GLO-10

AFO 2000

Chemical and Dynamical Characterisation of Air Pollution Episodes using a 3-D Eulerian Modeling System

A contribution to subproject GLOREAM

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INTRODUCTION

Chemistry Transport Models (CTMs) are used to calculate the formation, transport and deposition of atmospheric trace constituents. Models can be used to analyse the interaction of the different atmospheric processes to get a better understanding of the development of concentration fields and to characterize specific chemical regimes.

A complex CTM, the EURopean Air pollution Dispersion model (EURAD) has been used to simulate the formation of photooxidants during the first intensive measurement phase (July 20/21, 1998) of the Berlin Ozone Experiment (BERLIOZ).

The nesting technique has been applied to include the interactions between the European scale down to the urban scale in the Berlin/Brandenburg area.

Specific aims are the characterisation of air pollution episodes by chemical indicatos, sensitivity studies and the evaluation of chemical schemes (see also GUEST-9).

Specific emphasis is on processes (advection, chemical net production/loss, turbulent exchange, clouds, deposition) contributing to the mass budget of ozone and other photo-oxidants.

MODEL DESIGN FOR BERLIOZ

The following design of the EURAD modeling system has been used for the application of the model

Mother domain: Europe, grid size 54 km

Nest1: Central Europe, grid size 18 km

Nest2: Eastern Germany/Poland, grid size 6 km

Nest 3: Berlin/Brandenburg, grid size 2 km

Vertical resolution: 23 layers, 16 layers below 3000 m

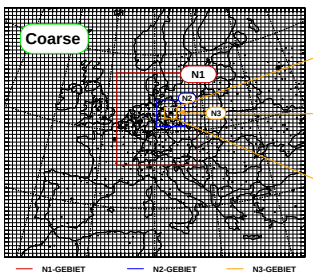
Thickness of lowest layer: about 40 m

upper boundary: 100 hPa (about 16 km)

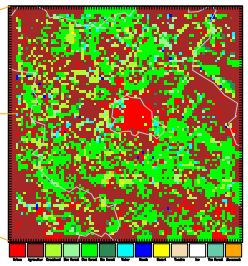
Meteorological model: MM5 (PennState/NCAR)

Chemical Mechanism: RADM2, RACM

Deposition: resistance model (Wesley 1995)



Modellgebiete für die Simulation



landuse for the region Berlin/Brandenburg

TEST CASE: BERLIOZ

BERLIn OZone experiment

Field campaign during July/August 1998 as part of the Tropospheric Research Programme TFS (BMBF)

First intensive measurement phase July20/21, 1998

Modeling continued within the AFO2000 (BMBF)

AIM

analysis of the processes which contribute to the formation of ozone and other photooxidants in the urban plume of Berlin

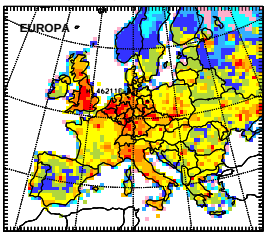
Modeling

Evaluation of CTMs

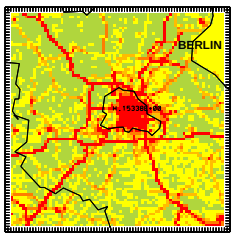
Improvement of chemical mechanisms (see GUEST-9)

better understanding of processes controlling the concentrations of ozone and other photooxidants in the urban plume of Berlin

NO-EMISSION 06 UTC, 20 July, 1998
MAX: 4.6 kg/(h km**2) EUROPA

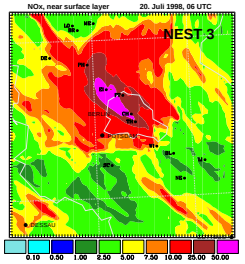


NO-EMISSION 06 UTC, 20 July, 1998
MAX: 153.4 kg/(h km**2) BERLIN



1 5 10 25 50 100 250 500 1000
g/(h km**2)

PRECURSORS: NOx and Alkenes



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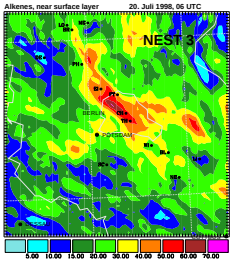

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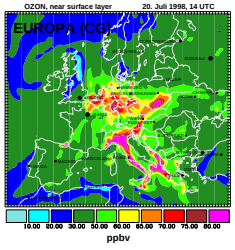
OZONE, BERLIN, JULY 20

Europe ---> Berlin (Nesting Application)

Shown are examples for the model results illustrating the interaction of different scales from Europe (mother domain) to the innermost nest (Belin/Brandenburg, Nest 3).

Europe (mother domain)/Nest1 allows for the analysis of larger scale structures, e.g. regions of enhanced ozone over western and central Europe and the mediterranean region (Po-valley). The Nest 1 region represents more clearly the areas with enhanced ozone south-eastward from Berlin, but gives also a first impression of the Berlin ozone plume.

Nest 2/ Nest 3 allows for a better view of the Berlin ozone plume. Evidently, parts of the Berlin ozone plume already has left innermost domain at the northern boundary.



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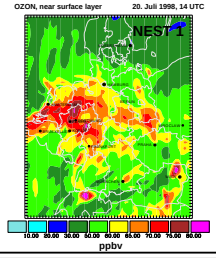

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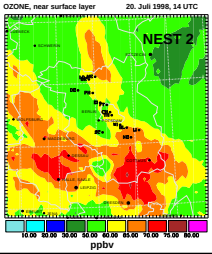

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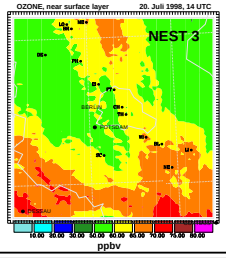

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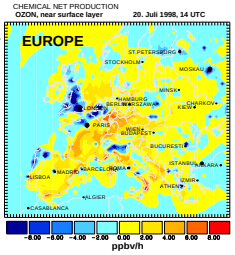
PROCESSES, BERLIN, JULY 20

The temporal change of a trace constituent is controlled by the different processes contributing to the mass continuity equation (advection, turbulent exchange, deposition, clouds, chemical net production/loss).

Shown here is the chemical net production/loss of ozone for the Nest 3 domain and the mother domain covering the whole of Europe. Shown are the lowest layer and a more elevated layer for an altitude of about 350 m. Chemical net production in the lowest layer is strongly controled by the emission of fresh NO into the system. In elevated layers and outside the source regions for ozone precursors the photochemical production of ozone can be more than 8 ppb/h.



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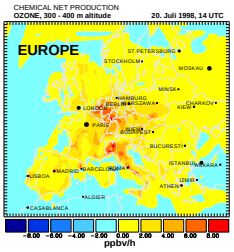

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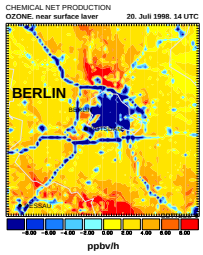

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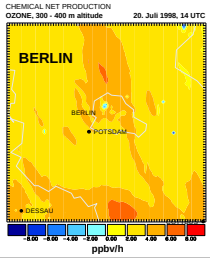

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OH-RADICAL, BERLIN, JULY 20

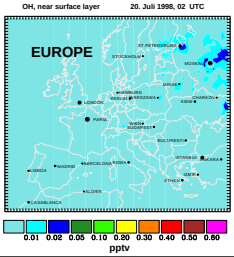
OH radicals plays the central role in the oxidation processes in the atmosphere. The main source of OH is given by

$$O3 + h\nu \rightarrow O(1D)$$
$$O(1D) + H2O \rightarrow 2OH$$

the main sink is given by

$$NO2 + OH \rightarrow HNO3$$

Displayed are the OH concentrations for Europe (mother domain; CG) and the highly resolved Berlin area (N3). A frontal system extending from the UK to the northwestern part of the Iberian Peninsula can clearly be identified by the patterns in the OH field during daytime. The daytime features for the Berlin area in the near-surface layer are very patchy due to strong inhomogenities (emissions, landuse) in the area. These patchy structures vanishes for more elevated layers.



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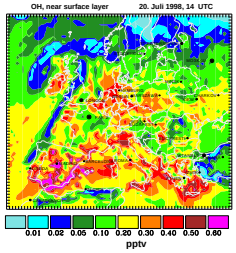

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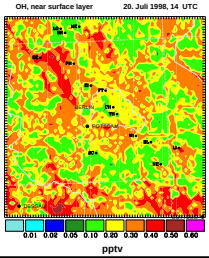

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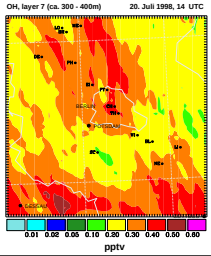

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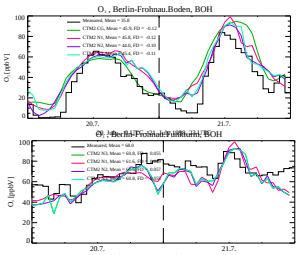
COMPARISON WITH MEASUREMENTS

The model results are compared with ozone concentrations at the Frohnauer Turm (altitude 328 m) and the corresponding near surface station Frohnau-Boden.

Displayed are results for all domains. The results for all domains look quite similar. There is a weak trend for Frohnau Boden that NO and NO2 show a better agreement with observations for the highly resolved Nest 2 and Nest 3. In particular NO is not in a good agreement for Frohnau-Boden for July 20. Ozone maxima are in quite good agreement for all domains, in particular for July 20.

Future work will include the specific measurements obtained during BERLIOZ.



SUMMARY and CONCLUSIONS

The first intensive measurement phase of BERLIOZ has been successfully simulated with the EURAD modeling system. The results have been used to characterise the episode on the basis of dynamical and chemical processes. The European scale has been considered together with the urban scale in the Berlin/Brandenburg area illustrating the effect of larger scale features on the ozone concentration in the Berlin plume. Ozone concentrations have been found to be in good agreement with the measured values. NO and NO2 show larger differences compared to the observed values. However there is a trend to better results with improved horizontal and vertical resolution.

Future work will aim on sensitivity studies with respect to emissions and evaluation of the chemical mechanism supported by measured data from SAPHIR (Simulation of Atmospheric PHotochemistry In a large Reaction Chamber; see GUEST-9 and GUEST-24) of the ICG-II, Research Center Juelich. The methods developed will be applied to other episodes under different meteorological and chemical situations. The episodes selected will be based on a cluster analysis of numerical forecasts of the DWD (see GLO-8). This work is part of the AFO2000 project IDEC.

Long-term runs with respect to scientific questions and to the recently established EU directives are currently performed (see AER-7 and TOR-8). The EURAD system is also used for daily air pollution forecasts (see GLO-6).

ACKNOWLEDGEMENTS

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