Application and inter-comparison of atmospheric chemistry mechanisms and advection schemes within the online-coupled regional meteorology chemistry model MCCM

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Objectives and Outline

Improvements in process descriptions are necessary to keep up with current developments. The effects of these improvements on the results of regional simulations should be investigated once a while.

Currents talk: two topics (somewhat nostalgic)

- ❖ Advection schemes
- ❖ Chemical mechanisms

- ➢ Introduction to the regional climate chemistry model MCCM
- ➢ Effect of three different advection schemes
- ➢ Effect of different versions of a chemistry mechanism on regional simulation results
- ➢ Summary

Online coupled climate chemistry model MCCM

MCCM (Mesoscale climate chemistry model)

Meteorological part
- Based on MM5
- Non-hydrostatic
- Nesting capability
- Soil and snow model

Online chemistry part
- RADM2 RACM RACM-MIM
- Photolysis model
- Aerosol module MADE/SORGAM
- Biogenic emission module

Input Any met. input suitable for MM5, initial concentrations of chemical compounds and hourly anthropogenic emissions in MM5-format

Output 3-d meteorological fields, snow height, photolysis frequencies, concentrations of chemical compounds in the gas and particle phase, …

Applications Episodes and sensitivity studies
Real time air quality simulations
Regional climate chemistry simulations

Grell et al. 2000, Atmospheric Environment

Advection schemes in MCCM

Advection schemes compared

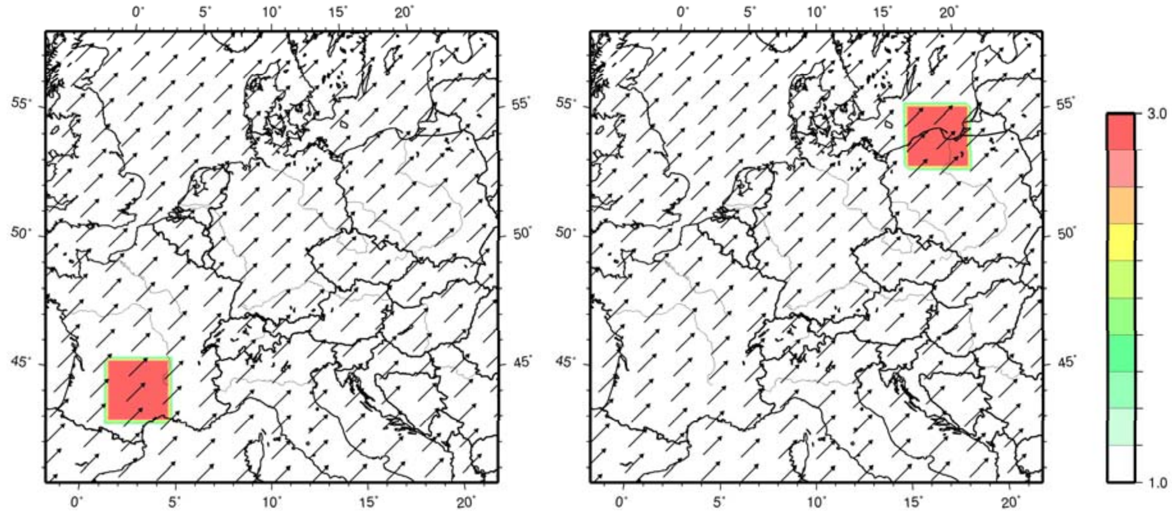
- **MPDATA**
  Modified Smolarkiewicz scheme (2nd order)
- **BOTTM**
  Monotonous Bott scheme (4th order)
- **BOTTP**
  Positive definite Bott scheme (4th order)

Advection schemes in MCCM

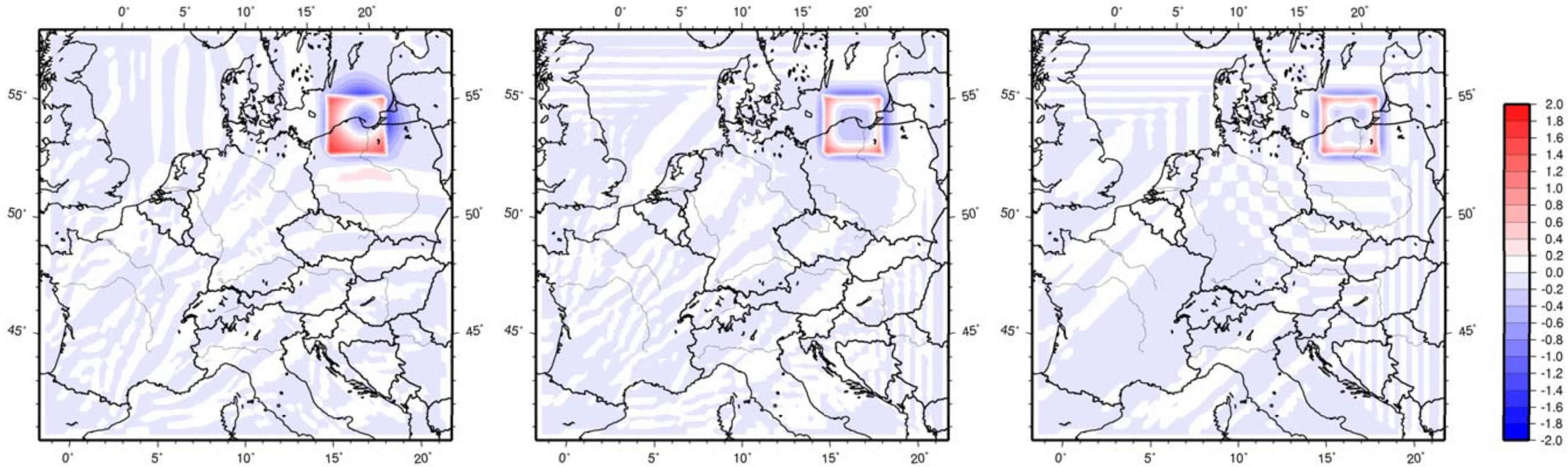
Advection test

Analytical solution for uniform wind field

Differences between analytical and numerical solution



MPDATA BOTTM BOTTP

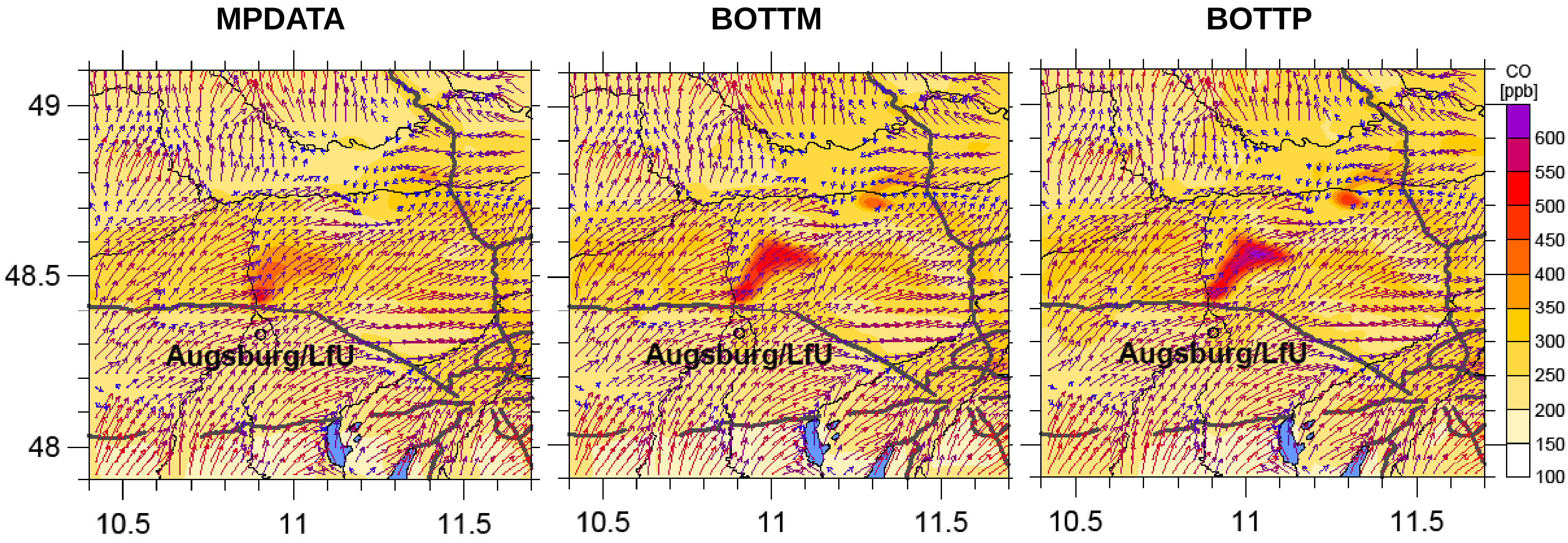


Advection schemes in MCCM

Implementation into MCCM for moisture and chemical compounds

Example: CO plume of the city of Augsburg

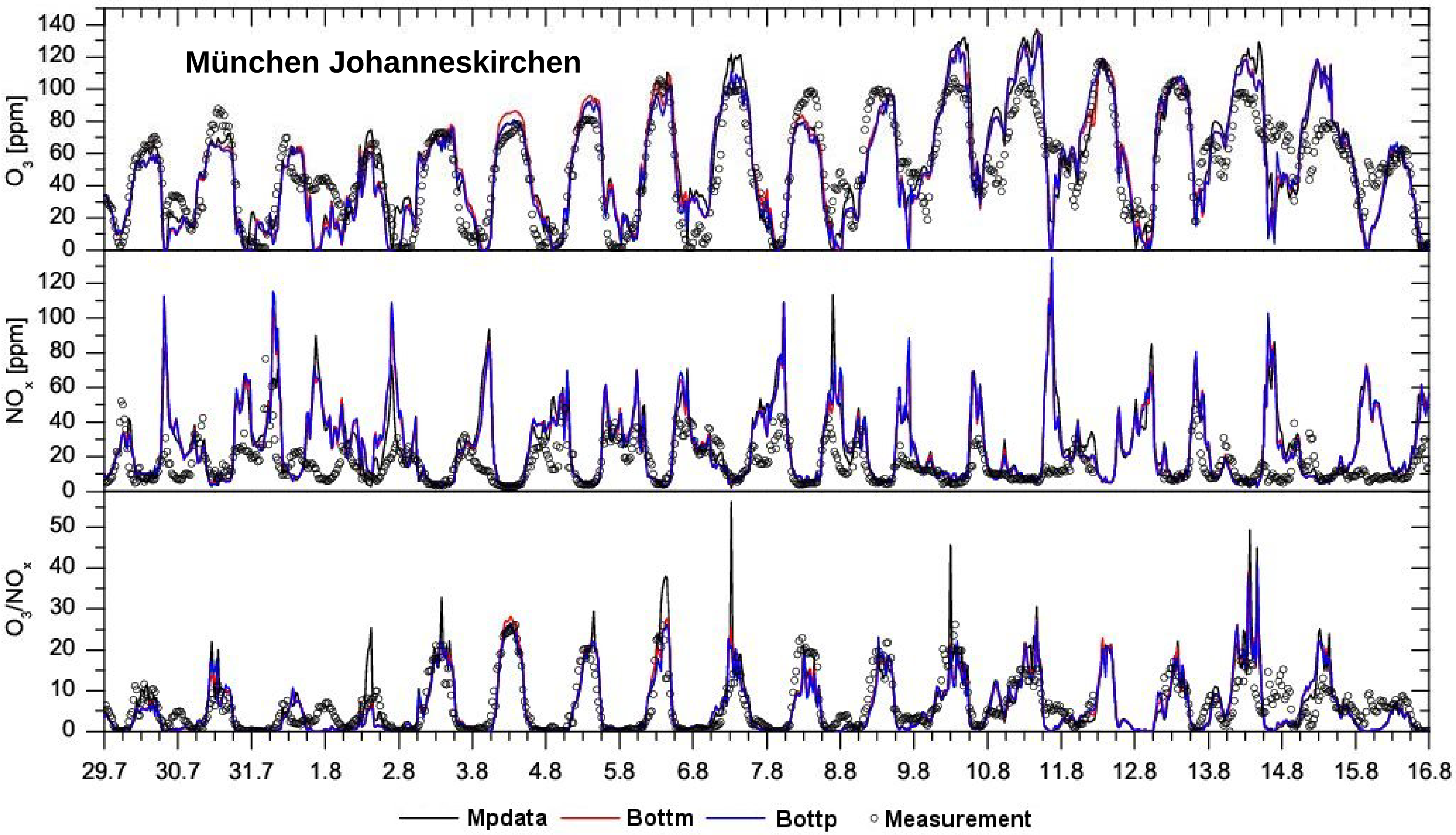
Results for July 30 2003, 4:30 h



Setup: 54-18-6-2 km grid, focus on Southern Germany
2 months episode in summer 2003

Advection schemes in MCCM

Comparison of observed and simulated diurnal course

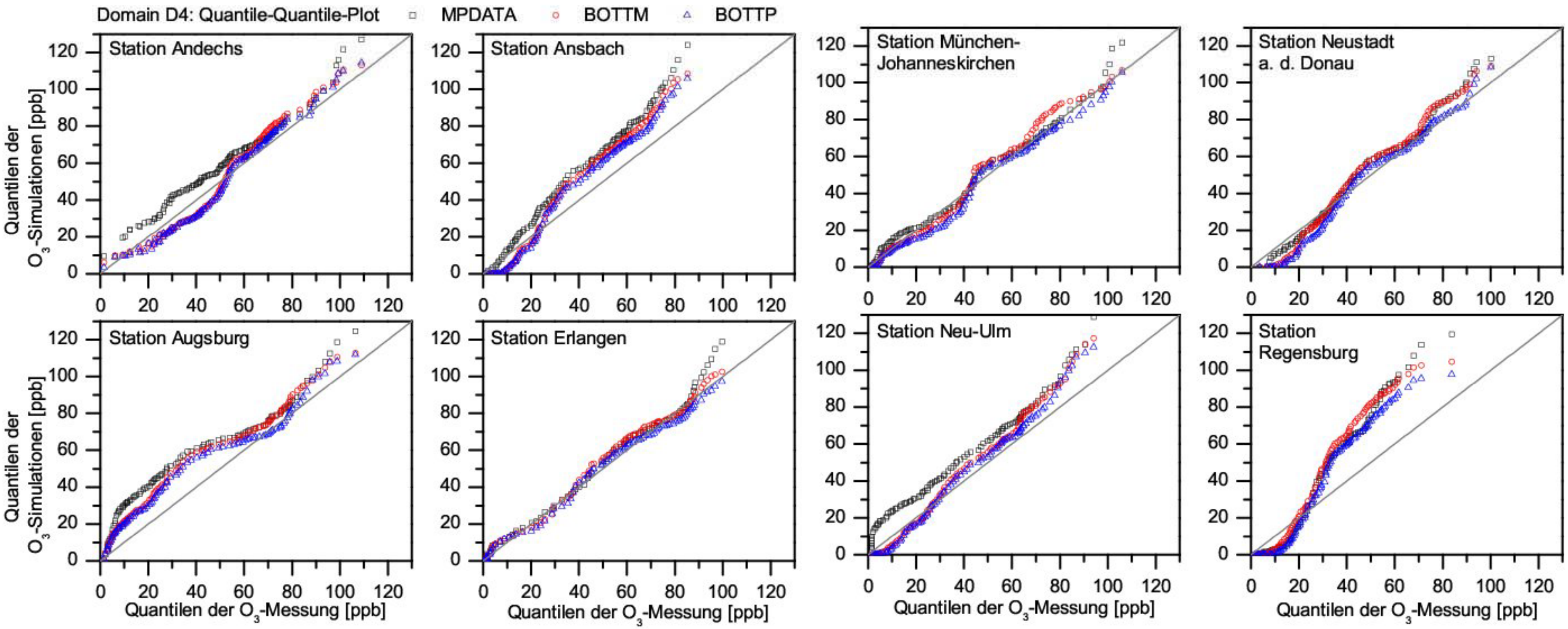


Measurements: LFU Bayern

Advection schemes in MCCM

Comparison against observations

Quantile-quantile plots for near surface ozone



Measurements: LFU Bayern

Advection schemes in MCCM

Summary

- Advection tests show significantly better results for monotone and positive definite Bott scheme
- Positive definite Bott scheme can produce oscillations in case of strong gradients
- However: Statistical analysis of regional simulations shows better agreement with observations for the positive definite Bott scheme
- Only the second best scheme shows best agreements with observations

Gas phase chemistry schemes in MCCM

Compared mechanisms

- **RADM2 (Stockwell et al. 1990)**
  63 chemical species, 21 photolysis reactions and 136 chemical reactions of higher order
- **RACM (Stockwell et al. 1997)**
  77 chemical species, 23 photolysis reactions and 214 chemical reactions of higher order
- **RACM-MIM (Geiger et al. 2003)**
  84 chemical species, 23 photolysis reactions and 221 chemical reactions of higher order
  (based on the MIM isoprene mechanism by Pöschl et al. (2000)
  This mechanism reflects a more advanced description of the chemistry of isoprene degradation

Gas phase chemistry schemes in MCCM

Main differences between the mechanisms

RACM

Updated and expanded version of RADM

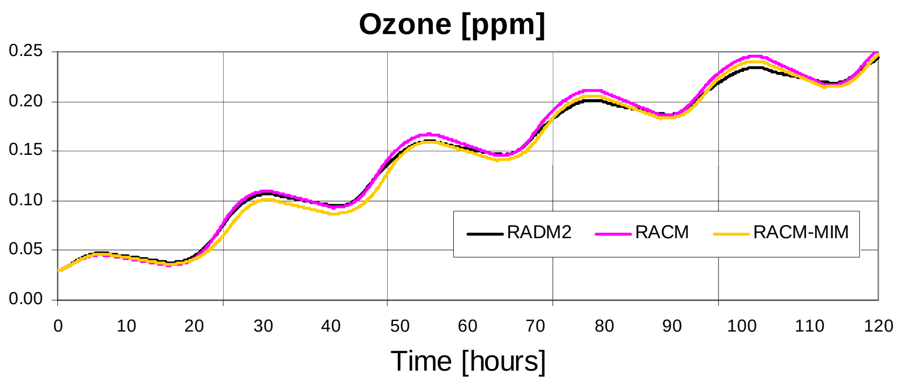
- Inorganic part: most changes related to NO_3 chemistry
- Inclusion of some typical isoprene degradation products
- Terpenes API and LIM
- Revised aromatic VOC and alkane chemistry
- New additional species for alkenes, dienes, unsaturated dihydroxycarbonyls
- Rate update for alcylperoxy radical with NO or NO_2 reaction, additional reaction with NO_3

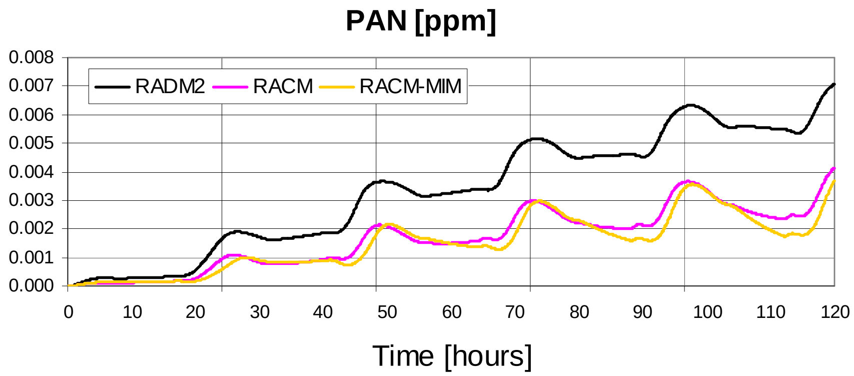
RACM-MIM

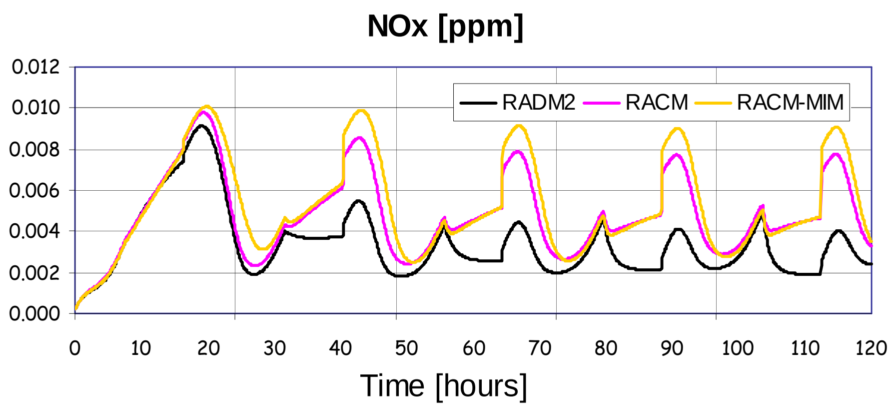
- More specific isoprene reaction products
- Additional peroxy-peroxy self-reaction

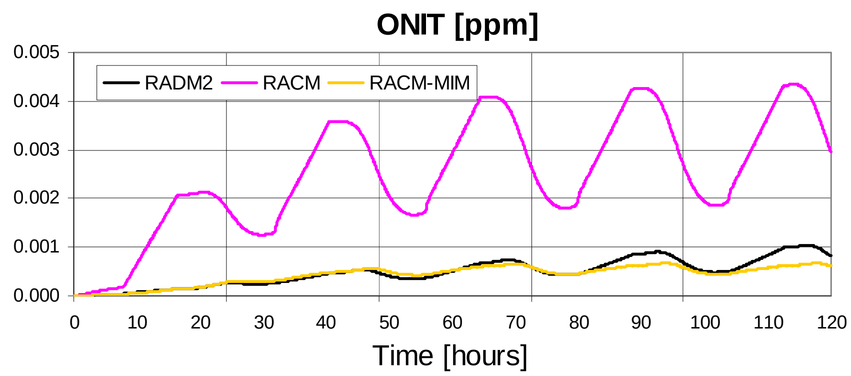
Gas phase chemistry schemes in MCCM

Box model simulations for standard scenario ´urban´





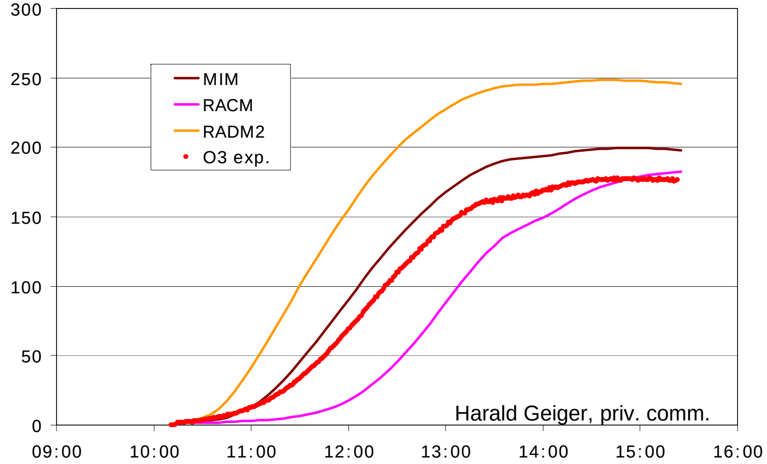




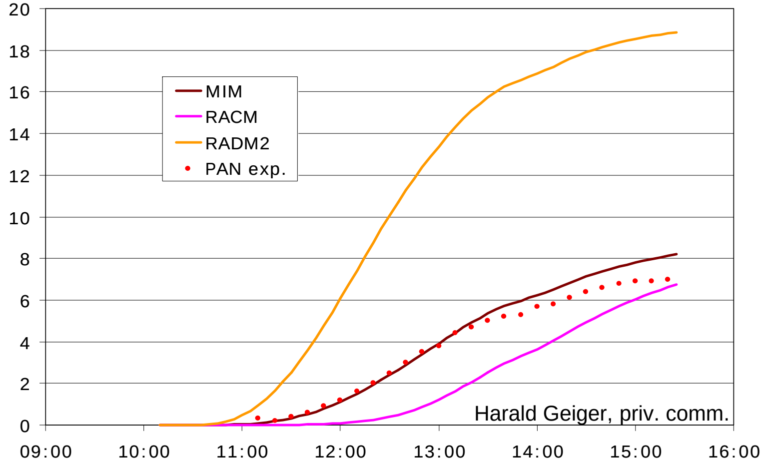
Gas phase chemistry schemes in MCCM

Box model simulations: Comparison with Euphore measurements

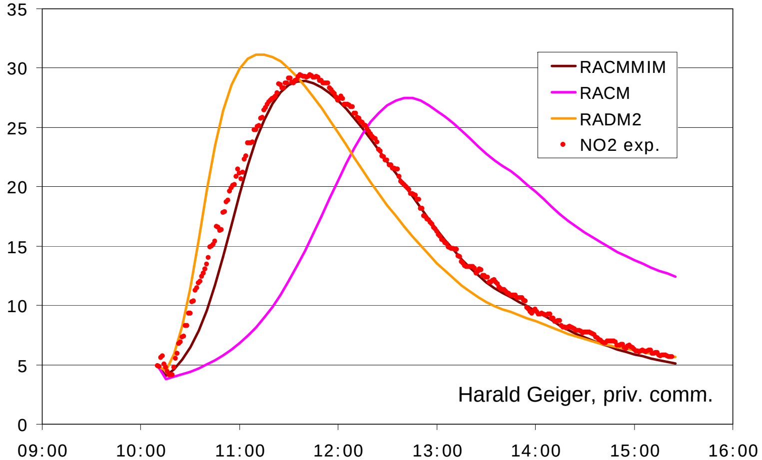
Ozone (ppb)



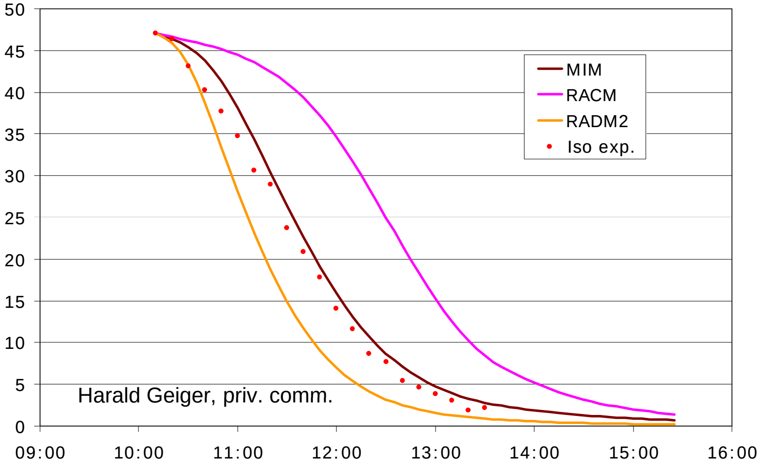
PAN (ppb)



NO_2 (ppb)



Isoprene (ppb)



Gas phase chemistry schemes in MCCM

Application within MCCM

Implementation in MCCM

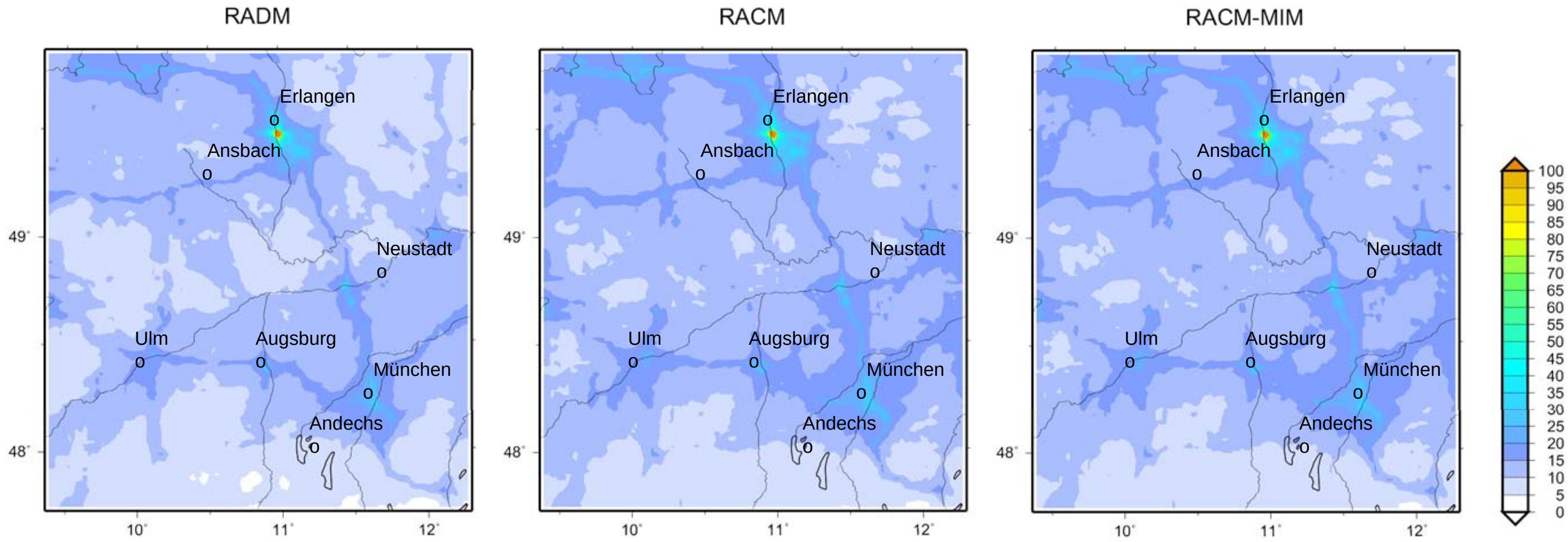
- KPP preprocessing (Sandu et al., 2003)
- Implicit ROS4 solver

Setup of the regional simulations

- 54-18-6-2 km grid, focus on Southern Germany
- 2 month period in summer 2003 (comparatively long for this type of study)
- Meteorology FDDA for first domain

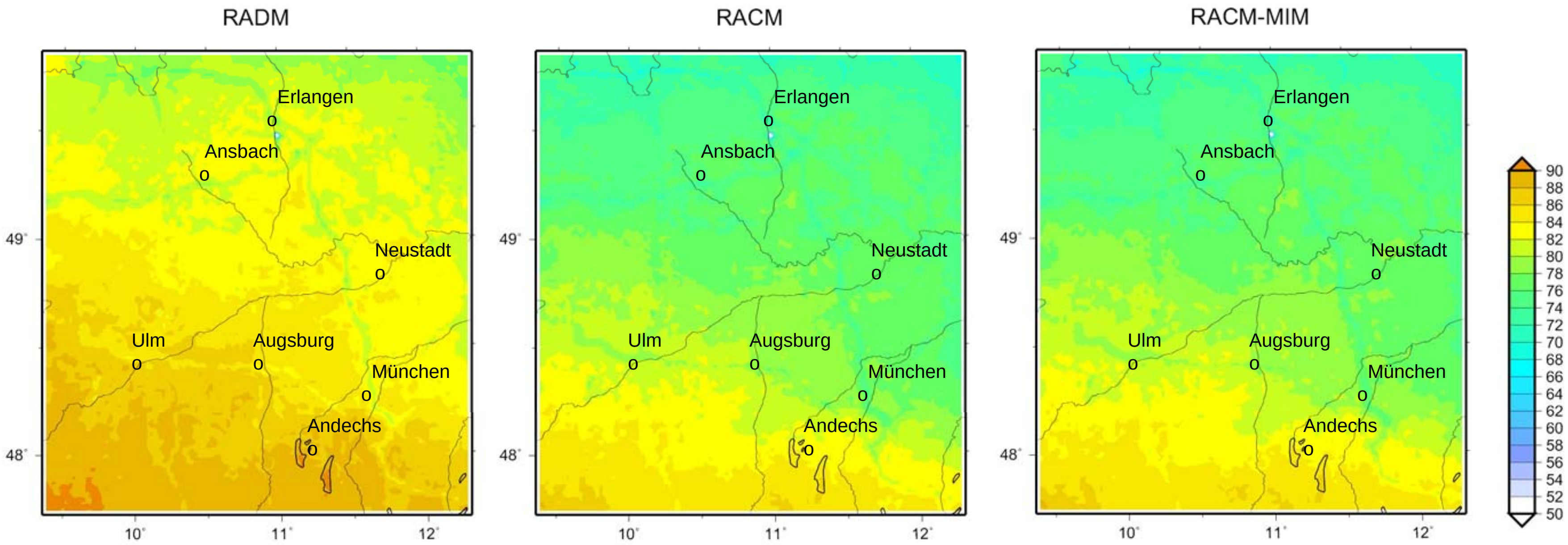
Gas phase chemistry schemes in MCCM

Mean NO_x in August 2003



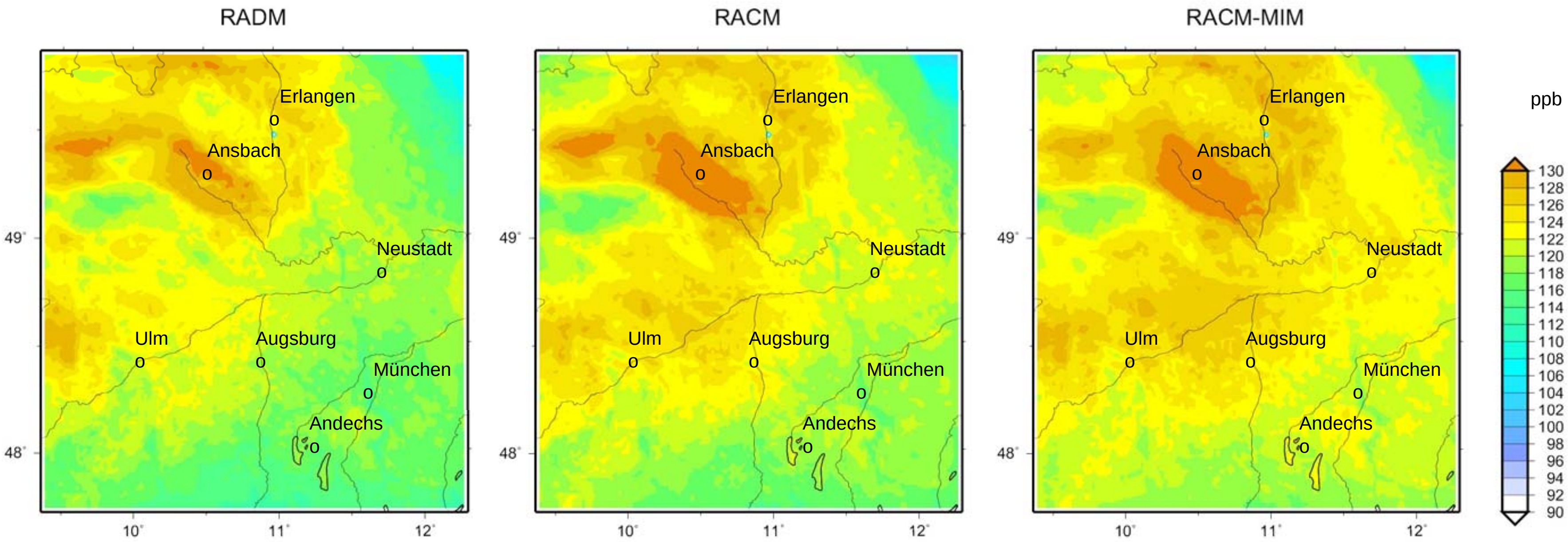
Gas phase chemistry schemes in MCCM

Mean ozone maximum in August 2003



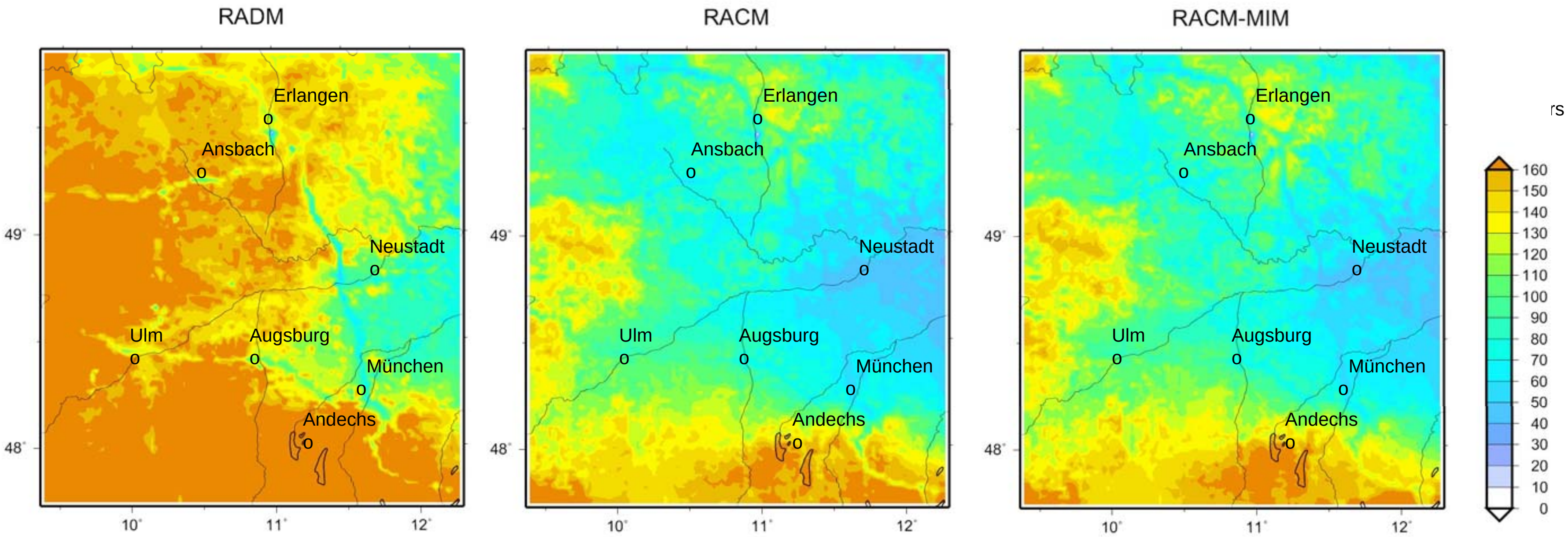
Gas phase chemistry schemes in MCCM

Ozone maximum on August 10 2003



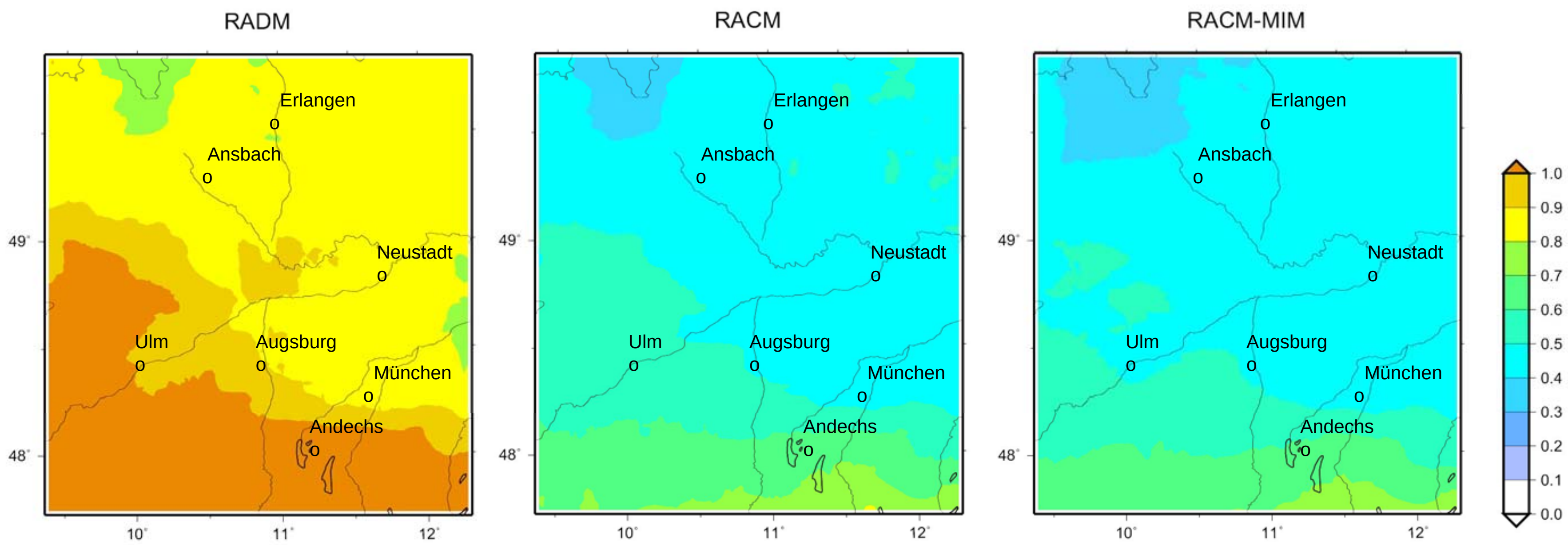
Gas phase chemistry schemes in MCCM

Hours with ozone > 90 ppb in August 2003



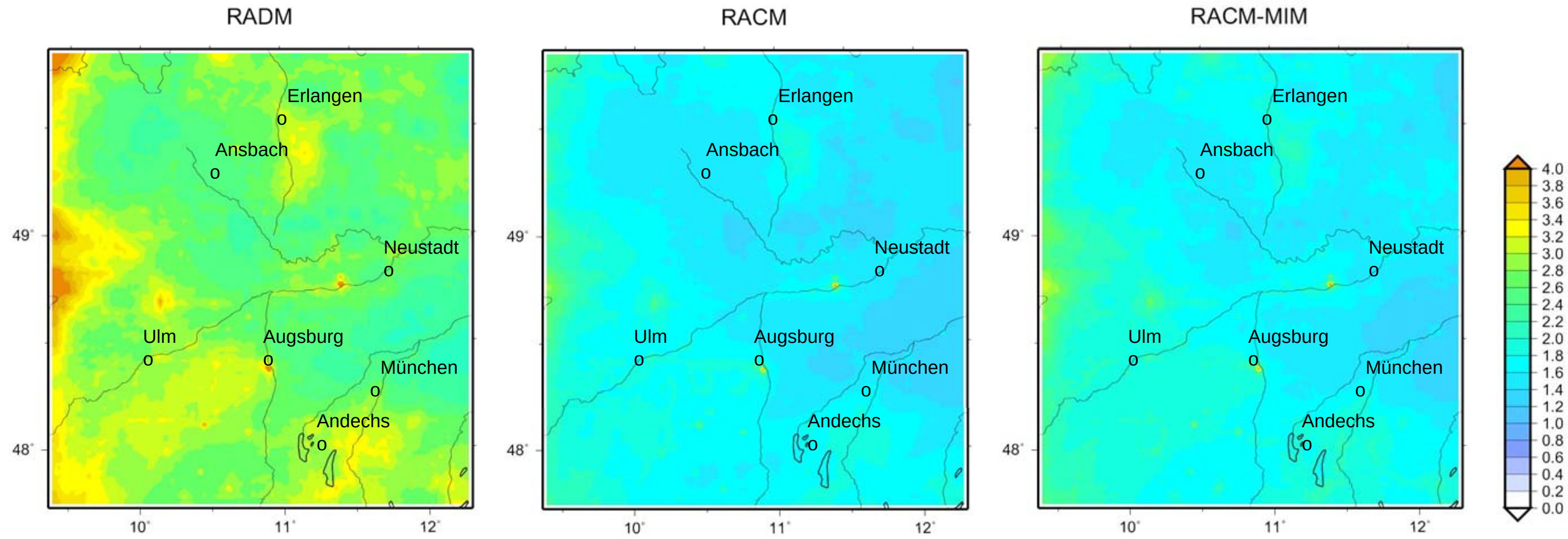
Gas phase chemistry schemes in MCCM

Mean PAN in August 2003



Gas phase chemistry schemes in MCCM

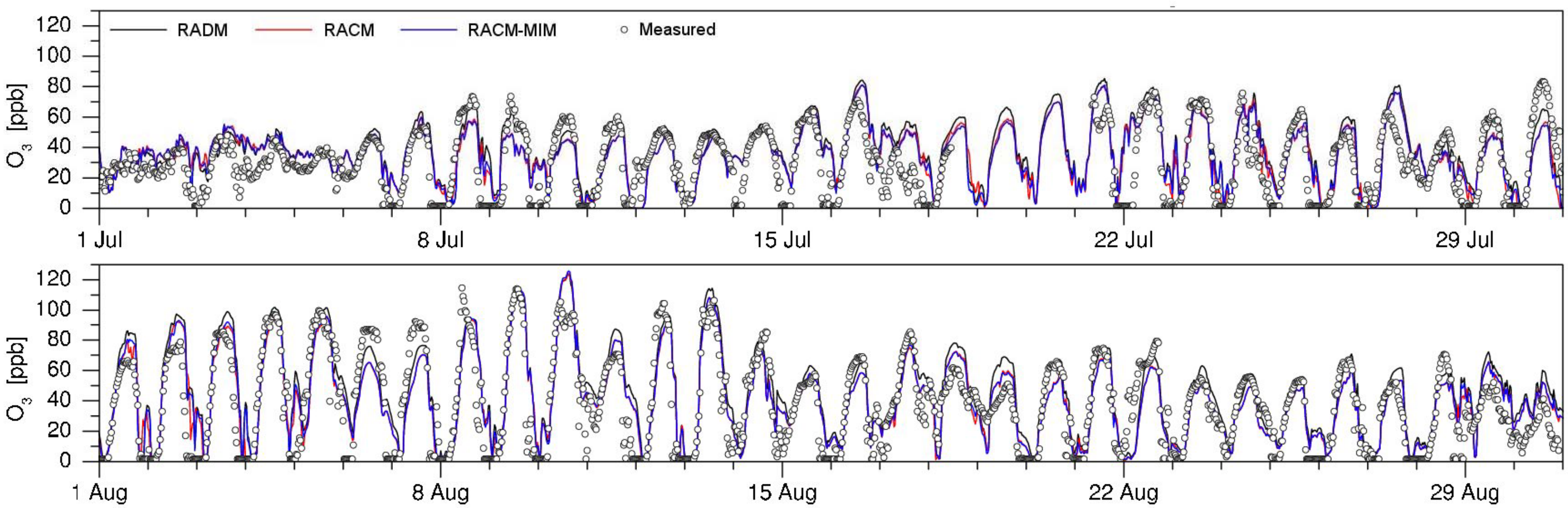
Mean HCHO in August 2003



Gas phase chemistry schemes in MCCM

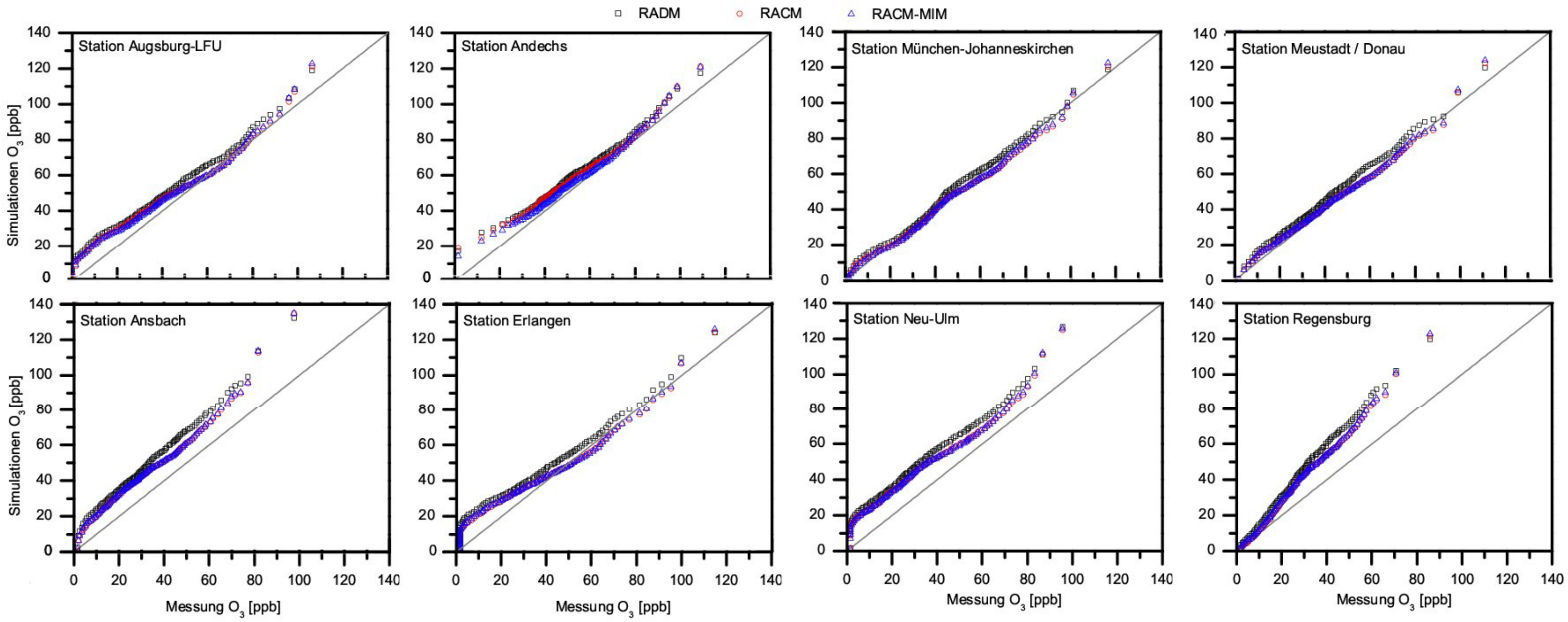
Comparison against observations

Domain D4, 2 km resolution: Station Erlangen



Gas phase chemistry schemes in MCCM

Comparison against observations



Gas phase chemistry schemes in MCCM

Comparison against observations

	RADM	RACM	RACM-MIM	observed
Mean ozone	49.3	45.7	45.4	39.5
Correlation	0.79	0.77	0.77	
Max. ozone	75.4	70.4	70.3	68.9
Correlation	0.77	0.74	0.73	

Average over 8 observational stations

Statistical evaluation according to EPA directive 450/91-1013,1991 shows best results for mean bias, root mean square error, mean normalized bias error, mean fractional bias, mean absolute gross error, etc …. for RACM-MIM

Gas phase chemistry schemes in MCCM

Summary

- In most cases higher ozone, HCHO, PAN, and H_2O_2 with RADM
- Higher ozone with RADM cannot be generalized
- Lower NO_x for RADM
- Practically no difference in simulated isoprene
- Statistical analysis of regional simulations shows better agreement for RACM and RACM-MIM
- Best agreement for RACM-MIM

Summary

- Best result for advection scheme:
  Positive definite Bott scheme
- Best result for chemistry:
  RACM-MIM
- Effect of improved schemes is sometimes ambiguous if only statistics is considered and less pronounced for regional simulations than for idealized conditions

Older schemes do not look that bad as long as they are not compared against better schemes

Question: RACM is quite old and RACM-MIM includes only limited modifications: What will result from further revisions in chemical schemes?