comparison of measured and modelled ozone production rates over Europe

10:05 - 10:30 Schell, B., Ackermann, I.J. and Hass, H.:
Particulate air quality over europe in the growing season of 1995 as simulated with the MADE/EURAD model

11:00 - 12:15   **Session 2: Regional modelling - BERLIOZ/FLUMOB**
Chairperson: Adolf Ebel, University of Cologne

11:00 - 11:25 Memmesheimer, M., Jakobs, H.J., Piekorz, G., Ebel, A., Kerschgens, M.J. and Tippke, J.:
Chemical and dynamical processes in the urban plume of Berlin during BERLIOZ and FLUMOB

11:25 - 11:50 Nester, K., Fiedler, F. and Zhao, T.:
Simulation of an episode of the BERLIOZ experiment and comparison with measured data

11:50 - 12:15 Becker, A. and Schaller, E.:
           Uncertainty analysis for trajectories (with application to the weather
           situation during the 1st intensive measuring period of BERLIOZ)

14:05 - 16:10   **Session 3: Regional modelling - Ozone forecasting**
Chairperson: Jørgen Brandt, NERI, Roskilde

14:05 - 14:30   Tilmes, S., Brandt, J., Flatøy, F., Langner, J. Bergström, R.,
                    Christensen, J.H., Ebel, A., Flemming, J., Friedrich, R., Frohn, L.M.,
                    Heidegger, A., Høv, Ø., Jacobsen, J., Jakobs, H.J., Reimer, E., Wickert,
                    B. and Zimmermann, J.:
                    Intercomparison of Eulerian ozone prediction systems within
                    GLOREAM for summer 1999 using the German monitoring Data

14:30 - 14:55   Reimer, E., Wiegand, G., Flemming, J. and Dlabka, M.:
                    A model system to forecast surface ozone maxima in Germany

14:55 - 15:20   San Josè, R., Salas, I., Pérez J.L., Pena, J.I. and González, R.M.:
                    Operational air quality modelling over Europe and Iberian peninsula by
                    using RSM, MM5 and CAXM modules

15:20 - 15:45   Heidegger, A., Tilmes, S. and Friedrich, R.:
                    Real time emission forecasting as the basis for operational air pollution
                    forecasts

16:15 - 18:20   **Session 4: Applications related (not only) to ozone**
Chairperson: Heinz Hass, FORD Forschungszentrum, Aachen

16:15 - 16:40   Stern, R., Flemming, J., Reimer, E. and Graff, A.:
                    Dispersion modelling within the European communities new air quality
                    frame directive

16:40 - 17:05   Carvalho, C., Barros, N. and Borrego, C.:
                    High ozone short-term episodes over the Iberian peninsula

17:05 - 17:30   Geernaert, G. and Zlatev, Z.:
                    Running the Danish Eulerian model with scenarios for biogenic
                    emissions

17:30 - 17:55   Smiatek, G.:
                    Land use data resolution and modelling

17:55 - 18:20   Jonson, J.E., Tarrason, L. and Bartnicki, J.:
                    Effect of international shipping on European pollution levels

19:15 - 21:15   **Steering group meeting**

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09:00 - 11:05   **Session 5: EUROTRAC-2 - General information, links among subprojects**
Chairperson: Peter Builtjes, TNO-MEP, Apeldoorn

09:00 - 09:25   Reuther, M. and Midgley, P.M.:
EUROTRAC-2 at mid term

09:25 - 09:50   Friedrich, R.:
Emission data - developments, trends and uncertainties

09:50 - 10:15   Moussiopoulos, N.:
SATURN - the state-of-play

10:15 - 10:40   Beekmann, M.:
Vertical exchange processes between the atmospheric boundary layer
and the free troposphere - an overview of the research performed within
the TOR-2 project

10:40 - 11:05   Herrmann, H.:
Connected Laboratory Studies and Mechanism Development in CMD:
Tropospheric Aqueous Phase Chemistry as an Example

11:35 - 13:15   **Session 6: Numerical aspects**
Chairperson: Zahari Zlatev, NERI, Roskilde

11:35 - 12:00   Djouad, R., Sportisse, B., Audiffren, N. and Charpentier, I.:
Modelling aqueous phase chemistry: Numerical integration and
sensitivity analysis

12:00 - 12:25   Ebel, A., Jakobs, H.J., Memmesheimer, M., Kessler, C. and Feldmann,
H.:
Experiments with subsequent nesting using the EURAD-CTM

12:25 - 12:50   Berkvens, P.J.F., Botchev, M.A. and Verwer, J.G.:
Efficient Treatment of Vertical Mixing and Chemistry in APM

12:50 - 13:15   Syrakov, D.:
A numerical advection scheme on non-homogeneous grid

14:30 - 17:30   **Visit (by bus) of the Open Mining region Jaenschwalde**

19:00 - 23:00   **Workshop dinner, Dubkowmuehle, Leipe**

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09:00 - 11:05 **Session 7: Model validation and improvement**
Chairperson: *A. C.* Carvalho, University of Aveiro

09:00 - 09:25 Schultz, M.G., Brasseur, G.P., Feichter, J. and Steil, B.:
MOZART/ECHAM: Present and future global atmospheric chemistry
modeling at the Max-Planck-Institute for Meteorology in Hamburg

09:25 - 09:50 Keller, J., Andreani-Aksoyoglu, S., Ritter, N. and Prévôt, A.:
Unexpected vertical pollutant profiles obtained by UAM-V over
complex terrain

09:50 - 10:15 Delobbe, L., Matthijsen, J., Mensink, C., Sauter, F. and Swart, D.P.J.:
A comparison of mixing heights derived from meteo data and inferred
from LIDAR measurements

10:15 - 10:40 Keller, J., Andreani-Aksoyoglu, S., Ritter, N. and Prévôt, A.:

Meteorological surface and sounding data: How do their spatial
resolutions alter the wind velocity, vertical diffusivity and ozone fields
modelled with SAIMM/UAM-V?

10:40 - 11:05 Schaller, E. and Wenzel, A.:
Testing of air quality modelling systems based on the TFS model
evaluation strategy

11:35 - 13:00 **Session 8: Data assimilation**
Chairperson: Annette Münzenberg, DLR, Bonn

11:35 - 12:00 Elbern, H. and Hölzemann, J.:
Chemical state analysis by two different data assimilation algorithms

12:00 - 12:25 Builtjes, P. and Canepa, E.:
Validation of the LOTOS model for August 1997

12:25 - 12:50 van Loon, M. and Segers, A.J.:
Improving model results by data assimilation

12:50 - 13:00 **Closing of the workshop**

Comparison of measured and modelled ozone production rates over Europe using data from the MAXOX Program

N.H. Savage, K. Law, P. Plantevin, F. O'Connor, S. Arnold, M. Cobb, J. Pyle: University of Cambridge, UK
T. Green, N. Brough, C.E. Reeves, G. Mills, B. Bandy, S.A. Penkett: University of East Anglia, Norwich, UK
S. Schmitgen, D. Kley: Forschungszentrum Julich, Germany
H. Richer, J. Kent, K. Dewey, I.D. Hawke, J. Foot:
UK Meteorological Office Research Flight, UK
Øystein Hov, Frode Flatoy: NILU, Norway

The aims of the GLOREAM project include the investigation of processes controlling the composition of the atmosphere and the evaluation and testing of models. Ozone is a highly important species in the troposphere due to both its role as a greenhouse gas and its central role in photochemical oxidation. Models still disagree on fundamental questions central to our understanding of tropospheric chemistry such as the magnitude of net photochemical production of ozone in the troposphere and even in some cases the sign e.g. see Kanakidou et al (1999). The MAXOX program was an EU funded program to evaluate MAXimum OXidation rates in the free troposphere. A series of aircraft measurements were made in the mid to lower troposphere using the UK Meteorological Office C-130 Hercules aircraft. Flights were made during spring and summer 1999 with a wide range of measurements relevant to chemical oxidant production being made on board the aircraft. The global off-line grid point model TOMCAT (Law et al, 1998) was run at T42 resolution and the concentrations of the measured species were output every 10s along the aircraft flight tracks. The rate of chemical ozone production was estimated using both measured and modelled data. This was calculated with the following equation, which describes the main processes in photochemical ozone production:

$$P(O_3) = k_1[HO_2][NO] + k_2[RO_2][NO] \hspace{3cm} (1)$$

Figure 1 shows a comparison of preliminary model results and measurements of peroxy radicals and derived ozone production rates calculated using measured and modelled data during the flight on the 26th of July. Laboratory tests have shown that HO_2 will be lost on the aircraft PFA inlet at the temperatures encountered during MAXOX. Thus the PERCA measures the total concentration of organic peroxy radicals (RO_2) which mostly consists of the methyl peroxy radical (CH_3O_2) at these altitudes. This is in good agreement with results from an in-situ steady state model constrained by other measured meteorological and chemical parameters. It therefore appears that concentrations of organic peroxy radicals modelled by TOMCAT are too high. Despite the model overestimating the organic peroxy radical concentrations it appears that the ozone production rates agree reasonably well with the rate determined from measurements (when it is assumed that PERCA data is a measure of organic peroxy radicals only). This probably indicates a trade-off between NO values, which are too low in the model, and RO2 concentrations, which are too high.

References

Kanakidou, M. et al., 3-D global simulations of tropospheric chemistry with focus on ozone distributions - results of the GIM/IGAC intercomparison 1997 exercise, European Union Rep. No. 18842, ISBN 92-828-5928-2, 1999.

Law, K.S., P.-H. Plantevin, D.E. Shallcross, H. Rogers, C. Grouhel, V. Thouret, A. Marenco and J.A. Pyle, Evaluation of modelled O3 using MOZAIC data, J. Geophys. Res.,103, 25721-25740, 1998.

Particulate air quality over europe in the growing season of 1995 as simulated with the MADE/EURAD model

B. Schell, I. J. Ackermann, H. Hass

In general proposed air quality standards for atmospheric particulate matter refer to particle mass below a spe-cific diameter, e.g. PM2.5 and PM10. If these standards are eventually exceeded it is important to know how much each aerosol compound contributes to the total aerosol mass. Design of the best strategy to improve air quality with respect to particulate matter requires on the one hand to identify what are the contributions of pri-ma-ry and secondary aerosol compounds. On the other hand the main contributors to either primary or secondary aerosol species have to be determined. These contributions may differ e.g. by region (country) and/or season. MADE (Modal Aerosol Dynamics Model for Europe) provides detailed information on the size distribution, primary and secondary contributions, as well as the chemical composition of atmospheric particles. Coupled to the three-dimensional Eulerian gas-phase air quality model EURAD (European Air Pollution and Dispersion Model) it is applied to simulate particle formation, transport and deposition during a long-term simulation over essentially the whole growing season in the year 1995. To take account of regional difference the model domain covers Europe in a sufficiently fine horizontal resolution (grid resolution: 27 km). The results of the simulation may additionally be compared to available measurements during the modeled period.

Chemical and Dynamical Processes in the urban Plume of Berline during BERLIOZ and FLUMOB

M. Memmesheimer, H.J. Jakobs, G. Piekorz, A. Ebel, M.J. Kerschgens, J. Tippke

The EURAD modeling system has been used to analyse chemical and dynamical processes in the urban plume of Berline during typical summer smog conditions. The FLUMOB episode (July 21 - July 29, 1994) and the first intensive measurement phase of the Berline Ozone Experiment (BERLIOZ; July 20/21, 1998) have been selected to investigate the importance of the different terms in the mass continuity equation for the temporal evolution of concentration patterns. The nesting technique has been applied to take the impact of the European scale processes on the plume into account. Horizontal grid sizes used are 54 km for the mother

domain (European scale) and 18, 6, and 2 km for the three nests. The eefect of different horizontal resolutions on the calculated concentration fields and processes is considered. The net chemical production of ozone has been calculated in the order of 4 - 8 ppb/h in the Berline plume. This is in quite good agreement with the observed values. Near the sources, in particular in the city and along major streets, a net chemical loss of ozone is found mainly due to tritration to NO2. The net chemical loss in the source regions is balanced by turbulent transport and horizontal advection of ozone from the net chemical production regions. Future plans aim on the analysis of other important photooxidants as PAN and HNO3 as well as the precursors.

Simulation of an Episode of the BERLIOZ Experiment and Comparison with Measured Data

K. Nester, F.Fiedler, H.-J. Panitz, T. Zhao

Institut für Meteorologie und Klimaforschung
Forschungszentrum Karlsruhe / Universität Karlsruhe

Introduction

The Berlin Ozone (BERLIOZ) Experiment has been carried out in the frame of the Troposheric Research Programme (TSF) in the period between July 13 and August 9, 1998. The experimental domain comprises the city of Berlin and an area with a radius of about 100 km around the city. The main aim of this experiment was to study the processes transport and chemical transformations in the urban plume of Berlin during photosmog conditions. The study was focused on the formation of ozone and other oxidants. But the data should also be used for the evaluation of Chemical Transport Models (CTM). Because the chemical formation of oxidants, especially ozone, depends on a great number of parameters, it is necessary to carry out a lot of experiments under various conditions in order to be able to analyse under which conditions the different processes are relevant. This is the reason why so many experiments have already been carried out. Urban plumes are of special interest because of their limited extend and the possibility to relate the plume to the emissions of the city. In contrast to other experimental sites in Europe, which are located in complex terrain, like e.g. Athens (Peleg et al., 1997), Madrid (Plaza et al., 1997), Milan (Prevot et al., 1997) and Vienna (Wotava et al., 1998), Berlin was selected because it is located in a flat environment extending about 100 km around the city. In many directions the urban plume is not influenced by greater, additional sources.

In this study we compare ozone concentrations measured at ground level stations and by aircraft along the urban plume with the results of the mesoscale CTM KAMM/DRAIS. Additionally, the ozone mass budget components are calculated. As it has been shown by other investigations (Memmesheimer et al., 1997), mass budget considerations allow the determination of the relevance of the processes in dependence on time and space. They provide more general results, because of their non-local character.

The model system KAMM/DRAIS

The model system KAMM/DRAIS (Fig.1) consists of the meteorological model KAMM (Adrian and Fiedler, 1991) and the dispersion model DRAIS (Nester and Fiedler, 1992). The non-hydrostatic Eulerian model KAMM solves the Navier-Stokes equations of motion, the continuity equation, and the heat equation in a terrain following coordinate system, which allows a better resolution close to the ground as compared to the upper levels. A soil-vegetation model (Schädler et al., 1990) describes the interaction between the soil and the atmosphere.

The dispersion model DRAIS solves the diffusion equation on a Eulerian grid using the same terrain following coordinate system as the KAMM model. The dry deposition of the different species is modelled by their dry deposition velocity (Baer and Nester, 1992). In order to simulate the chemical processes the gas phase chemical reaction mechanism of the RADM2 model (Stockwell et al., 1990) is applied.
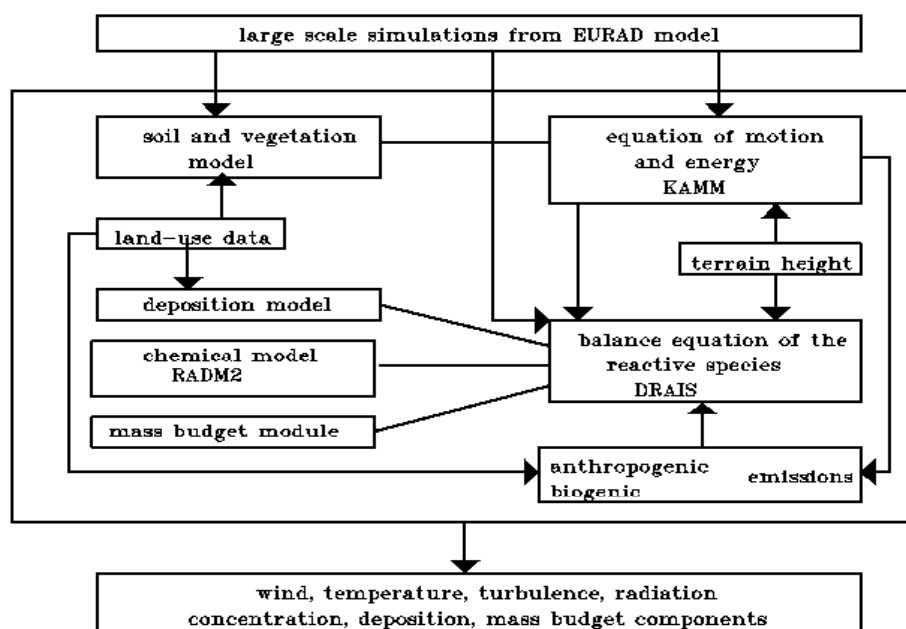

Fig. 1: Schematic representation of the model system KAMM/DRAIS

In the stable and neutral boundary layer a local first order approach is chosen for the vertical diffusion. In the convective boundary layer a non-local similarity approach is used (Degrazia, 1988).

With a special module the components of the mass budget can be calculated in predefined volumes for all species considered in the model (Panitz et al., 1997).

Performance of the simulations

Simulations with the model system KAMM/DRAIS have been carried out for the episode 20/21 July, 1998. The model domain had an extent of 200 km * 200 km and encloses the city of Berlin, which lies nearly in the centre of the domain. The horizontal grid resolution was 2 km. The external forcing for the KAMM model and the initial- and boundary conditions for the species concentrations in the DRAIS model have been determined from the results of the European scale model EURAD (Ebel et al., 1997). The grid size for this simulation was 18 km. The emission data for this episode have been provided by IER, Stuttgart. Land use and topography data are taken from the data base delivered by IFU, Garmisch. Two simulations

have been carried out. The first one uses the original boundary conditions delivered by the EURAD model. With the results of this run the model evaluation activities are performed. In the second run only the first day was simulated. For this run, the ozone profile in the upper levels (1.5-5) km has been modified corresponding to the measurements by the IBUF aircraft. Additionally, the nudging factor has been increased to get a better agreement between the measured and simulated wind speed and direction in the urban plume. With these modifications, an optimal result should be achieved concerning the formation of ozone in the urban plume. The results presented in this paper, except for the scatter diagram, refer to the second run.

The ozone concentration distribution near ground level at 15 UTC of July 20, 1998 shows a pronounced ozone plume downwind of the city of Berlin (Fig. 2). The maximum ozone concentration in this plume is 68 ppb. It occurs at a distance of about 70 km. Air masses with high ozone concentrations are transported over the southern boundary of the model domain.
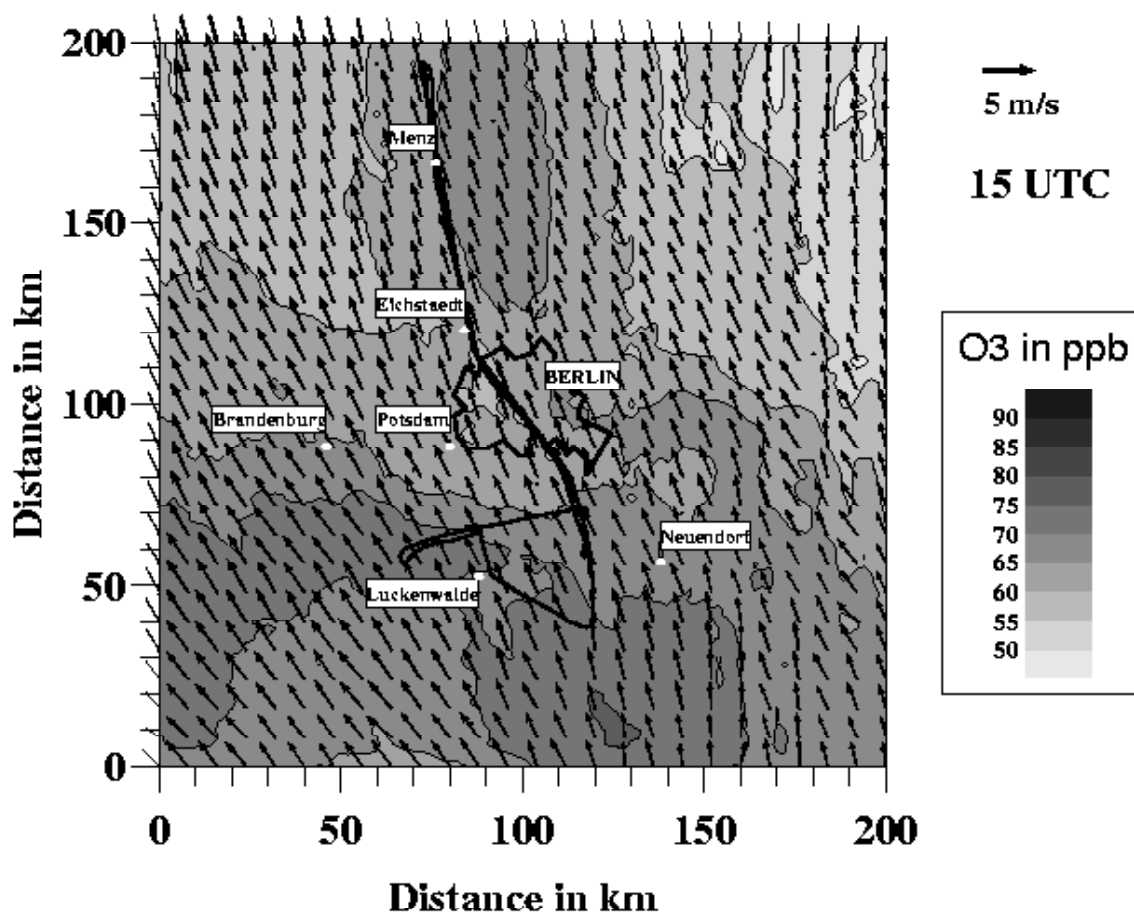

Fig. 2: Wind- and ozone concentration distribution near ground level for July 20, 1998 and afternoon flight track of the aircraft IBUF

The diurnal cycles of the ozone concentration at two stations are presented in Figure 3. At the station Eichstaedt, which is located about 30 km downwind of the city centre of Berlin, the simulated ozone concentrations fit quite well to the measurements. But at the station Menz, located about 70 km downwind of the city centre, the simulated ozone concentrations underestimate the measured ones. If we compare the ozone concentrations, measured along the flight track of the aircraft IBUF (see Fig. 2), with the corresponding simulated concentrations, a similar result is found. The main flight track begins on the upwind side
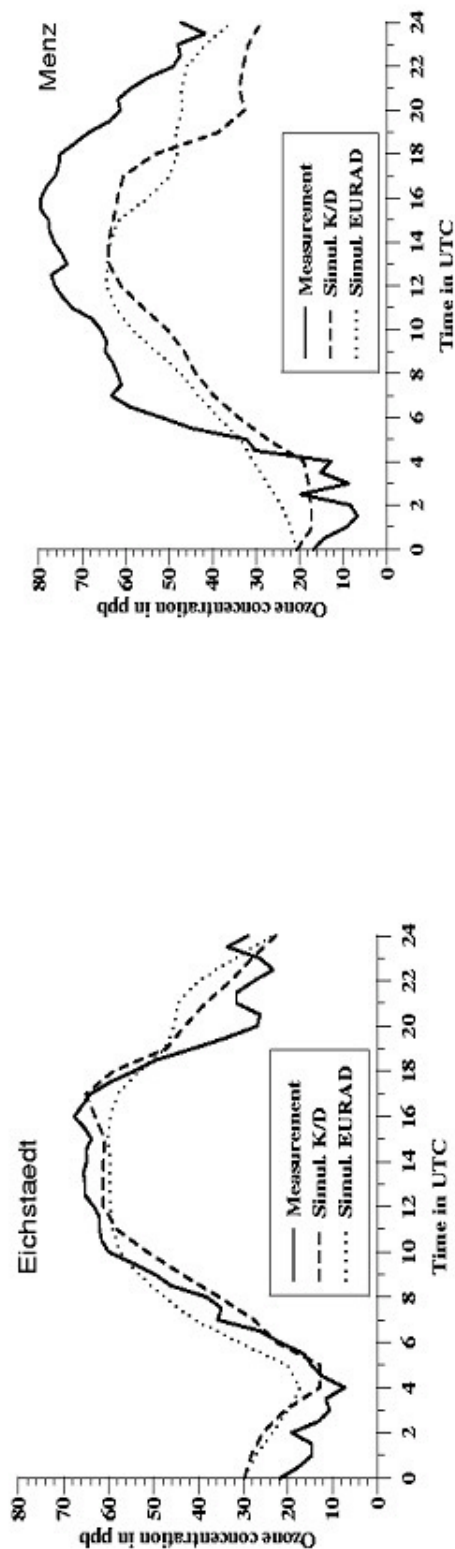
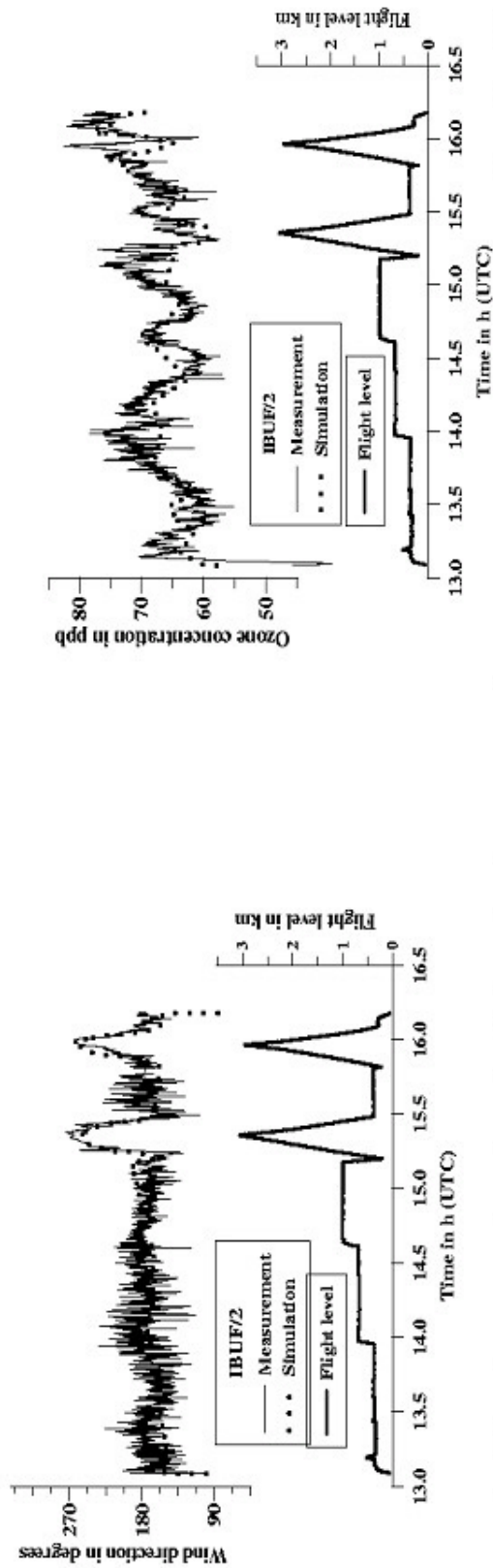Fig. 3: Diurnal cycle of the ozone concentration at ground level for the stations Eichstaedt and Menz

Fig.4: Wind direction comparison along the flight track of IBUF

Fig.5: Ozone concentration comparison along the flight track of IBUF

about 50 km south-west of Berlin, crosses the city, and ends at about 100 km downwind. Along this flight track the aircraft flew in different levels. As can be seen from Figure 4 the wind direction measured during the flight is well simulated by the model. A similar agreement is found for the wind speed. The simulated ozone concentration along the flight track agrees also quite well with the observations except for about two time periods (13.8 UTC and 15.1 UTC), where the model underestimates the measured ozone values (Fig.5). During these two periods the aircraft flew in the area around and north of Menz. This means that the simulation underestimates the ozone concentration in the plume of Berlin by about 10 ppb at larger distances although the meteorological conditions are well simulated.

For the period between 11 UTC and 16 UTC, a statistical evaluation has been carried out using measured data (half an hour means) from the ground level stations and the corresponding model results. The scatter diagram prepared with both data (not shown) reveals that the data are grouped around the agreement line. But the low correlation coefficient of 0.54 points to a great scatter around this line.

In 50% of the cases the difference between the measured and simulated ozone concentrations is less than 8 ppb.

The statistical results agree quite well with those of the episodes TRACT and FLUMOB. Therefore, they are combined. As can be seen from the scatter diagram (Fig. 6), the correlation is much better than for the individual episodes. The slope of the regression line and the correlation coefficient have acceptable values of 0.76 and 0.85, respectively. The difference between measured and simulated ozone concentrations (Fig. 7) is lower than 8 ppb in 50% of the cases being compared. 8 ppb is about 12 % of the average ozone concentration.

Mass budget components of ozone in four layers over three regions

The mass budget module in the model KAMM/DRAIS calculates the contributions of the different processes to the change of the mean concentration in a predefined volume (Fig. 8).
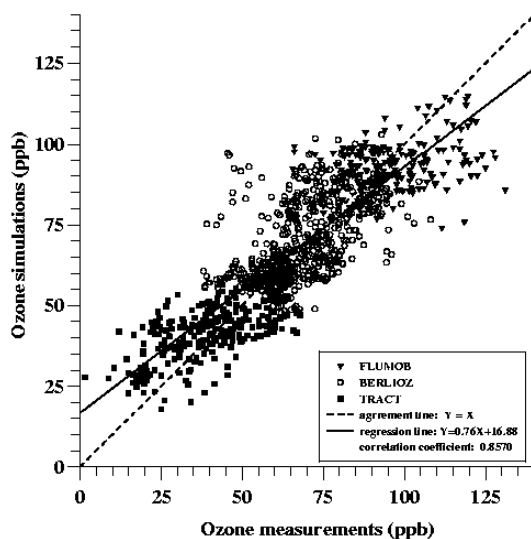

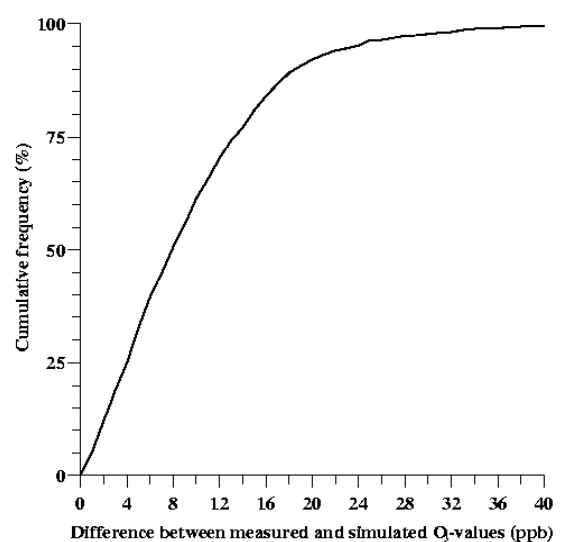Fig. 6: Comparison of measured and simulated ground level ozone concentrations (11 UTC till 16 UTC)

Fig. 7: Cumulative frequency distribution of the ground level ozone concentration difference (11 UTC till 16 UTC)
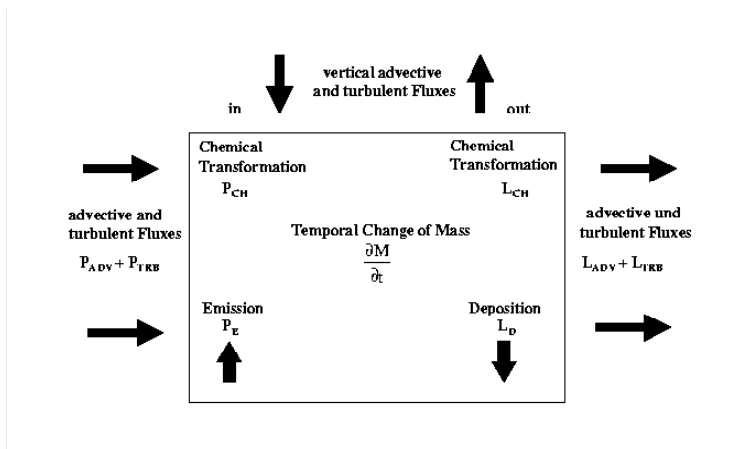
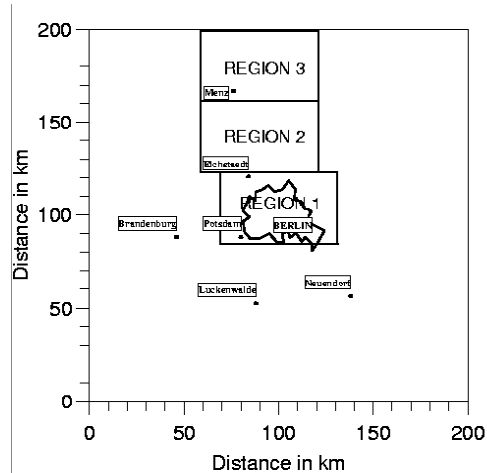Fig. 8: Illustration of the mass budget components   Fig. 9: Arrangement of the regions

These calculations have been performed for three regions. The first region comprises the city of Berlin and the other two are located north of the first one (Fig.9). They include the urban plume. The layers over these regions are:

Layer 1: 2000 m – 5000 m (free troposphere)
Layer 2: 1200 m – 2000 m (upper boundary layer)
Layer 3:   75 m – 1200 m (lower boundary layer)
Layer 4: ground –   75 m (surface layer)

Although all mass budget components are determined, only the changes of the ozone concentration due to chemical transformations are presented. The determination of this quantity was one of the aims of the experiment. Figure 10 shows the hourly change of the chemical ozone formation rate in dependence on the regions and the three layers (2-4). In the surface layer over the city a loss of ozone due to chemical reactions is found during the whole day. But nevertheless, the ozone concentration increases in this layer during the day caused by vertical mixing from the upper layer. In the regions two and three the behaviour of the diurnal variation of the ozone formation is quite similar, with a higher peak value (7.5 ppb/h) occurring in the second region. In the lower boundary layer (layer 3) over all regions, chemical ozone production occurs during daytime. As expected, it is most pronounced in region 2. The lowest production rate during the afternoon is found in region 3. For region 2, the peak values in layers 3 and 4 are similar. The formation of ozone is remarkably reduced in the upper boundary layer (layer 2). The strongest ozone formation (nearly 2 ppb/h) appears again in region 2. In all regions the change of the ozone concentration due to chemical processes in layer 1 is much smaller than in the other layers.

On the downwind side of the city, the formation of ozone in the urban plume, derived from the aircraft measurements (IBUF) in the afternoon, achieves a value of about (6.5 ± 1.0) ppb/h (Corsmeier et al., 2001). The aircraft flew in layer 3 in different levels and crossed region 2 and 3 several times. If the simulated formation of ozone is averaged over the crossing periods, the values 5.1 ppb/h and 3.5 ppb/h are found for the regions 2 and 3, respectively. Because layer 3 above region 2 represents a greater volume of air than the aircraft flight, this is still an acceptable agreement. The formation rate of ozone in region 3 is obviously too low. A corresponding comparison for the city provides the values (4.5 ±1.0) ppb/h and 5.0 ppb/h for the measured and simulated ozone formation rates, respectively.
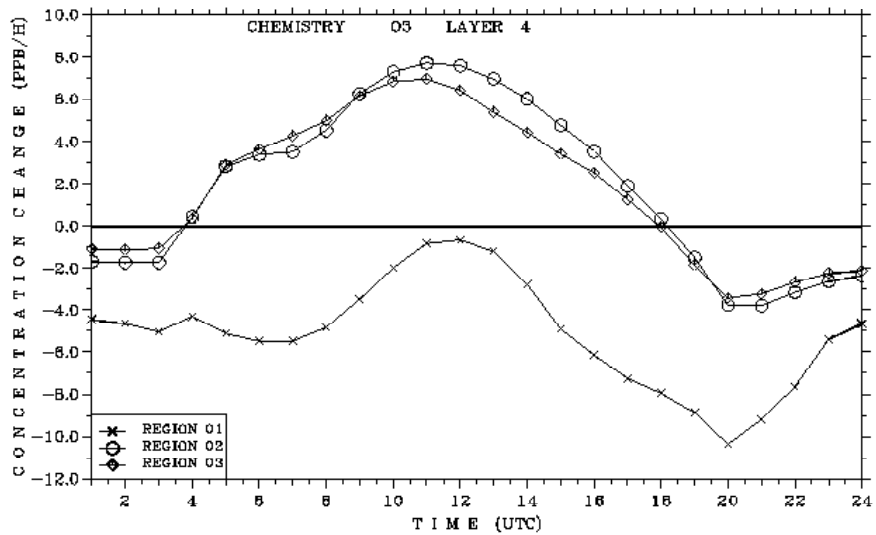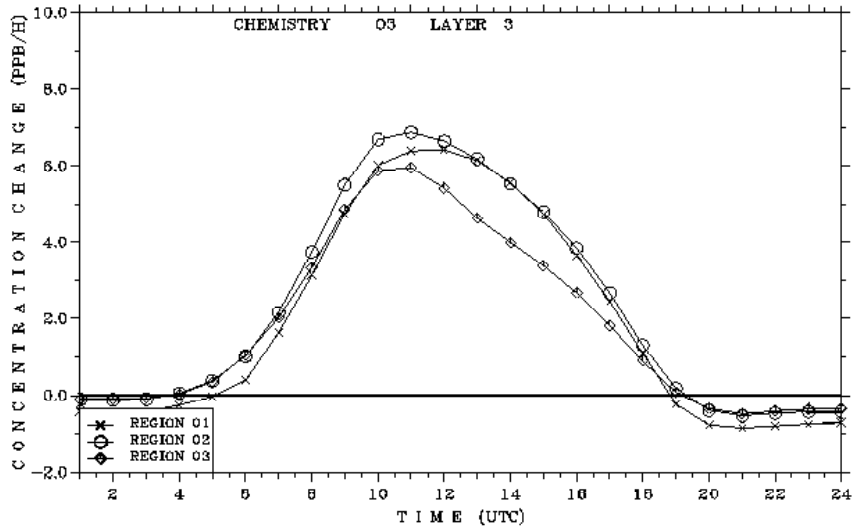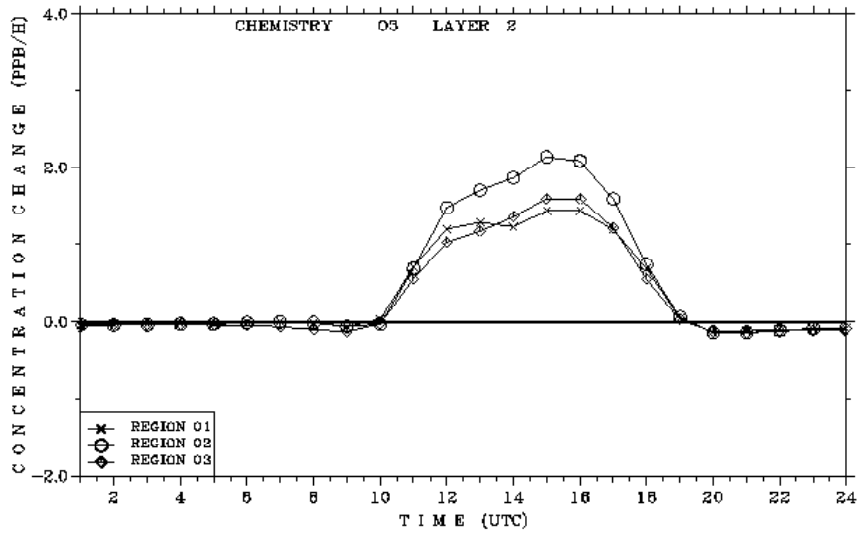
Fig.10: Diurnal cycle of the ozone formation rate caused by chemical reaction in three layers over three regions

Conclusions

At the first day of the simulated BERLIOZ episode, an ozone plume develops downwind of the city of Berlin. Although the meteorological conditions and the ozone concentrations on the upwind side of the city are well simulated by the model, the observed maximum increase of ozone in the plume is underestimated by about 10 ppb. To find the reason for this underestimation further comparisons with other relevant measured species are necessary.

The results of the statistical evaluations of the ozone ground level data for the BERLIOZ episode, based on the simulations with the KAMM/DRAIS model system, correspond to those for the episodes TRACT and FLUMOB. The result of the combined evaluation reflects the reliability of the model system KAMM/DRAIS with respect to ozone. The scatter diagram shows that there is no bias between the measured and simulated ozone concentrations. Most of the data are grouped around the agreement line. On an average, the model simulations underestimate the higher ozone concentrations and overestimate the lower ones. Especially the spatial variation of the ozone concentration is not good enough represented by the model results, although a horizontal grid resolution of 2 km is used.

The mass budget calculations for ozone show that the relevance of the different processes depends on the selected region and on the considered vertical layer. In the surface layer, deposition and vertical diffusion determine the change of the mean ozone concentration. Over the city, the chemical processes decrease the mean ozone concentration during the whole day. Nevertheless, an increase of the ozone concentration occurs during daytime, because air, carrying a higher ozone concentration, is mixed down from the layer above. In the mixing layer above the surface layer, chemical processes are mainly responsible for the change of the ozone concentration during daytime, independent of the considered region. In the late afternoon and the early morning the advection dominates the change of the ozone concentration in all layers. This is not only true, because the contributions of the other processes are reduced, but also because of changes in the wind field. As expected, the greatest increase of the mean ozone concentration due to chemical reactions occurs in region 2, which is located on the downwind side of the city. The maximum formation rate of ozone in the lower boundary layer was 7 ppb/h. This value occurs in the late morning (11 UTC).

The comparison of the simulated ozone formation rates with those derived from the IBUF aircraft measurements show an acceptable agreement over the city and the adjacent downwind region. In region 3 the formation rate is underestimated by the model. This result reflects the underestimation of the ozone concentration in the plume at farther downwind distances.

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Uncertainty analysis for trajectories (with application to the weather situation during the 1st intensive measuring period of BERLIOZ)

A. Becker and E. Schaller

The usability of air chemistry data gained at ground measuring stations for their intended purpose strongly depends on the spatial representativeness of the selected locations. In case of the BERLIOZ objectives, i.e. understanding the chemistry in the Berlin plume, the origin of the measured air during the sampling period is highly important. In other words, one wants to know the 4-D (spatial and temporal) catchment area of a receptor volume representing the ground measurement station during the observation period. A common method of source attribution is based on backward trajectories from wind fields gained by measurements or taken from Eulerian atmospheric models. However, there are two conceptual shortcomings on that method:

-The method usually lacks the information of the turbulent proportion of the wind field.

-Even with the knowledge of this turbulent proportion the temporal backward calculation of trajectories contradicts the principle of irreversibility connected with turbulent motion. Hence if the area of investigation lies within the PBL the uncertainty of turbulence neglecting backward trajectories has to be determined by another method of source attribution that

enounces on the calculation of backward trajectories. In doing so we carried out source-receptor relationships with the aid of a coupled Euler-Lagrange model system LaMM5 considering the import situation at the 13 ground measurement sites according to the BERLIOZ operation plan for the first day if intensive measurements, i.e. the 20th of July in 1998. Our method of investigation is to calculate a huge number of forward particle trajectories under recognition of turbulence. In connection with a suitable emission scenario, namely a quasi equally horizontally distribution of 4-D sources, and statistics of the particle properties 4D-release- and 4D-approach-location, raised at the boundaries of free selectable receptor volumes, their catchment areas are calculated and compared. These areas of relevant emissions for the regarded receptor are compared with the according result of a second run which is identical despite of the neglecting of turbulence within the Markov chains for the trajectory calculation. The deviations between both runs and the comparison to simple backward trajectories for the same period elucidate the role of the PBL turbulence on the representativeness of BERLIOZ ground measurement stations. Moreover these deviations determine the uncertainty of the backward trajectories.

Intercomparison of Eulerian ozone prediction systems within GLOREAM for summer 1999 using the German monitoring data

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Abstract

Within GLOREAM numerous activities are concerned with operational forecasting of ground level ozone concentrations in Europe. Comprehensive forecasting systems based on an Eulerian approach are driven for example by NERI, Denmark, DWD and FUB, Germany, NILU, Norway, and SMHI, Sweden. To apply such modeling systems, e.g. for regulatory purposes according to new EU directives, an evaluation and comparison of the model systems is fundamental in order to assess their reliability. One step in this direction is presented in this study: The model forecasts from all five systems have been compared to measurements of ground level ozone in Germany. The outstanding point in this investigation is the availability of a huge amount of data – from forecasts by the different model systems and from observations. This allows for a thorough interpretation of the findings and assures the significance of the observed features. Data from more than 300 measurement stations for a 5-month period (May – September 1999) of the German monitoring networks have been used in this comparison. Different spatial and temporal statistical parameters were applied in the evaluation. Generally, it was found that the most comprehensive models gave the best results. However, the less comprehensive and computational cheaper models also produced good

results. The extensive comparison made it possible to point out weak points in the different models and to describe the individual model behavior for a full summer period in a climatological sense. The comparison also gave valuable information for an assessment of individual measurement stations and complete monitoring networks in terms of the representativeness of the observation data.

1. Introduction

According to the proposal of the new EU directive relating to ozone in ambient air, every EU member state has to inform or warn the populations if the ozone concentration exceeds the information or alert thresholds of 90 ppb and 120 ppb, respectively. Furthermore, it is proposed that every member state will have to operate routinely forecasts of time period and geographical area of expected exceedances of information and/or alert threshold for ozone and to forecast the expected change in pollution (EU, 2000). Different air pollution forecasting systems have been developed and are presently in operational use in many European states; the systems range from simple statistical models to fully three-dimensional comprehensive Eulerian model systems directly coupled to numerical weather prediction (NWP) systems. To enable an adequate application of such systems their results must be of high and known quality. This implies keeping the systems state-of-the-art concerning the scientific formulations and operational environment. Therefore a thorough and continuous evaluation is desired.

Within GLOREAM, numerous activities are concerned with operational forecasting of ground level ozone concentrations. Comprehensive forecasting systems based on Eulerian approaches are driven, for example, by DWD (together with the Universities of Cologne and Stuttgart), Germany, FUB, Germany, NERI, Denmark, NILU, Norway, and SMHI, Sweden. All the systems use advanced and well-tested numerical algorithms and chemical schemes with more than 35 prognostic species. The main differences are in the setup of the systems, especially with respect to the horizontal and vertical resolutions and physical parameterizations. The setup of the DWD, NILU and SMHI systems are in terms of full three-dimensional description of vertical exchange and high vertical resolution. The FUB and NERI systems are quite similar in setup with only three vertical layers and simple vertical exchange processes. The horizontal resolution of the systems covers ranges from about 50 km × 50 km (NERI, NILU and SMHI) to about 20 km × 20 km (DWD, FUB). Comparison of the horizontal resolution of the models with respect to their performance is important in terms of the representativeness of the measurement stations.

Measurement data covering the period May to September 1999 were provided by the German Environmental Agency (UBA) and the corresponding institutions of the Federal States (UBA, 1999). The data are still preliminary, and overall uncertainties are assumed to be in the range of 5 – 10 % (Tilmes and Zimmermann, 1998). The data set consists of time series from more than 300 sites all over Germany. The data are uniformly related to 20 °C and UV calibration. The original half-hour values are averaged with the full hour in the center of the averaging interval. Only stations with data coverage better than 50 % are considered in this study. The spatial distribution is quite inhomogeneous, as are the local characteristics of the sites. A large number of stations are placed close to industrial or traffic emission sources. Therefore, the problem of the representativeness of the sites is serious and must be taken into account in the interpretation.

A summary of the air pollution forecasting systems is found in Tilmes et al., 2001. The DWD forecasting system is described in more detail in Hass (1991), Friedrich et al., (1999); Jakobs et al., (2000), Tilmes (2000), Tilmes and Zimmermann (1998), Tilmes et al., (2000a and

2000b). The FUB forecasting system is described in Flemming (2000); Flemming et al., (2000); Reimer et al., (1992; 2000); A description of the NERI system can be found in Brandt et al., (2000a; 2000b; 2000c; 2000d). The NILU system are described in Flatøy et al., (1995; 1996; 1997; 2000) and the system at SMHI is described in Langner et al., (1998a; 1998b); Robertson et al., (1999).

In this paper we will present results of a comparison of the performance of the five model systems for the period July – August 1999. Spatial and temporal statistics for ground level ozone concentrations will be shown for modeled and measured time series of daily maximum ozone data.

3. Model results and comparisons

The comparison of the five model systems and measurements resulted in several hundred visualizations. Only a few of them are included in this paper. In Figures 1 – 4 some of the model results and comparisons of the model results using different statistics are shown. However, all the visualizations can be found at the web page http://www.dmu.dk/atmosphericenvironment-/gloream/forecasts1999.

In Figs. 1-3 examples are given for the comparisons of the spatial distribution of the temporal statistics: bias, correlation coefficient and Root Mean Square Error (RMSE) calculated from time series at each monitoring station. Below each of these Figures 1-3, frequency distributions in relative numbers of the different parameters are given. These frequency distributions are collected and shown in Figure 4 for all statistics and all model systems for the period July 1 to August 31 for the daily maximum concentrations (maximum in the time between 11 UTC and 17 UTC). The DWD2 and FUB2 are the 25-48 hour forecasts. All the others (DWD, NERI, FUB, SMHI and NILU) are the 1-24 hour forecasts. The different results are described in the following. Fig. 1 shows a comparison between DWD and NERI of the spatial distribution of the bias at every measurement station. In Fig. 2 a comparison of the spatial distribution of the correlation coefficients are made between DWD and FUB and in Fig. 3 a comparison of NILU and SMHI is shown in terms of the RMSE.

The example of comparison of bias between DWD and NERI (Fig. 1) shows very good performance – nearly no overall bias for both models (see frequency distributions below the figures). The largest differences between the two model system appear within the area of North-Rhine-Westphalia (NRW), which is highly urbanized. The fact that NILU and SMHI also do not show such large negative biases in this area, point to local deficiencies in the emission data used by DWD as the reason for the biased DWD forecasts. At a number of coastal stations NERI has nearly no bias. The models show similar biases in larger parts of Saxony, where there is a mountainous region towards the Czech Republic and several sites are under strong urban influence. The same can be observed for NILU and SMHI (not shown here). This points to a limited representativeness of some of the measurement locations where large biases can be observed for most of the models. The models also perform similar for other urban areas like Berlin, and there are a large number of sites with similar good behavior all over Germany.

The comparison of DWD and FUB in terms of the spatial distribution of the temporal correlation coefficient at every measurement station is shown in Fig. 2. It should be noted here that it is hard to achieve correlation coefficients better than 0.9 when considering the spatial resolutions in the models (Tilmes et al., 2000b). DWD gives very good results for most of Germany except for Saxony. The performance of DWD is especially good for the urban sites of e.g. Hamburg, Berlin, Frankfurt and Mannheim. In most parts of Germany the

correlation of FUB is less good but it performs better in the area of NRW and in the mountainous parts of SW-Germany. In the mountainous areas an integral representation of the boundary layer may be an advantage compared to a vertically resolved boundary layer. Due to the relatively coarse horizontal resolution, the orography is flattened resulting in a lower height of the corresponding sites in the model than in reality. Thus, models might achieve better correlation coefficients, if the observations are compared to data from upper model layers. However, this is not seen in the area of Saxony where DWD have better performance compared to FUB. In the frequency distributions below the figures it is also seen that the general performance of DWD is quite good – with a maximum of the distribution above 0.7. FUB is slightly worse.

From the comparison of NILU and SMHI in terms of the RMSE (Fig. 3), it is seen that both models have relatively large values of RMSE in the NRW area. Whereas NILU has a large positive bias for NRW and SMHI has nearly none (not shown here). SMHI has a clearly better overall performance (see frequency distributions below figures). However, both model systems seem to have similar high RMSE at a number of single sites, but better scores for nearby surrounding stations. This is an indication of a limited representativeness of certain observation stations.

In Fig. 4 frequency distributions from the spatial maps of the temporal statistics for all the model systems are shown for the daily maximum values for the period July 1 to August 31. With respect to the bias DWD, DWD2, NERI, NILU and SMHI have flat but symmetric distributions. Both FUB and FUB2 produce an overall negative bias. The model systems also differ in the correlation coefficients. DWD, DWD2 and SMHI obtain the best results, with maximum above 0.7. The frequency distributions also show good performance for FUB, FUB2 and NERI. NILU produces a flat distribution. As for the bias, the DWD, DWD2, NERI, and SMHI results are very good and similar with respect to the RMSE. The results for NILU show a little worse performance and FUB and FUB2 show less good performance.

4. Conclusions and recommendations

Five different models from Denmark, Germany, Norway and Sweden have been compared using the ozone monitoring data from Germany including more than 300 measurement stations. All the models that participated in the comparison are comprehensive Eulerian based European scale models, however with different setup of the model systems. All the models were operational during the summer of 1999. The models have been compared using standard statistical measures. For all the models the 1-24 hour forecasts were compared. For the DWD and FUB also the 25-48 hour forecast were available. The DWD, SMHI and NILU models have high vertical resolution compared to the NERI and FUB models, which have a low vertical resolution (3 layers). The intention was not to evaluate the different individual processes in the model systems. But the extensive comparison showed to be of significant value for pointing out weak points in the different models.

The DWD, SMHI and NILU systems are comparable in comprehensiveness. The DWD and SMHI systems showed best overall performance, however the SMHI system underestimates the amplitude of the diurnal variation, which might be due to the coarser horizontal resolution or too strong vertical exchange during stable conditions. The NILU system has a less good performance in terms of the correlation. The NERI and FUB systems are less comprehensive with respect to vertical exchange and quite similar compared to the comprehensive models in the performance with respect to the correlation. However, the FUB system has a large overall bias and RMSE. The NERI system has a less pronounced diurnal variation but the daily maximum ozone concentrations are well described. For the chemistry-transport part the

horizontal resolution of FUB is a factor of four higher compared to the NERI system. Besides the coarse resolution, the small diurnal variation in the NERI system can be explained by a too simplified vertical exchange procedure with a too rough description of the nocturnal mixing height.

From the correlation coefficient and the RMSE the overall performance for all the models are better for the period July-August compared to the period May-September. The bias shows that the DWD tends to underestimate for the whole period compared to July and August pointing to too low concentrations at the lateral boundaries. The opposite can be observed for NERI and SMHI. The 1-24 hour forecasts are slightly better compared to the 25-48 hours forecast, both for DWD and FUB, however the drop of forecasting skill with forecasting length is stronger for FUB than for DWD.

The Scandinavian models included in this study (NERI, SMHI and NILU) were all run with a relatively coarse horizontal resolution (50 km-55 km) compared to the models from DWD and FUB which had resolutions of around 20 km-25 km. A tendency can be observed towards less diurnal variation in the coarser resolution models. The diurnal variation can be less pronounced due to resolution of emission data leading to a "dilution" of the pollutants, which makes the models more rural in a climatological sense.

At a number of single sites the forecast from all the models failed. This is a strong indication of a very poor representativeness of these observations since all the models perform better for nearby measurement stations. In some regions the performance of all the models is low. Two explanations for this are possible: either a large fraction of a network is not representative or the models have principal problems within the regions. We recommend to utilize modeled data of the kind presented in the paper for the assessment of monitor locations and the design of observation networks.

The importance of using a set of statistical parameters must be stressed, because different conclusions were reached from the different statistics. This was true both with respect to the single parameter statistics (e.g. the mean or standard deviations) and the difference statistics (as e.g. the correlation coefficient or RMSE).

From this study it turns out that evaluation studies have to be carried out comparing several model systems by using a large number of observations over a large period and domain in order to achieve general information about model performance and deficiencies. This cannot be accomplished to that degree by the comparison of simulations only against data of limited spatial and temporal extension. In the present case we only had access to ozone data from the German monitoring networks. But data from several countries, for longer periods and for more species (as e.g. NO_x) should be used for comparison studies like this. Furthermore, a model comparison of the vertical profiles from ozone soundings or data from commercial airliners would be of great interest. Therefore, a continuation of this work is desirable. Additionally, in order to achieve significant results it must be emphasized that the basis must be an observation data set of an adequate quality. Nevertheless, the comparison against data from field campaigns is necessary for detailed process studies. The evaluation process will be optimized, if both strategies would be building up one upon another.

Different air pollution models in Europe are in the process of being routinely operated. In view of the proposed EU directives, evaluation and comparison exercises should be a part of any forecasting system, like it is common practice in numerical weather forecasting. This would require real time data exchange and cooperation on the European scale. Furthermore,

model comparisons like this should be carried out in close cooperation with agencies operating the measuring networks to improve the monitoring networks.

Acknowledgements

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A model system to forecast surface ozone maxima in Germany

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Within the last four year an operational forecast system was developed at FU Berlin to forecast the daily surface ozone maxima in Germany. This system is a combination of statistical and Fuzzy models for local sites and the chemical transport model REM3 for the Middle European area. The meteorological forecasts are received from German Weather Service. For the development of the statistical and Fuzzy models timeseries from 1990 to 1998 at 350 stations from the German environmental agencies were used. The CTM REM3 was applied in a diagnostic mode from 1995 to 1998 for preparation and in forecast mode from 1997 up to now. Besides the separate use and presentation of all models there is special interest in the combination of these models. Therefore tests were made to use the ozone forecast from CTM REM3 in combination to regression technics MOS and Fuzzy-modeling. The system will be presented and the accuracy of all model components will be discussed. This project was funded by Umwelbundesamt, Germany.

Operational air quality modelling over europe and Iberian Peninsula by using the RSM, MM5 and CAMX modules

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In this contribution we will show preliminary information related to online and operational air quality modelling over Europe by using the RSM (Regional Spectral Model, NOAA), MM5 (PSU-NCAR) and CAMx models. The RSM is a limited area atmospheric numerical model system, which used primarily for daily weather forecasts, and climate simulation or forecasts. The initial motivation is from the authors' experiments with a limited-area grid-point model. Since spectral computation has higher accuracy in term of gradients and spectral interpolation. We switched from grid-point model to spectral model. The difficulty to do limited area model with spectral method is overcome by the time-dependent perturbation method. The extension of this perturbation method is used to step into the non-hydrostatic model from the existed hydrostatic model. The Fifth-Generation NCAR / Penn State Mesoscale Model (MM5) is the latest in a series that developed from a mesoscale model used by Anthes at Penn State in the early 70's that was later documented by Anthes and Warner (1978). Since that time, it has undergone many changes designed to broaden its usage. These include (i) a multiple-nest capability, (ii) nonhydrostatic dynamics, which allows the model to be used at a few-kilometer scale, (iii) multitasking capability on shared- and distributed-memory machines, (iv) a four-dimensional data-assimilation capability, and (v) more physics options. The model (known as MM5) is supported by several auxiliary programs, which are referred to collectively as the MM5 modeling system. The Comprehensive Air quality Model (CAMx) (ENVIRON Eulerian photochemical grid model that allows for integrated assessment of gaseous and particulate air-pollution over many scales, from individual point source impacts to urban-regional effects. CAMx simulates the emission, dispersion and removal of inert and chemical reactive pollutants in the lower troposphere by solving the pollutant continuity equation for each chemical species on a system of nested three-dimensional grids. The emission inven-tory is generated by using the EMEP, GEIA and

EDGAR emission inventories. The results show that it is possible to provide in an operational and on-line mode results from these two air quality modelling systems through the WWW.

Real time emission forecasting as the basis for operational air pollution forecasts

A. Heidegger, S. Tilmes, R. Friedrich

The purpose of the emission calculation module CAREAIR/ECM, which was developed within the German TFS, is the provision of anthropogenic and biogenic emission data in high temporal, spatial and species resolution as re-quested by air pollution modelling systems for any (past or future) modelling episode of a year and variable modelling areas in Europe. To be able to carry out short time forecasts, a forecast mode has been implemented within the TFS network model system at the DWD utilising present weather forecasts. A persistent basic data inventory for emission calculation is held at the IER containing basic data sets from various emission models. This database is updated regularly. On its base a platform independent interface between the emission inventory and the emission calculation module can be generated, called cache database. The cache database is containing all the basic data necessary for the generation of high-resolution emission data sets of a whole year. For each area of interest, each year and each geographical projection system a separate cache database is generated. The main task of the ECM is to calculate, split and then sum up emissions from all the different processes (road traffic, combustion plants, solvent use and so on) for each time step and each grid cell. Anthropogenic emissions are calculated by use of yearly emissions split into substance and source classes as well as by use of the associated time curves and spatial distribution tables and the VOC emission profiles. Biogenic emissions are calculated using the model of Steinbrecher (Fraunhofer Institut für Atmosphärische Umweltforschung, Garmisch-Partenkirchen, 1995). The ECM allows for calculating emission data for a variety of projection grids with the following specifications:

- arbitrary episodes of a year,
- daily or hourly temporal resolution,
- spatial resolution down to 1 km x 1 km,
- pollutants: SO2, NOx, CO, NH3, VOC (substance classes or single substances). The ECM has been directly coupled to the meteorological model LM of the Deutscher Wetterdienst and to the chemistry transport model EURAD/CTM of EURAD. We will show examples for the temporal development of emission rates. Also we will present a brief intercomparison between real-time emission forecasts using ECM in forecast mode and emission calculations based on climatological meteorology using ECM in hindcast mode. The influence on the resulting ground level ozone values will also be discussed.

Dispersion modelling within the european communities new air quality frame directive

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The new ambient air quality framework directive 96/62/EC of the European Commission provides an EU-wide framework for national, regional and local measures to improve or maintain air quality. According to the directive, the Member States have assess air quality through-out their territory. Besides direct measurements, the use of other techniques as air quality modelling is intended. Air quality models shall be applied in regions where the ambient concentrations are low or where measurements not sufficient informations to fulfil the requirements of an air quality assessment. In addition, models are the only tools that allow to predict the likely effects diffe-rent measures on air quality. In an ongoing project sponsored by the German and carried out at the Free University of Berlin the development of an integrated modelling system, fulfils all requirements of the EU air framework directive is under way. The system dispersion models for the following scales: The regional scale (European wide) for calculating the national background concentrations with a 3-dimensional large scale photochemical model in a spatial resolution of ca. ¥° lat. by ½°lon. (30 x 30 km²). These concentrations simultaneously serve background for the agglomeration regions to studied with a 3-dimensional urban photochemical modelin a resolution of 2 x 2 km² least. Urban scale modelling interacts with the micro that is resolved with a 3-dimensional micro scale model for city quarters or with a 2-dimensional street canyon model for single streetcanyons as a link to 'hot spot' related air problems. Measurements will be introduced into this air quality assessment system for validating modelling results and for data assimilation and Kalman-filtering. Currently the integrated (REM3, CALGRID, MICRO-CALGRID and CPB) are upgraded to the latest state-of-the-art chemistry, aerosol modeling and numerical methods. First results are presented of the application of photochemical long range transport model REM3 to assess nationwide O3, NO2 and PM10 concentration levels and of a test case considering all scales involved.

High ozone short-term episodes over Iberian Peninsula

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Abstract

During the night and early morning of 29 of April 2000, a high ozone short-term episode has occurred over Madrid, Spain. This type of episode is unusual. Nevertheless, several similar episodes with very high ozone concentration during only a few hours have been observed also over Lisbon region some years ago (e.g. 12 hours above 400 μg.m^{-3} between 8 pm and 8 am, 21 – 22 June 1989 or 4 hours above 530 μg.m^{-3} – with a maximum of 867 - between 11 am and 14 pm, 4 April 1990). Nevertheless, a cause-effect link is usually difficult to attain due to two main constrains: (i) is a local phenomena (in Lisbon, for several times, the phenomenon

was recorded only at a single station, being a sensor error the logical and the acceptable answer, as a first attempt); (ii) lack of information to formulate an hypothesis explaining the phenomenon.

In the present case, the phenomenon had a larger amplitude (has been recorded in several air quality stations of Madrid) and was immediately identified. With this rapid reaction, become possible to get all the necessary atmospheric information in order to formulate hypothesis to explain the phenomenon.

Some meteorological phenomena are related with tropopause fold. This mechanism can be responsible to bring down into the troposphere air from the stratosphere. This air is identified, among others characteristics, by a high ozone concentration level and high radioactivity, due to nuclear bomb testing.

The measured concentrations in Madrid network indicated that the ozone episode had occurred during the night and the reached values are, at some stations, more than one order of magnitude above background ozone concentration, which can indicate the possibility of occurrence of the process above described.

Trying to explain this particular ozone episode using the hypothesis of tropopause fold, a west-east vertical section for potential temperature and wind velocity has been done, based on radio-sondes data, between the 25th and 29th of April of 2000. The analysis of this vertical section has been made in conjunction with surface pressure maps, with fronts represented and 200 hPa surface maps (in order to evaluate the jet stream position). It was also under consideration the atmospheric radioactivity measured over that location for the same period of meteorological data analyses.

Although the data gathered for analysis is being object of complementary treatment, first results indicate that the hypothesis of ozone stratospheric intrusion may be valid.

1. Introduction

The exchange of ozone between the different layers of the atmosphere, mainly between the atmospheric boundary layer, free troposphere and lower stratosphere, is a common scientific topic on the calculation of the tropospheric ozone budget. Also it is important to have an estimate of how much of the stratospheric ozone is important when one wants to model the tropospheric chemistry (Elbern *et al*, 1997, Beekmann *et al*, 1997, Kentarchos *et al*, 1999 and Bian *et al*, 1999). Moreover, the stratospheric-tropospheric exchange have an important role on the distribution of other atmospheric constituents such as aerosols and greenhouse gases and the rate of transport between both layers affecting their chemical balance. (http://see.gsfc.nasa.gov/edu/SEES/strat/class/Chop_6/6_5.htm)

Studies on this subject were already done by EUROTRAC subproject Tropospheric Ozone Research (TOR) (Hov, 1997).

In Warneck, 1987, there are four processes responsible for air exchange across the tropopause:

    (a) seasonal adjustment of the average tropopause level;

    (b) organized large-scale mean motions due to meridional circulation

    (c) turbulent exchange processes via tropopause gaps or folds associated with jet streams

    (d) small scale eddy transport across the entire tropopause

Following Beekmann *et al*, 1997, tropopause folding constitutes an important event for air mass exchange between stratosphere and troposphere. These tropopause folding can be related with the seasonal displacement of the tropopause. This displacement is considered (Warneck, 1987) of extreme importance on the exchange of air masses between the tropopause and stratosphere. In winter, above 30º N the mean tropopause level is lowered, introducing tropospheric air into the stratosphere. Below 30 º N tropopause level is common in higher levels, bringing into the troposphere stratospheric air, rich in ozone.

Studies point out that the most effective eddy induced transfer processes in the extra tropics are mesoscale phenomena such as tropopause folds and cut-off lows. These events are the more effective on the intrusion of stratospheric air masses into the tropopause (Elbern et al, 1998).

Elbern *et al*, 1998, studied the climatology of tropopause folds, based on a ten years routine global analysis data set from the ECMWF. The authors came to the conclusion that significant occurrence of tropopause foldings are restricted to pole-ward 30 ºN in latitude and the regions with the great activity of this event are eastern Canada and north-western Atlantic, northern Pacific, and central to eastern Europe. Tropopause folds activity is stronger in the Northern Hemisphere (N.H.) and decrease during the summer of the N.H.

Davies and Schuepbach (1994) indicates that stratospheric air masses can appear near the ground although such intense events are scarce even above regions of high probability of tropopause folds and cut-off lows (North-eastern of North America and Japanese Sea). These facts are in accordance with studies made upon time average zonal wind speed that states strong zonal wind maxima near 30 ºN above the eastern part of the Asian and North America Continents (Holton, 1992). And related to the development tendency of the synoptic-scales disturbances in the regions of maximum time mean zonal winds over the western Atlantic and western Pacific and to propagate downstream along the storm track that follows the jet axes.

As stated in Beck *et al*, 1997, the air within the troposphere is transported and redistributed by the atmospheric dynamical processes, sometimes related, namely:

- Large scale downward movements due to anticyclonic circulation;
- Convective growth of the boundary layer (entrainment);
- Convective clouds (cumulus);
- Large scale upward motions induced by cyclones;
- Frontal systems;
- Stratus clouds;
- Rain scavenging;
- Downward flux from the stratosphere;
- Orographic effects;
- Land and sea breezes;
- Heat island effects;

Particularly, the mechanisms that seem responsible for the transportation of stratospheric air into the lowermost levels of the boundary layer in the downward motions related to frontal passages are (Johnson and Viezze, 1981, in Beck *et al*, 1997):

- Dissipation of a stratospheric intrusion by general mixing and diffusion into the free troposphere;

- Persistence of the intrusion down to the atmospheric boundary layer, where the lower portion of the intrusion is mixed down to the ground by turbulent eddies and convection at the top of the boundary layer;

- Coupling of the intrusion to the frontal zone associated with a cold front, with direct transport of the stratospheric ozone to the ground by frontal downdrafts;

- Similar to the previous process, but in this last case the stratospheric air become entrained in organized frontal and pre-frontal convection, which then transports it to the surface in connections with rain showers or thunderstorm downdrafts.

2. Case study: Ozone episode over Madrid, Spain

During the night and early morning of 29 of April 2000, a very high ozone short-term episode has occurred over Madrid, Spain. Although this is a rare event, several similar episodes with very high ozone concentration during only a few hours have been observed also over Lisbon region some years ago (e.g. 12 hours above 400 μg.m^{-3} between 8 pm and 8 am, 21 – 22 June 1989 or 4 hours above 530 μg.m^{-3} – with a maximum of 867 - between 11 am and 14 pm, 4 April 1990). Nevertheless, a cause-effect link is usually difficult to attain due to two main constrains: (i) is a local phenomenon; (ii) lack of information to formulate a hypothesis explaining the occurrence. The phenomenon was record only at a single station, being a sensor error the logical and the acceptable answer, as a first attempt. As examples, ozone episodes above 300 μg.m^{-3}, were recorded at Monte Velho (Mvelho, an EMEP station located southern Lisbon) and also at Rua do Século (an air quality station located in the centre of the city of Lisbon and are listed in table 1).

From the analysis of table 1, it can be observed that during the year of 1989, ozone episodes were very frequent and most of them are associated to cyclonic circulation during autumn and spring. Most of the ozone episodes were registered during the afternoon, but some have been recorded in the morning and early morning. Although only ozone values above 300 μg.m^{-3} were identified more ozone episodes above 180 μg.m^{-3} were recorded for this period (Barros, 1999).

For the ozone episode over Madrid, high ozone concentrations were measured between 2 and 8 am in 29th of April 2000 by some of the air quality stations of the Madrid Community Area. The periods of elevated ozone concentrations measurements varied from station to station, but in some of the periods of 2-3 hours were recorded (San Jose, 2000).

2.1 Methodology

The data used in this study are the measurements taken in the radiossonding over Lisbon (Portugal), Barajas (near Madrid, Spain), Baleares Islands (Spain) and Corsega (France), at 00H00 and 12H00 UTC (see Figure 1). In table 2 the latitude and longitude of each station is reported.

2.2 Discussion

The below discussion is made on basis of the interpolation of the vertical profiles measured in the above cited locations. Due to the lack of space, it is impossible to show all the figures although they exist.

On the 25th of April, a cold front is passing through the Iberian Peninsula, which is confirmed by the downslop of the isentropics and an increasing of relative humidity coming from the

Atlantic Ocean. A very dry air mass is located between 700 and 600 hPa descending for 850 to 750 hPa at noon. This low value for water vapour can be related with anticylonic conditions verified on previous day.

Table 1: List of ozone episodes above 300 $\mu g.m^{-3}$ registered in the Lisbon air quality measurement network, between 1989-1997.

Date	Nº of Hours	Period (hours of occurrence)	Local	Circulation	O$_3$ Hourly Average Conc. ($\mu g.m^{-3}$)
1 Out 90	1	15	MVelho	Cyclonic	307
23 Out 89	1	9	MVelho	Cyclonic	418
12 Nov 90	4	13-16	MVelho	Cyclonic	441
14 Nov 89	3	15-17	MVelho	Cyclonic	505
18 Nov 89	4	15-18	MVelho	Cyclonic	422
22 Nov 89	4	13-16	MVelho	Cyclonic	464
25 Nov 89	3	(4+8+9)	MVelho	Cyclonic	354
30 Nov 89	4	13-16	MVelho	Cyclonic	620
8 Dez 89	3	9-11	Século	Cyclonic	499
16 Dez 89	4	15-18	MVelho	Cyclonic	555
4 Apr 90	4	(11-14)	MVelho	Cyclonic	689
22-23 Jun 89	17	14 +15+(18-8)	Século	Anticyclonic	379

Figure 1: Location of the radiossonding sites analysed (University of Wyoming, United States - http://www-das.uwyo.edu/upperair/index.html).

Table 2: Latitude and longitude of each station considered.

Station	WMO ID	Latitude (°)	Longitude (°)	Z (m)
Lisbon	8579	38.77	9.13	105
Barajas	8221	40.45	3.55	582
Baleares	8301	39.55	2.62	6
Corsega	16560	39.25	9.05	1

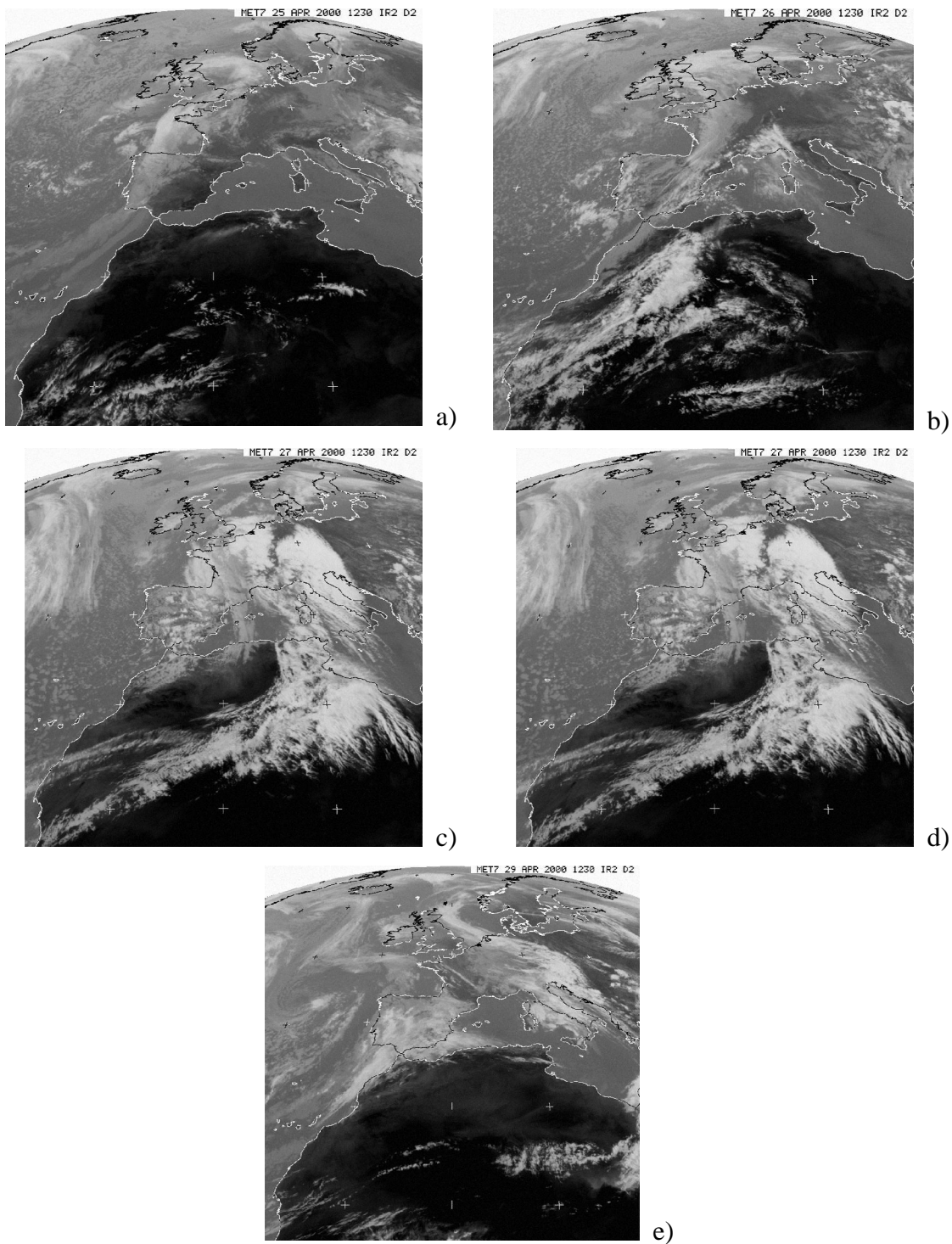The data were interpolated using the nearest neighbour interpolation method.

Figure 2: Images from the METEOSAT satellite at 12H30 UTC, between the 25th and 29th of April (http://www.infomet.am.ub.es/arxiu/meteosat).

On the 25th of April starts to form a cut-off low NW of the Iberian Peninsula. This cut-off low is completely formed in the 26th of April at 00H00 UTC. Its centre starts to move southward and on the 27th of April, 12H00 UTC is over Madrid. At this time, the cut-off low is part of a complex frontal system that extends from Great Britain to Marroc, with another cut-off low centred in the North of Ireland. The cut-off low centred in the Iberian Peninsula moves to the east and the one centred over Ireland moves to the South until the 29th of April 00H00 UTC,

breaking apart between 00H00 UTC and 12H00. Although the 300 hPa charts are not represented in this report, this situation can be followed by the satellite images in figure 2.
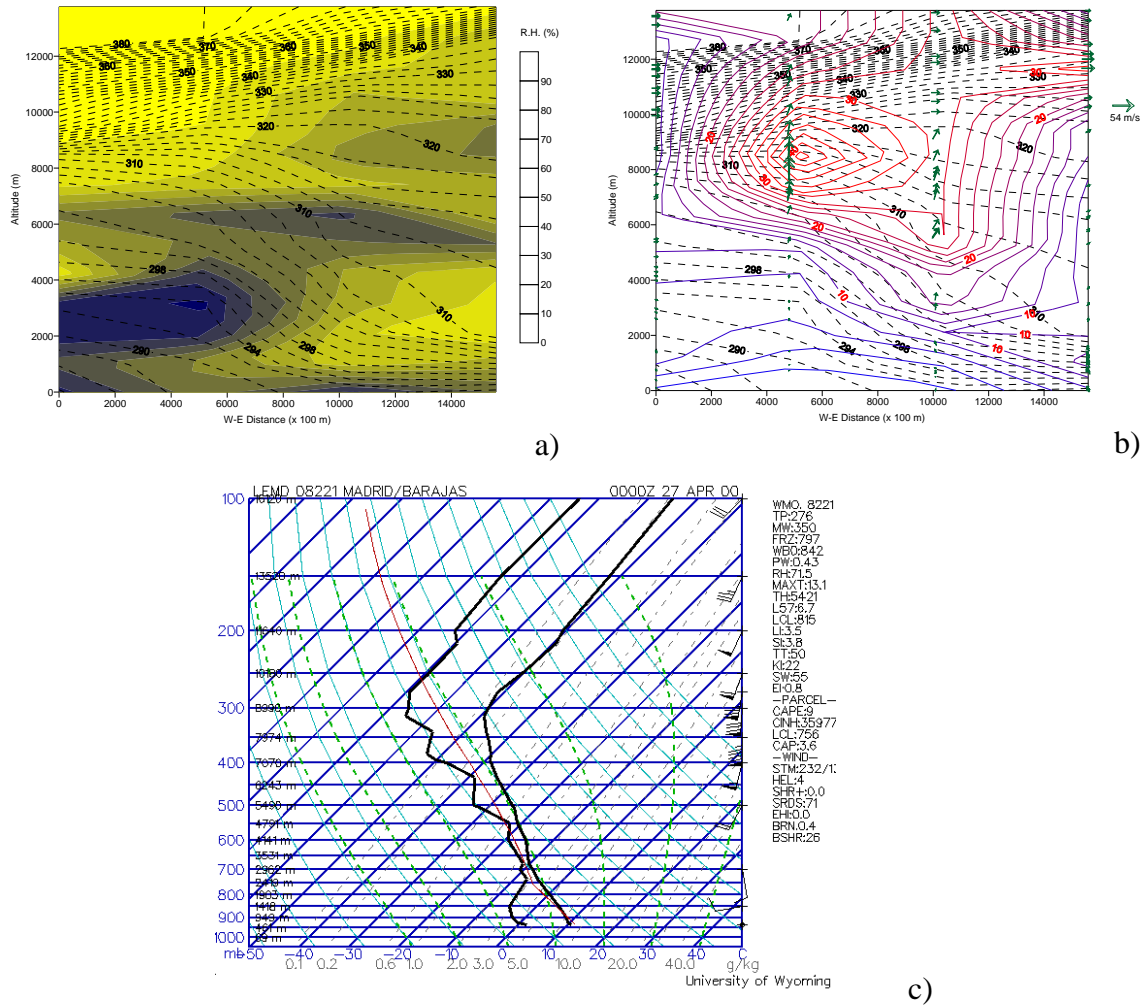

a)

b)

c)

Figure 3: a) Interpolated potential temperature and humidity, b) Wind speed, potential temperature and vertical wind vectors over Lisbon, Madrid, Baleares and Corsega (from West to East), c) radiosonde data; 27th of April of 2000, at 00H00 UTC.

In the 25th of April, the jet stream starts to intensify and to gain a very strong meridional component over the region in analysis. Between the 27th of April 00H00 and 12H00 UTC, the jet stream is totally meridional over and east of Madrid. After this period, the jet stream changes direction and becomes NW, rotating to SW until 12H00 of the 29th of April 2000, favouring an anticyclonic situation to form at surface. The largest observed vertical wind shear over Madrid is between 00H00 UTC of 26th and 27th of April, also at 00H00.

Although the isentropic potential vorticity had not been calculated, figure 6 appears to have good conditions for tropopause folding due to the intensification of the isentropics slopes over the region under analysis. The isentropics of 300 K is at 8000 m on altitude over Lisbon and around 2000 m over Corsega.

After the 28th of April warm advection is observed in the vertical potential temperature profiles. In this figures, the air is characterised by high values for relative humidity. At 00H00 of the 29th of April, the pressure gradient is favourable to a relative high formation in the centre and south east of Madrid. This anticyclonic situation can be the principal responsible

for the downward movement to the surface of the stratospheric air intruded in the 27th of April.

Also, it tried a correlation between tropopause high and radioactivity data, over Madrid. The obtained correlations were low (table 3) and there was an attempt to correlate only with Berilum 7 radioactivity measurements, but this particular data is not yet available for comparison.

Table 3: Correlation between radioactivity data and tropopause high over Madrid between the 25th and 30th of April 2000.

Radiation	Tropopause high
Alfa (Bq/m3)	0.11
Beta (Bq/m3)	0.13
Radon(Bq/m3)	0.46
Iodos (Bq/m3)	0.67
Gamma(uSv/h)	-0.24

3. Conclusions

The authors are convinced, base on this preliminary work, that strong vertical movements of ozone rich air masses could explain this type of short-term ozone episodes over the Iberian Peninsula. The Madrid episode is a clear evidence of this. Nevertheless, a long and hard work should be done in order to fully prove the hypothesis. The introduction of modelling tools could be a very useful help and will be implemented as soon as possible.

Acknowledgments

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STUDYING THE INFLUENCE OF THE BIOGENIC EMISSIONS ON THE AOT40 LEVELS IN EUROPE

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Abstract

It is well known that the uncertainties in the determination of the biogenic emissions are very large (some authors claim that these emissions are under-estimated in certain areas up to ten times). A long series of runs with different biogenic emissions was performed. The results obtained in this study show clearly that the biogenic emissions must be taken into account when control strategies are developed for reducing the anthropogenic emissions in order either to reduce some high pollution levels to prescribed critical levels or to keep them under the critical levels.

1. Creating sets of biogenic emissions

Consider an arbitrary area within the space domain of consideration (this area could be a grid-square, a country, a group of countries or a whole continent). In our particular study the space domain is the whole of Europe with parts of Asia, Africa and the Atlantic Ocean. Consider also M vegetation categories (as, for example, forests, crops, etc.). Then the *VOC* emissions in the selected area that are emitted from the selected vegetation category j, $j = 1,2,\ldots,M$, can be described in the following generic form containing **a product of three terms** in its right-hand-side (this form for representing the biogenic emissions is very similar to that discussed in [6]):

where
- E_j is the *VOC* emission, which is emitted in the area under consideration from vegetation category j during a time-period of N hours,
- $PORTION_{ij}$ is the portion of the area selected, which is covered by the vegetation category j at hour i (it should be mentioned that very often this factor is assumed to be a constant),
- $EMISFACT_{ij}$ is the emission from vegetation category j, which is emitted at hour i, standardized for temperature of $30^0 C$ (in [6] also for full sun light).
- $TEMPFACT_{ij}$ is a factor dependent on the temperature, which is used to transform the standardized emission $EMISFACT_{ij}$ from vegetation category j to the actual emission at hour i (in [6] this factor is assumed to depend also on the solar radiation),

Different algorithms for calculating the biogenic VOC emissions are obtained by making different assumptions about the three factors in the right-hand-side of formula (1). The following assumptions were used in this study:

- $PORTION_i$ is obtained by using land-use inventories downloaded from the Internet,
- $TEMPFACT_{ij}$ is obtained by using formulae that are similar to those proposed in [5],
- $EMISFACT_{ij}$ is obtained by using values similar to those proposed in [6].

It should be mentioned that the algorithm used in [3], [7] and [8] is similar to that proposed above. It should, furthermore, be stressed that several different algorithms for varying $TEMPFACT_{ij}$ are discussed in [6]. The differences resulting from different choices of $TEMPFACT_{ij}$ are fully discussed in [6]. However, from the section about uncertainties (Section 4 in [6]), it becomes clear that the major uncertainties are caused by the lack of knowledge for the values of the important third factor, $EMISFACT_{ij}$. Therefore, the main aim in this study is **to show the impact of the uncertainties in the determination of $EMISFACT_{ij}$ on the ozone pollution levels**. This will be done by applying three scenarios for producing the biogenic emissions that are based on the use of three different choices of $EMISFACT_{ij}$. The temporal variations of the biogenic emissions are important. Therefore, these variations will be discussed before the detailed definition of the scenarios used.

2. Temporal variations of the biogenic emissions

The major part of the biogenic VOC emissions is coming from the forest areas (see, for example, [6]). During the last 5-10 years, however, more and more scientists are proposing to take into account also biogenic emissions from other kinds of vegetation (these emissions will

be called here biogenic emissions from crops only in order to use a shorter name). The temporal variation of the 1995 VOC emissions from forests and from crops emitted in the space domain on the Danish Eulerian Model, [7], are shown in Table 1. The units used in Table 1 are *Ktonnes per area per year*.

Table 1: Temporal variations of the biogenic emissions from forests and from crops

Month	Forests	In percent	Crops	In percent
January	265	2.3 %	0.606	0.38 %
February	260	2.3 %	0.716	0.45 %
March	327	2.8 %	1.150	0.72 %
April	605	5.2 %	4.450	2.80 %
May	1411	12.3 %	20.800	13.10 %
June	2130	18.5 %	38.200	24.00 %
July	2341	20.3 %	43.900	27.60 %
August	1989	17.3 %	32.100	20.20 %
September	1015	8.8 %	11.300	7.10 %
October	658	5.7 %	3.800	2.40 %
November	295	2.6 %	1.130	0.71 %
December	217	1.9 %	0.672	0.42 %
1995	**11513**		**159.00**	

It is seen that the biogenic emissions during the period from April to September (including here both April and September) are much greater than the biogenic emissions for the remaining months. This is especially true for the biogenic emissions from crops. The actual values of the emissions in the period from April to September are:
- 9491 Ktonnes for the biogenic emissions from forests (i.e. 82.4%),
- 150.75 Ktonnes for the biogenic emissions from crops (i.e. 94.8%).

The biogenic emissions emitted from crops are much smaller than those emitted from forests. However, it should be emphasized that the former emissions seem to be much more uncertain. The example given in Section 4 in [6] indicates that if the evaluations of the $EMISFACT_{ij}$ factors proposed in [2] are used, then this will lead to an increase of the biogenic emissions from crops by a factor of 20.

3. Scenarios for biogenic emissions

As mentioned in the end of Section 1, three scenarios for creating biogenic emissions in Europe are used in this study:
- Normal Biogenic Emissions (obtained by using $EMISFACT_{ij}$ factors similar to those in [6]).
- High Biogenic Emissions (increasing the biogenic emissions by using $EMISFACT_{ij}$ factors similar to those proposed in [2]). The High Biogenic Emissions from forests become about 5 times greater than the corresponding Normal Biogenic Emissions from forests for this choice of the $EMISFACT_{ij}$ factors. The increase of the High Biogenic Emissions from crops is by a factor of about 20. It should be mentioned that the same factors (5 and 20) are quoted in Section 4 of [6].
- Low Biogenic Emissions (decreasing the biogenic emissions by using the same factors as in the previous case). The Low Biogenic Emissions from forests become about 5 times less than the corresponding Normal Biogenic Emissions from forests. The corresponding factor for the Low Biogenic Emissions from crops is 20.

4. Scenarios for the anthropogenic emissions

Following the Seventh Interim Report prepared at IIASA (see [1]), four different scenarios for variation of the anthropogenic emissions have been considered:

- **Basic Scenario** (the results are computed by using meteorology for 1995 as well as the actual EMEP emissions for 1995; see [4]).
- **Scenario 2010** (the results are obtained by reducing the EMEP emissions for 1990 by the IIASA factors given on pp. 14-15 in the Seventh Interim Report, [1]; furthermore, this scenario is run by using meteorology for 1995).
- **Central Scenario H1** (as Scenario 2010, but the emissions of the 15 EU countries are further reduced by the factors given on p. 37 in the Seventh Interim Report, [1]; also this scenario is run by using meteorology for 1995).
- **Maximum Feasible Reduction (MFR) Scenario**, where the EMEP emissions for 1990 are reduced by the IIASA factors given on pp. 14-15 in the Seventh Interim Report, [1]; this scenario is again run by using meteorology for 1995).

Four additional scenarios for the anthropogenic emissions have been applied. These additional scenarios are defined as follows:

- **Scenario Basic-1** (the NO_x anthropogenic emissions are as in Scenario 2010, the others as in the Basic Scenario). We shall refer to this scenario also as **Scenario REFA**.
- **Scenario Basic-2** (the *VOC* anthropogenic emissions are as in Scenario 2010, the others as in the Basic Scenario). We shall refer to this scenario also as **Scenario REFB**.
- **Scenario 2010-1** (the NO_x anthropogenic emissions are as in the MFR Scenario, the others as in the Scenario 2010).
- **Scenario 2010-2** (the *VOC* anthropogenic emissions are as in the MFR Scenario, the others as in the Scenario 2010).

Each of these eight scenarios for the anthropogenic emissions was run with the three scenarios for the biogenic emissions (NORMAL, HIGH and LOW; see the previous section). This means that the total number of scenarios used in this study was 24. Each of these 24 scenarios was run for the 12 months of 1995. Thus, the total number of runs needed to obtain results concerning the impact of biogenic emissions on the ozone pollution levels in 1995 was 288. This is a very comprehensive computational task. It was possible to resolve this task only because a highly efficient code was prepared and run on high-speed parallel computers. The total amount of data produced in these runs is several Gbytes. Only a few percent of these data were used until now. Some results concerning the AOT40 levels in Europe are given in the next section.

5. Ozone levels in Europe for different biogenic emission scenarios

As mentioned in the end of the previous section, we are not able here to report all findings from the runs with the selected 24 scenarios. Therefore, we shall try to show the influence on higher biogenic emissions on the AOT40 levels in Europe. More precisely, we shall perform the following comparisons:

- We shall study the transition **from the Basic Scenario to Scenario 2010** for both normal and high biogenic emissions.
- We shall study ratios **(Basic Scenario – Scenario 2010)/(Basic Scenario)** for both normal and high biogenic emissions (and the same for the case where Scenario 2010 is replaced with Scenario MFR.
- We shall study two important cases, where (i) the anthropogenic NO_x emissions are reduced, while the anthropogenic VOC emissions are kept unchanged and (ii) the

anthropogenic NO_x emissions are kept unchanged, while the anthropogenic VOC emissions are reduced.

5.1. The Basic Scenario vs Scenario 2010

Results concerning the change of the AOT40 levels in the transition from the Basic Scenario to Scenario 2010 are given in Fig. 1. The two upper plots in Fig. 1 are for the scenario with basic anthropogenic emissions, while the two lower plots are for the scenario with 2010 anthropogenic emissions. The two plots on the left-hand-side are for the normal biogenic emissions, while the two plots on the right-hand-side are for the high biogenic emissions.

The transition from the 1995 anthropogenic emissions to the 2010 anthropogenic emissions results in reductions of the size of the highly polluted areas in Europe (both when the normal and the high biogenic emissions are used; compare the upper plots in Fig. 1 with the lower ones).

The transition from the normal biogenic emissions to the high biogenic emissions results in increasing the size of the highly polluted areas in Europe both when the 1995 and 2010 anthropogenic emissions are used; compare the plots in the left-hand-side in Fig. 1 with the plots in the right-hand-side).

5.2. Comparison of the size of the changes

The ratios (Basic Scenario – Scenario 2010)/(Basic Scenario) and (Basic Scenario – Scenario MFR)/(Basic Scenario), which are obtained when both normal and high biogenic emissions are applied, have been studied in order to evaluate the size of the changes when different scenarios are used. Some results are given in Fig. 2.

It is seen that if the reductions of the anthropogenic emissions are larger (this is the case when Scenario MFR is used), then the areas where big reductions of the AOT40 values are observed become larger (compare the two lower plots in Fig. 2 with the two upper plots).

The size of the changes does not vary too much when the high biogenic emissions are used instead of the normal biogenic emissions. This is true both when Scenario 2010 is used and when Scenario MFR is applied (compare the plots on the left-hand-side of Fig. 2 with the plots on the right-hand- side).

There are areas in Eastern Europe where the AOT40 levels are increased when Scenario 2010 is used. These areas become larger when the High Biogenic Emissions are used instead of the Normal Biogenic Emissions (compare the two upper plots in Fig. 2). When the reductions of the anthropogenic emissions become larger (when the MFR Scenario is used instead of Scenario 2010), then this phenomenon is practically vanished (see the two lower plots in Fig. 2).

5.3. Reductions of NO_x emissions vs reductions of *VOC* emissions

The ratios (Basic Scenario – Scenario REFA)/(Basic Scenario) and (Basic Scenario – Scenario REFB)/(Basic Scenario) obtained when both normal and high biogenic emissions are used have been studied in order to evaluate the size of the changes when (i) the NO_x emissions are reduced, but the VOC emissions are kept unchanged and (ii) the NO_x emissions are kept unchanged, but the VOC emissions are reduced. Some results are given in Fig. 3.
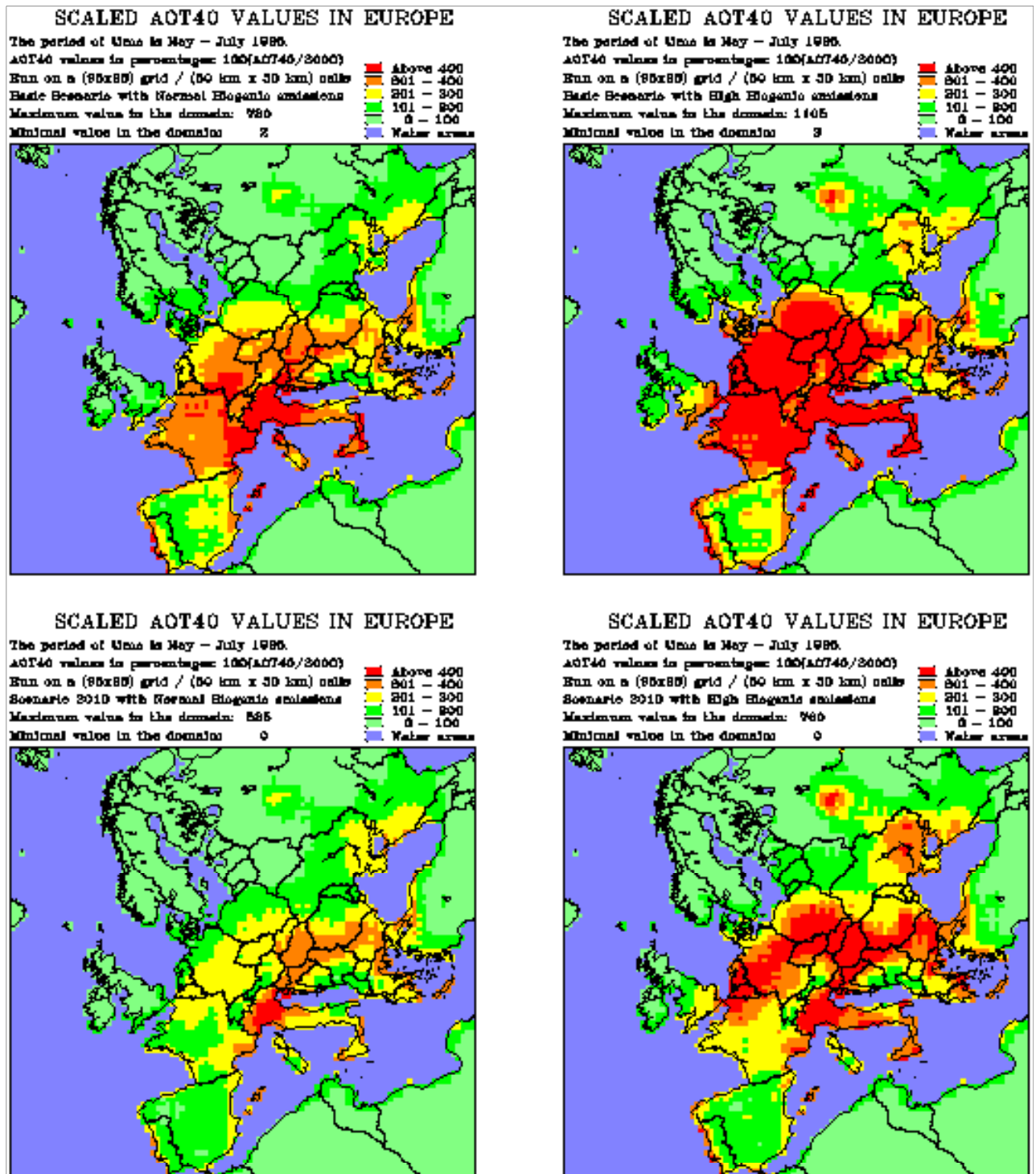
Figure 1:
Scaled AOT40 values, 100(AOT40)/3000, in Europe, obtained by using: (a) the Basic Scenario for the anthropogenic emissions and normal biogenic emissions (upper, left-hand-side), (b) the Basic Scenario for the anthropogenic emissions and high biogenic emissions (upper, right-hand-side), (c) Scenario 2010 for the anthropogenic emissions and normal biogenic emissions (lower, left-hand-side), (d) Scenario 2010 for the anthropogenic emissions and high biogenic emissions (lower, right-hand-side).
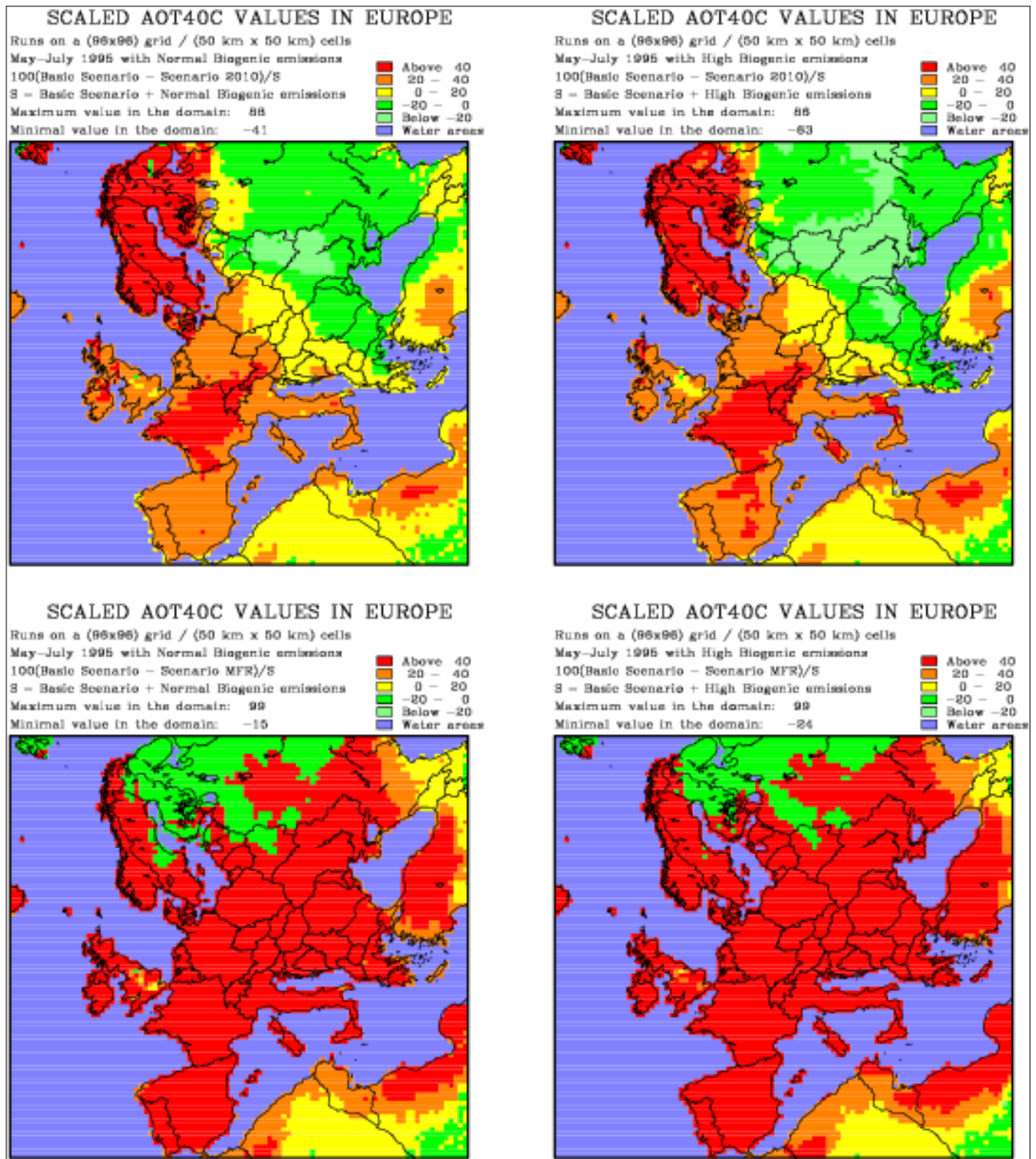
Figure 2:
Ratios related to AOT40 values that are obtained by using the formulae: (a) (BN-SN)/BN (upper,left-hand-side), (b) (BH-SH)/BH (upper, right-hand-side), (c) (BN-MN)/BN (lower, left-hand-side) and (d) (BH-MH)/BH (lower, right-hand-side), where BH stands for the Basic Scenario for the anthropogenic emissions with normal biogenic emissions, BH stands for the Basic Scenario for the anthropogenic emissions with high biogenic emissions, SN stands for Scenraio 2010 for the anthropogenic emissions and normal biogenic emissions, SH stands for Scenraio 2010 for the anthropogenic emissions and normal biogenic emissions, MN stands for Scenraio MFR for the anthropogenic emissions and normal biogenic emissions, MH stands for Scenraio MFR for the anthropogenic emissions and normal biogenic emissions.
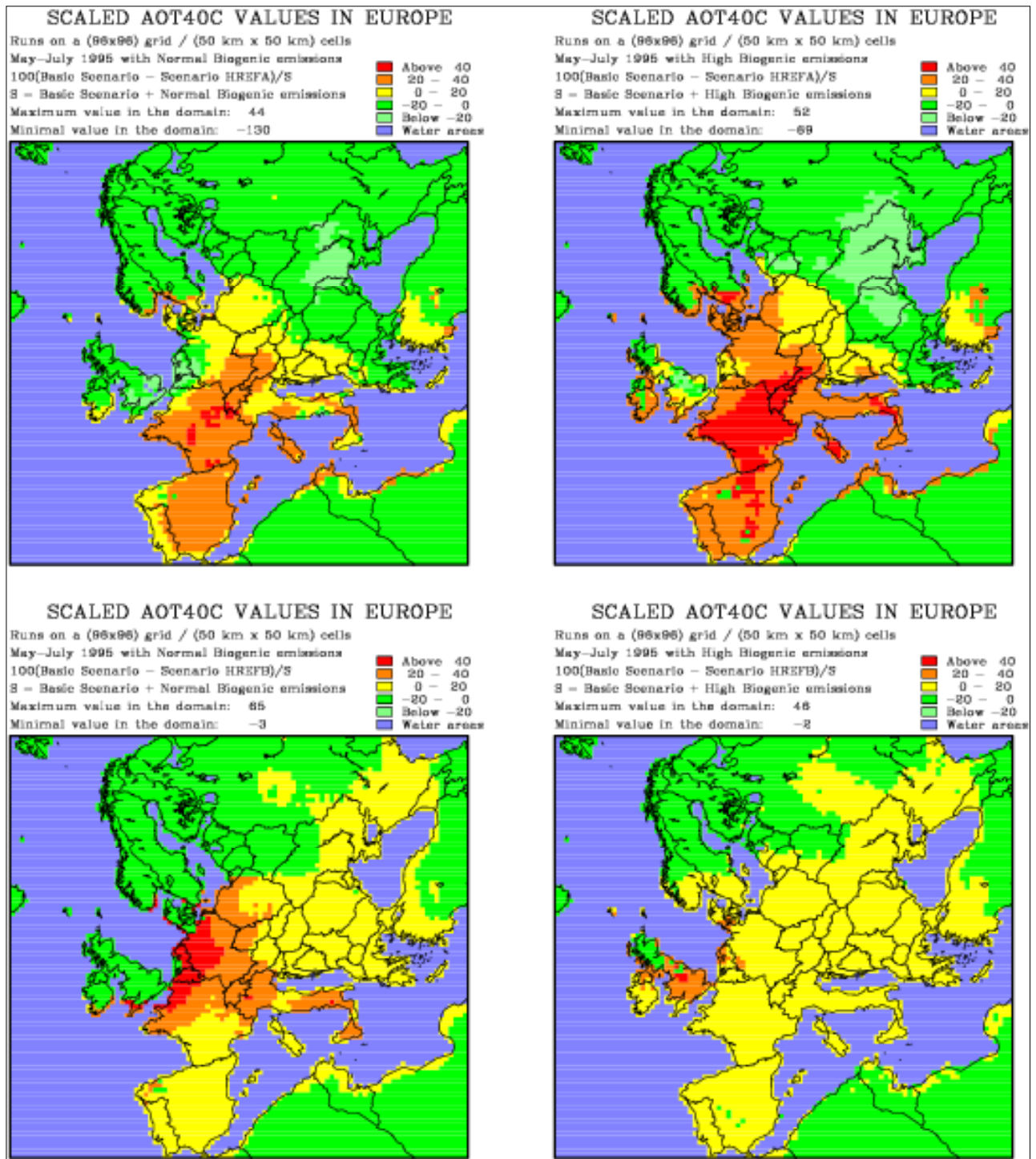
Figure 3:
Ratios related to AOT40 values obtained by using the formulae: (a) (BN-RNN)/BN (upper,left-hand-side), (b) (BH-RNH)/BH (upper, right-hand-side), (c) (BN-RVN)/BN (lower, left-hand-side) and (d) (BH-RVH)/BH (lower, right-hand-side), where BH stands for the Basic Scenario for the anthropogenic emissions with normal biogenic emissions, BH stands for the Basic Scenario for the anthropogenic emissions with high biogenic emissions, RNN stands for Scenraio REFA for the anthropogenic emissions and normal biogenic emissions, RNH stands for Scenraio REFA for the anthropogenic emissions and normal biogenic emissions, RVN stands for Scenraio REFB for the anthropogenic emissions and normal biogenic emissions, RVH stands for Scenraio REFB for the anthropogenic emissions and normal biogenic emissions. REFA: NO_x reduced as in Scenario 2010, while VOC kept as in the Basic Scenario. REFB: NO_x kept as in the Basic scenario, VOC reduced as in Scenario 2010.

If the anthropogenic NO_x emissions are reduced then the changes are larger when the high biogenic emissions are used (compare the two upper plots in Fig.3). If the anthropogenic VOC emissions are reduced, then the results become opposite. In fact, the results become very insensitive to changes of the anthropogenic *VOC* emissions when the High Biogenic Emissions are used (see the lower right-hand-side plot), because the relative part of the reduction of the anthropogenic *VOC* emissions is in this case a smaller part of the total *VOC* emissions (compared with the case where the Normal Biogenic Emissions are used). If only the NO_x emissions are reduced, then there are again areas in which the AOT40 levels are increased (mostly in the Eastern Europe but also in some parts of England, Belgium and The Netherlands, see the upper two plots in Fig. 3). If only the *VOC* emissions are reduced, then this phenomenon is practically vanished (see the lower two plots in Fig. 3).

6. Discussion of the results obtained by using biogenic emissions scenarios

6.1. Increasing the importance of the biogenic *VOC* emissions

The fact that the anthropogenic emissions in Europe (not only the anthropogenic *VOC* emissions) have been reduced considerably during the last decade shows clearly that the relative part of the biogenic emissions is in general increasing. In addition, since biogenic *VOC's* have had greater uncertainty than anthropogenic *VOC's*, the overall uncertainty of ozone predictions naturally increases, due to this shift of weights towards biogenics.

6.2. Need for extensive studies concerning the biogenic emissions

The great uncertainties in the evaluation of the amount of the biogenic emissions have always been a source of concern in making scenarios and/or predicting future ozone concentrations. However, because the relative contribution of biogenic *VOC's* is increasing, the difficulties in evaluating different scenarios in support of decision-making are also increasing. Therefore, it is necessary to study more carefully the impact of the biogenic emissions on the pollution levels in Europe under different scenarios, where inventories for the biogenic *VOC* emissions are treated with more care and detail, as anthropogenic emissions are steadily reduced in time.

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Land use data resolution and modelling

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Development, operation, validation and comparison meteorology-chemistry models and integrated assessment models are only possible if high input geo-data on land use is available. In order to overcome memory problems in handling the amount of the high resolution data, is has to be resampled to much coarser resolution, i.e. 10 minutes. Also, the transformation process from geographic projection to the coordina-tes of a specific model run introduces additional errors. Both can substantial influence on the models results. This question has been investigated using the MM5 Results covering meteorological parameters as well as biogenic VOC emissions will be presented.

Effects of international shipping on European polution levels

J.E. Jonson, L. Tarrason, J. Bartnicki

Emissions from international shipping, estimated by Lloyd's Register of Shipping, representative for 1990 for NOx, SO2, CO and NMVOC are now available for all sea areas surrounding Europe. The effects of emissions on European pollution levels has been calculated with the EMEP Eulerian model. There are two versions of this model, the Photochemistry version and the Acid Deposition version. With the Acid deposition version the effects on acidification and eutrophication are calculated (for 1998) and with Photochemistry version the effects on boun-dary layer ozone are calculated (for 1996). Our calculations show that in European countries close to major routes significant fractions of the depositions can be attributed to emissions from ships. For coun-tries the contribution to the depositions of sulphur and oxidized nitrogen are close to or than 10%, even in areas with large land-based emissions as Belgium and the Netherlands. increase in the depositions caused by international shipping also contribute significantly to exceedances of critical levels for acidification and nutrient nitrogen in Europe as defined in the protocol to "Abate Acidification, Eutrophication and ground level ozone". There are also marked effects in ozone levels and in the exceedances of threshold values for ozone Increases in ozone levels, and accumulated levels for ozone exposure, are mainly confined to coun-tries with a Mediterranean coastline. In and around the English Channel, the North Sea and Baltic Sea, a combination of moderate to high emissions and low insolation, leads to decreases in mean July concentrations and accumulated critical levels for this component.

EUROTRAC-2 at Mid-term

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The aim of this contribution to the GLOREAM Workshop at Cottbus, September 2000, is to present the EUROTRAC-2 project as a whole with its structure, organisation, tasks, and the scientific work within the EUROTRAC-2 subprojects. The new, recently approved subproject TROPOSAT will be mentioned and the status of the ongoing "mid-term review" of the EUROTRAC-2 subprojects will be highlighted.

Structure of EUROTRAC-2

EUROTRAC-2 is a co-ordinated interdisciplinary research project studying the transport and transformation of environmentally relevant trace constituents in the troposphere over Europe. As in all EUREKA projects, there is no central funding. It has the overall objective to provide an improved scientific basis for the quantification of source-receptor relationships for photo-oxidants, acidifying substances, aerosols, mercury and persistent organic pollutants (POPs) to support the further development of abatement strategies within Europe. The second phase, EUROTRAC-2, started in 1996 and is scheduled to finish at the end of 2002.

EUROTRAC-2 is a "bottom up" project, based on several scientific subprojects. Financial support for scientific work within EUROTRAC-2 comes from research institutes, national governments and funding agencies as well as from the the European Commission. Three bodies ensure project management (International Executive Committee - IEC), scientific quality (Scientific Steering Committee -SSC) and environmental policy management (Environmental Assessment Group - EAG). The International Scientific Secretariat (ISS) is responsible for the overall co-ordination of EUROTRAC-2. It maintains contacts with the subproject co-ordinators, principal investigators, and the three committees, implements their decisions and arranges meetings (see Fig. 1). The ISS is also responsible for the publication of reports and newsletters and organises the biennial EUROTRAC Symposium. A detailed EUROTRAC-2 description is given in the EUROTRAC-2 project description and handbook (ISS, 1998) as well as on the web page (*http://www.gsf.de/eurotrac*).

EUROTRAC-2 Tasks

The scientific tasks of EUROTRAC-2 refer to

- Emission: to quantify natural and anthropogenic emission sources of substances contributing to formation and destruction of pollutants

- Formation processes: to establish and quantify the processes contributing to formation in the gas phase and multiphase system

- Transport and distribution: to determine the spatial distribution, transport and temporal variation of photo-oxidants, precursors and intermediate products

- Deposition: to establish the pattern and amount of deposition in major ecosystems as well as the response to changing emissions

- Model development: to develop and implement validated models for application in scientific interpretation and policy

- Quality control / instrumentation: to maintain and improve the quality and capability of in-situ and remote field measuring activities

- Synthesis and integration: to evaluate and highlight the results obtained within the project for scientific purposes and policy application

Scientific work within EUROTRAC-2

The scientific work within EUROTRAC-2 is carried out by well over 300 research groups from 30 European countries. It is thematically divided in 13 subprojects. Each subproject has a common organisation structure, clearly formulated goals and is conducted within research networks that are international and interdisciplinary linked.

Some subprojects focus on chemical mechanisms, on formation processes of photo-oxidants, including clouds and aerosols, the biosphere/atmosphere exchange of trace substances, and air pollution in urban and in coastal areas. Others deal with atmospheric cycling of mercury and POPs, eutrophication, generation and evaluation of emission data, regional atmospheric processes and modelling. Including the countries from Eastern Europe long- and short-term ozone variation and trends and air quality control measures are covered by the scientific programmes.

A new subproject in the field of using satellite data was proposed in Spring 2000, considered in the EUROTRAC-2 committees and accepted in June 2000. It focuses on the development of retrieval algorithms, the use of satellite data for understanding atmospheric processes, synergistic use of different instrumentation and the validation of tropospheric satellite data (ISS, 2001).

EUROTRAC-2 Mid-term review

A mid-term review of EUROTRAC-2 was carried out during the year 2000. Given that EUROTRAC-2 is originally a "bottom up" project, the mid term review should not be seen as a instrument of control on the scientific work. Its tasks are to help the subprojects to achieve their scientific goals, to advise on any required changes in the programmes in order to provide high quality and relevant scientific results and to assist scientists in defining the policy relevant and applicable outcomes of their work (ISS, 2000).

With the background of establishing research progress against the project description, the following three questions were the guidelines of the review:

1. What is the scientific quality and innovativeness of the research activities and findings?

2. Is there relevance for environmental policy application?

3. What is the level of co-ordination and co-operation?

The questions were addressed according to following criteria:

Scientific quality:

- Is the research performed of high quality?

- Have the research activities resulted so far in significant publications?

- What are the most important issues addressed in the subproject?

- How much of the research performed is innovative?

- Realism and focus of the subproject?

- Will the goals be achieved in the timeframe of the project?

- Have the scientific objectives of the subproject been changed with respect to the original ones?

- Are there interactions within the subproject and with other subprojects?

- Will the results be usable after/outside EUROTRAC-2?

- Do the activities result in creating new or updating existing databases of wider interest?

- Does the model development yield new or updated model tools for a better simulation of processes?

Policy relevance:

- Is the research carried out relevant for policy developers or implementers?

- Are the results useful for assessing the state of the environment in Europe?

- Are the results relevant to link the pressures to the impacts on the environment?

- Have the policy objectives been changed with respect to the original ones?

- Do contacts between the subproject and policy developers or implementers exist?

- What are the most important policy relevant issues addressed in the subproject?

- Realism and focus of the subproject?

- Will the goals be achieved in the timeframe of the project?

- Are the application results of high quality?

Co-ordination and Co-operation:

- Was the co-operation between individual groups promoted to an adequate level?

- Was the structure of the subproject adequate and effective in promoting co-operation?

- Was the exchange of information within the working groups, the subproject and/or EUROTRAC-2 satisfactory?

- Have there been interactions between the subproject and other relevant subprojects?

- Has the research activity resulted in joint publications between research groups?

- How results are being disseminated?

- Added-value of the bottom-up approach applied in EUROTRAC-2?

- Has the collaboration resulted into collaboration within other fora (EU...)?

- Would the subprojects have expected stronger internal communication with the EUROTRAC-Committees?

The review process was based on the current Annual Reports of the subprojects, Subproject Description and statistics, presentations given at the EUROTRAC-2 Symposium 2000 in Garmisch-Partenkirchen and interviews of the subproject co-ordinators. The procedures were carried out by the SSC, mainly reviewing the scientific quality and relevance of the work within the subprojects, and the EAG to assess the policy relevance. The ISS was involved with the organisation of the review process and compiling the results. Presented to the IEC at their 10th meeting in Ljubljana, February 2001, the mid-term review report was accepted. A final "synthesis and integration" phase will be needed to evaluate the results from basic and applied research and to bring the EUROTRAC-2 project to a successful conclusion.
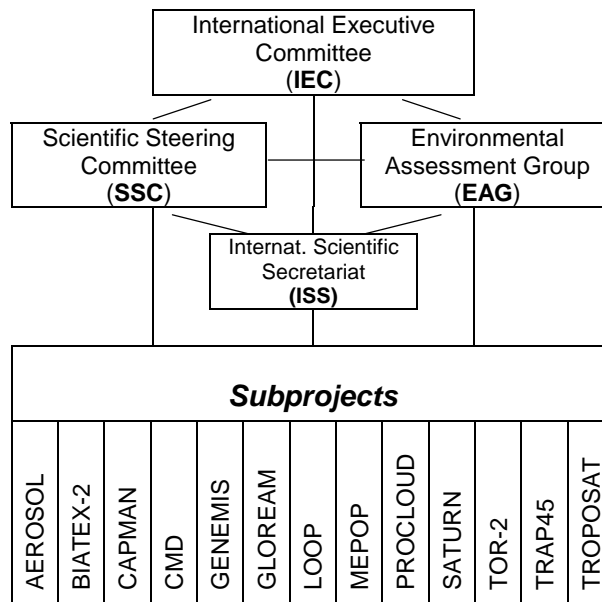
Figure 1: EUROTRAC-2 organisation scheme

Figure 1: Organisational scheme of EUROTRAC-2

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Emission data - developments, trends and uncertainties

R. Friedrich

For using atmospheric models emission data of and known quality is needed. The subproject GENEMIS has the objective to improve the quality of emission data and to assess the accuracy of these data. Progress has been made - inter alia - in estimating VOC split factors, solvent use and particulate matter emissions and emissions from road transport Furthermore a scenario of future emissions for was developed showing reductions of VOC and NOx emissions; a comparison with the thresholds of the National Emissions Ceiling Directive will be made. The last part of the presentation will deal with uncertainties of emission data; as well results of a statistical error analysis as compa-risons calculated emission data and data derived from ambient measurements will be shown. This includes the results of the EVA experiment.

Vertical exchange processes between the atmospheric boundary layer and the free troposphere - an overview of the research performed within the TOR-2 project

M. Beekmann

I will present an overview over current reserch performed within the TOR 2 project on vertical uplifting of continental boundary layer emissions into the free troposphere. Within TOR, we have formed a task group dealing with this topic and we have established an integrated research plan. This plan buit on four major

* case study analysis of airborne observations of vertical uplifting processes including mesoscale modelling studies,

* climatological analysis of vertical ozone sounding and mountain station data,

* climatological trajectory analysis in order to assess processes of vertical uplifiting, in particular related to frontal systems,

* integrating climatological model studies assessing the chemical consequences of transport of ozone precursors into the free troposphere. The purpose of my presentation is to seek and to initiate collaboration with the GLOREAM project. In particular, modelling support from GLOREAM related to the last topic "integrated modelling studies" which implies the use of global or continental scale models for climatological time periods would be wellcome.

Connected Laboratory Studies and Mechanism Development in CMD: Tropospheric Aqueous Phase Chemistry as an Example

H. Herrmann

The concepts of multiphase and chemistry as well as the physical appearance and role of particles containing liquid water as a matrix for tropospheric chemical conversions will be discussed in short. An overview on recent laboratory studies of aqueous phase chemistry relevant for the understanding of multiphase and heterogeneous conversions in aqueous tropospheric particles is given. Examples regarding radical- as well as non-radical reactions will be shown. A possible treatment of chemical reactions under high electrolyte conditions as encountered in deliquescent aerosols will be outlined. In the second part it will be demonstrated how results of laboratory studies are directly used in mechanism development. The current chemical aqueous phase radical mechanism (CAPRAM 2.4) will be outlined and some implications of cloud and aerosol chemical conversions on the tropospheric system as a whole as identified by box model studies. Current restrictions and lines of further research, especially the design of chemistry modules, will be discussed. This may serve as a basis of connecting GLOREAM and CMD activities.

Modelling aqueous phase chemistry. Numerical integration and sensitivity analysis

R. Djouad, B. Sportisse, N. Audiffren, I. Charpentier

The presence of clouds can substantially modify the chemical kinetics and thus the rates of destruction and production of the chemical species. For the ozone concentration, when considering only gas phase chemistry, this can lead to strong overestimates. In this paper we focus on two major points: A. Integration efficiency:
The mathematical models describing heterogeneous chemistry can present additional stiffness. This is due to the sudden apparition or the disappearance of the liquid phase. The mass transfer occuring at the interface between the two phases and the chemical reactions taking place into the water drops have timescales of different magnitudes and can present a strong slow/fast dynamical behaviour. We propose to solve the new system of ODE's using the non-autonomous order-2 Rosenbrock method. Comparison is made with LSODE solver.
B. Sensitivity analysis:
The atmospheric models including both gas and aqueous phases are often complicated because of the many physical phenomena they describe (molecular diffusion, gas and aqueous chemical reactions, ionization, mass transfer to the liquid-gas interface ... etc). This induces the use of a large number of kinetic and microphysical parameters. In these models, all the parameters have not the same importance and a sensitivity analysis is useful. In this paper we propose to study the sensitivity of the gas/aqueous model with respect to some parameters (aqueous reactions, PH, droplet radius, ...etc) by using the multiphase code developed at CEREVE and its linear tangent code produced by Odyssée (an automatic differentiation software developped by INRIA).

Experiments with subsequent nesting usind the EURAD-CTM

A. Ebel, H. J. Jakobs, M. Memmesheimer, C. Kessler, H. Feldmann

The EURAD model system enables the application of the technique of subsequent nesting of the chemical as well as the meteorological part of the system. Experiments, i. e. sensitivity studies, have been carried out for various episodes aiming at the assessment of the effects of the nesting procedure on the estimation of the concentration of atmospheric pollutants, in particular ozone. Results concerning the role of lateral boundary values, changes of land use characteristics and increased resolution of emission sources will be discussed. The dependence of simulated transformation and transport processes on the (horizontal) resolution of the nested models will be demonstrated.

Efficient Treatment of Vertical Mixing and Chemistry in APM

P.J.F. Berkvens, M.A. Botchev, J.G. Verwer

We address the implicit treatment of vertical transport and (photo)chemistry, as a subproblem (i.e. without advection) in large-scale Eulerian Air Pollution Modelling (APM) as in e.g. the TM3 model. Spatial discretization of the governing PDEs leads to a huge system of coupled stiff ODEs. Standard stiff ODE solvers need far too much CPU time to solve the ODE system. A standard way to overcome this is by using operator splitting: the various physical processes are solved consecutively in substeps within a time step rather than simultaneously. This is easy, cheap, and stable if stable methods are used for the substeps. But in reality the processes act simultaneously and a disadvantage is the occurrence of splitting errors caused by the operator splitting. Another disadvantage is that the initial condition for a stiff chemistry substep (which is often the result of a substep with a different process), may be far from chemical equilibrium, and this hampers the work of the chemistry solver. We start from a method employed in a version of TM3. It uses 6-hour timesteps with two 3-hour vertical transport substeps and three 2-hour substeps of emissions, chemistry, and depositions; the substeps of the processes are arranged symmetrically. The 2-hour chemistry substeps consist of seven smaller substeps each. Our aim is to compare this standard approach with three seemingly better alternatives which reduce or remove the oprator splitting. First, we incorporate emissions and depositions in the chemistry (we will call these three processes together chemistry). Second, we decrease the timestep size from 6 hours to 0.5 hour and replace the seven chemistry substeps with one 0.5 hour step. This gives the first alternative method, called STRANG. The second alternative, called SOURCE-SPLIT, is obtained from STRANG by`feeding' the changes by vertical transport as sources to the chemistry process. The third alternative, called ROS2-AMF, results from removing operator splitting completely and using Approximate Matrix Factorization (AMF) in the time integrator ROS2. Indeed, we use ROS2, which stems from the stiff-ODE field, as the underlying time integrator for all processes in the above methods. We apply these methods to an air column above the tropical rain forest in the Amazon region in March 1997, when strong vertical mixing occurs and large emissions take place, thus creating a difficult scenario. We observe the following:
* standard operator splitting with 6-hour timesteps and 3 and 2-hour substeps give large splitting errors;
* all alternative methods with 0.5-hour time steps perform well;
* in general ROS2-AMF performs clearly better than SOURCE-SPLIT, which is slightly better than STRANG;
* all alternative methods have the same cost, but are more expensive than the standard method;
* in the alternative methods the largest errors occur at sunrise, sunset, and at meteorology updates;
* clipping of negative concentration values occurs occasionally in all methods, but causes little harm.
We conclude:
* the large errors in the standard method seem unacceptable for air pollution modelling;
* the main error source in the standard method is the large timestep size;
* the errors in the alternative methods are acceptable;
* the larger errors with SOURCE-SPLIT and STRANG as compared to ROS2-AMF are caused by operator splitting;
* a fixed time-step size can be used (advantageous for load balancing);
* ROS2-AMF is a viable candidate for the chemistry and vertical transport processes in APM.

A numerical advection scheme on non-homogeneous grid

D. Syrakov

Numerical integration of the advection equation is still a challenge for modellers. A great number of advection scheme are proposed and used in the numerous numerical models. As to describe adequately the transport of pollution specie the numerical advection scheme must possess properties as conservativity, positive definiteness, transporting ability, low (or no) numerical viscosity and fast performance. One of the most popular schemes is the one of Bott. It calculates the one step change of tracer concentration in a fixed grid cell as a difference of advective fluxes through the cell edges. The fluxes are computed utilizing the integrated flux concept - the concentration in some neighboring grid points are fitted by suitable polynomial used as integral core. The fluxes are normalized and then limited by upper and lower values. The produced scheme is conservative and positively definite with small numerical diffusion. These properties make the Bott scheme very attractive for further improvements and optimizations. Some modifications of Bott scheme are elaborated in the frame of GLOREAM subproject (Syrakov and Galperin, 1997,1999) and the best one is the so called TRAP scheme. In this scheme, instead of integrating, the flux area is supposed trapezoidal. The flux is determined as a product of the Courant number and a single value of the approximating polynomial referring the middle of the passed distance. New type of fitting polynomial - Bessel one - is proposed decreasing the number of influencing points. Big number of tests show that displaying the same properties as Bott's scheme, the TRAP-scheme turns out to be rather faster. Here, a non-homogeneous grid version of the TRAP scheme is described and tested. Ist performance is compared with the homogeneous one. In addition, the case of variable_with_space wind is considered and divergence corrections are introduced in the scheme. The TRAP performance over log-linear grid for instantaneous sources with gaussian, triangle and point profiless is demonstrated below.

MOZART/ECHAM: Present and future global atmospheric chemistry modeling at the Max-Planck-Institute for Meteorology in Hamburg

M. G. Schultz, G. P. Brasseur, J. Feichter and B. Steil

The talk will give an overview about the global atmospheric CTM Mozart and present results from a 1-year simulation driven by ECMWF reanalysis fields for 1990. The discussion will focus on the evaluation of the model results and the predicitve capabilites of Mozart for simulating ozone in Germany. Finally, plans for future Mozart developments including a coupling to the general circulation model ECHAM will be presented.

Unexpected vertical profiles obtained by the UAM-V air quality model over complex terrain

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1 INTRODUCTION

After having used the Urban Airshed Model (UAM) for air quality modelling at PSI for the last few years, we procured the updated version UAM-V with variable grid capability (SAI, 1999). The meteorological data required by UAM-V are prepared by the pre-processor SAIMM (Systems Applications International Mesoscale Model). The model package is widely used in the U.S. in the frame of air quality programs. The model domain, however, was usually applied to flat domains (see e.g. Jang et al., 1998). UAM-V creates two output data sets for each pollutant: the mixing ratio [ppb] in the lowest layer averaged over 1 hour, and the instantaneous concentration [μmol / m^3] in all layers at the end of each hour. We tested the SAIMM / UAM-V package for the complex Swiss topography. The size of the model domain was 470 km x 385 km with 5 km grid cell size and 8 atmospheric layers up to 3000 m a.g.l.

2 UNEXPECTED VERTICAL CO PROFILES

Using the long-lived CO as a tracer, we found that the instantaneous mixing ratio increased inexplicably with height. For instance, a test run was initialised at noon with 160 ppb CO in the layers 1 and 2 and 140 ppb in the layers 3 to 8. After 2 hours of simulation the mixing ratio increased up to 200 ppb in the upper layers. In addition, the Swiss topography was mirrored in the horizontal CO distribution (Figure 1). The concentration field (in μmol / m^3), however, did not show this effect. After numerous calculations it became evident that UAM-V does not take into account expansion and compression of trace gases when they are transported from one pressure level to another. In applications linked with air quality regulations it is usually sufficient to consider the lowest layer only. On the one hand the mixing ratios in this layer are strongly influenced by the emissions. On the other, most model domains investigated so far do not exhibit large altitude variations. Under these conditions the shortcomings mentioned above are invisible.

We converted the trace gas concentrations of each grid cell to a common pressure and temperature before the mixing processes due to vertical and horizontal turbulent exchange, advection and entrainment occur. After these modifications the pressure and temperature dependence of the mixing ratios completely disappeared.

3 Conclusions

For the first time the original version of UAM-V was applied time to the complex Swiss topography. We found that the mixing ratio of CO increased with height above ground and that the topography is mirrored in the spatial pattern of the upper layers. This is due to the fact that the model neglects pressure and temperature changes when the trace gases are transported between different altitudes. These shortcomings disappeared when expansions or contractions of the air is taken into account. These features have probably not been detected yet because the model domains of the simulations done so far were usually flat.
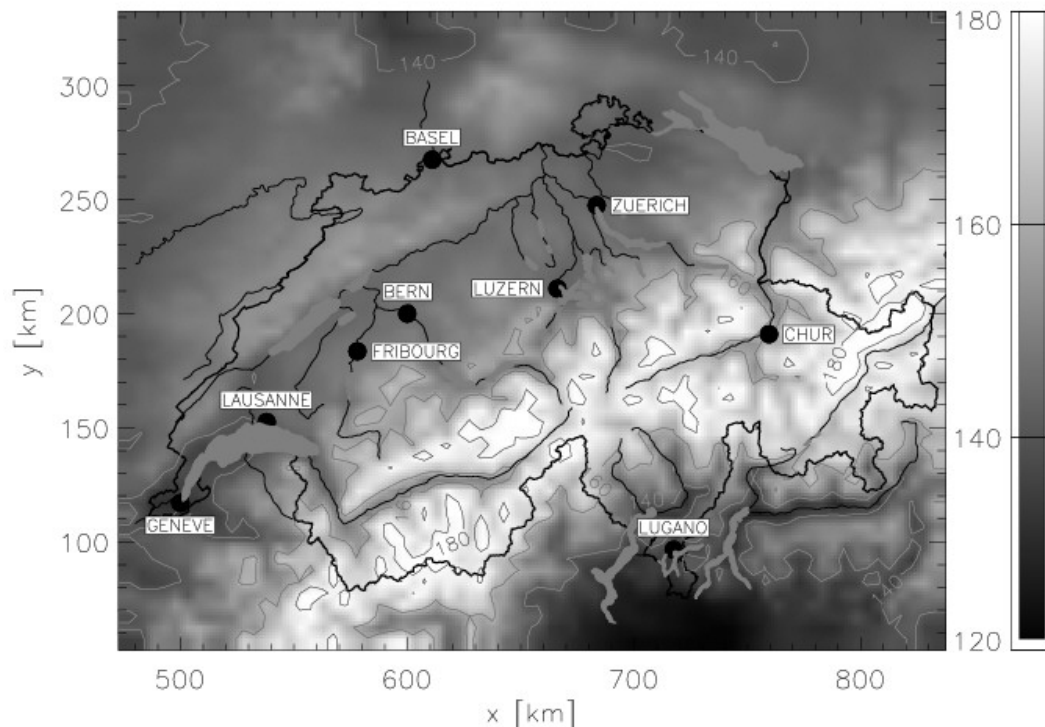
Figure 1: CO mixing ratio [ppb] of layer 7 (2000 to 2500 m a.g.l.) on July 28, 1993, 14:00 CET. The simulation started 12:00 with a constant mixing ratio of 140 ppb.

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A comparison of mixing heights derived from meteo data and inferred from LIDAR measurments

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Introduction

The mixing height (MH) is a fundamental parameter in many air pollution models. Its practical determination is often based on simple parameterizations, which only need a few input meteorological parameters. For validation purpose, it is useful to compare the results of these parameterizations with more sophisticated methods and with measurements

In this study, we compare the mixing height evolution at Bilthoven (The Netherlands) for August 1997 estimated in 3 different ways: (1) from the parameterization used in the photo-chemical smog model EUROS, developed at RIVM.(van Loon, 1996), (2) as derived by the VITO from the ECMWF vertical profiles using a Richardson number method, (3) from the LIDAR measurements at RIVM (Bilthoven).

Methods used for the determination of the mixing height

Euros formulation

In EUROS, the MH (H) is calculated from the friction velocity (u*), the Monin-Obukhov length (L) and the surface sensible heat flux (h_s), using simple parameterizations found in the literature (Nieuwstadt, 1981; Holtslag and Westrhenen,1989; Tennekes, 1973). Three cases are considered.

Stable conditions :
$$\frac{H}{L} = \frac{c_1 \, u_* \, /fL}{1 + c_2 \, H/L} \qquad (1)$$

Neutral :conditions :
$$H = c_1 \, u^* \, / f \qquad (2)$$

Unstable conditions :
$$\frac{\partial H}{\partial t} = \frac{h_s}{\gamma \, H} \qquad (3)$$

In these expressions γ is the potential temperature gradient above the convective boundary layer and f is the coriolis parameter. The surface meteorological parameters u^*, L, and h_s are calculated using a software library developed at KNMI (Beljaars and Holtslag, 1990). Input parameters are wind velocity (at 10 m for example), surface air temperature (at 2 m), aerodynamic roughness length and cloud cover from synoptical observations. These data are taken from the gridded NCAR synop observations (referred to as ODS, observational data set).

Richardson Number method applied on ECMWF vertical profiles

This method allows estimating the mixing height from the vertical profiles of temperature, moisture and wind. It has been used by numerous authors (e.g., Troen and Mahrt, 1986; Vogelezang and Holtslag, 1996; Sorensen et al.,1996). The top of mixing height is given by the top of the layer defined by:

$$Ri_B = \frac{g \, z \left(\theta_v - \theta_{vs}\right)}{\theta_{vs} \left(U^2 + V^2\right)} \leq Ri_{critical} \qquad (4)$$

with g the gravity constant, z the height above the surface, U and V the horizontal wind components, θ_v the virtual potential temperatures at the height z, and θ_{vs} the surface value of θ_v . In convective conditions, several authors recommend to include in θ_{vs} a surface excess temperature which is dependant on the surface sensible heat flux . Since the heat flux was not available in our data set, the excess temperature has not been applied.

As described in Delobbe et al. (2000), this Richardson method fails when the meteo data exhibit a thin and slightly stable layer near the ground under an unstable layer. To remedy this

shortcoming, a modified method has been used, which combines the standard Richardson method with a criterion based on the vertically integrated buoyant energy.

LIDAR measurements

The third estimate of the MH is based on the LIDAR measurements carried out at the RIVM (Bilthoven, The Netherlands). The LIDAR determination of the MH is based on the backscatter of a laser beam by aerosol particles present in boundary layer (van Pul et al., 1994). The top of the MH is marked by a discontinuity in the backscatter profile.

Comparison and discussion

The comparison has been carried out for August 1997. The results are illustrated in Figure 1 for a specific week. Significant discrepancies are found. For most days, the EUROS MH is 100 m during the night and grows in a motonic way up to a value around 1000 m in the late afternoon. The LIDAR and ECMWF estimates exhibit a much larger day to day variability. In the night, ECMWF values are comparable with the EUROS estimate while the LIDAR values significantly differ. It must be noted that the lowest MH that can be detected by the LIDAR is about 200 m. If the actual ML top is lower than 200 m, the LIDAR may consider the top of a residual layer as the ML top leading to unrealistically high MH values.
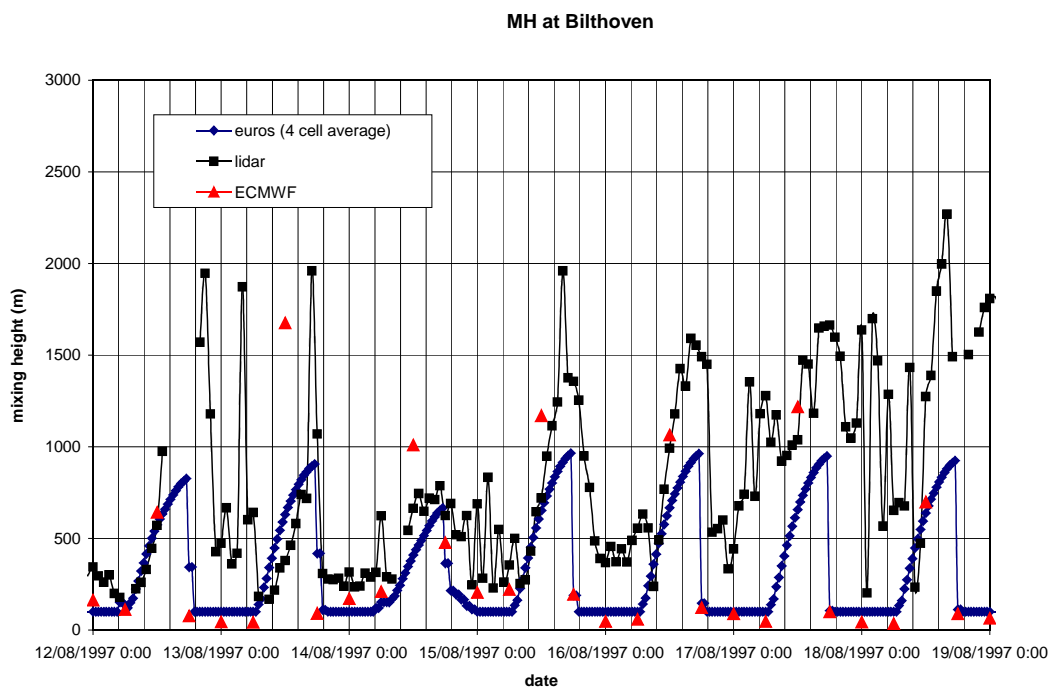

Figure 1: Mixing height eution at Bilthoven (The Netherlands): (1) as calculated by the EUROS model, (2) as derived from the LIDAR measurements at RIVM, (3) as estimated from the ECMWF data using a Bulk Richardson method.

During day time, the EUROS MH is usually small in comparison with the ECMWF and LIDAR values. The ECMWF estimates are only available at 00, 06, 12, and 18 UT but the MH value at 12 UT is systematically higher than the EUROS estimate. The LIDAR provides hourly estimates of the MH. Large variations between two successive hours are regularly found. The LIDAR values averaged over 11, 12 and 13 UT have been compared with the ECMWF estimate at 12 UT for the month August. Figure 2 shows that the LIDAR values are usually higher than the ECMWF values.
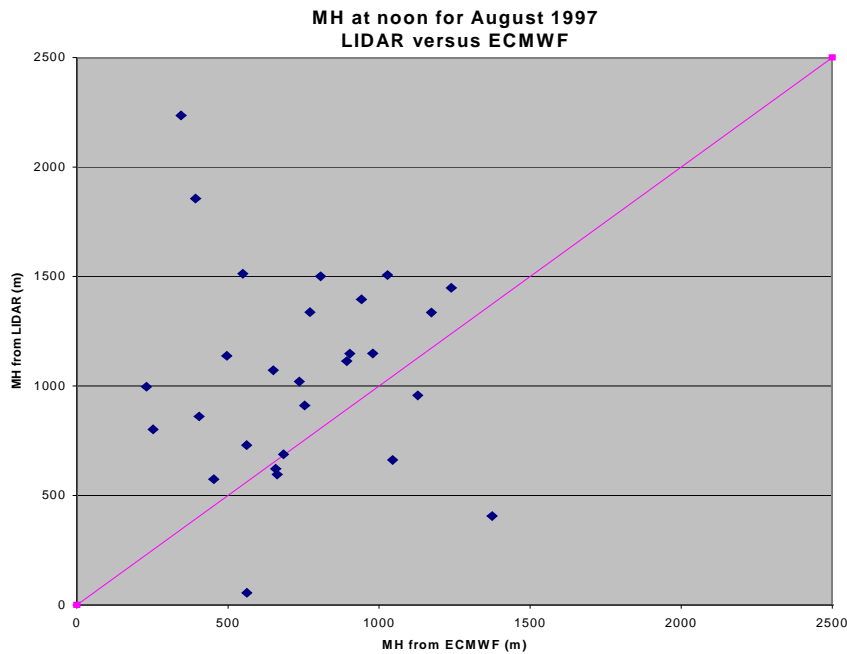
Figure 2: Mixing height at Bilthoven (The Netherlands) around noon in August 1997: LIDAR estimate averaged over 11, 12 and 13 UT versus ECMWF estimate at 12 UT.

Several causes of discrepancies between the three MH estimates can be mentioned. First of all, the method used in EUROS for the calculation of the MH has its own limitations. Errors may arise from the calculation of the surface meteorological parameters (Obukhov length, friction velocity and heat flux) but also from the determination of the MH from these parameters using expressions (1), (2) or (3). The meteo input used for the calculation of the surface meteo variables, for example the 2m-temperature and the 10-m wind, also induce some errors. The meteo input used in EUROS results from a spatial interpolation from synoptic observations and a time interpolation from the 4 input times of these synoptical observations (00, 06, 12, 18 UT). This interpolation partly explains the fact that the MH diurnal cycles simulated by EUROS are much smoother than the observed diurnal cycles from the LIDAR. Another possible cause of discrepancies arises from the fact that the LIDAR observations are local while, for ECMWF and EUROS, the estimate is an average over a grid cell, whose size is about 60 x 60 km^2 (for both models). The LIDAR measurements are much more sensitive to local conditions such as updraft or downdraft in convective conditions.

Concerning the estimates from ECMWF using a Richardson number method, a first source of error results from the relatively coarse vertical resolution of the ECMWF data: around 400m in the boundary layer. The Richardson method exhibits also some shortcomings (e.g., Seibert et al., 2000). In this study, the surface excess temperature has not been applied which may induce significant underestimation of the MH in convective situations. A previous study has shown the high sensitivity of the MH estimate to the surface temperature used in (4) (Delobbe et al., 2000).

The determination of the MH from LIDAR measurements has also its limitations. We have already mentioned the minimal detectable value of 200 m, which may results in large errors for the night estimates. Another shortcoming is the large inaccuracies in case of rain or if the amount of aerosol or trace gas in the boundary layer is too low.

Conclusions

This study brings a contribution to the validation of MH parameterizations used in air quality models. It has been found that the EUROS formulation tends to underestimate the MH values

and the day to day variability. Besides, the estimate based on a Richardson number method applied on ECMWF vertical profiles is generally lower than the LIDAR estimate. Our study underlines the need to test new formulations proposed in the literature. The present study has also shown that the comparison between various MH data sets is not straightforward which makes the validation procedure quite difficult.

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Meteorological surface and sounding data: How do their spatial resolutions alter the wind velocity, vertical diffusivity and ozone fields modelled with SAIMM / UAM-V?

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1 Introduction

The Urban Airshed Model with variable grid, UAM-V (Morris and Myers, 1990), is used at PSI for air quality modelling in Switzerland. For the preparation of the gridded meteorological data (pressure, temperature, wind, vertical turbulent exchange coefficient (diffusivity)) a pre-processing package including the Systems Applications Inc. Mesoscale Model (SAIMM) is available. This package requires surface data and vertical soundings as

well as an initial sounding for the whole domain. A nudging procedure forces the simulated meteorological quantities towards the input fields. For most applications these input data are available only for specific locations and time intervals. The spatial distribution of operational sounding stations, for instance, is very coarse and the balloons are launched only in 6 or 12 hours intervals. For simulations in the current UAM-V model domain of Switzerland (370 km x 285 km, 5km x 5km grid cell size, 8 vertical layers up to 3000 m a.g.l.), hourly data of the meteorological network ANETZ operated by the Swiss Meteorological Institute are used as surface inputs. The vertical soundings are taken from the hourly output of the Swiss prognostic Model (SM) used for the operational weather forecast (about 14 km x 14 km grid cell size). These data are pre-processed by SAIMM in an enlarged model domain (470 km x 385 km, 19 layers up to 9000 m a.s.l., see topography in Figure 1). The objective of this study is to answer the following questions:

- How are the SAIMM wind and vertical diffusivitiy fields distorted in the complex topography of Switzerland if only a few surface and/or sounding input data are available?

- How is the short term summer air quality in Switzerland affected by these distorted fields?
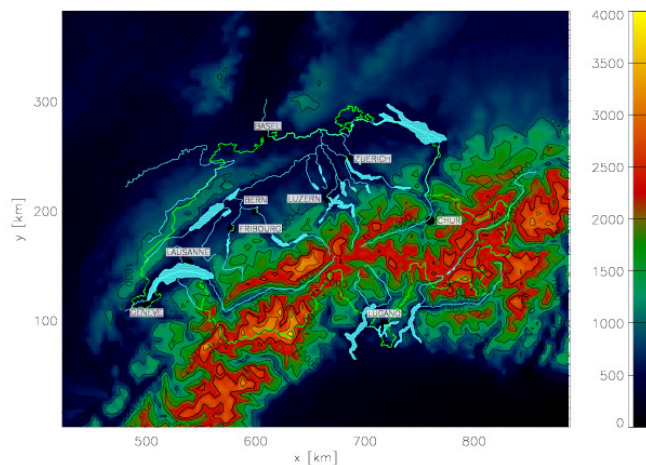

Figure 1: Topography of the SAIMM domain of Switzerland (m a.s.l)

2 Sensitivity study

In the model domain there are 68 ANETZ stations and 29 x 20 SM grid cells (Figure 2). The test period was July 28 – 30, 1993, the intensive operation phase of the Swiss field experiment POLLUMET. In the maximum case, all input data were used. In the next step, the spatial resolution of the SM grid was decreased by skipping an increasing number of grid cells. In the minimum case, only 1 surface station (Payerne, located in the western part of the country) and 1 sounding (in the south-west corner of the domain) were taken (Figure 2). These data sets were processed by SAIMM. Subsequently, the 3-dimensional output was used as input data set for UAM-V. The emission inventory was the same as used in previous studies (e.g. Andreani and Keller, 1998). July 29 was selected for the intercomparison of the mixing ratios of key substances such as ozone. A pre-run of the model was performed for 12 hours of the previous day.
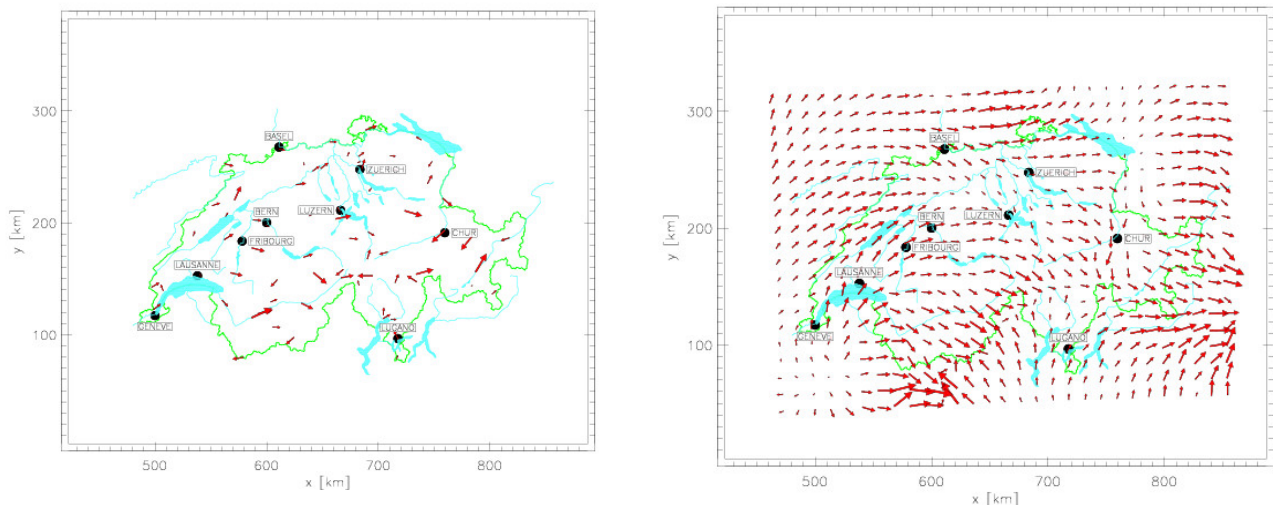
Figure 2: Surface and sounding wind data for July 29, 1993, 16:00 CET used as input for SAIMM. Left part: 68 surface stations (ANETZ), right part: 29x20 SM grid cells, layer 1 (layer top at about 30 m a.g.l.).

3 Results

In Figure 3 the wind fields in layer 1 (0 to 50 m a.g.l.) at 16:00 CET are shown. The full input data set (68 surface stations, 29x20 soundings) is compared with the set based on 1 surface and 1 sounding only. Figure 4 shows the distribution of the vertical diffusivities k_v. The ozone mixing ratios in layer 1 is depicted in Figure 5.

If all surface and sounding data are included in the input data set for SAIMM (maximum case), the *wind pattern* of the model is very similar to the SM wind field because of the strong nudging effect. The distance of the centers of two adjacent SM grid cells is about 14 km, i.e only about 3 times the distance of the UAM -V grid cells. Hence, there is a strong forcing towards the SM dat a and the capability of the model to adapt to the 5 km terrain decreases. The topography used by the SM, however, is much coarser than the data used in SAIMM. On the other hand, it is obvious from Figure 3 that the wind field is substantially distorted and the average wind speed increases if only 1 surface and 1 sounding data are used. This is particularly the case for the eastern region of the model domain which are far from the surface station and the sounding grid cell. The inclusion of all 68 surface st ations and of 1 sounding (not shown) decreases the wind speed due to the lower surface velocities, but the pattern is similar. We found an optimum number of 8 x 5 SM soundings corresponding to a distance of about 70 km between two adjacent grid cells. The difference to the maximum case is not significant; this is valid for all layers.

The *vertical diffusivity* k_v in the complex domain of Switzerland is highly variable. At the top of layer 1 (50 m a.g.l.), the maximum amounts to about 20 m^2/s at nighttime (n ot shown). In the afternoon, we found values up to 150 m^2/s over water and >350 m^2/s over land (Figure 4). At that time the diffusivity is usually higher over mountain ridges than over flat terrain and water surfaces. There is a significant vertical profil e at daytime. At topographic elevations below 1000 m a.s.l. the diffusivity increases with height up to about 500 m a.g.l., the maximum often exceeding 600 m^2/s. If the model runs with minimum nudging (1 surface station, 1 sounding) the distribution is dis torted and the absolute values decrease in the lower layers. The vertical profiles change as well, leading to modified mixing conditions in the lower troposphere. There is no clear trend of k_v with the number of stations or sounding grid cells. The diffusi vity may decrease or increase in the upper layers depending on location and time leading to smaller or larger mixing heights, respectively. Including all surface stations

affect the surface distribution of the diffusivity, but has a minor effect compared t o the minimum case.

The combination of a distorted windfields and a modified mixing layers influence significantly the transport of pollutants. As an example, Figure 5 shows the distortion of the city plumes of *ozone*. The mixing ratio at a specified site may decrease or increase by up to 20 ppb if this site is located outside or inside the plume, respectively. This variation may be crucial if model results are compared to measurements. Another influence is the cleaning effect of stronger winds. Higher mixi ng ratios in layer 5 (not shown) can be partly attributed to an increased mixing height.
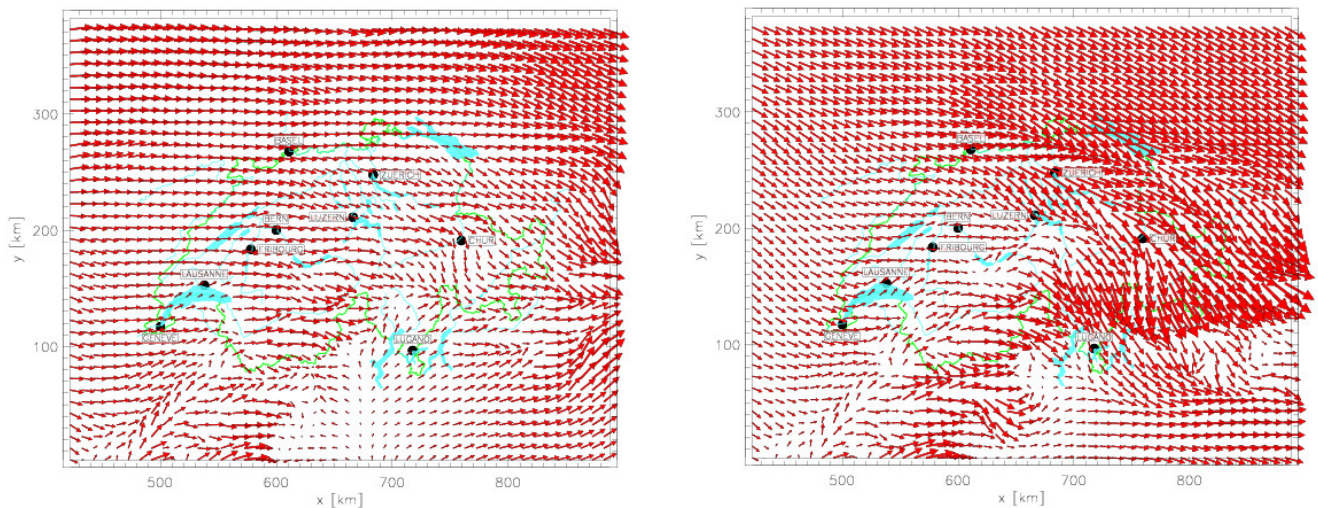
Figure 3: Wind fields in layer 1 (0–50 m a.g.l.) for July 29, 1993, 16:00 CET.
Left: 68 surface stations, 29 x 20 soundings   Right: 1 surface station, 1 sounding.
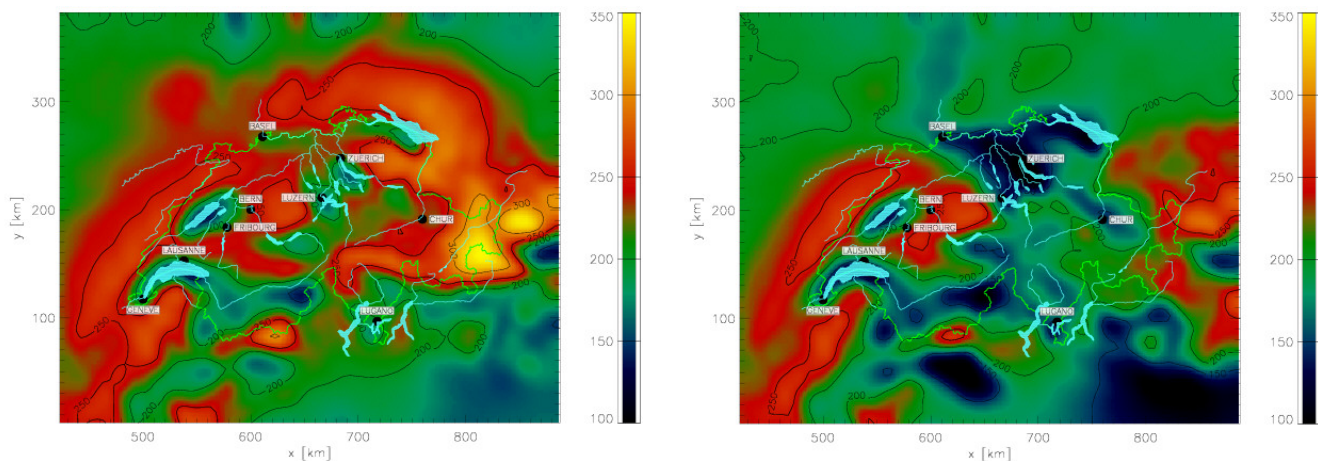

Figure 4: Vertical diffusivity k_v [m^2/s] at the top of level 1 (50 m a.g.l.) for July 29, 1993, 16:00.

Left: 68 surface stations, 29x20 soundings.   Right: 1 surface station, 1 sounding.

4 Conclusions

We conclude that much attention has to be paid to control the mesoscale model with as many external data as possible. This is particularly true for a complex terrain. If only a few sparse soundings are available, the wind field and the v ertical diffusivity may be significantly

distorted leading to modified distribution of trace gases such as ozone. For Switzerland 8x5 SM grids will be used for further simulations.
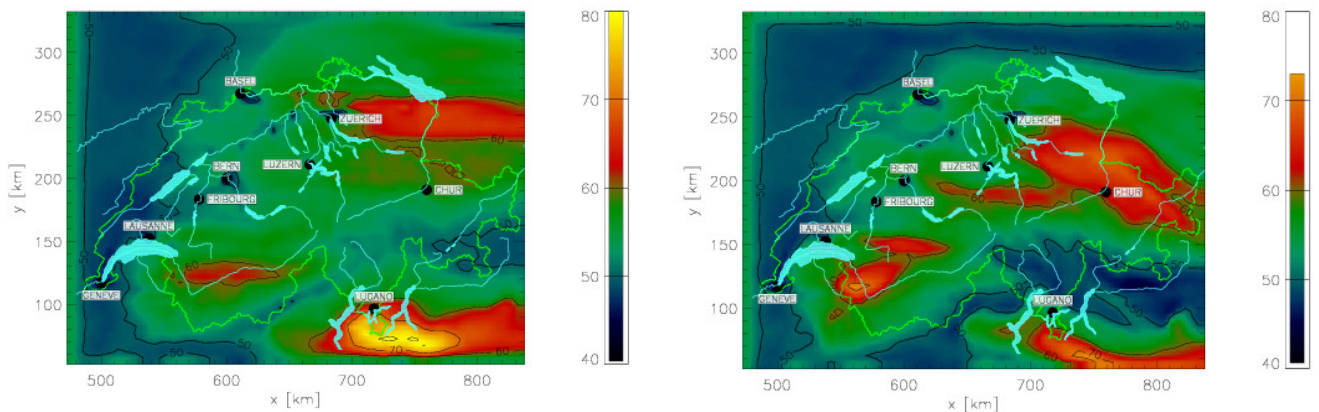

Figure 5: Ozone mixing ratio [ppb] in layer 1 (0-50 m a.g.l.) for July 29, 1993, 16:00 CET. Left: 68 surface stations, 29x20 soundings   Right: 1 surface station, 1 sounding.

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Acknowledgements

Chemical State Analysis by two Different Data Assimilation Algorithms

H. Elbern and J. Hölzemann

An analysis of synoptic chemical states of the atmosphere cannot be based only on usually sparse observations. A means to provide additional information to an analysis system requests secondary knowledge, which is available prior to actual measurements. These include amassed statistical data or forecasts by models. Advanced data assimilation algorithms also include process knowledge as far as they are available in existing model formulations. This measure allows for inclusion of observations scattered in time. The present study compares two data assimilation algorithms, one of which representing a variant of a spatial analysis method (Physical-space Statistical Analysis System, PSAS). The other, considerably more complex algorithm is the four-dimensional variational data assimilation system (4D-var), which, for the first time, has been developed for an Eulerian model at EURAD. Comparison of the analysis skill will be made in terms of observations withheld from the respective

assimilation algorithm. Further, an advanced data assimilation algorithm like 4D-var is able to evaluate systematic model biases. Results of this issue will be presented as well.

Validation of the LOTOS model for August 1997

P. Builtjes and E. Canepa

Ozone observations have been collected for the test-period of august 1997, the period which is intended as the general test-period of GLOREAM. Modelled ozone concentrations are compared with observations using statistical indices, qualitiy indicators which have proven their adequacy in previous studies. The results obtained will be discussed with emphasis on the spatial representativeness of the measuring stations and in relation to the results of data-assimilation studies performed with LOTOS also for (a part of) August 1997. Preliminairy results will be shown of calculated sulfate, nitrate and ammonium concentrations using an extension of the LOTOS-model. Some conclusions will be drawn baded on a comparison between calculated and measured concentrations.

Improving model results by data assimilation

M. van Loon and A. J. Segers

Sometimes large differences between modelled and measured concentrations of air pollutants occur. For several reasons, this is undesirable, for example in the case the model serves as starting point for scenario calculations. To improve the model results, data assimilation can help: by combining the model with available measurements, this technique is able to improve the modelled concentrations not only at measurement locations, but at other locations as well. In this work a special implementation of the Kalman Filter is used. It will be shown by application to the atmospheric transport chemistry model LOTOS that based on a proper specification of the uncertainties in the model and its input, this technique is able to decrease the residues (modelled minus measured concentrations) significantly.