Nesting applications of the EURAD modeling system to Berlin and North-Rhine-Westphalia

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Introduction

Comprehensive regional-scale air quality models (AQMs) are an important tool to understand the physical and chemical processes controlling the concentration of atmospheric pollutants and their deposition to the surface. Numerical simulations with AQMs can be used for scientific research (e.g. planning of field experiments and data interpretation) and the development of air pollution abatement strategies. Analysis and interpretation of observed data from operational networks and field experiments using AQMs support the understanding of the measured data and help to evaluate and improve the parametrization of the processes in the modeling system. An evaluated modeling system can be used to investigate the impact of changing conditions in the environment, e.g. anthropogenic emissions or landuse. The results of the model simulations (concentration fields, deposition) allows to fill the gaps in measurement networks and to estimate the current and future status of air quality.

Two examples for applications of the EURAD modeling system (Hass et al., 1997; Memmesheimer et al., 1997; Jakobs et al., 2001) will be given. One example show results obtained for the first intensive measurement phase of the Berlin Ozone Experiment (BERLIOZ, Corsmeier et al., 2001), the second application has been focussed on the highly populated region of North-Rhine-Westphalia (NRW; Memmesheimer et al., 2000) including the simulation of atmospheric particles using the MADE model (Ackermann et al., 1998, Friese et al., 2000, Schell et al., 2001). Both examples include the application of nesting to couple the regional-scale (Europe) to the local scale (Berlin, North-Rhine-Westphalia).

Model Design

The nesting configuration used for the BERLIOZ simulation covers the European scale with a horizontal grid size of 54 km (N0 domain), the numerical simulations for the local scale of Berlin has been carried out with a grid size of 2 km (N3 domain). Two additional nest levels close the gap between N3 and N0: The N1 domain covers most parts of Central Europe with a horizontal grid resolution of 18 km, the N2 domain covers the eastern part of Germany and parts of Poland with a grid size of 6 km.

The NRW case has been simulated with a nesting ratio of five instead of three (BERLIOZ) - horizontal grid sizes are 125 - 25 - 5 - 1 km. The results presented here are from N0 (125 km) and N1 (25 km) model calculations. Work for the other domains (N2, N3) is currently underway and not finished yet. The model design for the NRW case is also used for daily air pollution forecasts which are available on the EURAD web site (www.eurad.uni-koeln.de).

23 layers are used for the BERLIOZ as well as for the NRW case in the vertical between the surface and 100 hPa (ca. 16 km); about 16 layers are below 700 hPa, the lowest layer has a thickness of about 40 m.

Results

Figure 1 shows the ozone concentration as calculated with the model for the lowest layer, which is about 40 m thick. The results for July 20, 1998, 14 UTC are shown for all of the four model domains used in the numerical simulation. Regions of high ozone concentrations could be found along the mediterranean coastlines, in particular Italy, Greece and the former Yugoslavia. The other regions of increased ozone concentrations are found over Germany and Southern Poland. The numerical simulation show the urban plumes of large cities as Vienna, Berlin, Munique with a gridsize of 18 km (N1 domain). Increased ozone concentrations are found in the Benelux-Rhein-Ruhr area extending towards the Frankfurt region. The increased ozone values southward of Berlin are clearly present in all nest levels. Air masses with increased ozone concentrations moved over the Berlin area in the evening and during the night of July 20 to July 21, 1998.

Net photochemical production of ozone is shown for all nest levels in figure 2, again for the lowest layer. Regions of high emissions of nitrogen oxides show net chemical loss of ozone due to titration of ozone to NO_2. Net chemical production in the order of 4 - 8 ppb/h is found outside the main source regions. The results for N3 show special features as the highways in the Berlin area which act as net chemical loss regions (conversion of O_3 to NO_2.) The net chemical production in more elevated layers is shown in figure 3 for layer 7 of the model which is in an altitude range of 300 - 400 m, approximately the height of the Frohnauer Turm located in the northern part of Berlin. Chemical net production rates are found to be more than 8 ppb/h in Central Germany and Switzerland and 4 - 6 ppb/h in the plume of Berlin. Comparison with measured values of net chemical production derived from airplane observations show good agreement with the values calculated by the model for the BERLIOZ campaign (Corsmeier et al., 2001).

Comparison of model results and observed values at the special BERLIOZ measurement site Pabstthum are shown as time series for July 20 and 21 in figure 4 for NO, NO_2 and ozone. The plume of nitrogen oxides show to high values and seems to be to sharp in the model calculations for the morning hours of July 20. However, the total amount of nitrogen oxides integrated about the morning hours seems to be in the order of the observed values. Ozone concentrations show a quite good agreement with model results at Pabstthum for July 20 but is overestimated in the afternoon of July 21. Figure 5 show comparison with observations as scatter plots for Pabstthum for CO, NO, NO_2, NO_y, O_3 and HNO_3 but for N3 only. The agreement between measured and calculated data again is quite good, except for the night and early morning hours.

As mentioned in the introduction atmospheric particles have been included in a second application focussed on the federal state of North-Rhine-Westphalia. The PM_{10} mass concentration is shown as an example for August 13, 1997 as vertical cross section for the lower part of the N1 model domain which has a horizontal grid size of 25 km in this case. The development of PM_{10} mass concentration during this warm summerday is shown by a sequence of vertical cross sections for 06, 10, 14, 18 and 22 UTC. The increased turbulent mixing during the day can be seen in the concentration fields. Values of more than 70 microgram/m^3 are found in the near-surface regions. Figure 7 shows a comparison of measured and calculated concentration data for the network of North-Rhine-Westphalia. Shown are NO_x, SO_2, O_3 and PM_{10}.

The model results has been evaluated with respect to the model accuracy requirements given in the EU directive 96/62 and its daughter directive 99/30. The hit rate for the N1 calculations is given in table 1 (from Memmesheimer et al., 2001):

Run	*NO2*	*NOx*	*SO2*	*PM10*	*O3*
N0-15	80.00	57.78	26.37	100.00	57.58
N0-23	83.33	70.00	26.37	100.00	78.79
N1-15	92.22	75.56	36.36	97.83	81.82
N1-23	91.11	81.11	34.07	97.83	86.36

Table 1: Hit rate of simulated daily averaged concentrations compared with observations from the LUQS network operating in Nordrhein-Westfalen. Presented is the hit rate for model uncertainty of 50% (EU directive). All values are percentages. Extension -15, -23 indicates the number of vertical layers. N0 is coarse grid (125 km grid size), N1 - Nest 1 domain (25 km grid size).

Conclusions and future plans

The modeling work for the numerical simulation of the BERLIOZ episode will be continued within the framework of AFO 2000 in close cooperation with the Research Centre Jülich and the German Weather Service. BERLIOZ will serve as a test case to develop methods which allows for a characterization of chemical regimes under different meteorological conditions. Emission scenario runs will be performed to characterize VOC and NOx sensitive regimes and appropriate indices to characterize these regimes (e.g. Sillmann -factors as H_2O_2/HNO_3). Data measured in the field will be considered, in particular volatile organic compounds and radicals, and compared with model results. The chemical gas phase reaction mechanism will be improved and evaluated in cooperation with the ICG-II of the Research Centre Jülich. The gas phase chemistry used in the EURAD system will be evaluated by comparison with data measured in the atmospheric simulation chamber SAPHIR of the ICG-II, Research Centre Jülich (see: http://www.kfa-juelich.de/icg/icg-ii/).

Long-term runs will be performed with respect to the year 1997, including atmospheric particles and focused to the region of North-Rhine-Westphalia. The data of these long-term runs will be used together with operational forecasts from the German Weather Service (Tilmes et al., 2001; Jakobs et al., 2001) to built a data archive for different air pollution regimes.

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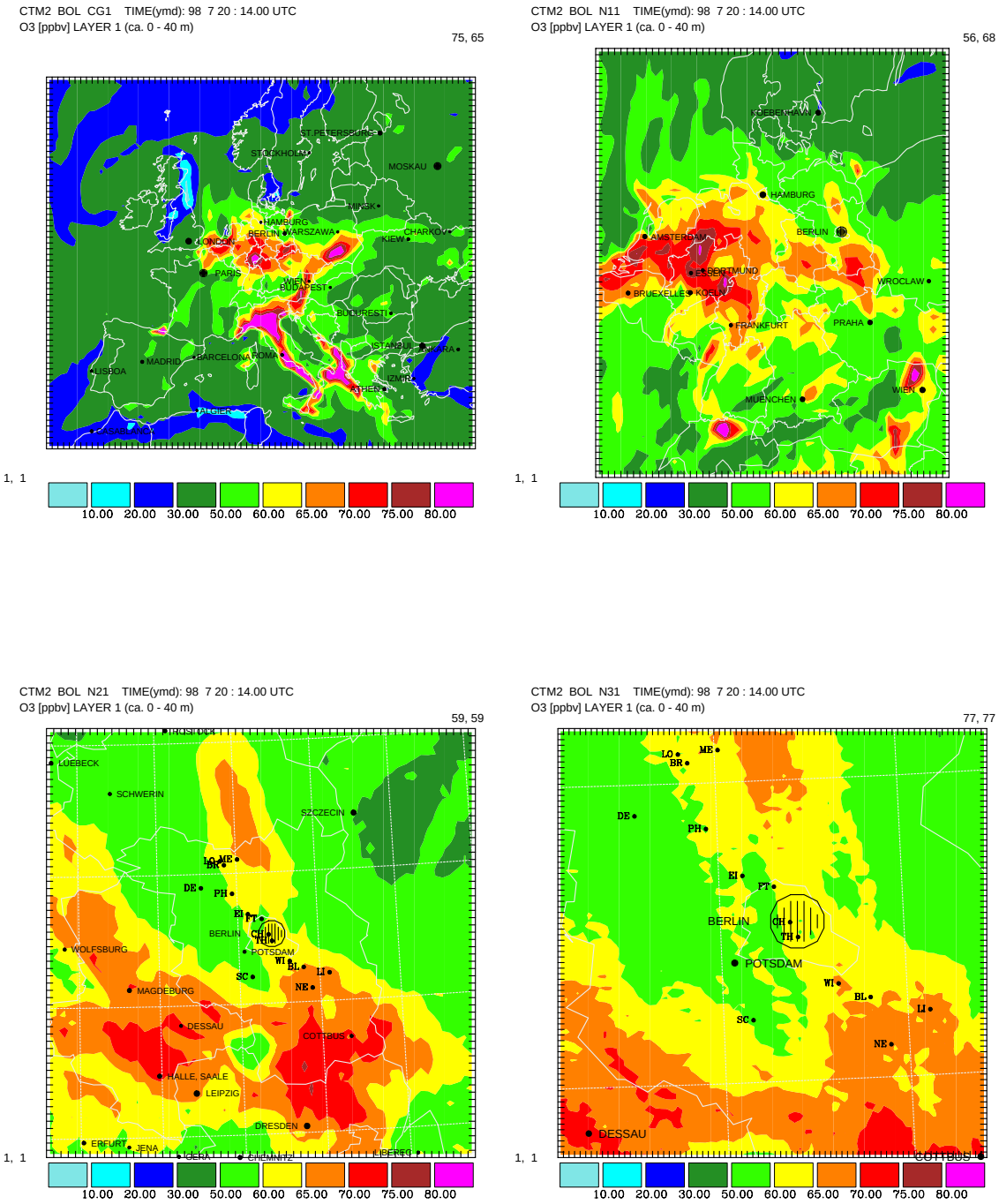

Figure 1: Ozone concentration [ppbv] as calculated with the EURAD modeling system during the first phase of the BERLIOZ experiment (July 20/21, 1998). Shown are the results for the first layer of the model for July 20, 14 UTC, for the different modeling areas N0, N1, N2 and N3 with a horizontal grid resolution of 54, 18, 6 and 2 km, respectively. The first layer is about 40 m thick. Areas with increased ozone pollution over the whole of Europe (upper panel; N0, N1) as well as for the Berlin area can clearly be identified. The special mesearement sites for BERLIOZ are indicated by black dots in the plots of N2 and N3 (lower panel).

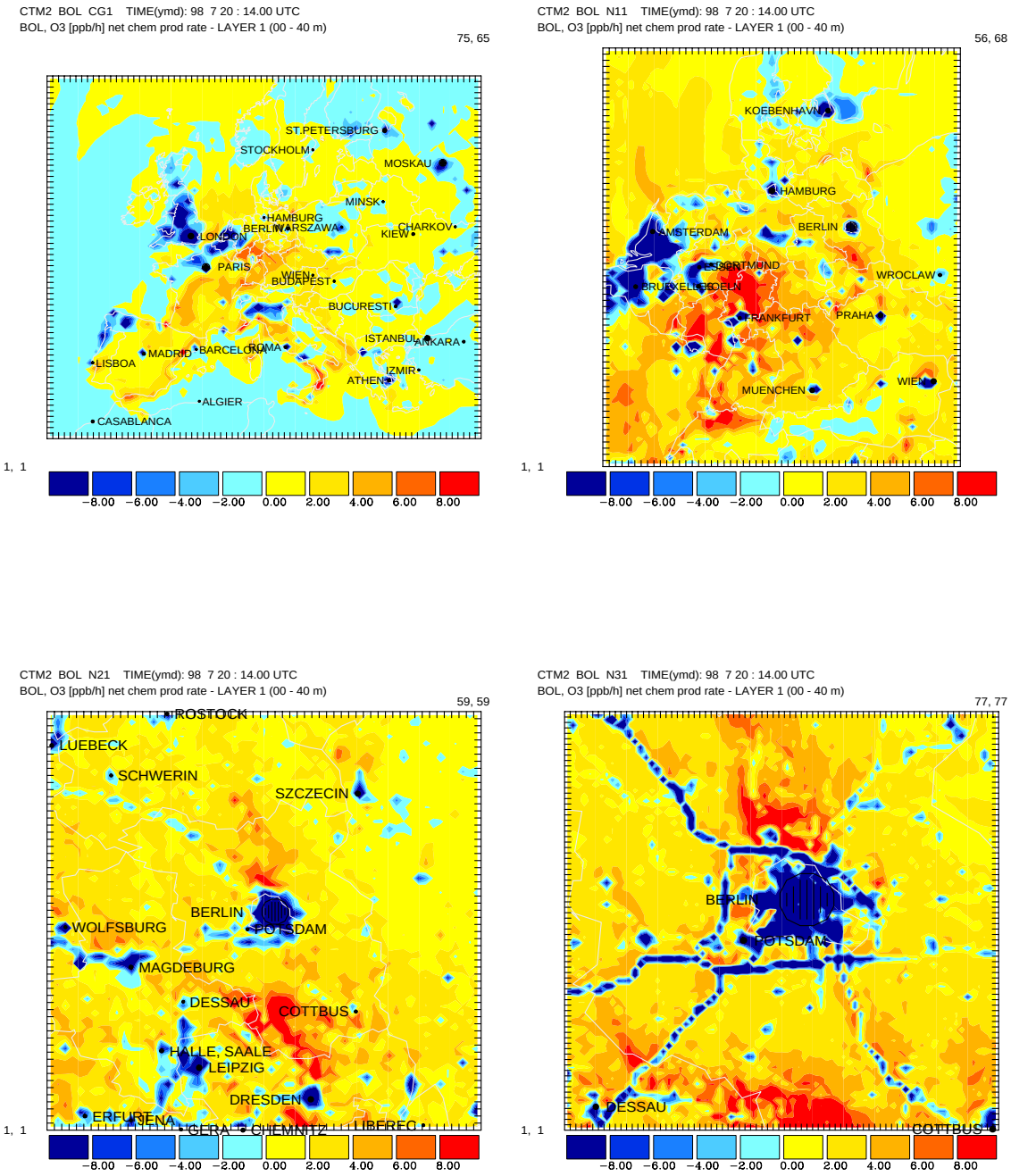

Figure 2: as figure 1, but for the net chemical production rate of ozone [ppb/h] integrated over one hour, i.e. 14 UTC means the net chemical production rate of ozone integrated from 14 UTC - 15 UTC. Those areas in Europe with high emissions of NO_x clearly show a net ozone loss, mainly due to titration of ozone to NO_2 which is a very fast process dominating in the near source regions with high NO-emissions. It also can be seen that a horizontal grid resolution of 18 km (N1) resolves the major cities horizontally as e.g. Berlin, Praha, München, Wien and others with respect of net ozone loss due to tritration in the city centers and ozone net chemical production downwind of the city. N2 and N3 (lower panel) show the ozone loss in Berlin and the major cities of Saxonia southward of Berlin as well as ozone production downwind of the source regions.

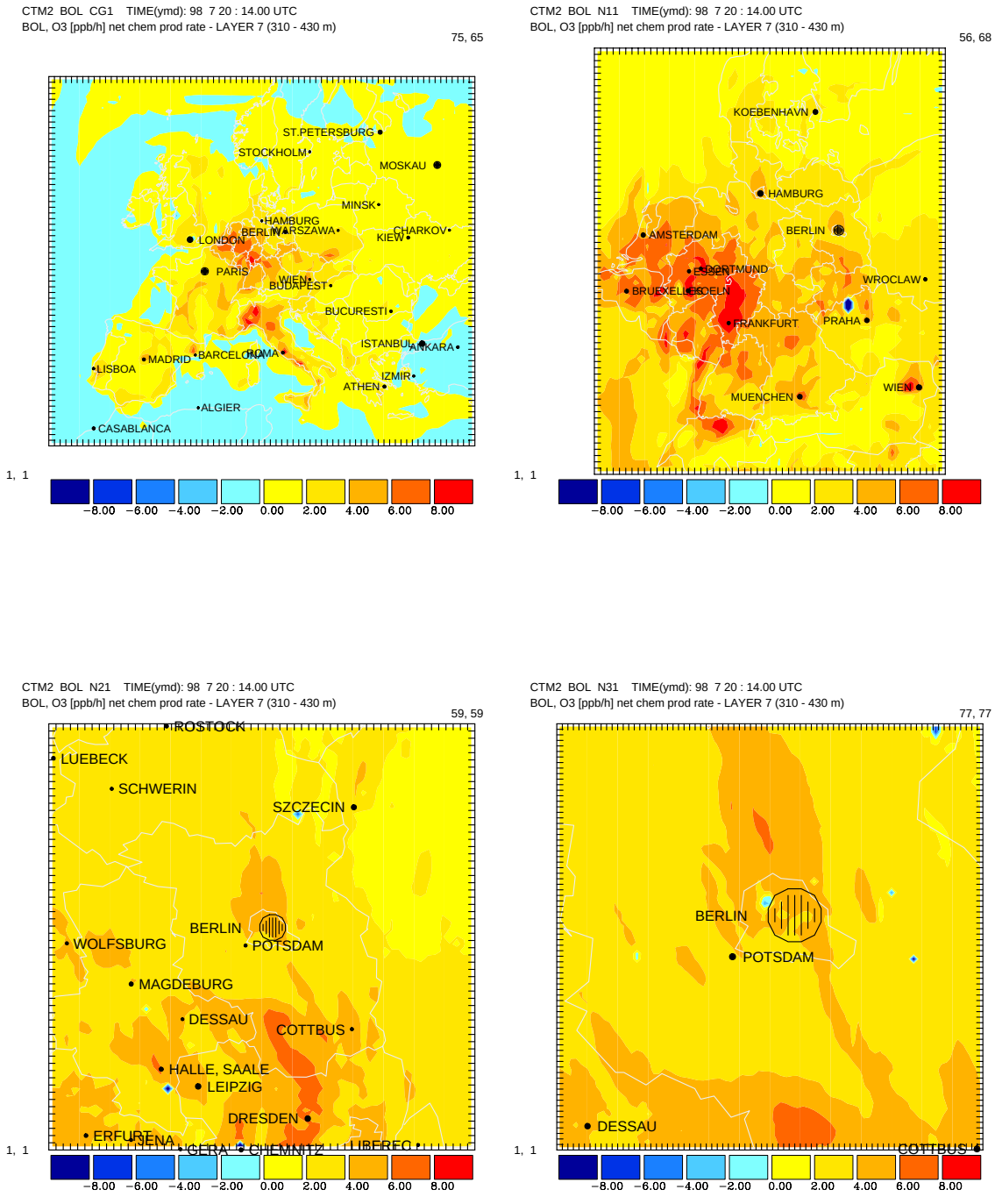

Figure 3: as figure 2 but for layer 7 (310 -430 m) which is approximately the height of theFrohnauer Turm in the northern part of Berlin (indicated by FT in the N2, N3 plots in the lower panel of figure 1). Ozone prodution of about 5 ppb/h can be seen throughout this layer in the plumes of larger cities, more than 8 ppb/h in the western part of Germany.

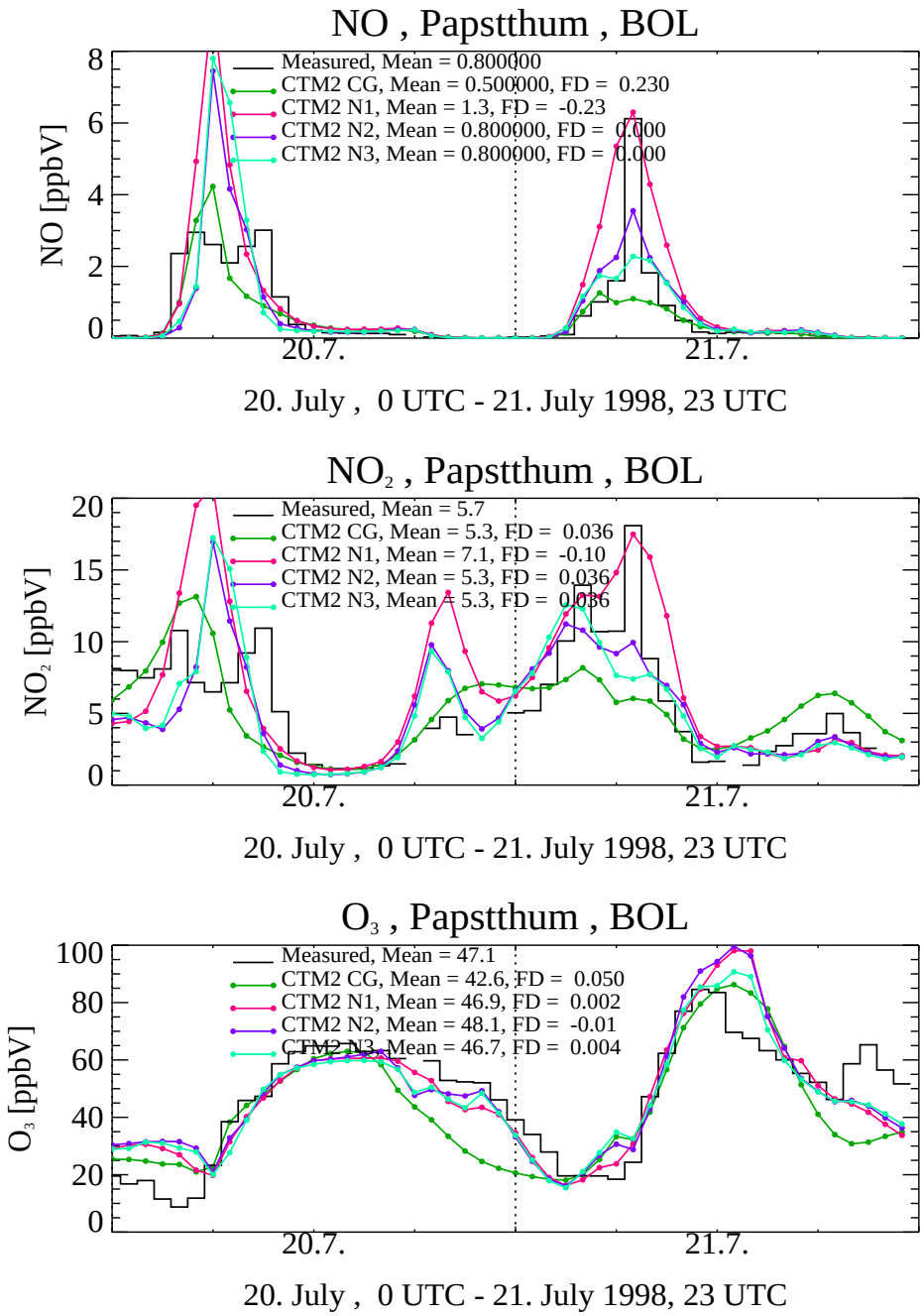

Figure 4: Comparison of EURAD model results with measured data for NO, NO_2 and ozone at the special measurement site Pabstthum. The model results are shown for all for areas used in the model simulation (N0, N1, N2, and N3). The differences of N2 and N3 simulations (grid resolution 6 km and 2 km, respectively) are quite small. The improved quality of the model simulation due to refined horizontal resolution can not be resolved by a comparison with one stations. Even the complete network of measurement sites is not able to resolve small scale structures as highways or single point sources in a simple way. Measured data kindly have been provided by Heiner Geiß, ICG2, Research Centre Jülich.

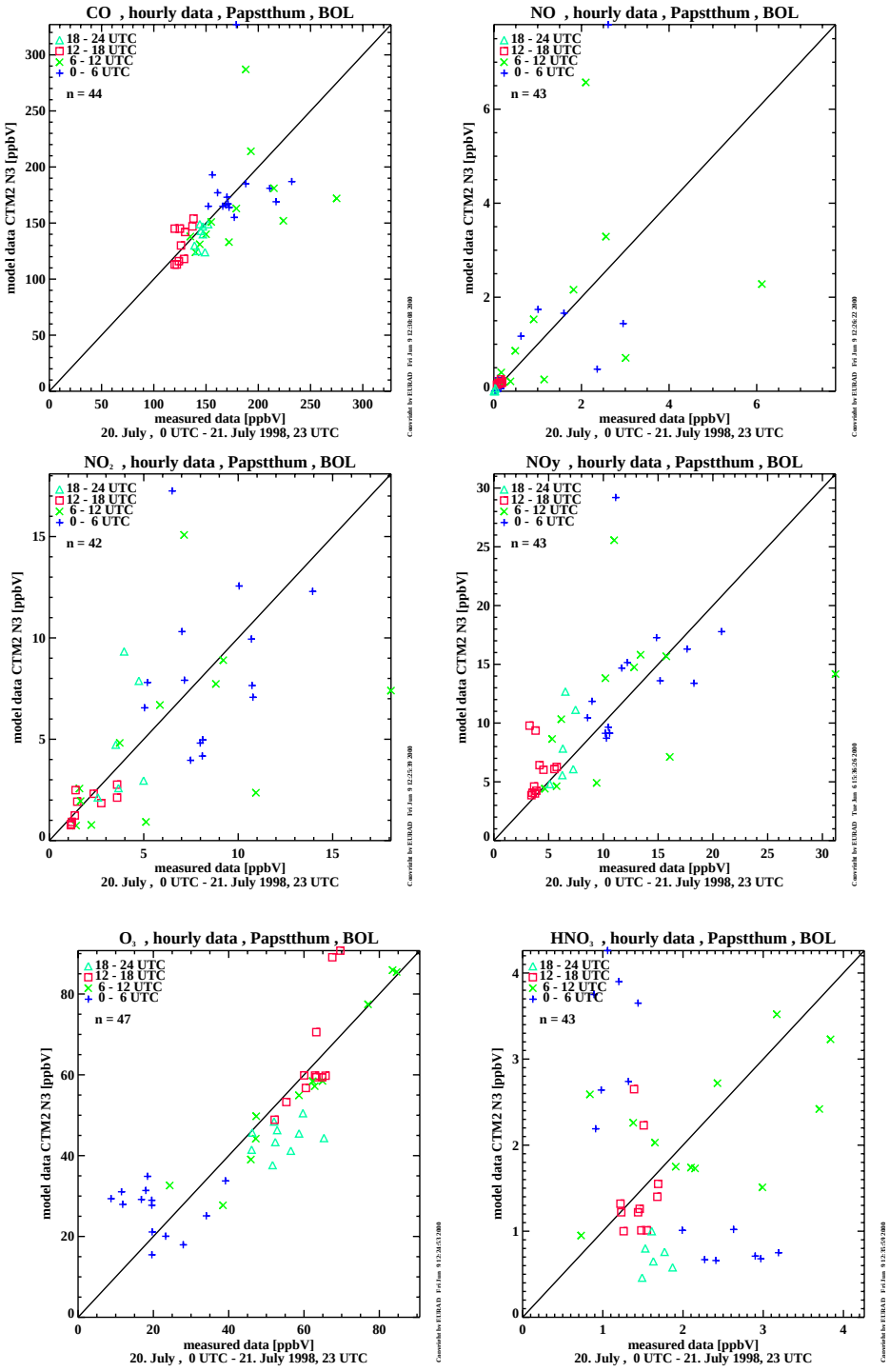

Figure 5: Comparison of model results with observations at the site Pabstthum for July 20/21, 1998. Only results for N3 are shown for CO, NO, NO_2, NO_y, O_3 and HNO_3.

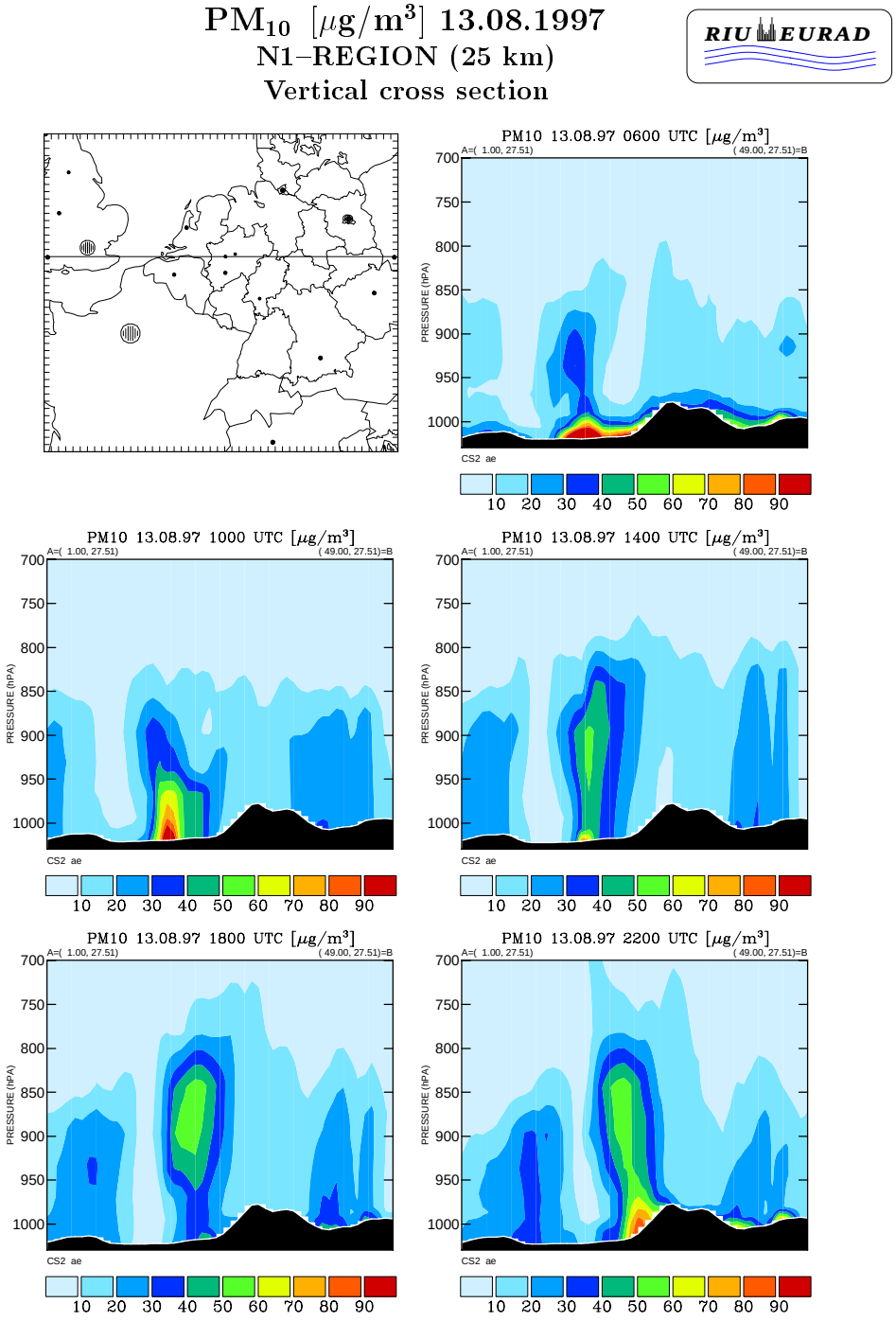

Figure 6: Vertical cross section of PM_{10} as calculated by the EURAD modeling system along the line London - Rhein-Ruhr are - Poland for N1 of the COSIMA model design (25 km grid resolution) for August 13, 1997. The accumulation of PM_{10} during the night (0600 UTC), and the mixing during the day can be found in the model calculations. The vertical scale covers the approximately the atmospheric boundary layer from the surface till 700 hPa, which is about 3000 m altitude.

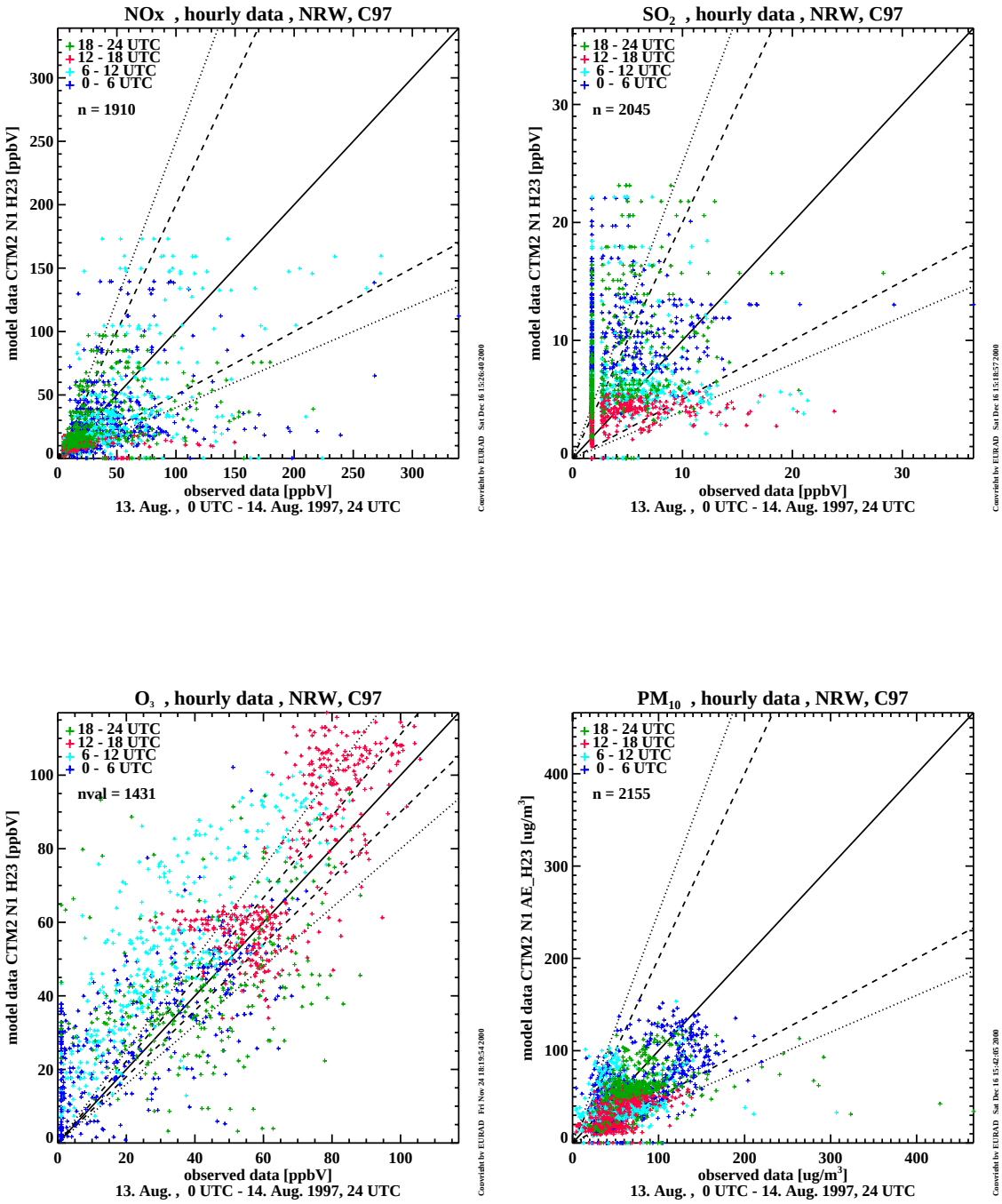

Figure 7: Comparison of measured and modeled data for NO_x, SO_2, O_3 and PM_{10} for the observational network of the Environmental Agency of the Federal State of North-Rhine-Westphalia (LUA). The measured data have been kindly provided by the LUA-NRW.