AFO 2000

A contribution to the AFO2000 Project IDEC

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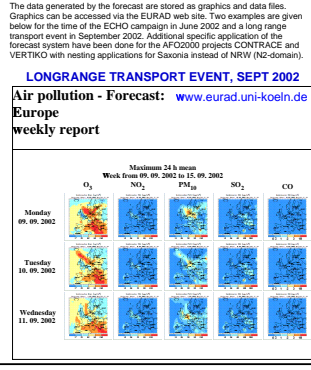Bundesministerium für Bildung und Forschung

RIU EURAD

SENEVA

OBJECTIVES

MAIN OBJECTIVE

Improvement and evaluation of the complex air quality modeling system EURAD as a tool for air pollution prediction, an instrument for scientific research on the interaction of chemical and dynamical processes and the planning of air pollution abatement strategies.

SPECIFIC AIMS

Investigation of the impact of changing emissions on the concentrations of airpollutants for selected reference cases. The choice of reference cases will be based on statistical methods developed by the German Weather Service (DWD).

Improvement and evaluation of the chemical mechanism in close cooperation with the ICG-II of the Research Center Jülich and based on measurements obtained in the atmospheric simulation chamber SAPHIR. Starting point are the chemical mechanisms RADM2 and RACM.

A better understanding of the interaction of dynamical and chemical processes based on 3D applications of EURAD to the selected reference cases. Different meteorological and chemical conditions for different seasons will be investigated to improve the scientific basis of the modelling system.

The first intensive measurement phase of the Berlin Ozone Experiment during July 20/21, 1998 will be used as first test case, Northrhine Westphalia is another area of special interest.

MODEL DESIGN AND APPLICATIONS

Two domains have been selected for the 3D applications: BERLIN and Northrhine Westphalia (NRW) and subdomains within NRW. Episodic calculations have been performed for the Berlin area, the numerical simulations for NRW additionally aims on annual model calculations and daily short-term forecasts of air pollution.

The following model designs have been used for the numerical simulations

	BERLIOZ	FORECAST & LONG-TERM
Mother domain (CG):	Europe, grid size 54 km	Europe, grid size 125 km
Nest1 (N1):	Central Europe, 18 km	Central Europe, 25 km
Nest2 (N2):	East Germany, 6 km	NRW, 5 km
Nest3 (N3):	Berlin, 2 km	Duisburg, 1 km

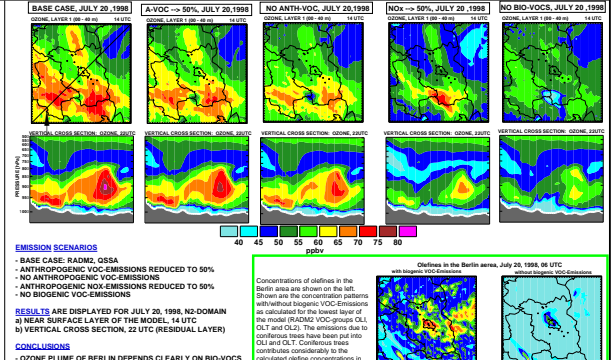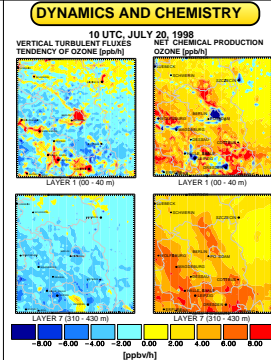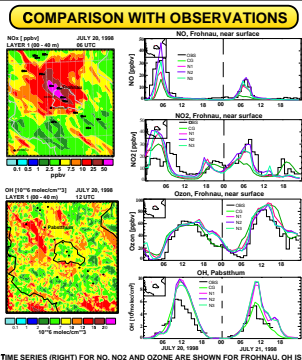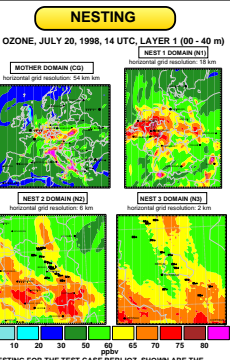| Vertical Resolution:	23 layers, 10 layers below 3000m
Thickness of lowest layer:	about 40 m
Upper boundary:	100 hPa
Meteorological Model:	MM5 (PennState/NCAR)
Chemical Mechanisms:	RADM2, RACM
Aerosols:	MADE with SORGAM
Deposition:	resistance model (dry), wet deposition (clouds)
Emissions:	IER, University Stuttgart, EMEP, LUA-NRW
Landuse:	IFU, Garmisch-Partenkirchen

DAILY SHORT-TERM FORECAST, DATA BANK AND ARCHIVE

The EURAD air pollution system has been started with first tests in spring 2001. The system starts automatically with the download of the AVN global meteorological forecast via ftp at around 3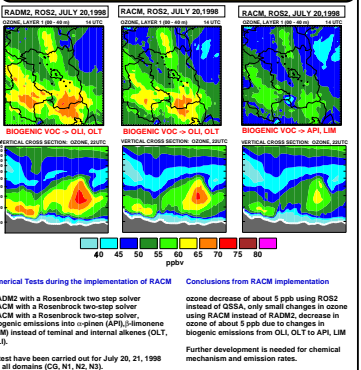:30 UTC every morning. The forecast is finished at around 9:00 UTC and the results are updated and displayed on the EURAD web site. The forecast system calculates fields for meteorological parameters and concentrations of air pollutants including atmospheric particles.

The data generated by the forecast are stored as graphics and data files. Graphics can be accessed via the EURAD web site. Two examples are given below for the time of the ECHO campaign in June 2002 and a long range transport event in September 2002. Additional specific application of the forecast system have been done for the AFO2000 projects CONTRACE and VERTIKO with nesting applications for Saxonia instead of NRW (N2-domain).

DURING THE ECHO-CAMPAIGN, JUNE 2002

Air pollution - Forecast: www.eurad.uni-koeln.de
Central Europe weekly report

LONGRANGE TRANSPORT EVENT, SEPT 2002

Air pollution - Forecast: www.eurad.uni-koeln.de
Europe weekly report

BERLIN PLUME DURING BERLIOZ

NESTING

OZONE, JULY 20, 1998, 14 UTC, LAYER 1 (00 - 40 m)

NESTING FOR THE TEST CASE BERLIOZ. SHOWN ARE THE OZONE CONCENTRATIONS AT NOON (14 UTC) FOR JULY20, 1998. THE OZONE PLUME OF THE CITY CAN BE SEEN NORTHWARD (DOWNWIND) FROM THE CITY, HIGH OZONE IS PRESENT ALSO SOUTHWARD IN THE INDUSTRIALIZED REGION THERE.

COMPARISON WITH OBSERVATIONS

TIME SERIES (RIGHT) FOR NO, NO2 AND OZONE ARE SHOWN FOR PABSTTHUM. SIMULATED VALUES FOR ALL NEST-LEVELS (CG, N1, N2, N3), FROHNAU AND PABSTTHUM ARE INDICATED IN THE NOX- AND OH FIELDS AS CALCULATED BY THE MODEL. OH RADICAL IS OVERESTIMATED AT PABSTTHUM. ON THE LEFT SNAP-SHOTS OF NO2 (06 UTC) AND THE OH (12 UTC) ARE SHOWN.

DYNAMICS AND CHEMISTRY

10 UTC, JULY 20, 1998

TENDENCY OF OZONE AT 10 UTC (12 CEST) DUE TO THE DIVERGENCE OF VERTICAL TURBULENT FLUXES AND NET CHEMICAL PRODUCTION. UPPER PANEL: NEAR SURFACE LAYER, LOWER PANEL: LAYER 7. OZONE PRODUCTION OUTSIDE THE EMISSION REGIONS CAN BE SEEN.

SENSITIVITY TO EMISSIONS

EMISSION SCENARIOS
- BASE CASE: RADM2, QSSA
- ANTHROPOGENIC VOC-EMISSIONS REDUCED TO 50%
- NO ANTHROPOGENIC VOC-EMISSIONS
- ANTHROPOGENIC NOX-EMISSIONS REDUCED TO 50%
- NO BIOGENIC VOC-EMISSIONS

RESULTS ARE DISPLAYED FOR JULY 20, 1998, N2-DOMAIN
a) NEAR SURFACE LAYER OF THE MODEL, 14 UTC
b) VERTICAL CROSS SECTION, 22 UTC (RESIDUAL LAYER)

CONCLUSIONS
- OZONE PLUME OF BERLIN DEPENDS CLEARLY ON BIO-VOCS
- ANTHR. NOX REDUCTION MORE EFFECTIVE THAN VOC-RED.
- OZONE PLUME APPEARS EVEN WITHOUT ANTHR. VOCS
- LAYERS ABOVE THE PBL ARE NOT VERY MUCH EFFECTED
- ALL RESULTS AVAILABLE FOR OTHER DOMAINS AND DAYS

Olefines in the Berlin aerea, July 20, 1998, 06 UTC with biogenic VOC-Emissions / without biogenic VOC-Emissions

Concentrations of olefines in the Berlin area are shown on the left. Shown are the concentration patterns with/without biogenic VOC-Emissions as calculated for the lowest layer of the model (RADM2 VOC-groups OLI, OLT and OL2). The emissions due to coniferous trees have been put into OLI and OLT. Coniferous trees contributes considerably to the calculated olefine concentrations in the Berlin area and evidently increase the ozone concentrations. Aldehydes, which are not shown here, show similar concentration patterns.

EU DIRECTIVES AND LONG-TERM APPLICATIONS

SENSITIVITY RADM2-RACM-QSSA-ROS2

Numerical Tests during the implementation of RACM
- RADM2 with a Rosenbrock two-step solver
- RACM with a Rosenbrock two-step solver
- RACM with a Rosenbrock two-step solver, biogenic emissions into α-pinene (API), β-limonene (LIM) instead of teminal and internal alkenes (OLT, OLI).

All test have been carried out for July 20, 1998 and all domains (CG, N1, N2, N3).

Conclusions from RACM implementation

ozone decrease of about 5 ppb using ROS2 instead of QSSA, only small changes in ozone using RACM instead of RADM2, decrease in ozone of about 5 ppb due to changes in biogenic emissions into OLI, OLT to API, LIM

Further development is needed for chemical mechanism and emission rates.

The recently established directive 96/62 of the European Comission on air quality and its daughter directives prescribes specific limit values on air pollutants e.g. atmospheric particles (PM10), NOx, Ozone, NO2 and CO. The limit values are mainly based on annual statistics of air pollutants and have to be achieved within given time spans. For model applications to assess air quality or emission scenarios therefore the extension from episodes to an annual time-scale is necessary.

In close cooperation with the Environmental Agency of Northrhine-Westphalia (NRW) an application of the EURAD modelling system has been performed with the specific aim to calculate the air quality in NRW. The results of the study have also been used for additional scientific studies within SENEVA and the related EUROTRAC subprojects as GLOREAM, AEROSOL and TOR-2.

Nesting capability of the model is used to perform calculations on the European as well as on the local scale for NRW. The model design is the same as for the daily air pollution forecast. In the case of the annual run for 1997 the RACM gas chemical scheme has been used together with the Modal Aerosol Dynamics Model for Europe (MADE) which accounts also for the formation of secondary aerosols. Formation of secondary organic aerosols also have been considered, including the contribution of biogenic emitted precursors handled in the RACM as α-pinene and β-limonene (API, LIM).

LONG-TERM SENSITIVITY STUDY

Results from the annual runs for PM10 and Ozone (left panel above) and comparison with observations from the local network of the LUA-NRW (right panel above).

The six plots on the right compare the base case calculations for ozone on the European scale for the year 1997 with the results from a calculation where only the emissions have been changed to the values of 1987. This calculation is a contribution to the model intercomparison study of EUROTRAC-2 (GLOREAM, TOR-2). It could be shown that the annual maxima of ozone decrease with decreasing emissions from 1987 to 1997. The average values however show an increase in Central and Western Europe.

The results of the numerical calculations have been compared with measurements from the local available network in NRW. Some results are shown as scatter plots.
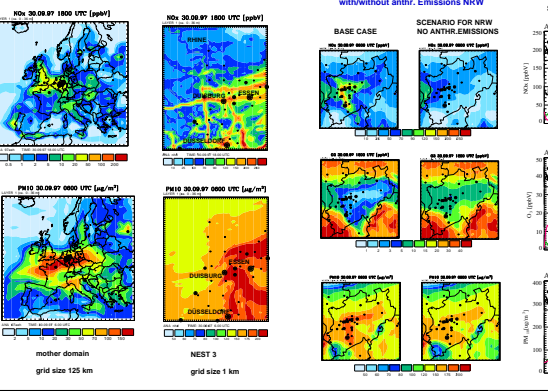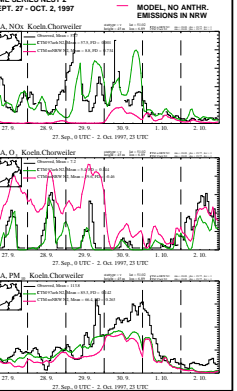
SUMMARY AND CONCLUSIONS

The EURAD modelling system has been considerably improved scientifically and technically since the beginning of the SENEVA project. The most important milestones achieved until now are:

Higher flexibility of the modelling system
Quasi-operational use on LINUX-PC is demonstrated by daily short-time forecasts of air pollutants including atmospheric particles. Data from the daily forecast are stored and can be accessed on the EURAD web site (AFO2000 campaigns CONTRACE, VERTIKO (Saxonia)) Additional basis for the selection of reference cases for different meteorological and chemical conditions.

Emission sensitivity show the strong importance of biogenic emissions, in particular for the ozone plume of Berlin during BERLIOZ, which was used as a reference case.

Implementation and testing of the RACM gas phase chemical scheme. Sensitivity studies with respect to numerical solver, biogenic emissions Ozone concentration calculated are highest for RADM2 with QSSA solver, somewhat lower for RACM with ROS2 solver. Changes in biogenic emissions to account for α-pinene and β-limonene decrease ozone considerably.

Long-term application to the year 1997 (EUROPE → NRW; in cooperation with the LUA-NRW) using RACM (a necessary prerequisite to handle the formation of secondary organic aerosols from α-pinene and β-limonene).

Long-term nesting application show an underestimation of NOx during summer, an underestimation of ozone during March and April 1997, improvement with increasing horizontal resolution for all species (as expected) except for high ozone maxima (not expected) probably due to uncertainties in biogenic and anthropogenic VOC-emissions.

Long-term sensitivity for emission changes from 1987 to 1997 show a decrease in ozone maxima with decreasing emissions, but an increase of annual average ozone values in Central and Western Europe.

Harmonization and high quality emission with high temporal and spatial resolution would be very helpful, in particular for VOCs.

FUTURE PLANS

Further development of the chemical mechanism in cooperation with the ICG-II, Research Center Jülich, SAPHIR measurements, in particular a better treatment of biogenic VOCs using extensions of RACM (close cooperation within AFO2000, e.g. Uni. Wuppertal, Geiger).

Update and improvement of the emission rates used for biogenic VOC (close cooperation within AFO2000).

3D model application to selected days from the ECHO measurement campaign with 1 km grid resolution. Comparisons with data measured during the campaign.

Extension of the modeling system to the hemispheric scale in close cooperation with other AFO2000 projects (e.g. ATMOFAST) to account for transcontinental transport. This is considered to be important for long-term applications in the context of recently established EU directives on air quality.

Further emission sensitivity studies for additional reference cases to beselected. Accessibility of the results via the EURAD web site.

NORTHRHINE WESTPHALIA (NRW)

A specific episode has been selected from the annual run for 1997 to be investigated in more detail. The episode covers the time span from Sept. 27 - Oct. 02, 1997. The meteorological conditions are dominated by high pressure over Central and Western Europe. This leads to high values of primary emitted air pollutants. As an example the concentrations of NOx and PM10 are displayed for Sept. 30, 06 UTC and 18 UTC, respectively.

The horizontal resolution for the selected episodes has been refined to 1 km for domains of specific interest, in that case for the region near the cities Duisburg, Essen and Düsseldorf (Nest 3 domain). The effect of the refinement is also shown for NOx (18 UTC) and PM10 (06 UTC) as an example. The major cities and the river Rhine can be seen in the NOx concentration patterns. The It is planned to simulate selected days for the ECHO campaign with the same horizontal resolution for the Jülich area.

An emission scenario for the selected episode has been calculated for NRW. The aim of the emission scenario is to quantify the contribution of air pollutants transported towards NRW during that episode. Therefore a calculation without anthropogenic emissions in NRW has been performed. As examples the concentration fields for NOx, Ozone and PM10 are displayed for the N2-domain (grid resolution 5 km) as snap-shots for Sept. 30, 06 UTC (NOx, PM10) and 12 UTC (Ozone). Time series are shown for the measurement site Köln-Chorweiler. It could clearly be seen that NRW is acting as a sink for ozone during that episode. NOx and in particular PM10 seems to be strongly influenced by transport.

with/without anthr. Emissions NRW

mother domain / grid size 125 km

NEST 3 / grid size 1 km

TIME SERIES NEST 2 SEPT. 27 - OCT. 2, 1997

ACKNOWLEDGEMENTS