Influence of grid resolution and meteorological forcing on air quality simulations: A sensitivity study with the modelling system COSMO-MUSCAT

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Outline

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- Motivation
- Main features of COSMO-MUSCAT
- Description of different model setups
- Model study (focus on Central Europe)
  - Statistical analysis
  - Impact of wild land fires
  - Influence of grid size
  - Influence of meteorology / meteorological driver
- Summary and outlook

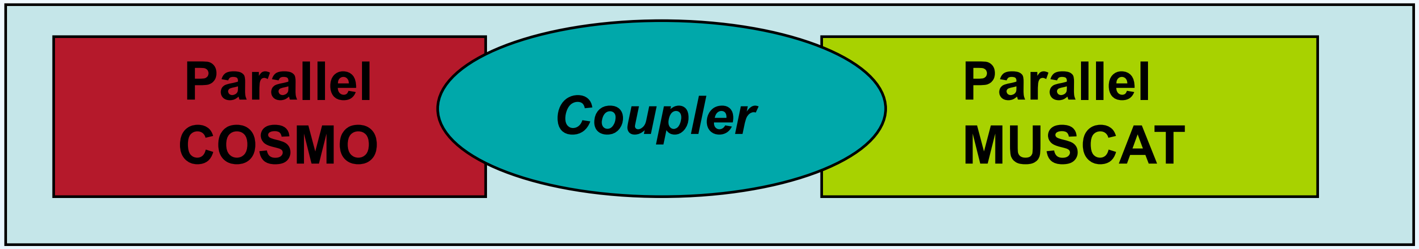
Motivation

- Check the sensitivity and robustness of COSMO-MUSCAT against "technical" changes in the model setup
- Varying the grid size ➔ Influence on meteorological forcing as well as the calculated emission and deposition fluxes
- Studies of the effect of grid resolution in literature (e.g. Salvador et al., 1999; Geco et al., 2005), not always an improvement in the results (Mass et al., 2002)
- To get feeling for observed model "feedbacks" in relation to other model variations
- Simulation of the year 2006 on the European domain in AQMEII shows
  - Periods with very elevated PM concentrations are observed.
  - COSMO-MUSCAT can not capture these peaks.
- ***Different setups are investigated for the two corresponding periods (21 April – 20 May, October) to analyze especially the influence of grid resolution and the meteorological forcing.***

Chemistry-Transport Model MUSCAT

(« MUltiScale Chemistry Aerosol Transport »)

- **Transport and chemical transformation of gas phase pollutants and particles in the atmosphere**
- **Online coupling with COSMO (*version 4.18*)**



- **Applied from regional to urban scale**
- **Mainly used in forecast mode without data assimilation and nudging**
- **Direct and semi-direct feedback are implemented.**

Chemistry Transport Model System COSMO-MUSCAT

Gas phase ("*read in*"):

- **RACM** *(Stockwell et al., 1997)* **+**
- **MIM2** *(Karl et al., 2006)*
  (98 species and over 250 reactions
- *Other modules (e.g., amine chemistry)*

Aerosol model:

- **Mass-based approach (e.g., *EMEP*)** *or*
- **Modal approach M7** *(Vignati et al, 2004)*:
  - 4 internal-mixed and 3 external modes
  - sulphate, sea salt, dust, EC, OC

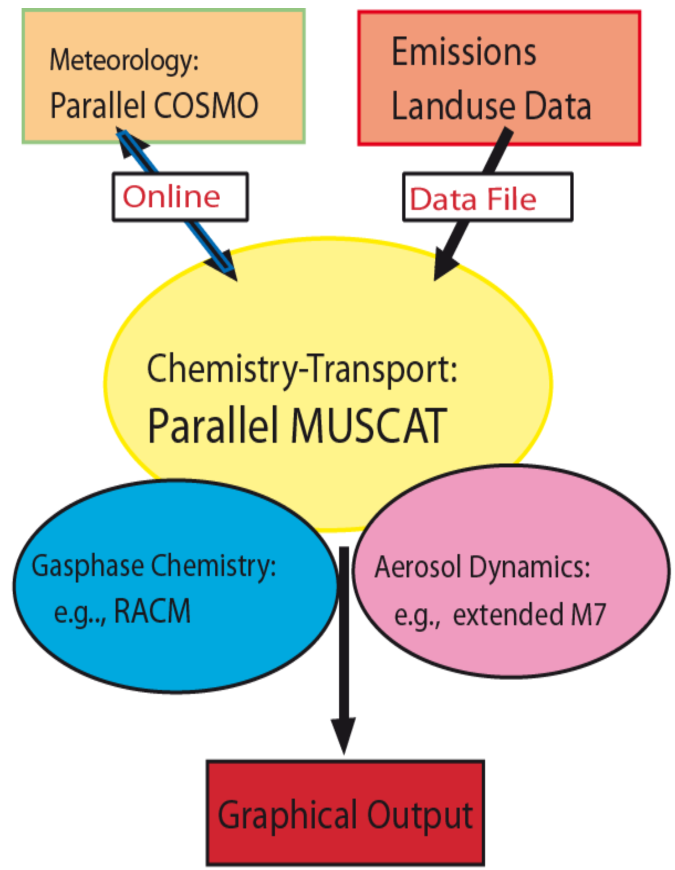
  extended by
  - nitrate and ammonium
  - SIA by *ISORROPIA* *(Nenes et al., 1998)*
  - SOA by SORGAM *(Schell et al., 2001)*
- **Dust: sectional (5 bins)**

Dry and wet deposition, sedimentation

Emissions:

- **Anthropogenic (11 snaps, area + point, fires)**
- **Biogenic** *(Günther et al., 1993)*
- **Seasalt** *(Long et al., 2011)*

➔ *see also Poster of Stefan Barthel !!*

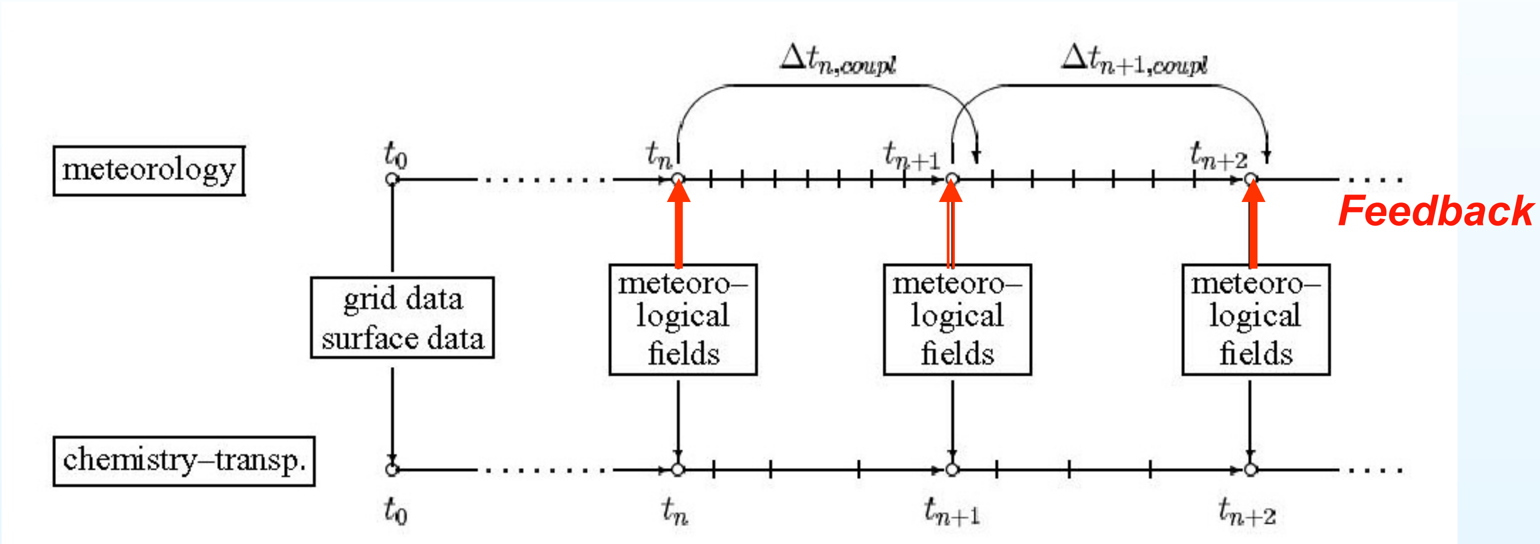


The coupled model system COSMO-MUSCAT

Numerical methods

- **Space discretization**
  - ***Staggered grid. Finite-volume techniques.***
  - ***Multiblock approach*** (different grid resolutions in the domain)
  - ***Advection: Third-order upwind***
- **Time-integration: IMEX scheme** *(Knoth & Wolke, 1998)*
  - ***Explicit second-order Runge-Kutta for horizontal advection***
  - ***Second order BDF method for the rest:*** *Jacobian is calculated explicitly, linear systems by Gauss-Seidel iterations or AMF*
  - ***Automatic step size control***
  - ***Multirate approach (Schlegel et al., 2012)***
- **Parallelization**
  - ***Domain decomposition***
  - ***Dynamical load-balancing by redistribution of blocks***

Coupling Scheme (+ feedback to COSMO)



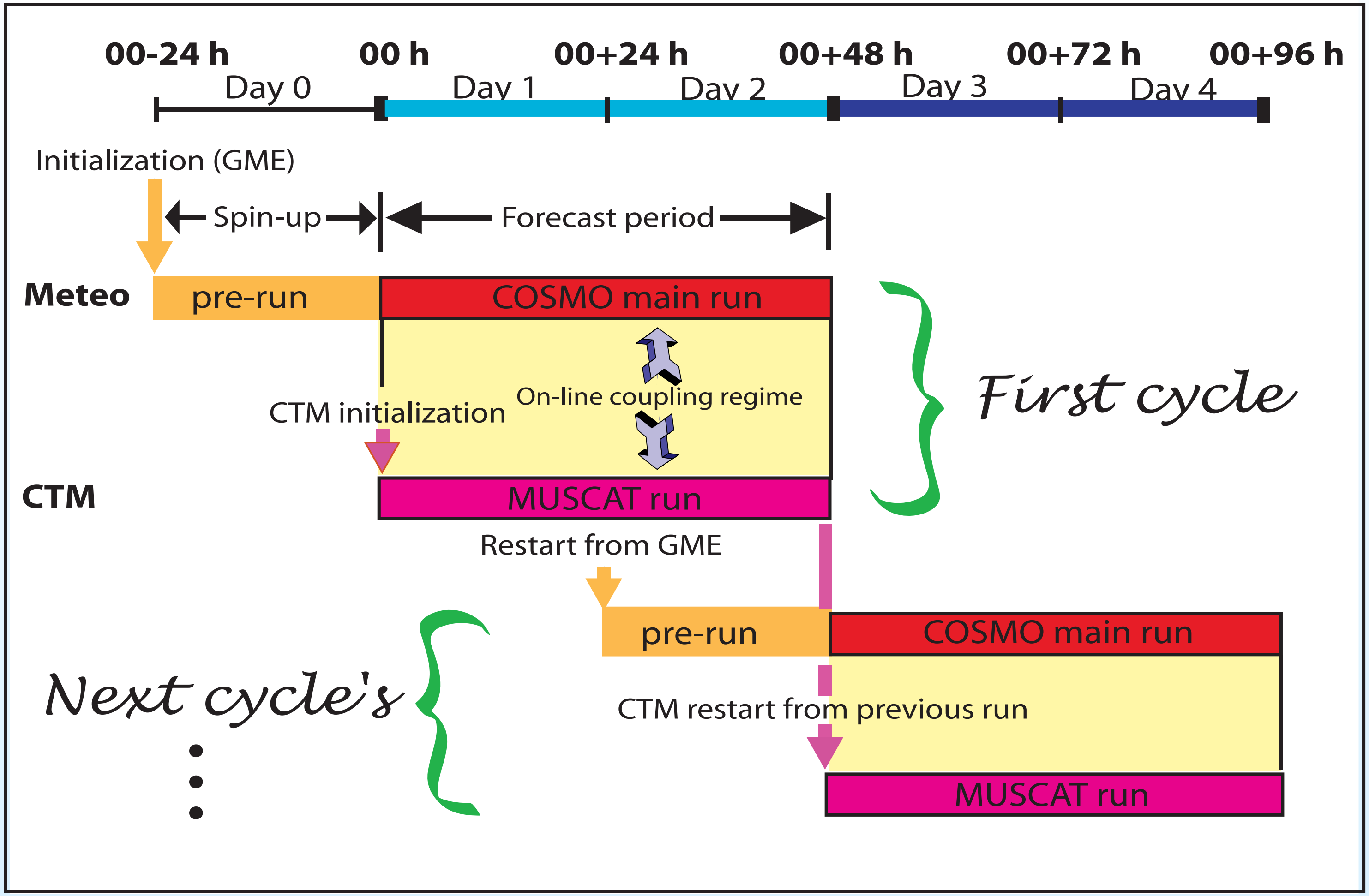
- Time interpolation of the meteorological fields:
  - Linear interpolated in $[t_n, t_{n+1}]$: Temperature, Density,….
  - Time-averaged values on $[t_n, t_{n+1}]$: ***Projected*** wind field

  ➔ ***ensures mass conservation (elliptic equation by cg-method) !!***
- Separate time step size control for COSMO and MUSCAT

Model Study

- Performed in the framework of
  AQMEII (EU+NA): *"Air Quality Model Evaluation International Initiative"*
  Phase 1: *"Operational & dynamic evaluation"* ➔ NA + Europe: 2006
  (20 different groups have participated in phase 1!)
  Phase 2: *only online-coupled models, feedback* ➔ NA + Europe: 2006 + 2010
- Simulations are performed for the EU domain and 2006. The annual simulation is included in the ENSEMBLE data base (JRC Ispra) and involved in the joint analysis.
- Anthropogenic emissions (TNO), fire emissions (FMI) and CTM boundary conditions (GEMS) provided by the AQMEII community.
- This study: 7 different setups are compared, contribution to the *"Special Issue"* of *Atmos. Environ.*
- Focus on Central Europe and on 2 one-month periods (21 April – 20 May 2006 and **October 2006**)
- Simulations are performed in the forecast mode without feedback, nudging and DA
- Cyclic time schedule with one day spin-up of the COSMO model
- COSMO is forced by reanalyzed GME data provided by the DWD
- Simulation results are compared with ground-based measurements, radiosonde and satellite data. Statistical analysis only for ground data.

Time schedule for model runs



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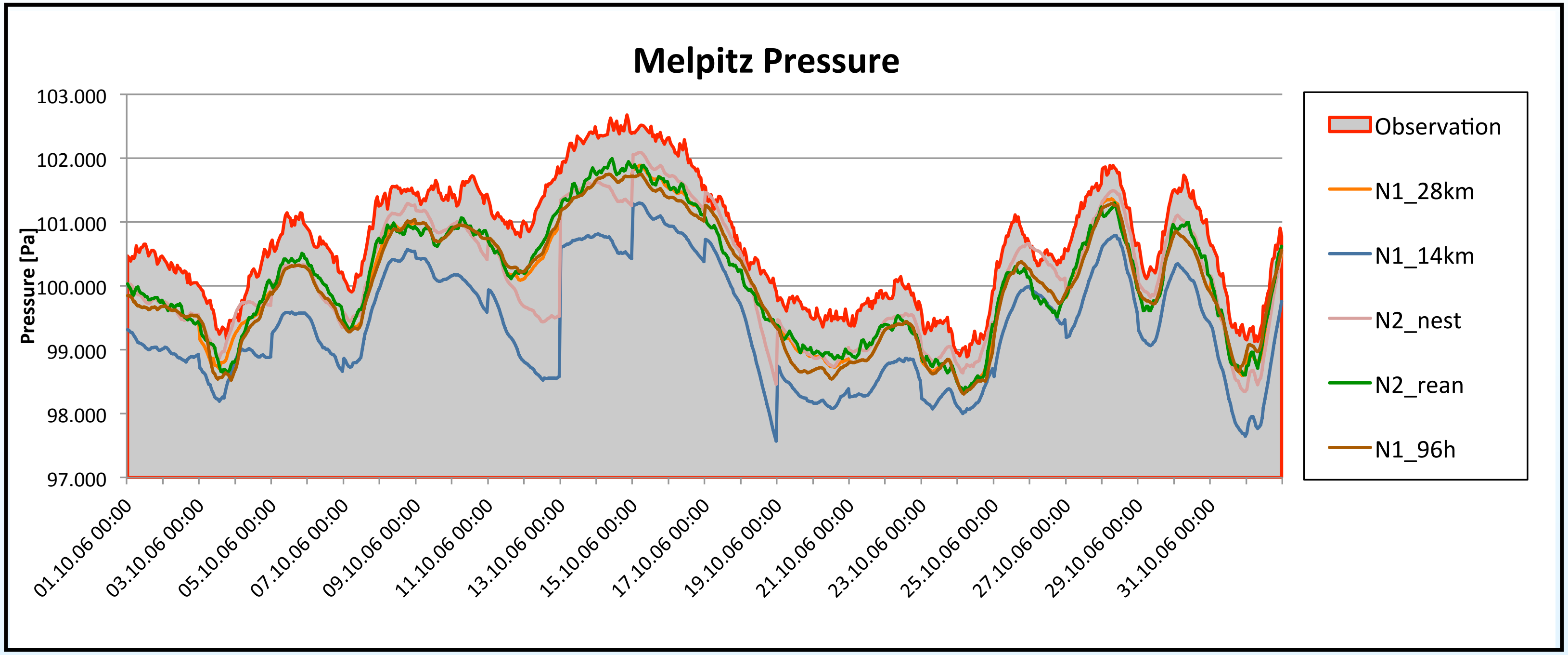
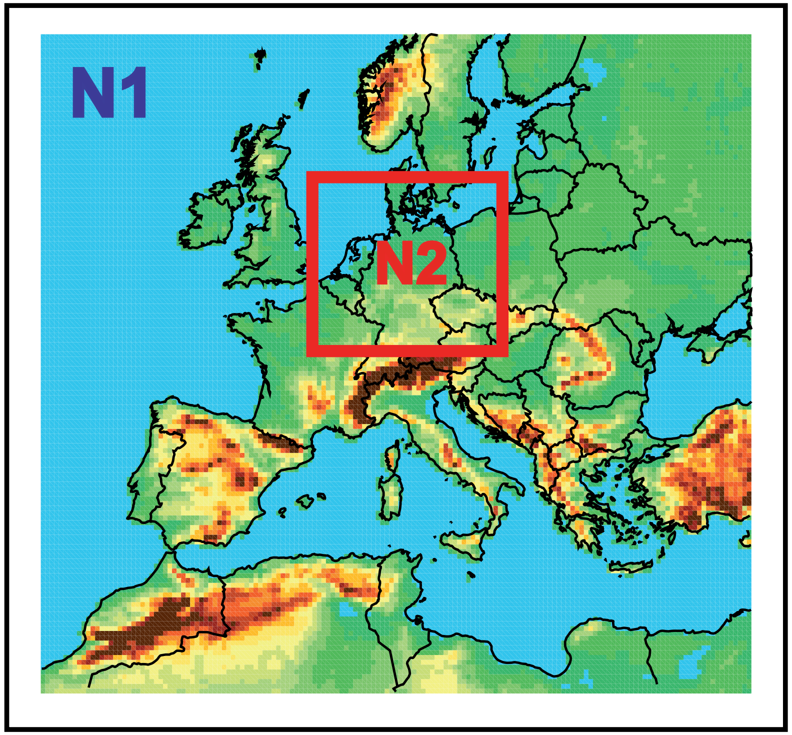


Problems:

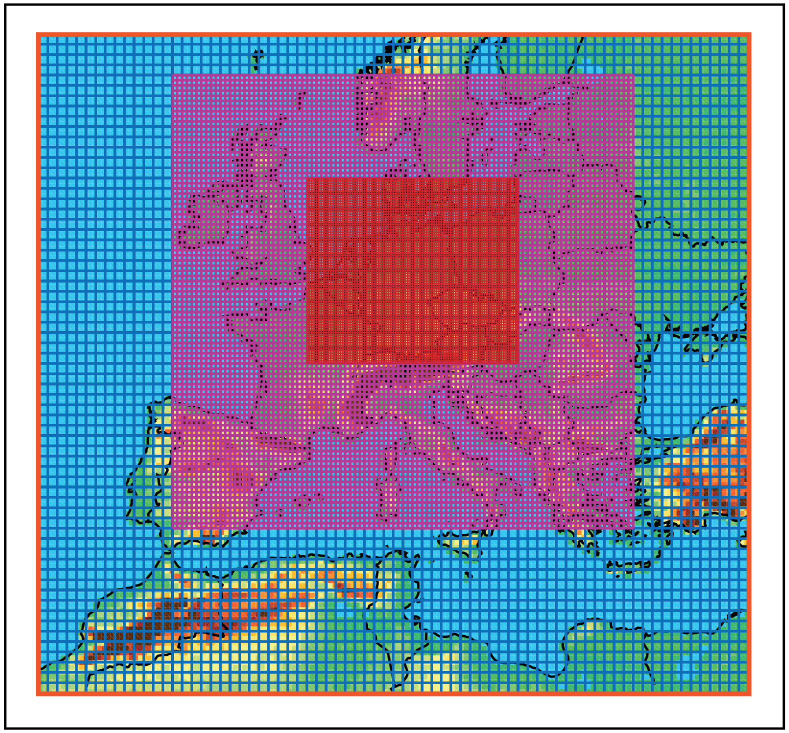
- *Jumps by restart of meteorology*
- *Differences in orography between the 28km, 14 km, and 7 km resolution*
- ***Regime for analyzing "feedback": Initialization interval, assimilation ?***

COSMO-MUSCAT Setups

COSMO grid nesting



MUSCAT N1_multi grid



Uniform grid resolution:

N1: 14 km x 14 km, 40 layers

N2: 7 km x 7 km, 50 layers

Different grid resolutions:

28 km - 14 km - 7 km, 22 layers

Comparison of different model setups: Grid resolution

	Meteorology Model COSMO			Chemistry Transport Model MUSCAT				cycle length
	horizontal grid	vertical grid	forcing	horizontal grid	vertical layers (first layer)	boundaries	aerosol modul	
N1_28km	28 km	40 layers	GME reanalysis	uniform 28 km	22 (approx. 60 m)	GEMS	mass-based	48 h
N1_14km	14 km	40 layers	GME reanalysis	uniform 14 km	22 (approx. 60 m)	GEMS	mass-based	48 h
N1_multi	14 km	40 layers	GME reanalysis	multiscale (Figure)	22 (approx. 60 m)	GEMS	mass-based	48 h
N2_nest	7 km	50 layers	nested in N1	uniform 7 km	32 (approx. 20 m)	N1_multi	mass-based	48 h
N2_rean	7 km	50 layers	COSMO reanalysis	uniform 7 km	32 (approx. 20 m)	N1_multi	mass-based	48 h
N1_96h	28 km	40 layers	GME reanalysis	uniform 28 km	22 (approx. 60 m)	GEMS	mass-based	96 h
N1_aero	28 km	40 layers	GME reanalysis	uniform 28 km	22 (approx. 60 m)	GEMS	extended M7	48 h
N1_nofire	same configuration as ***N1_48km***, but without ”wildland fire“ emissions							

Comparison of different model setups: Meteorological forcing

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Comparison of different model setups: Cycle length

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Comparison of different model setups: Aerosol model

	Meteorology Model COSMO			Chemistry Transport Model MUSCAT				cycle length
	horizontal grid	vertical grid	forcing	horizontal grid	vertical layers (first layer)	boundaries	aerosol modul	
N1_28km	28 km	40 layers	GME reanalysis	uniform 28 km	22 (approx. 60 m)	GEMS	mass-based	48 h
N1_14km	14 km	40 layers	GME reanalysis	uniform 14 km	22 (approx. 60 m)	GEMS	mass-based	48 h
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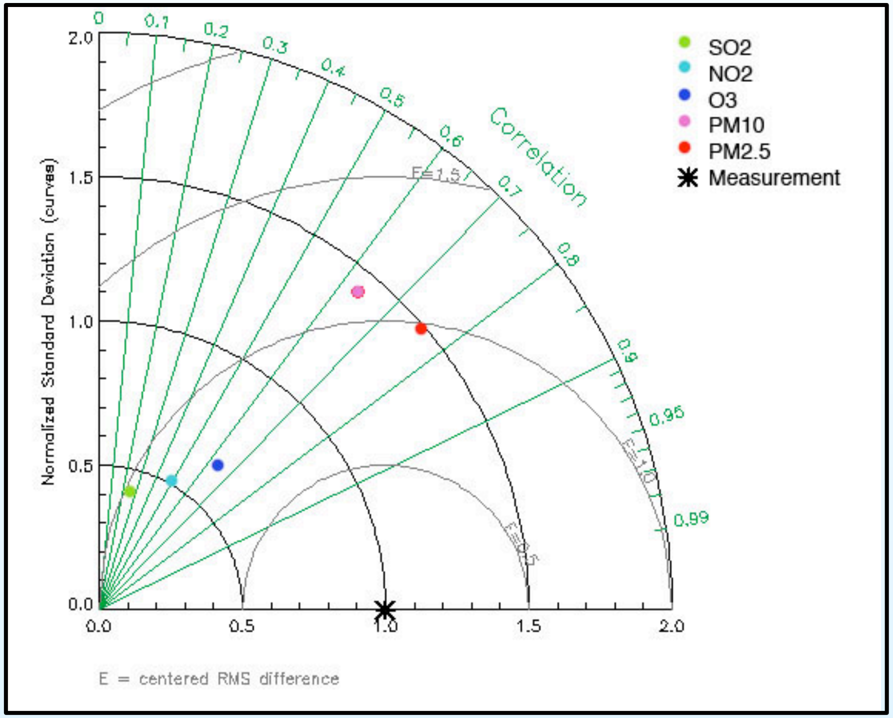
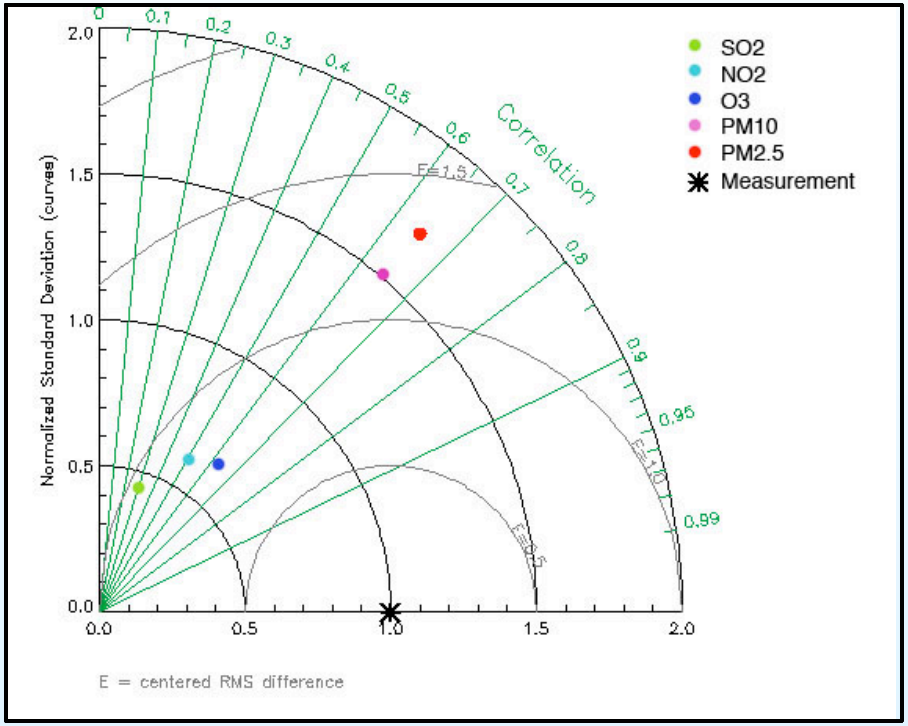
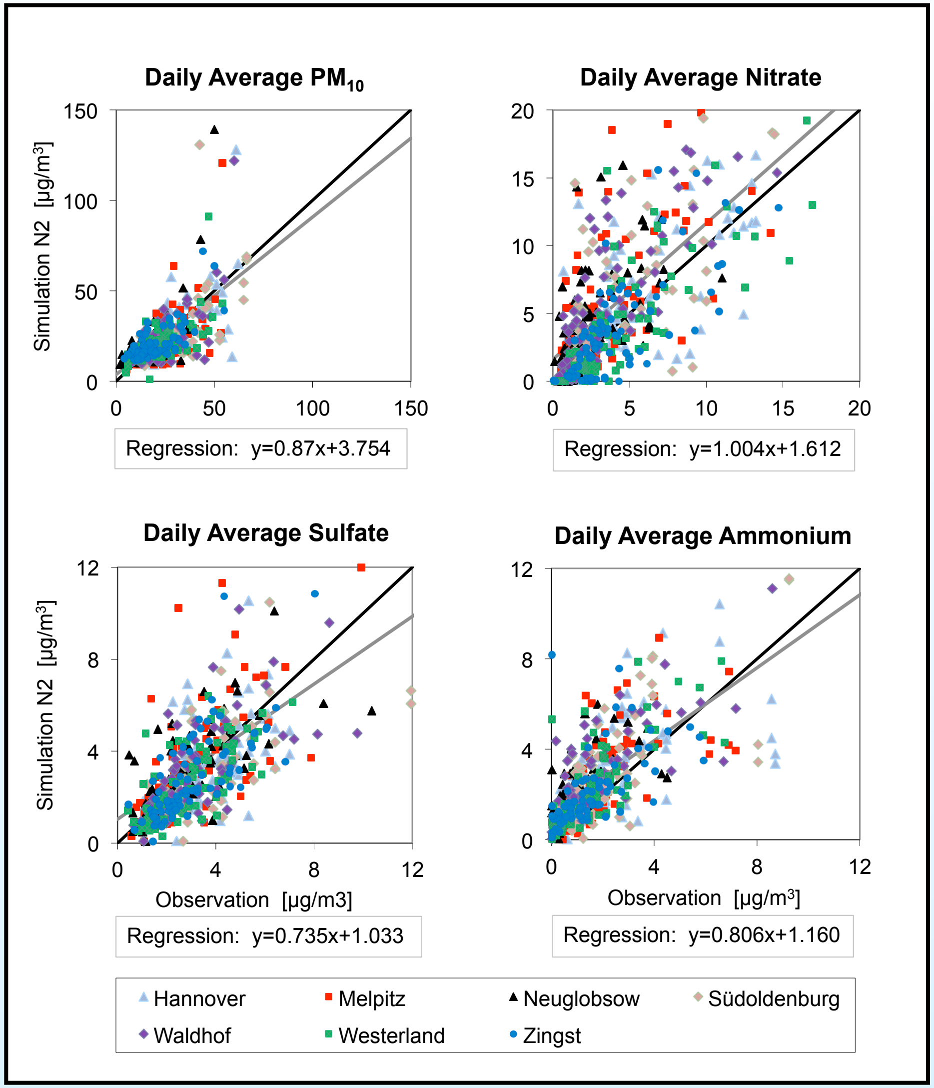
Normalized Taylor diagrams for the annual N1_28km run (ENSEMBLE analysis, JRC Ispra)



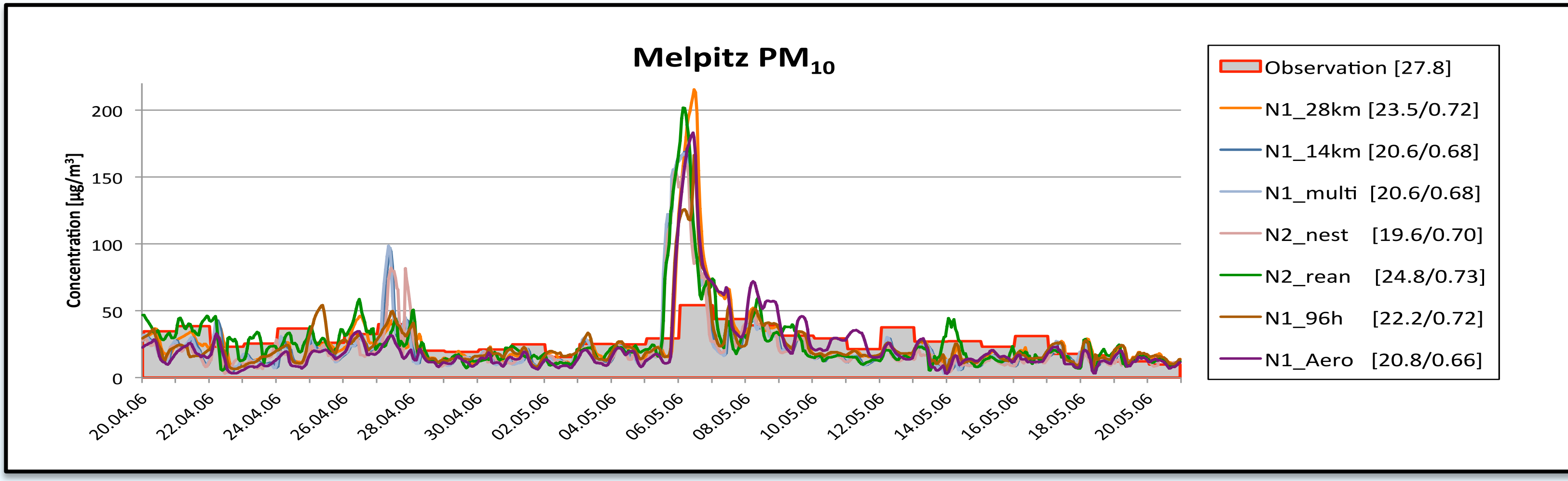


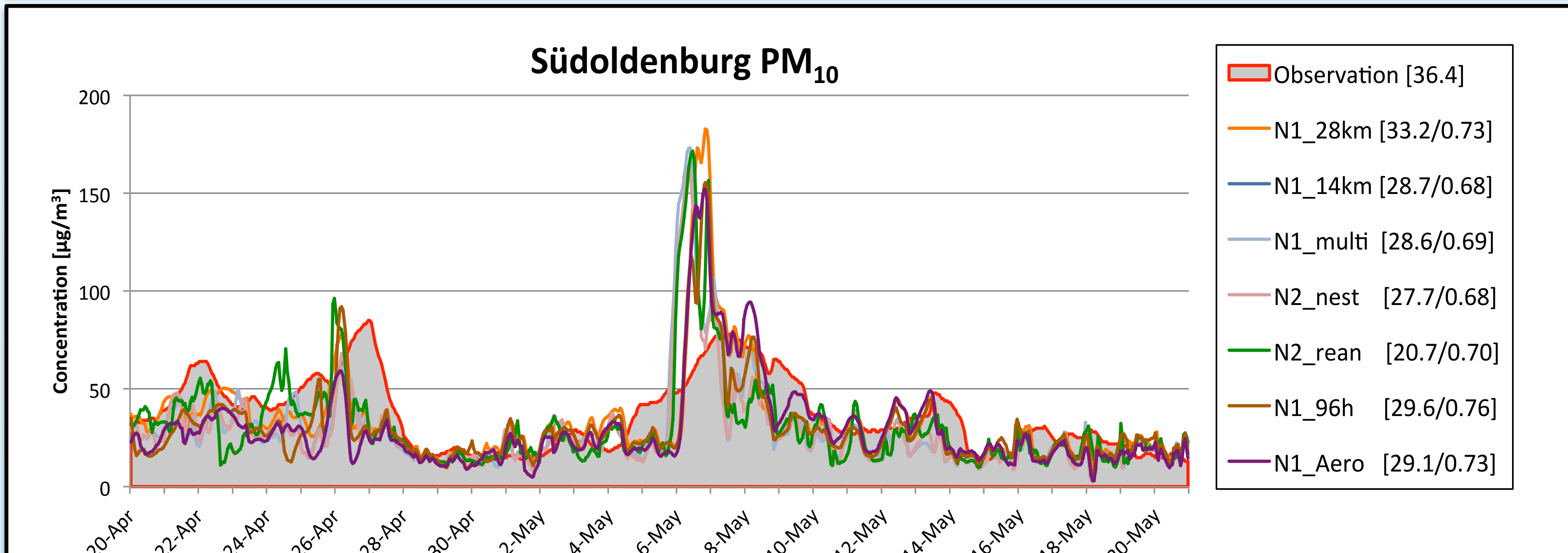
October 2006 for over 100 stations in Europe: rural (left) and suburban (right)

Comparison (both episodes): N2_rean vs. measurements

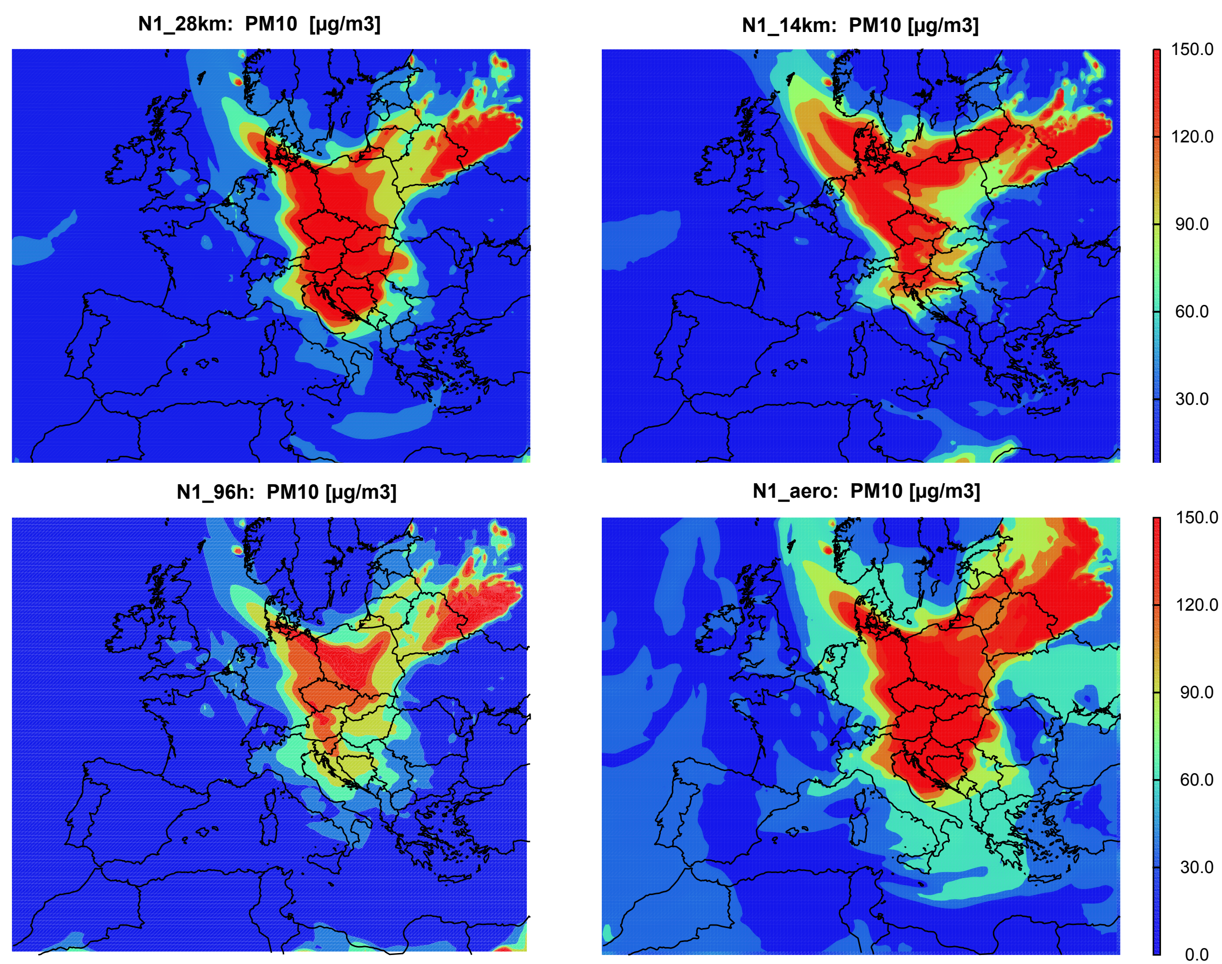


Comparison of the mean particle concentrations (April / May 2006)



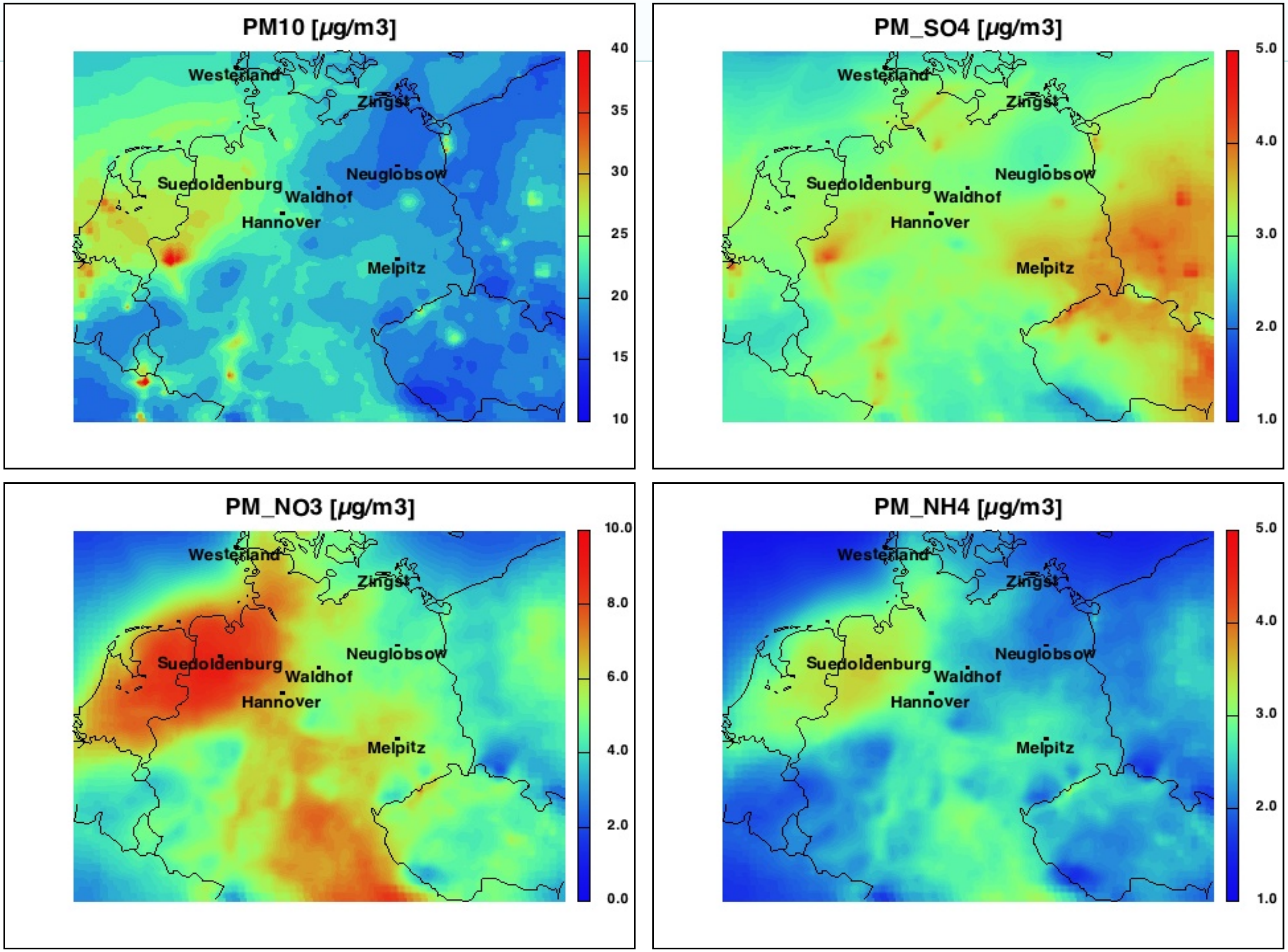


Comparison of PM10 over Europe computed with different setups

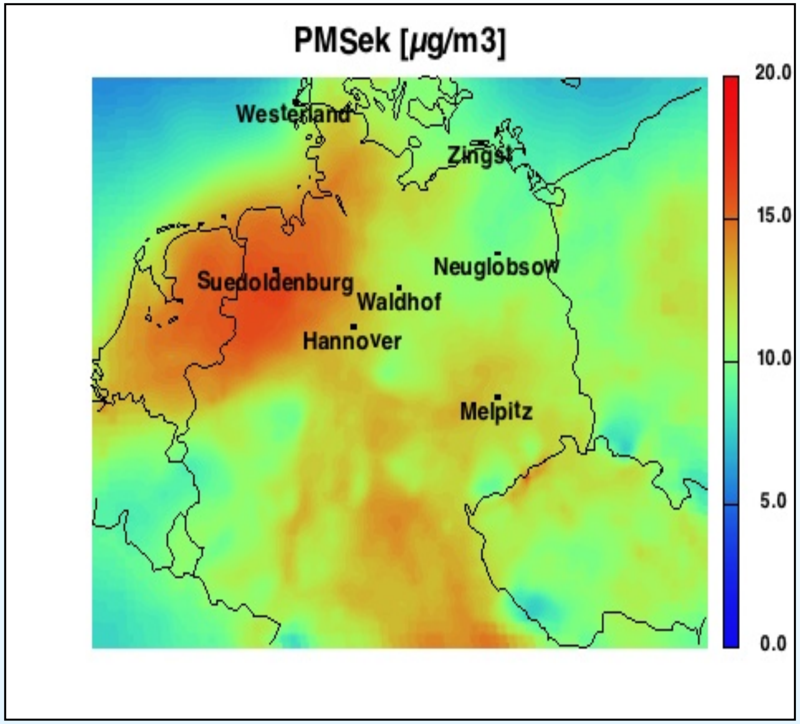


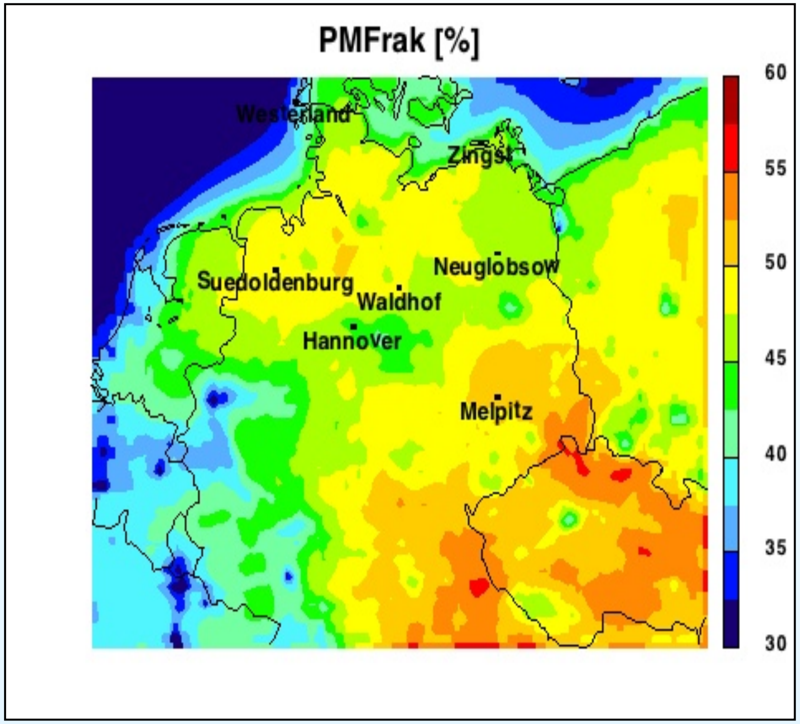
6th May 2006, 1:00 UTC

AQMEII (October 2006): PM



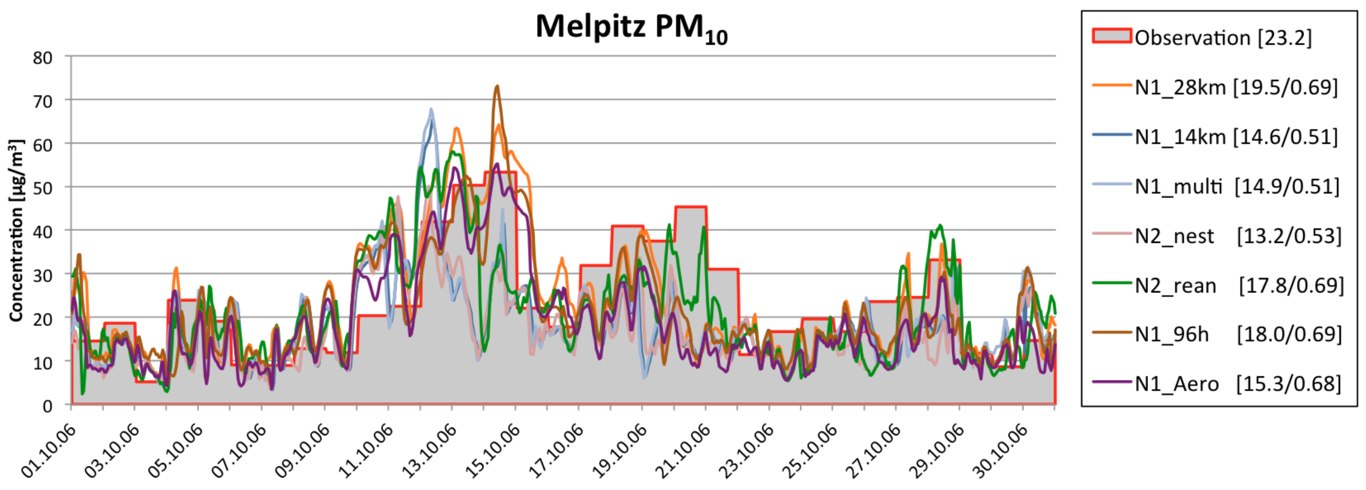
AQMEII (October 2006): PM

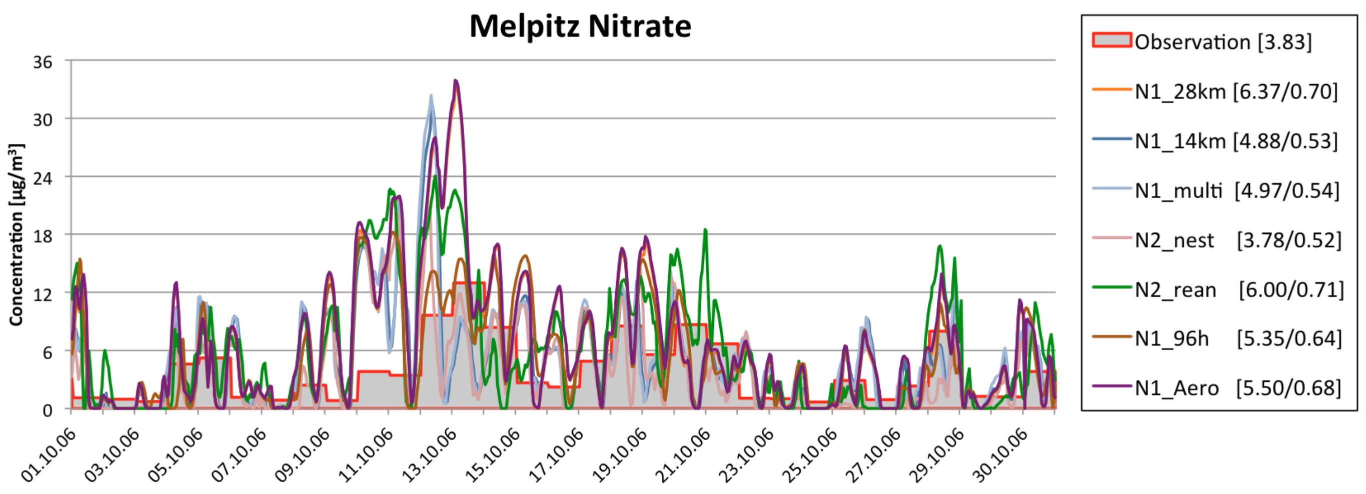




PMSek = total secondary formed organic and inorganic mass
PMFrak = PMSek / PM10

Comparison of the mean particle composition in Melpitz





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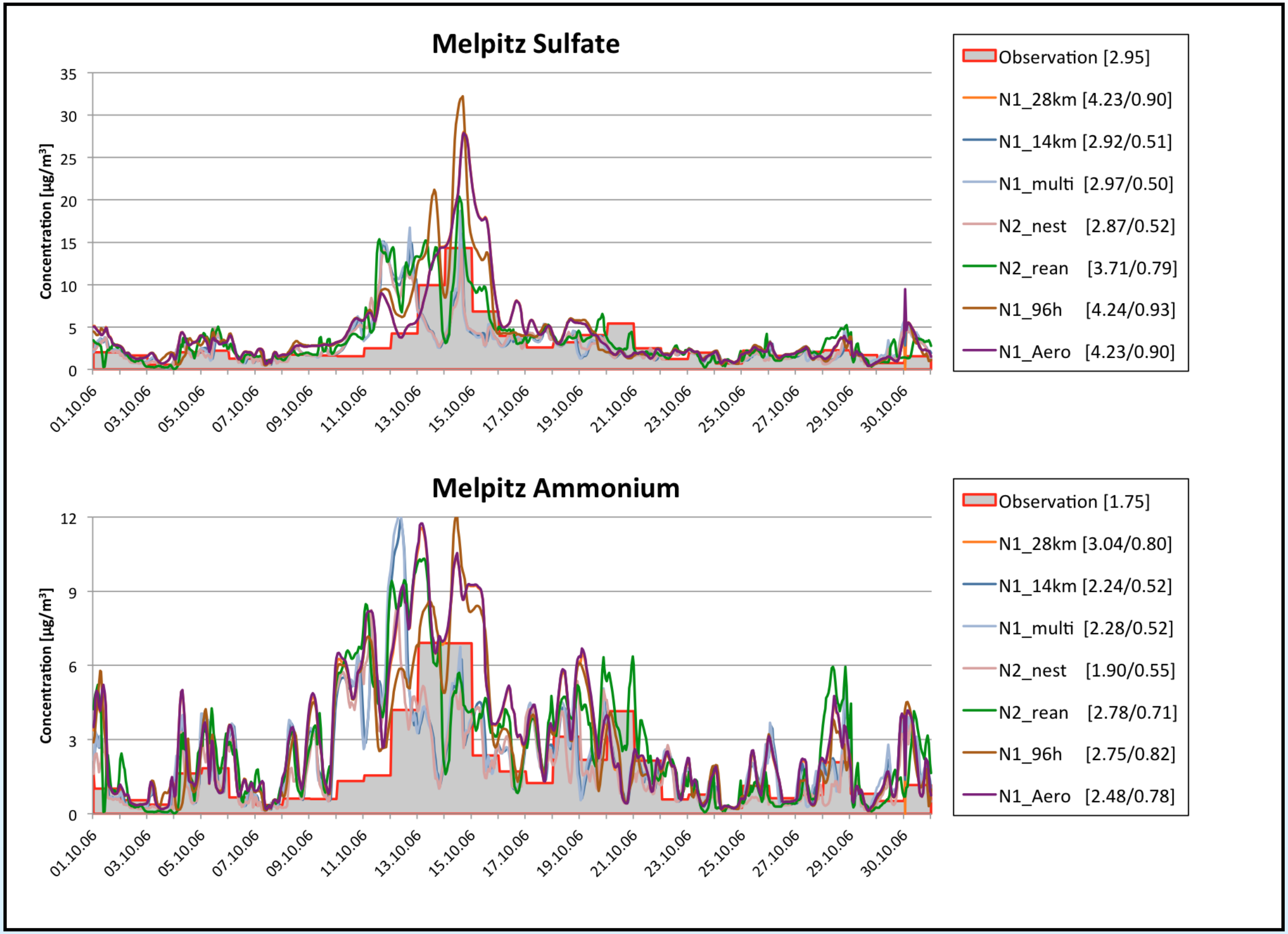
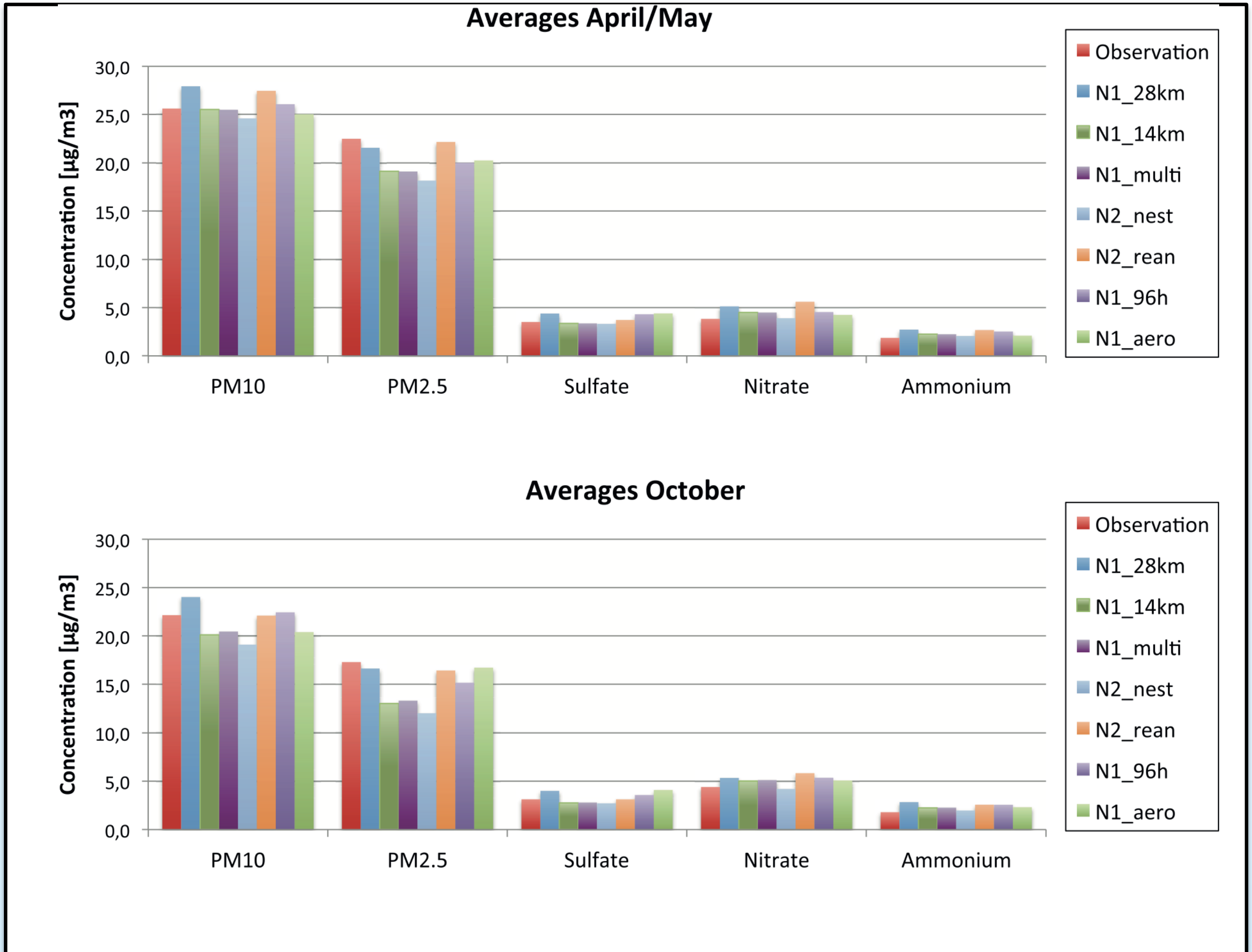


Comparison of monthly mean values: Measurements vs. different setups



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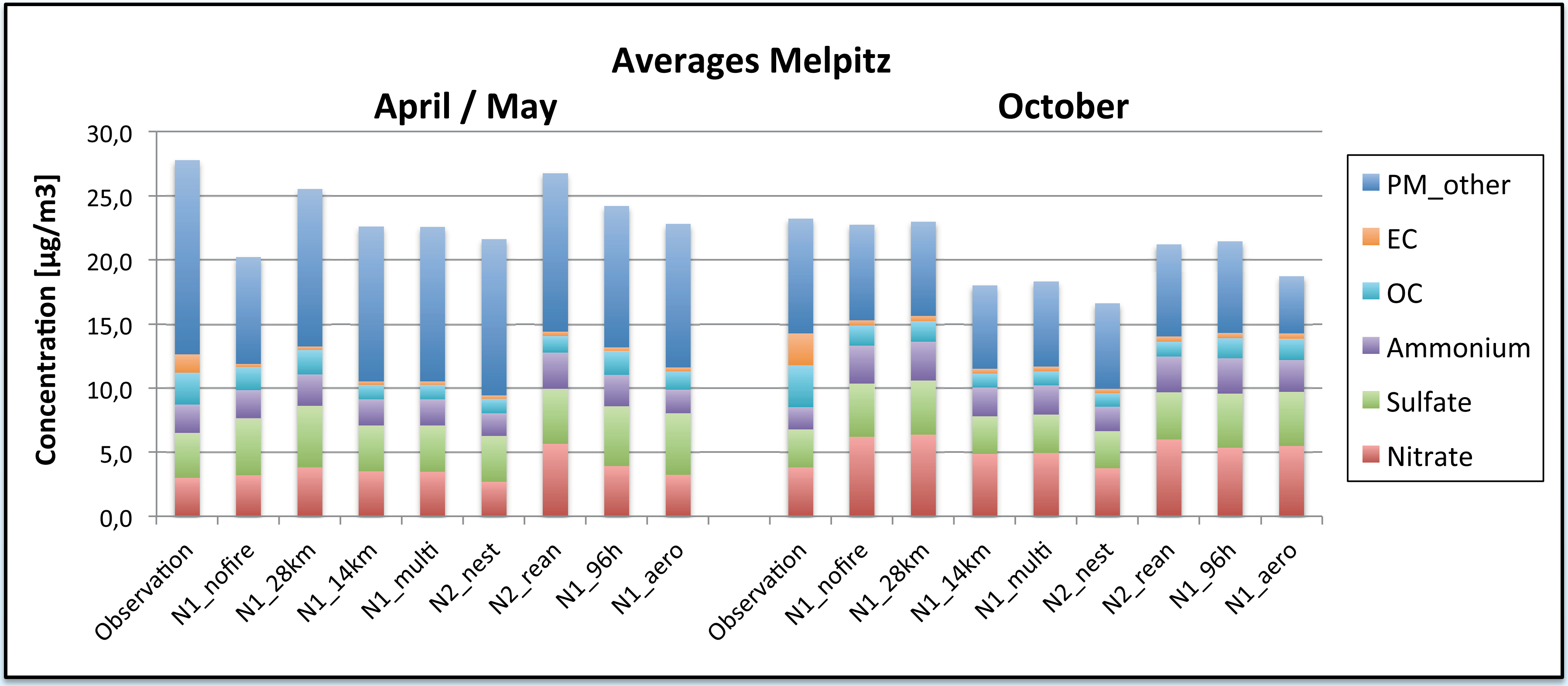

Comparison of different setups: Statistical analysis

	Particulate Matter				Composition						
	PM10 *(14 stations)*		PM2.5 *(10 stations)*		Sulphate *(7 stations)*		Nitrate *(7 stations)*		Ammonium *(7 stations)*		SIA
Model Setup	Average [µg/m3]	PCC	Average [µg/m3]	PCC	Average [µg/m3]	PCC	Average [µg/m3]	PCC	Average [µg/m3]	PCC	[%|
							21 April - 20 Mai 2006				
Observation	27.81		20.12		3.49		3.95		1.90		33.6
N1_28km	28.29	0.73	22.12	0.74	4.39	0.49	5.13	0.44	2.72	0.51	43.2
N1_14km	25.48	0.74	19.17	0.75	3.36	0.49	4.50	0.48	2.25	0.52	39.6
N1_multi	25.17	0.75	19.06	0.75	3.36	0.49	4.49	0.47	2.24	0.49	40.1
N2_nest	24.33	0.75	18.16	0.75	3.32	0.49	3.90	0.54	2.06	0.52	38.1
N2_rean	28.35	0.77	21.90	0.79	3.72	0.60	5.61	0.58	2.67	0.64	42.3
N1_96h	26.28	0.75	20.43	0.75	4.31	0.47	4.54	0.54	2.52	0.55	43.3
N1_Aero	24.80	0.75	20.24	0.66	4.40	0.51	4.24	0.36	2.09	0.42	43.3
							1 - 31 October 2006				
Observation	21.17		15.54		3.11		4.36		1.78		43.7
N1_28km	20.13	0.78	17.53	0.77	4.00	0.88	5.90	0.72	2.83	0.79	63.3
N1_14km	18.35	0.58	13.91	0.55	2.75	0.60	5.03	0.55	2.23	0.52	54.5
N1_multi	18.39	0.57	14.12	0.53	2.79	0.59	5.11	0.55	2.26	0.51	55.3
N2_nest	17.84	0.63	12.80	0.59	2.71	0.63	4.19	0.63	1.98	0.59	49.8
N2_rean	19.19	0.78	15.55	0.75	3.12	0.76	5.83	0.77	2.57	0.73	60.0
N1_96h	19.51	0.73	16.19	0.74	3.57	0.84	5.36	0.66	2.56	0.74	58.9
N1_Aero	17.85	0.78	16.01	0.74	3.98	0.89	5.06	0.68	2.29	0.77	63.5

Comparison of different setups: Statistical analysis

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N2_nest	17.84	0.63	12.80	0.59	2.71	0.63	4.19	0.63	1.98	0.59	49.8
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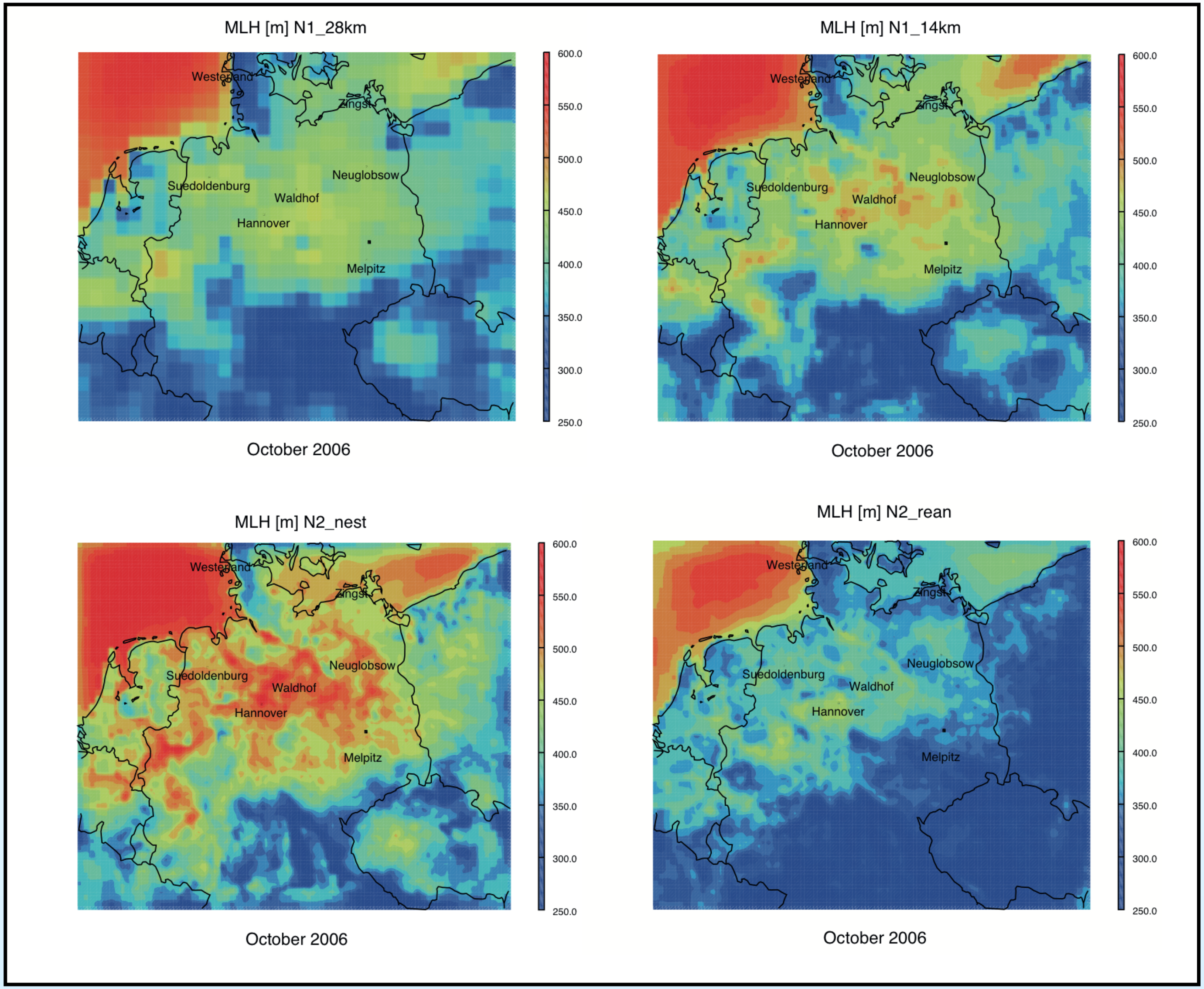
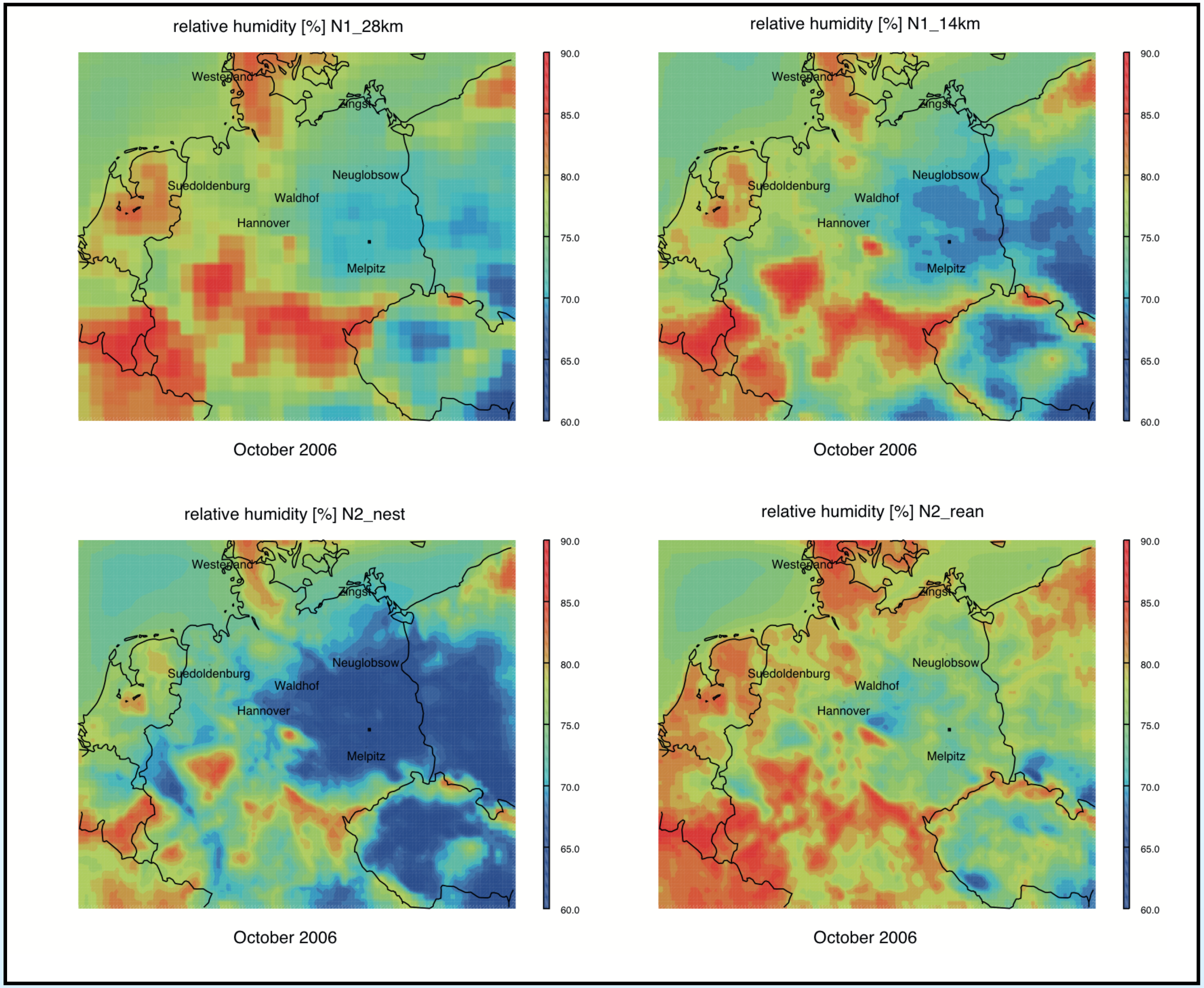
N1_96h	19.51	0.73	16.19	0.74	3.57	0.84	5.36	0.66	2.56	0.74	58.9
N1_Aero	17.85	0.78	16.01	0.74	3.98	0.89	5.06	0.68	2.29	0.77	63.5

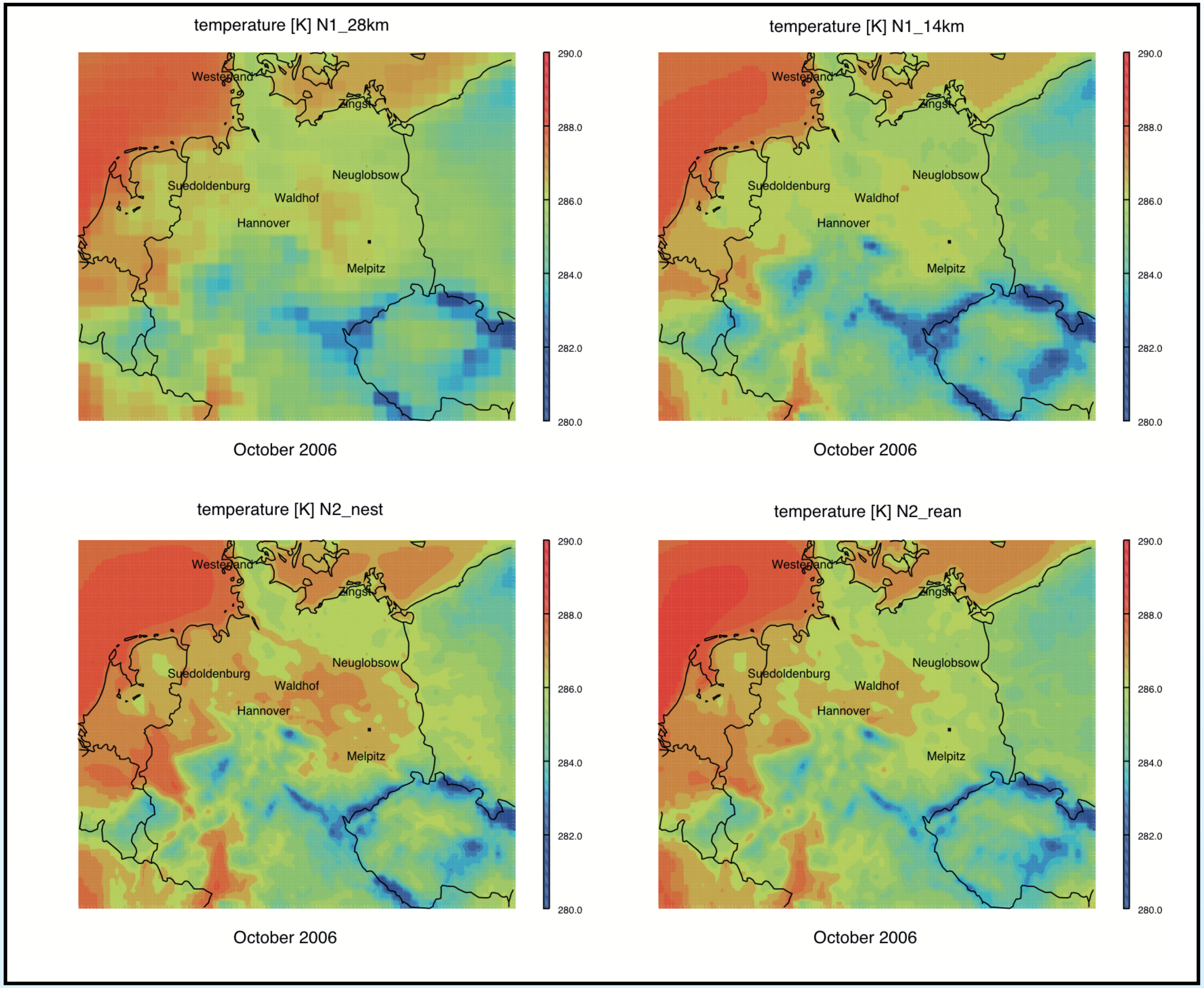
Simulated monthly mean values of PBL height for October 2006



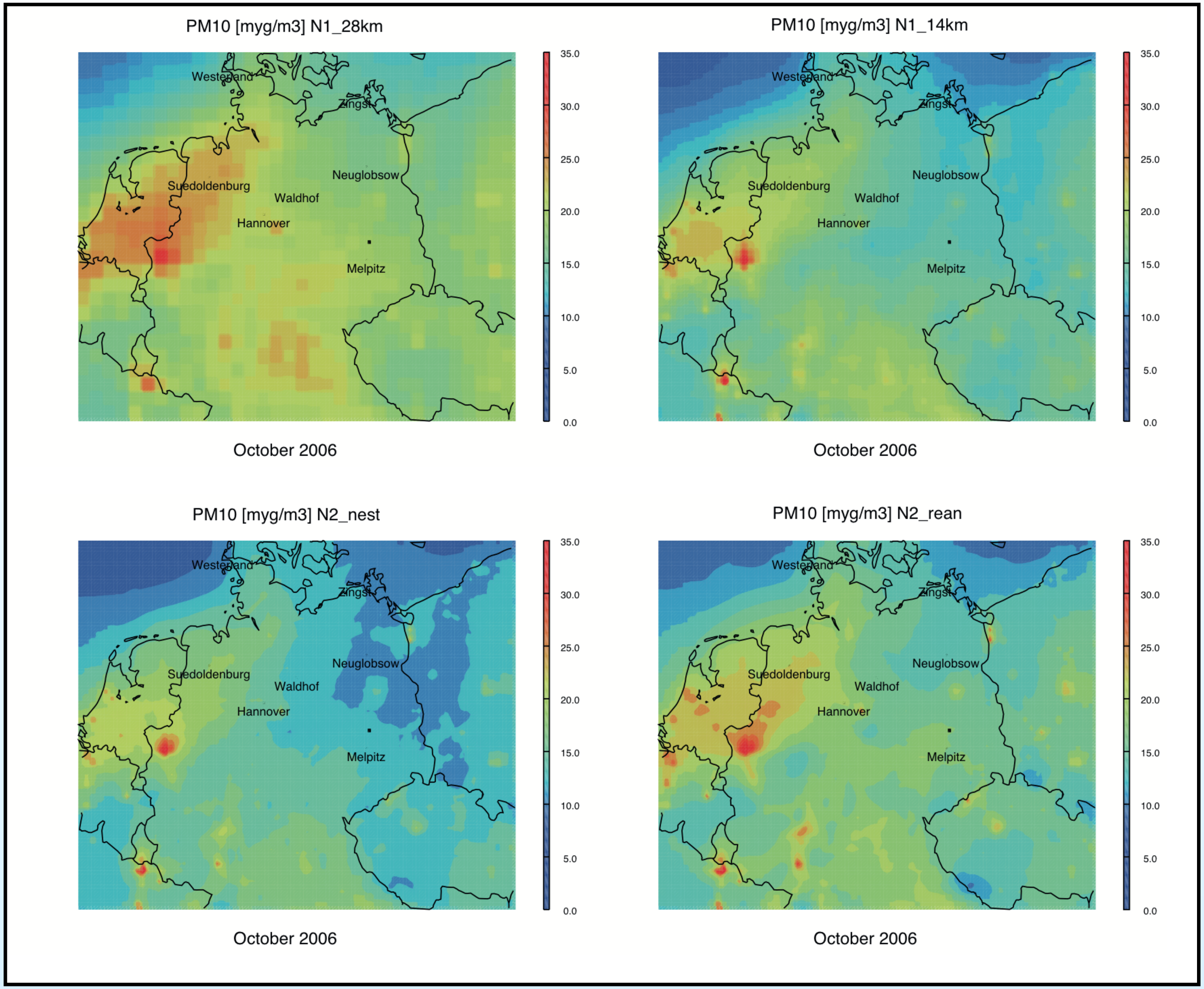
Simulated monthly mean values of relative humidity for October 2006



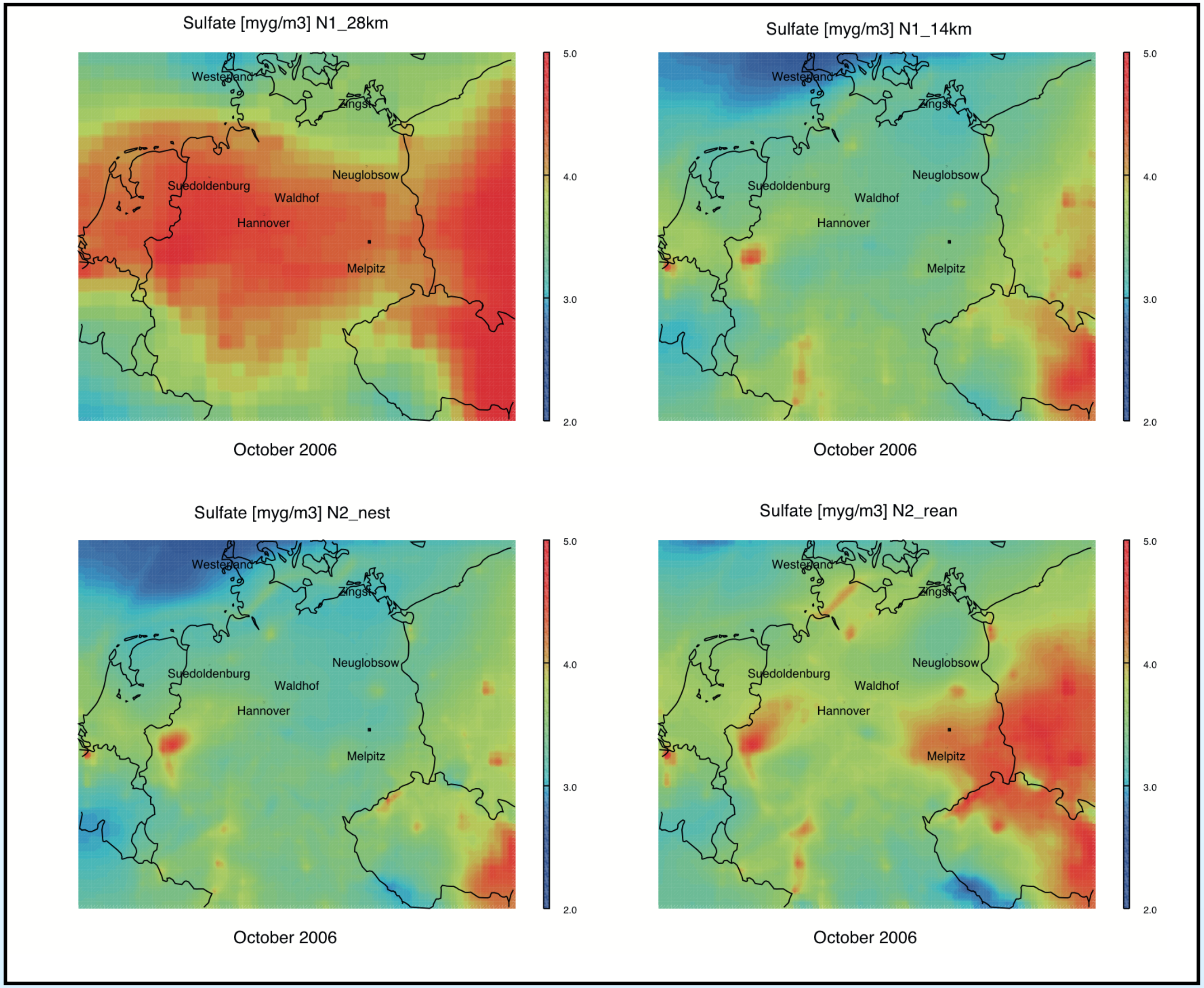
Simulated monthly mean values of temperature for October 2006



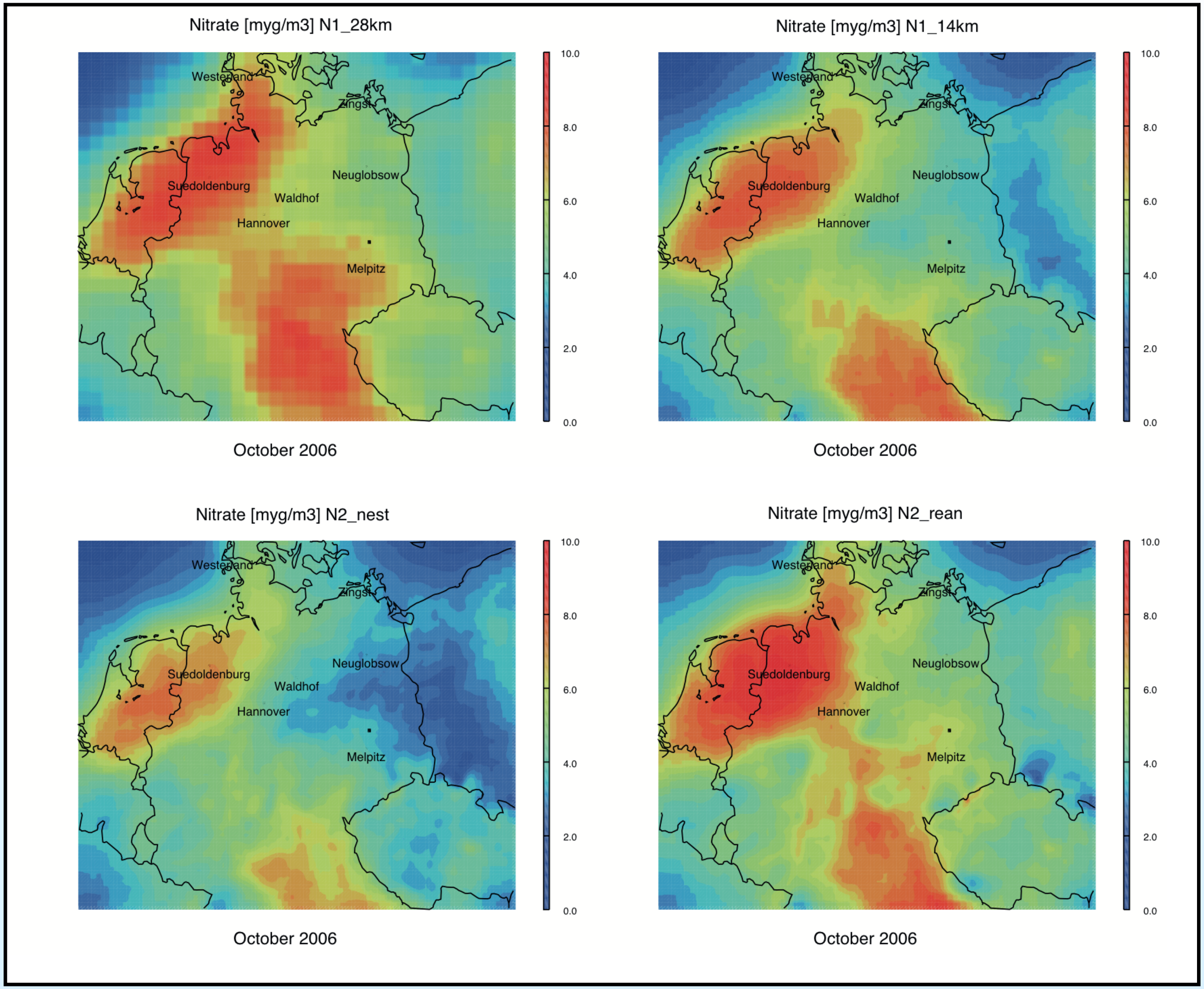
Simulated monthly mean values of PM10 for October 2006



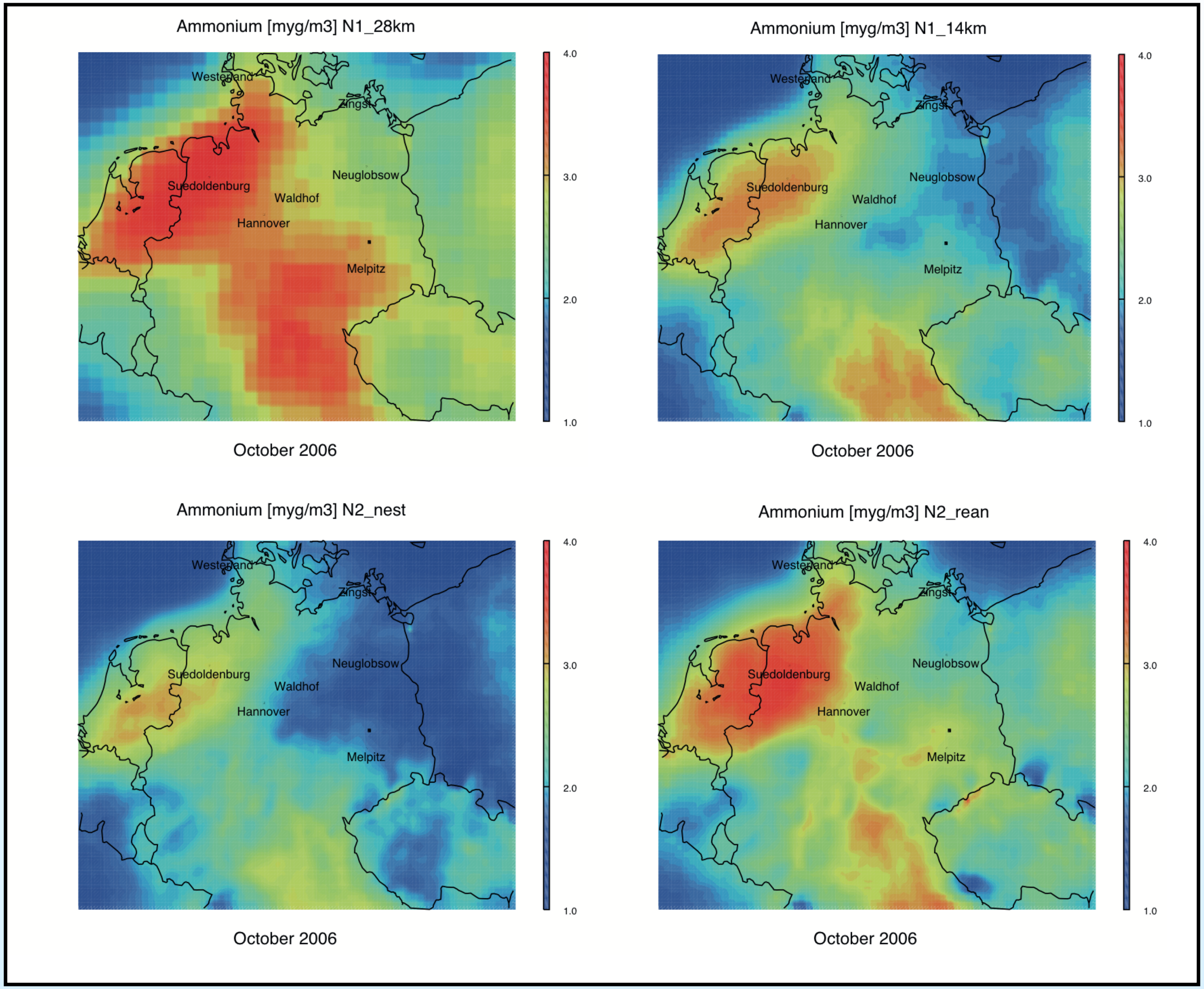
Simulated monthly mean values of sulfate for October 2006



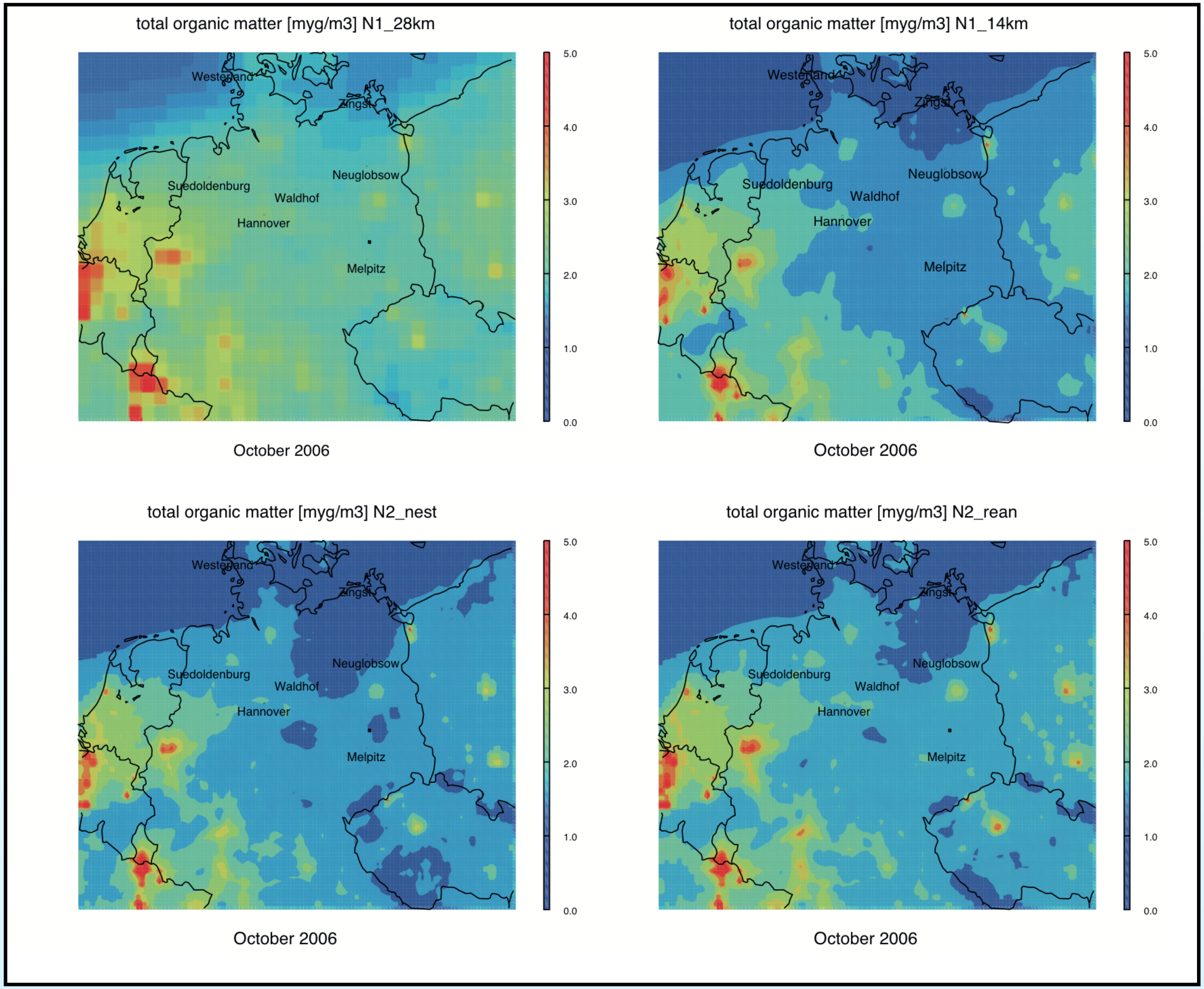
Simulated monthly mean values of nitrate for October 2006



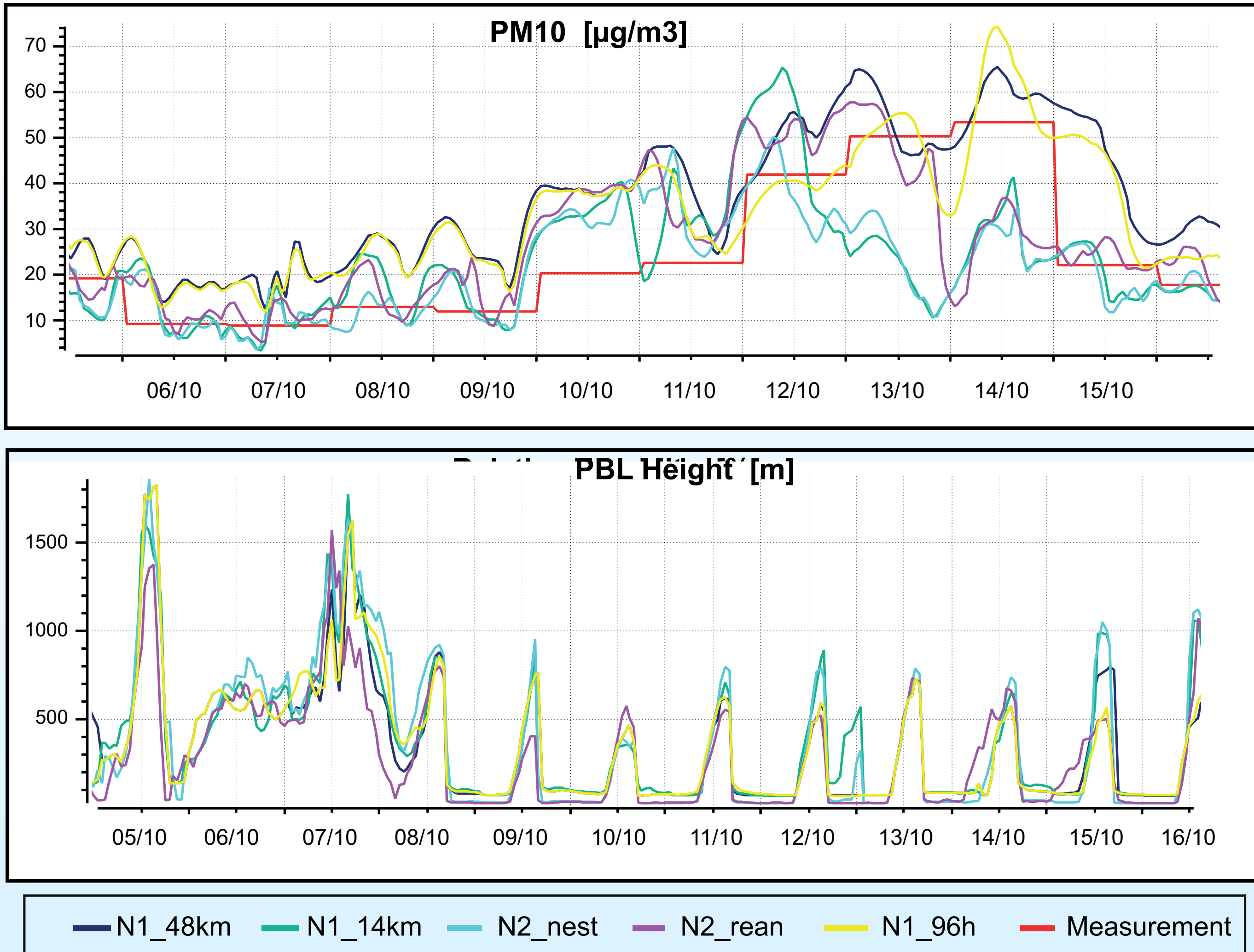
Simulated monthly mean values of ammonium for October 2006



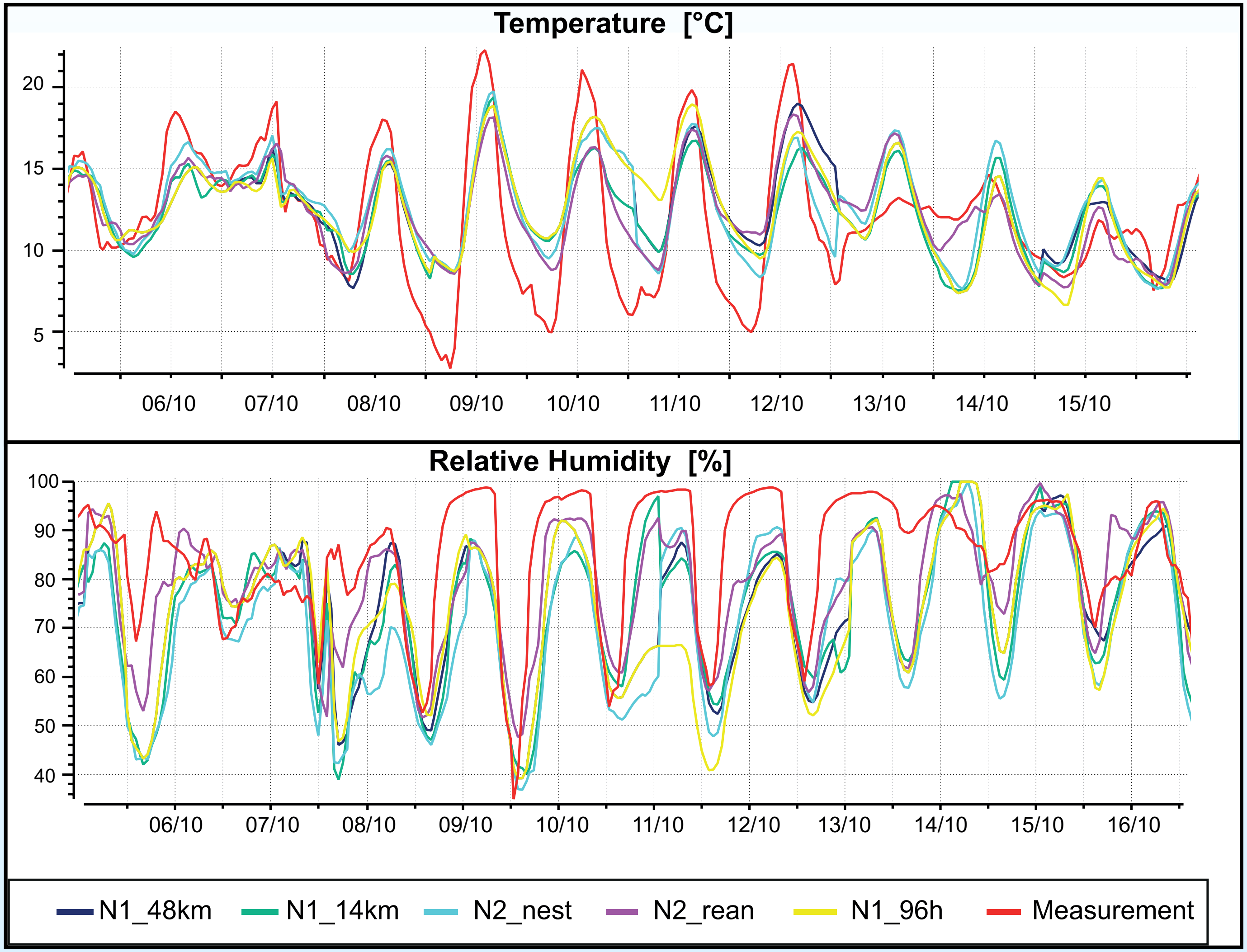
Simulated monthly mean values of total organic matter for October 2006



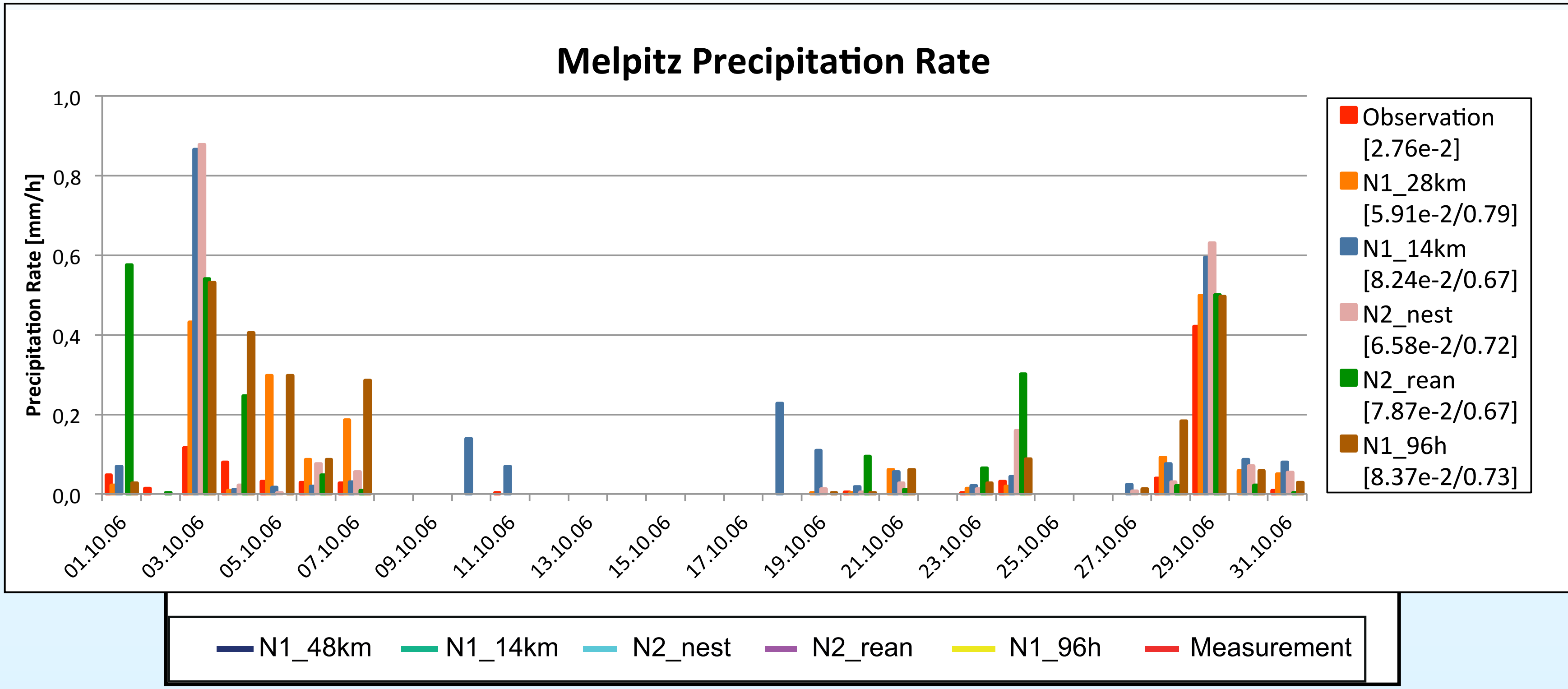
Time series in Melpitz during the period with high PM10 in October 2006



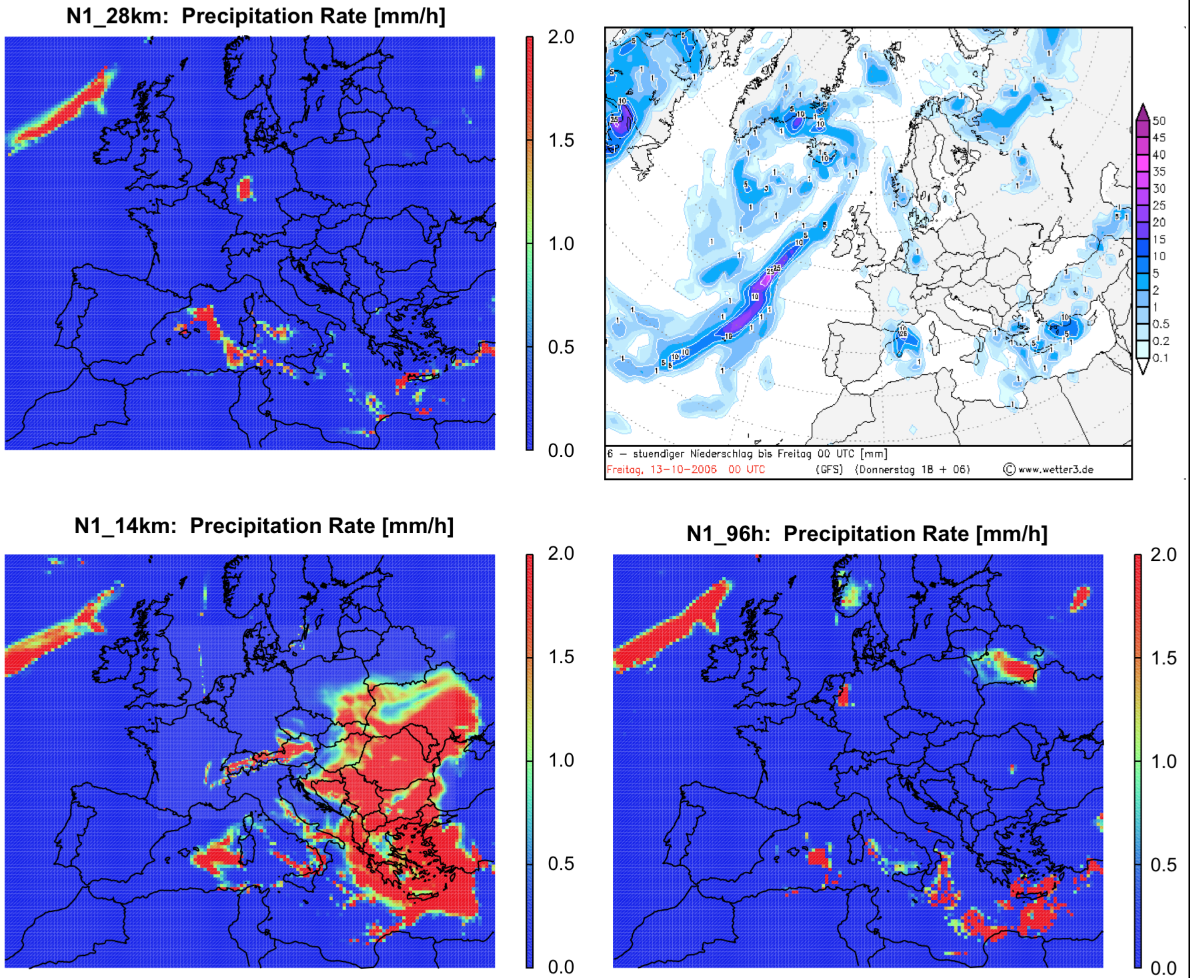
Time series in Melpitz during the period with high PM10 in October 2006



Time series in Melpitz during the period with high PM10 in October 2006



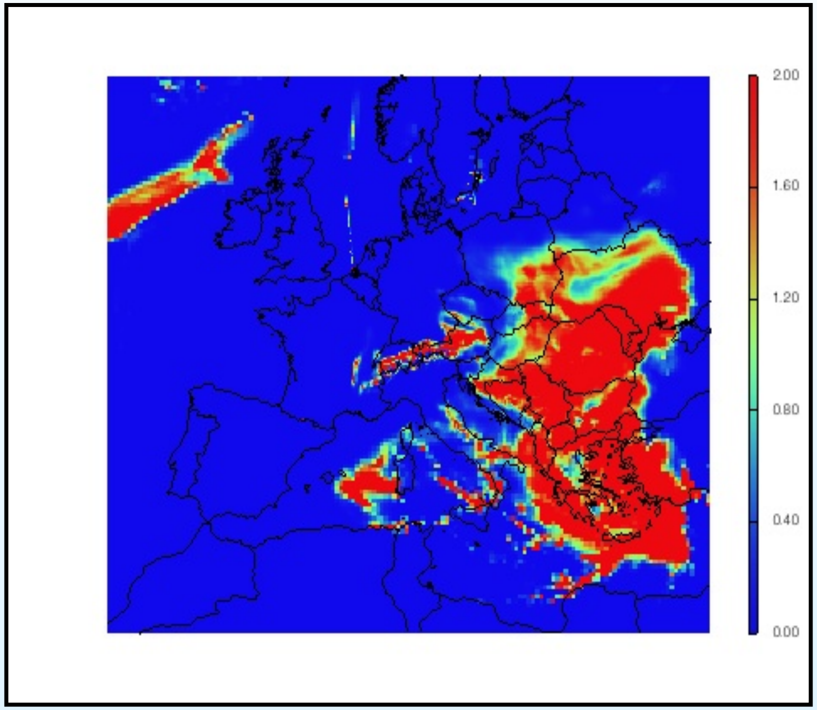
Comparison of simulated precipitation fields with 6-hour GFS forecast



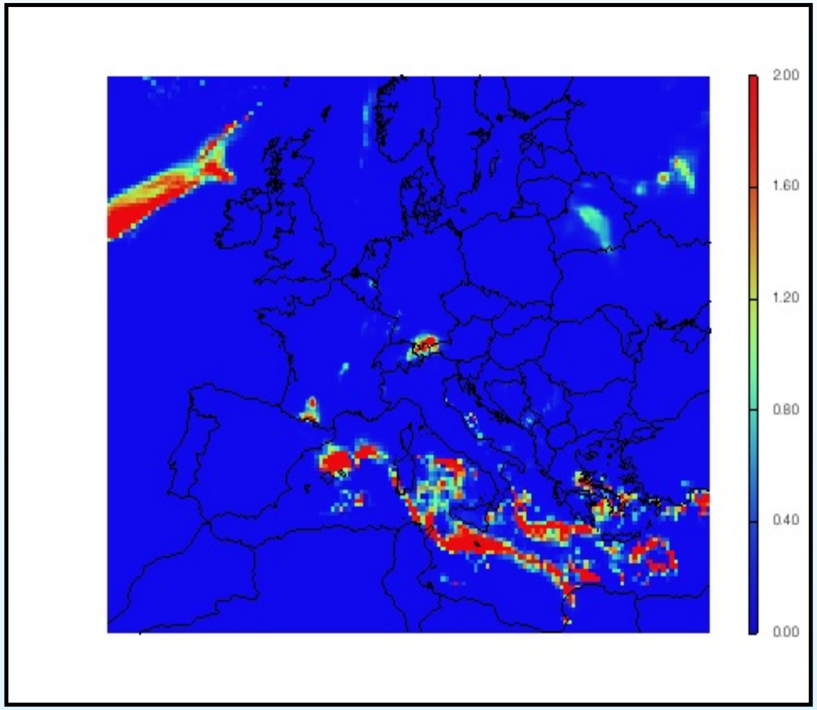
13th October 2006 (0:00 UTC)

Influence of cycle length: N1_14 km

N1_14 km (48 hours cycles)



N1_14km (24 hours cycles)



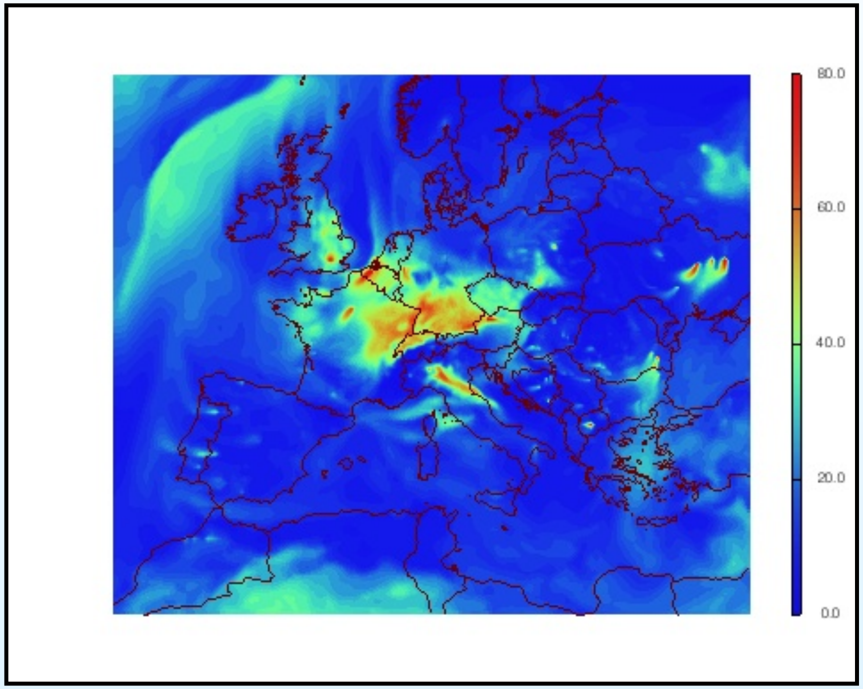
Precipitation rate [scale: 0 – 2 mm/h] at 13th October 2006, 12:00 UTC

Comparison of different model setups (modified)

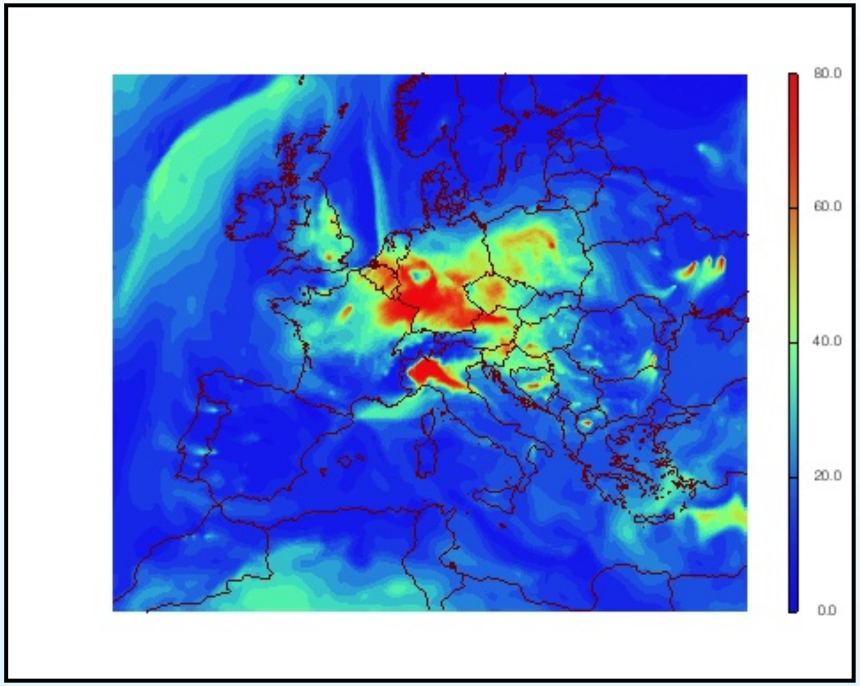
	Meteorology Model COSMO			Chemistry Transport Model MUSCAT				cycle length
	horizontal grid	vertical grid	forcing	horizontal grid	vertical layers (first layer)	boundaries	aerosol modul	
N1_28km	28 km	40 layers	GME reanalysis	uniform 28 km	22 (approx. 60 m)	GEMS	mass-based	48 h
N1_14km	14 km	40 layers	GME reanalysis	uniform 14 km	22 (approx. 60 m)	GEMS	mass-based	**24 h**
N1_multi	14 km	40 layers	GME reanalysis	multiscale (Figure)	22 (approx. 60 m)	GEMS	mass-based	**24 h**
N2_nest	7 km	50 layers	nested in N1	uniform 7 km	32 (approx. 20 m)	**N1_multi (24 h)**	mass-based	**24 h**
N2_rean	7 km	50 layers	COSMO reanalysis	uniform 7 km	32 (approx. 20 m)	**N1_multi (24 h)**	mass-based	**24 h**
N1_96h	28 km	40 layers	GME reanalysis	uniform 28 km	22 (approx. 60 m)	GEMS	mass-based	96 h
N1_aero	28 km	40 layers	GME reanalysis	uniform 28 km	22 (approx. 60 m)	GEMS	extended M7	48 h
N1_nofire	same configuration as ***N1_48km***, but without ”wildland fire“ emissions							

Influence of cycle length: N1_14 km

N1_14 km (48 hours cycles)



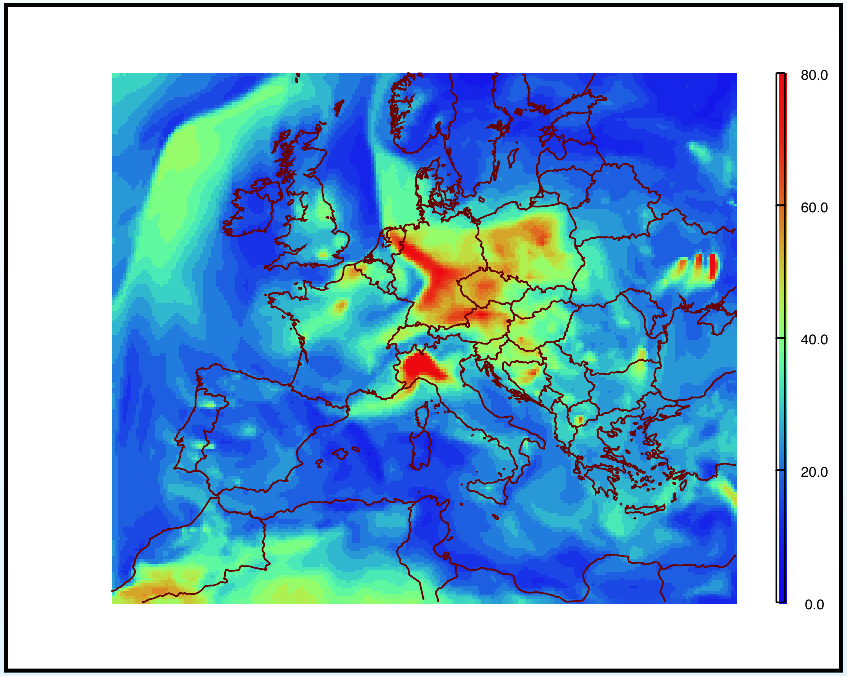
N1_14km (24 hours cycles)



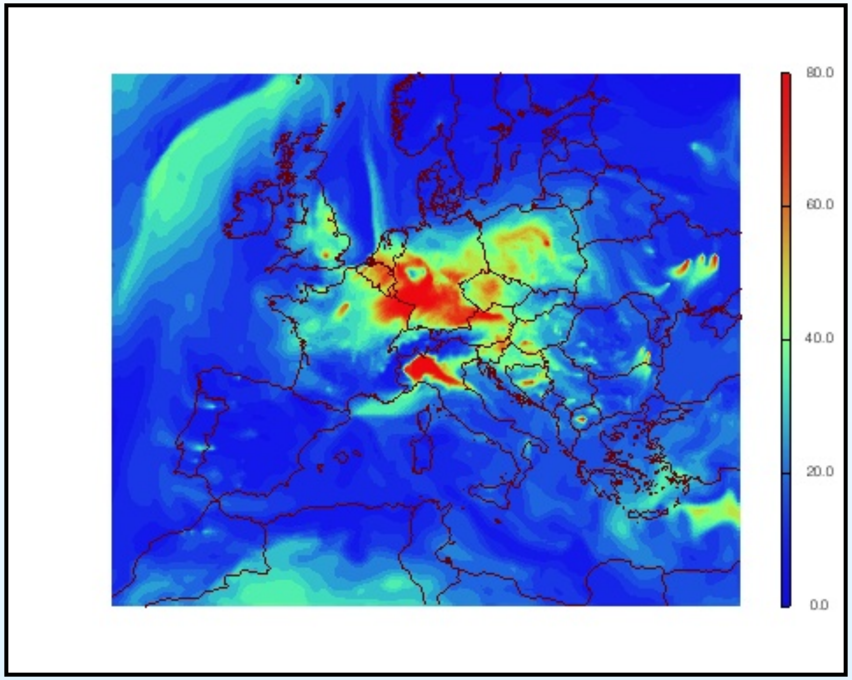
PM10 [scale: 0 - 80 µg/m^3] at 13th October 2006, 12:00 UTC

Influence of grid resolution: N1_28 km vs. N1_14 km

N1_28 km (48 hours cycles)



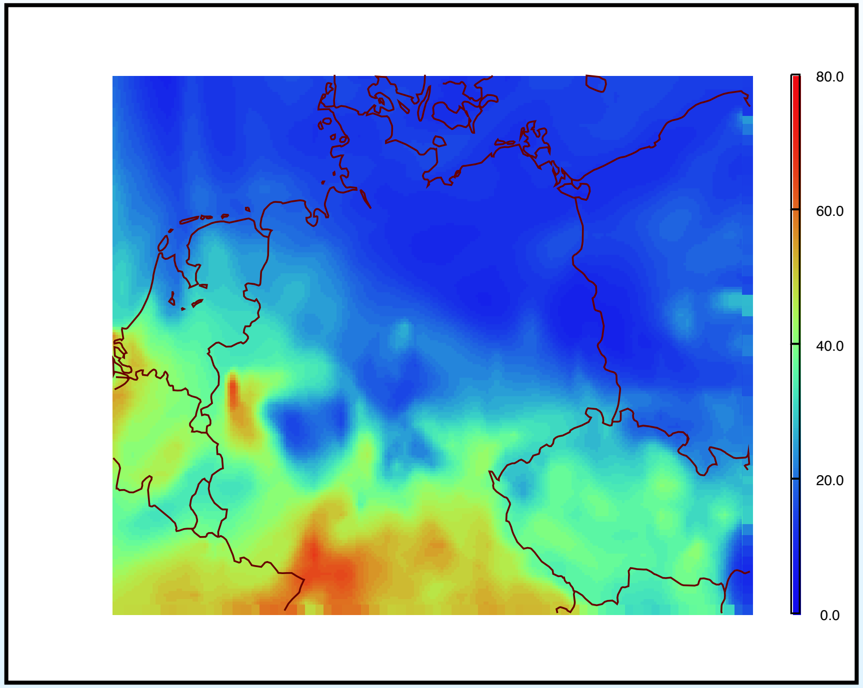
N1_14km (24 hours cycles)



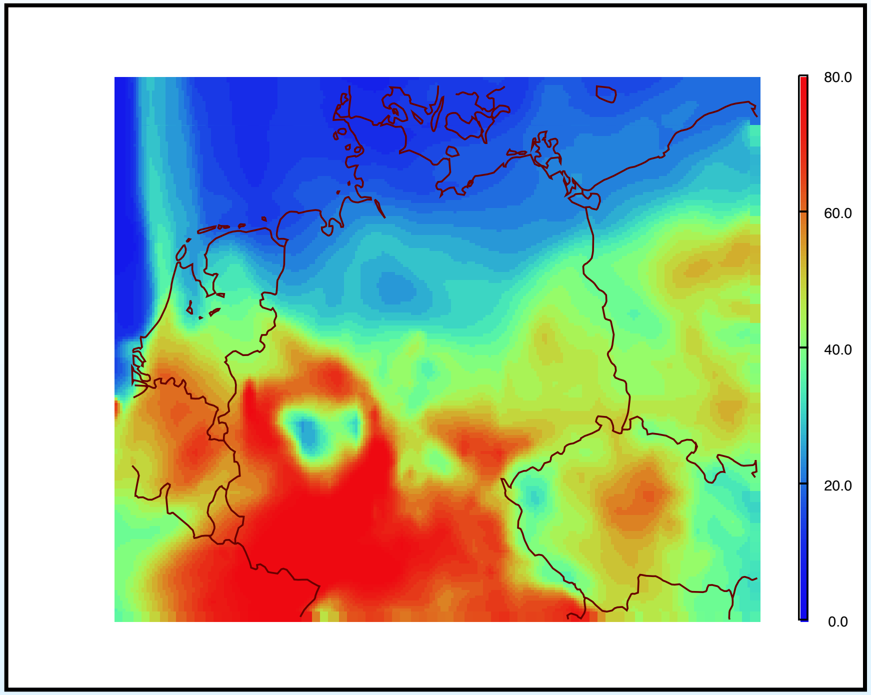
PM10 [scale: 0 - 80 µg/m^3] at 13th October 2006, 12:00 UTC

Influence of cycle length: N1_14 km run (zoomed for N2)

N1_14 km (48 hours cycles)

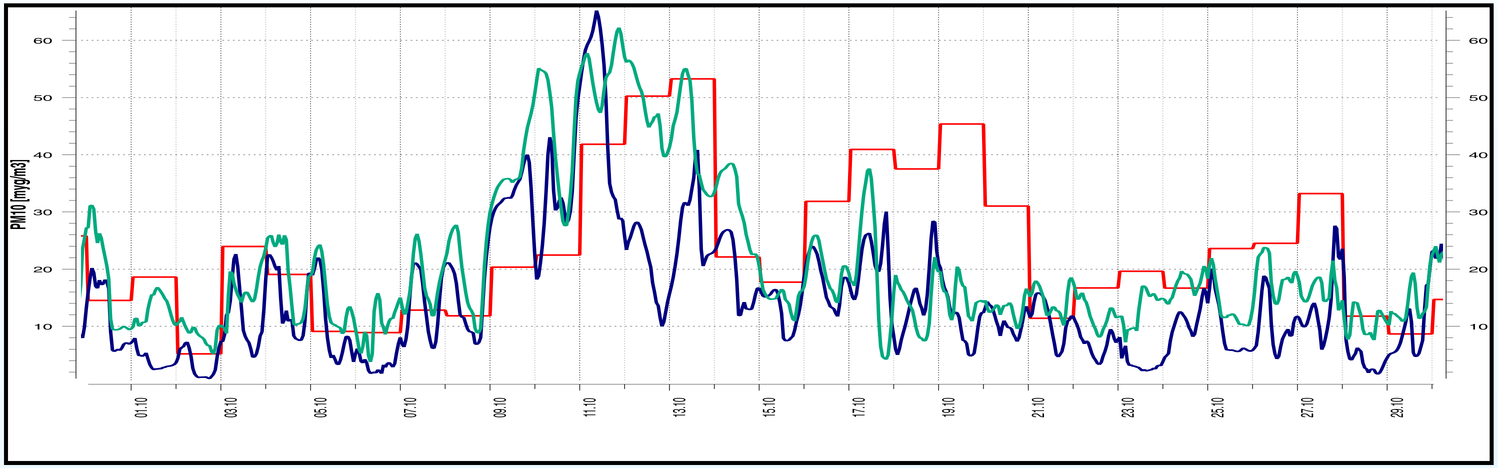


N1_14km (24 hours cycles)



PM10 [scale: 0 -80 μg/m^3] at 13th October 2006, 12:00 UTC

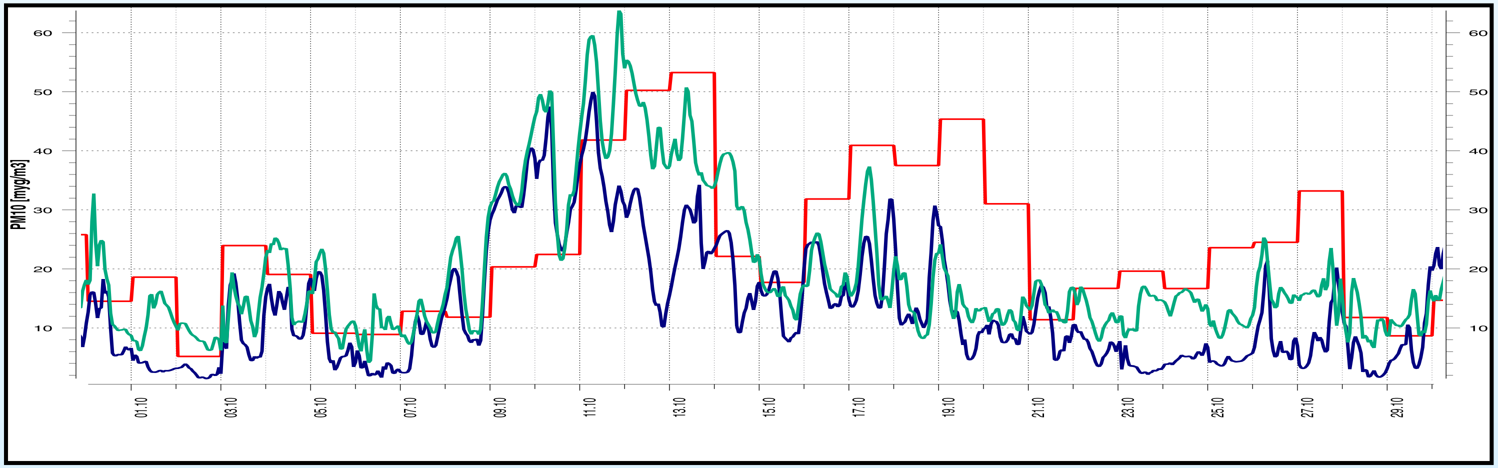
Influence of lateral boundaries and cycle length



Measurement
23.2

N1_14km (48 h)
14.6 / 0.51

N1_14km (24 h)
20.2 / 0.50

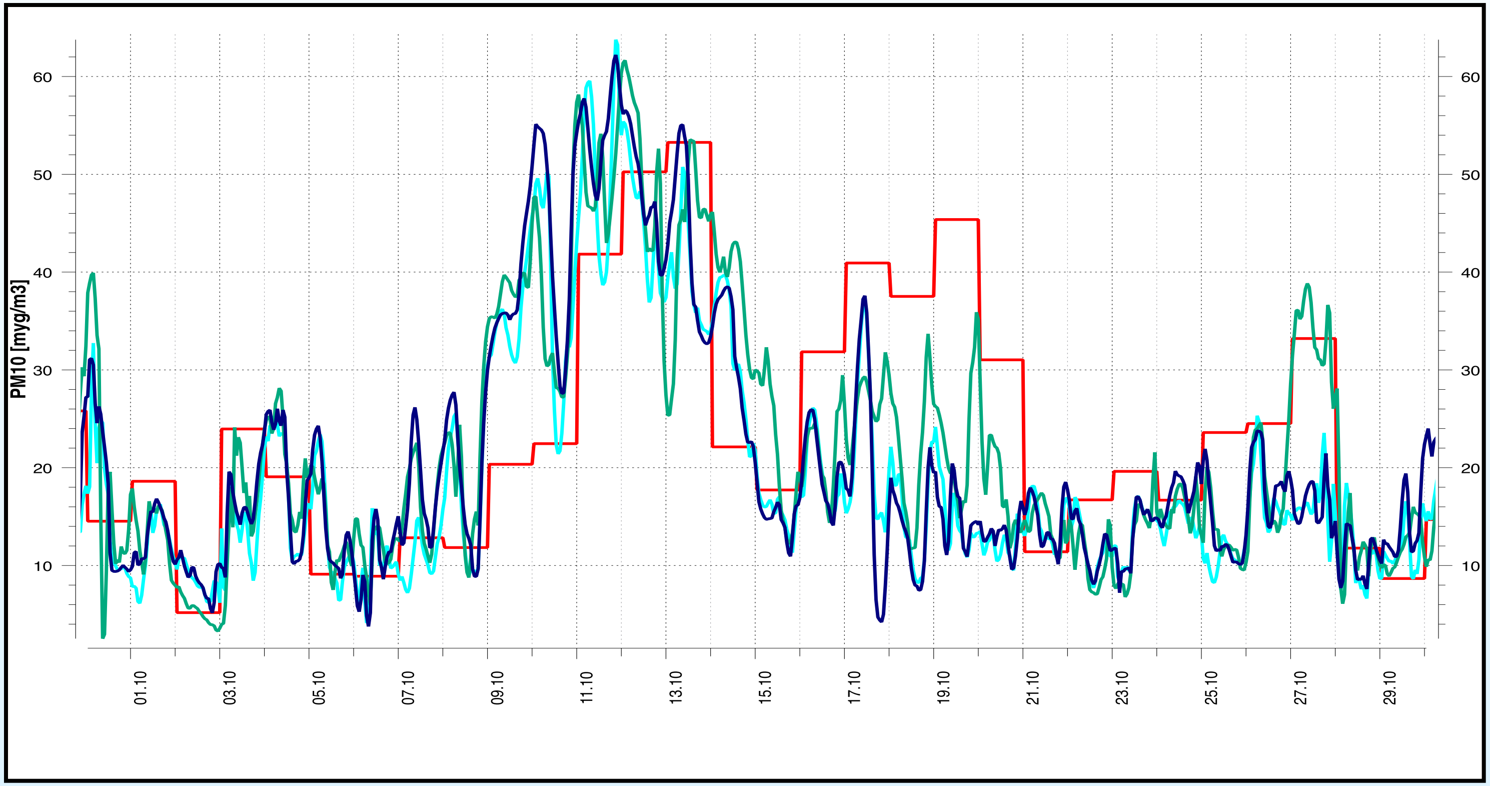


Measurement
23.2

N2_nest (48 h)
13.2 / 0.53

N2_nest (24 h)
18.73 / 0.54

Influence of grid size and meteorological forcing



Measurement
23.2

N1_14km (24 h)
20.2 / 0.50

N2_rean (24 h)
21.10 / 0.58

N2_nest (24 h)
18.73 / 0.54

Comparison of different setups: Statistical analysis

	Particulate Matter				Composition						
	PM10 *(14 stations)*		PM2.5 *(10 stations)*		Sulphate *(7 stations)*		Nitrate *(7 stations)*		Ammonium *(7 stations)*		SIA
Model Setup	Average [µg/m3]	PCC	Average [µg/m3]	PCC	Average [µg/m3]	PCC	Average [µg/m3]	PCC	Average [µg/m3]	PCC	[%|
					1 - 31 October 2006						
Observation	21.17		15.54		3.11		4.36		1.78		43.7
N1_28km	20.13	0.78	17.53	0.77	4.00	0.88	5.90	0.72	2.83	0.79	63.3
N1_14km	20.35	0.75	15.18	0.70	3.35	0.80	5.43	0.75	2.53	0.72	55,6
N1_multi	20.39	0.78	15.22	0.73	3.39	0.79	5.18	0.75	2.52	0.74	54,4
N2_nest	20.43	0.78	15..27	0.73	3.41	0.81	5.29	0.73	2.48	0.73	54,7
N2_rean	20.54	0.80	15.85	0.79	3.32	0.85	5.70	0.79	2.42	0.78	57,6
N1_96h	19.51	0.73	16.19	0.74	3.57	0.84	5.36	0.66	2.56	0.74	58.9
N1_Aero	17.85	0.78	16.01	0.74	3.98	0.89	5.06	0.68	2.29	0.77	63.5

Summary and outlook

TROPOS
Leibniz Institute for Tropospheric Research

- Sensitivity and robustness of results against grid resolution and meteorological forcing was investigated. A set of 7 different setups was used.
- Simulations of COSMO-MUSCAT are compared with measurements. The “ensemble” of setups can capture the range and variability of PM10.
- One key finding is the relatively high responsivity concerning changes in the model configuration. Clear and unexpected large spreading of the results.
- The influence of meteorological forcing seems to more significant than the better resolution of emission and deposition fluxes.
- Online coupled vs. offline forcing with reanalyzed data: Feedback studies, forecast, process studies?

Acknowledgement

This work was supported by the AQMEII consortium, TNO, NIC Jülich and the ZIH Dresden. Furthermore, we thank the DWD for good cooperation.

Thank You!