Simulating with CMAQ the transport of PAHs over Europe

First application to Benzo(a)Pyrene

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Research Objectives

- Investigation and assessment of air pollution , i.e. persistant organic pollutants (POPs) in Europe

- Deposition of POPs into the North and Baltic Sea

- Focus on coastal regions

- Evaluation of past and forecast of future developments (scenarios)

- Assessment of the impact of regulations

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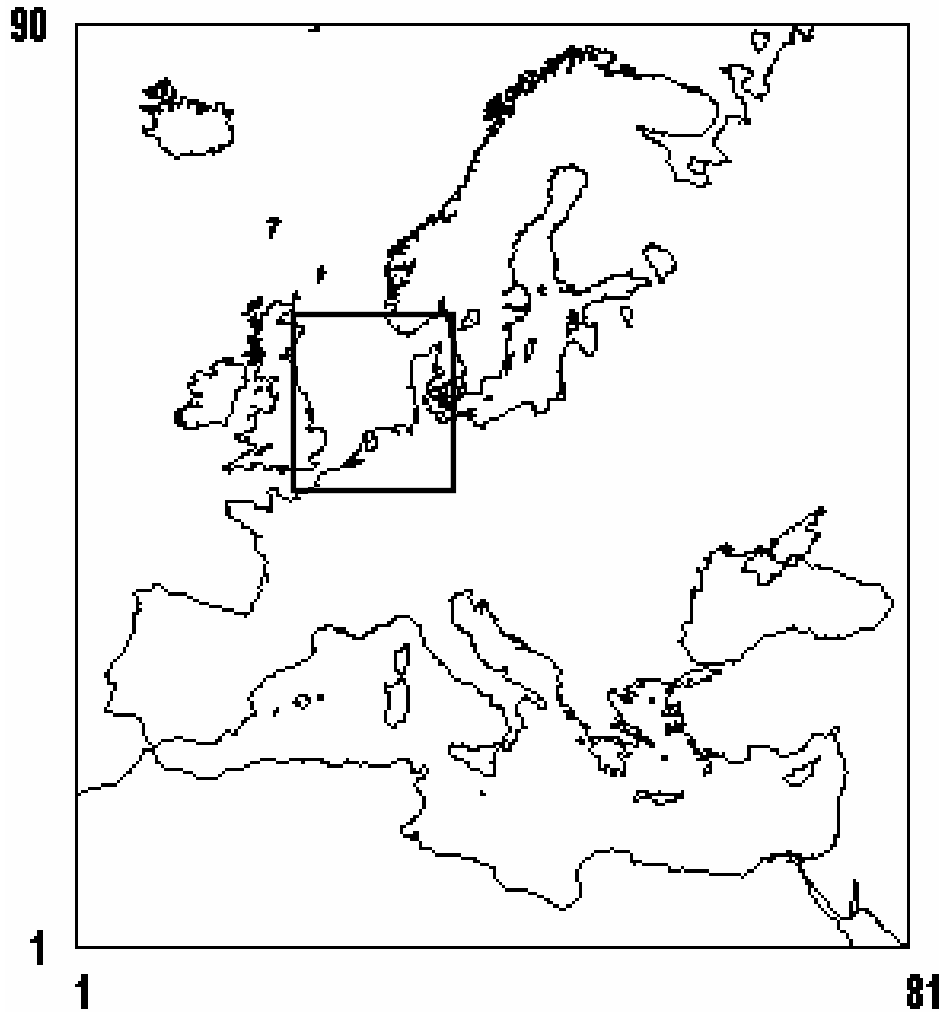
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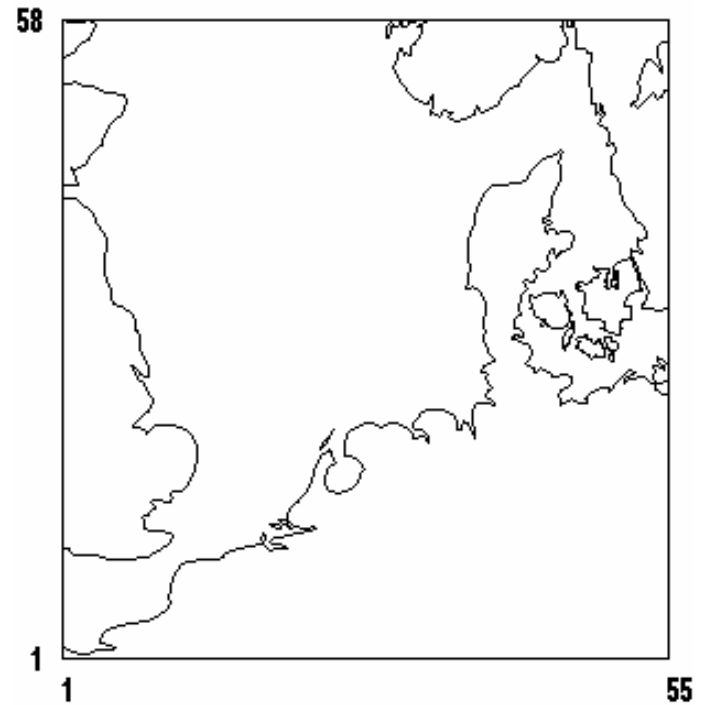
BaP
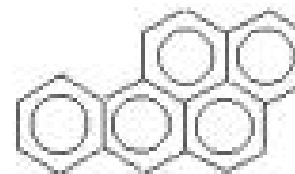
Benzo(a)pyren

- Belongs to PAHs
- Main sources anthropogenic
- Incomplete combustion of fossil fuels
- Carcinogenic
- Cause birth defects
- Impair reproduction
- Impair immune system

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CMAQ model domain and nest

54x54 km² grid

18x18 km² grid

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Meteorology

Meteorological fields are calculated with MM5

- <u>Boundary Layer:</u>

MRF (Hong and Pan, 1996), based on Troen and Mahrt (1986) nonlocal diffusion concept.

- <u>Microphysics:</u>

Reisner2, incl. ice, snow and graupel (Reisner et al., 1998).

- <u>Cumulus:</u>

Kain Fritsch 2, conservation of mass, thermal energy, total moisture and momentum (Kain and Fritsch, 1993)

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Emissions

- BaP emissions of 1993, provided by Dr. Knut Breivik on the 50 x 50 km² polar stereographic EMEP grid. Emissions in September are assumed to be ¼ of the average monthly emissions.

- Hourly emissions of of June 1 2001 for NO_x, SO_2 and NMVOC on the 54 km and 18 km CMAQ grid provided by the IER Stuttgart re-used for each simulation day.

- Yearly emissions of coarse and fine particles (PM10 and PM2.5) as well as CO and NH_3 from EMEP database (WEBDAB) EMEP grid.

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Emissions

BaP emissions september 1993

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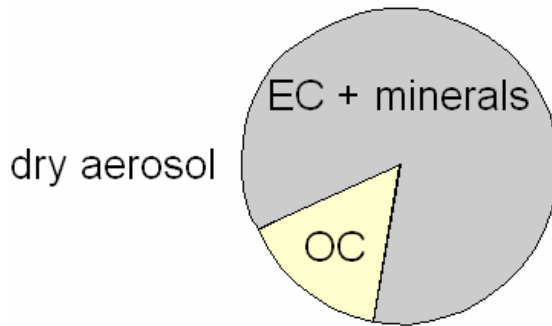
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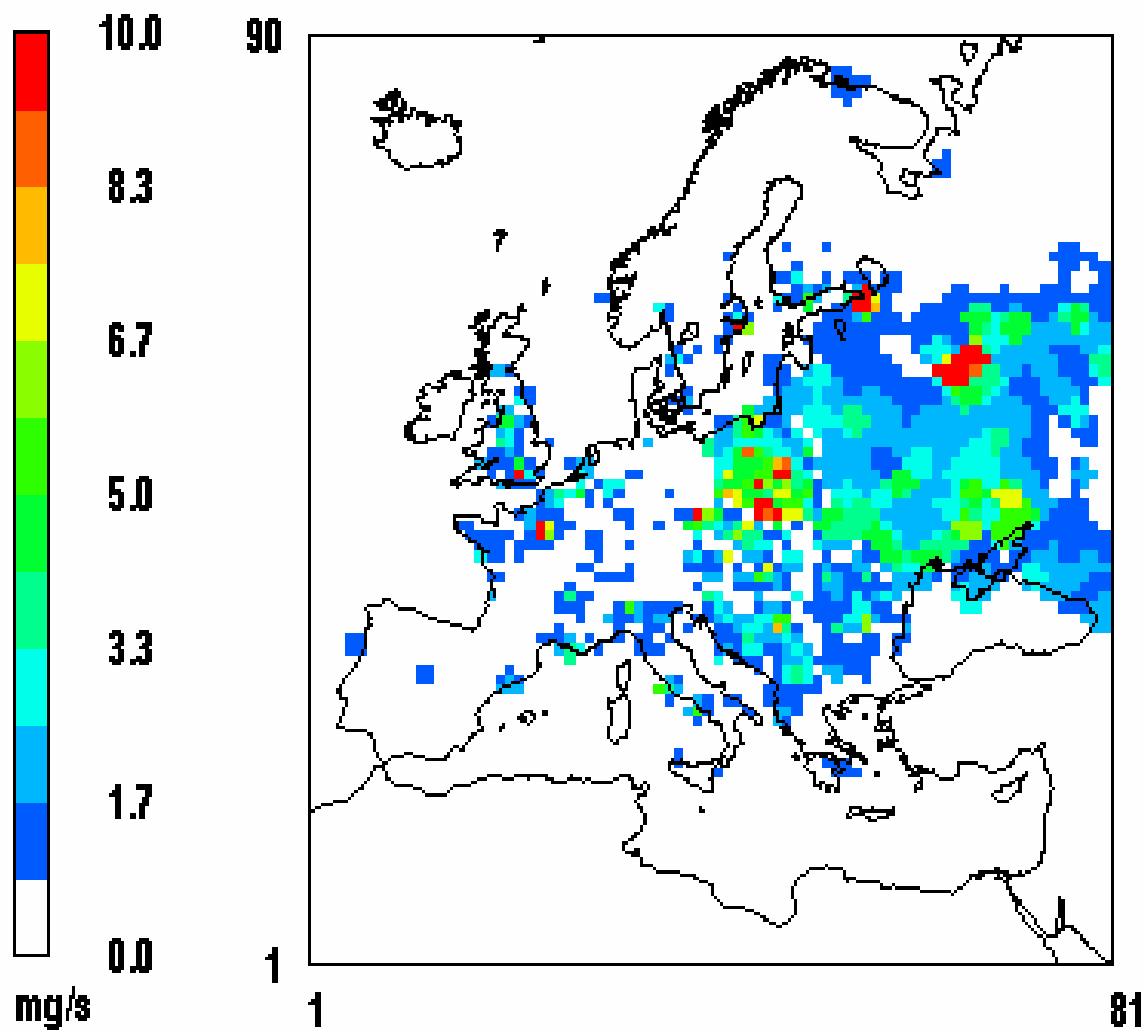
Processes

- Emitted as accumulation mode aerosol (with 0.1% in Aitken-mode)

- Gas-particle partitioning (Junge-Pankow concept)

- Dry deposition, scavenging and wet deposition

- No photolytical and chemical degradation so far

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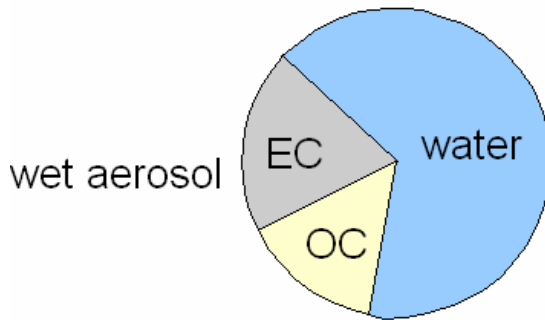FORSCHUNGSZENTRUM

Partitioning

processes | phys-chem. properties

dry aerosol

adsorbtion to elemental carbon and minerals

absorbtion into organic carbon

vapor pressure

octanol-air partitioning coefficient

Henry's law constant

wet aerosol

adsorbtion to elemental carbon

absorbtion into aerosol water

absorbtion into organic carbon

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Adsorption to dry surface

$$\phi_{ad} = \frac{c\,\theta}{pL + c\,\theta}$$

Φ_{ad} adsorbed fraction of compound

c Junge parameter

θ surface of adsorbat

pL subcooled liquid vapor pressure

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Absorption into organic matter

$$\log(Kp) = \log(K_{OA}) + \log(f_{OC}) - 11.91$$

$$\phi_{ab} = \frac{TSP \times Kp}{TSP \times Kp + 1}$$

Φ_{ab}	absorbed fraction of compound
Kp	gas/particle partition constant
Kp	octanol/air partition constant
f_{OC}	fraction of organic carbon
TSP	total suspended particles mass

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Absorption into aerosol water

$$\log(Kp) = \log(K_{WA}) + \log(f_{AQ}) - 12.0$$

$$\phi_{aq} = \frac{TSP \times Kp}{TSP \times Kp + 1}$$

Φ_{aq} absorbed fraction of compound
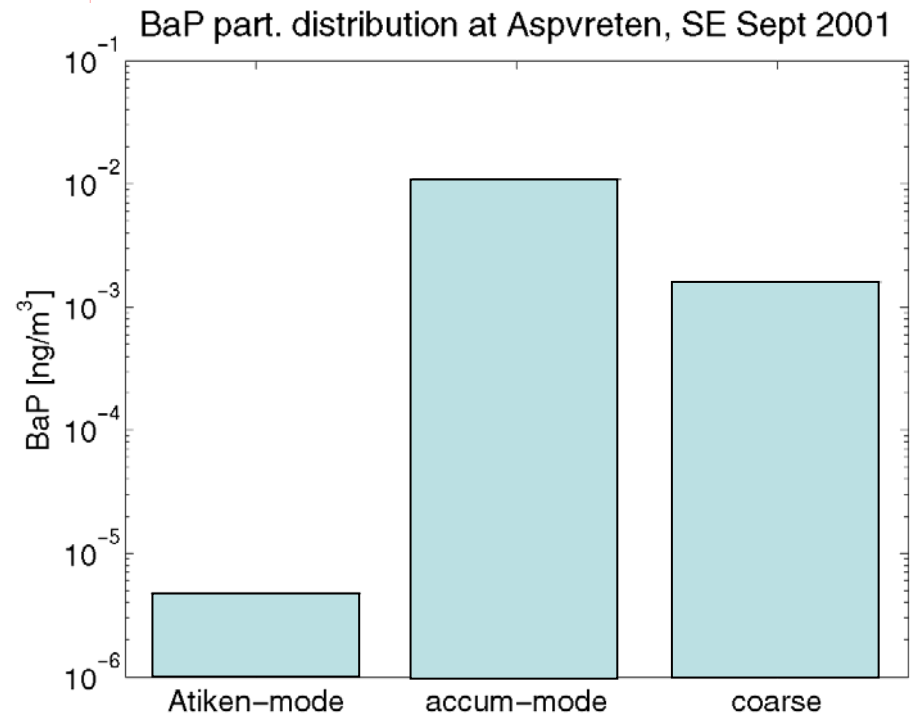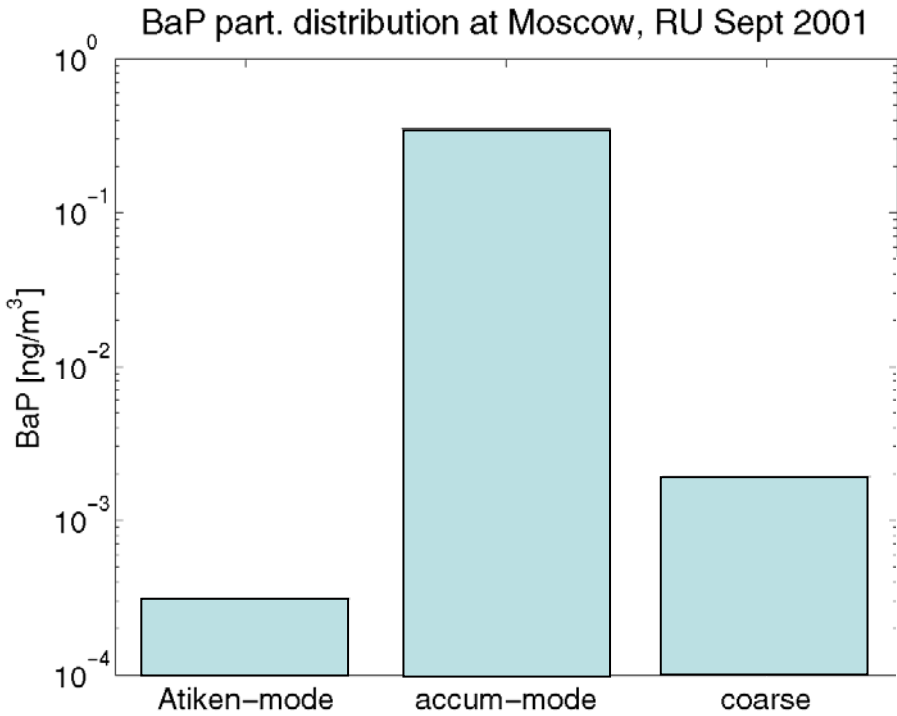
Kp gas/particle partition constant
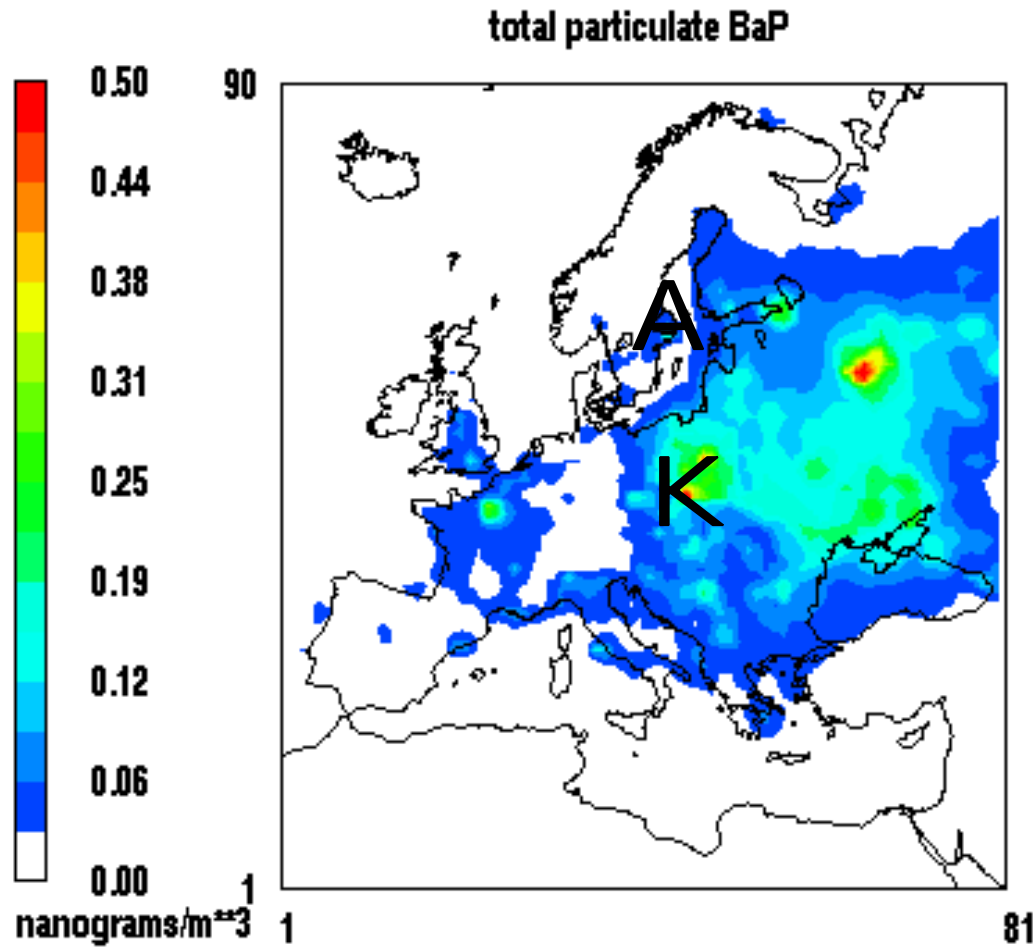
Kp water/air partition constant

f_{OC} fraction of aerosol water

TSP total suspended particles mass

Size distribution

BaP part. distribution at Moscow, RU Sept 2001

BaP part. distribution at Aspvreten, SE Sept 2001

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Simulated particulate BaP concentrations in September 2001

total particulate BaP

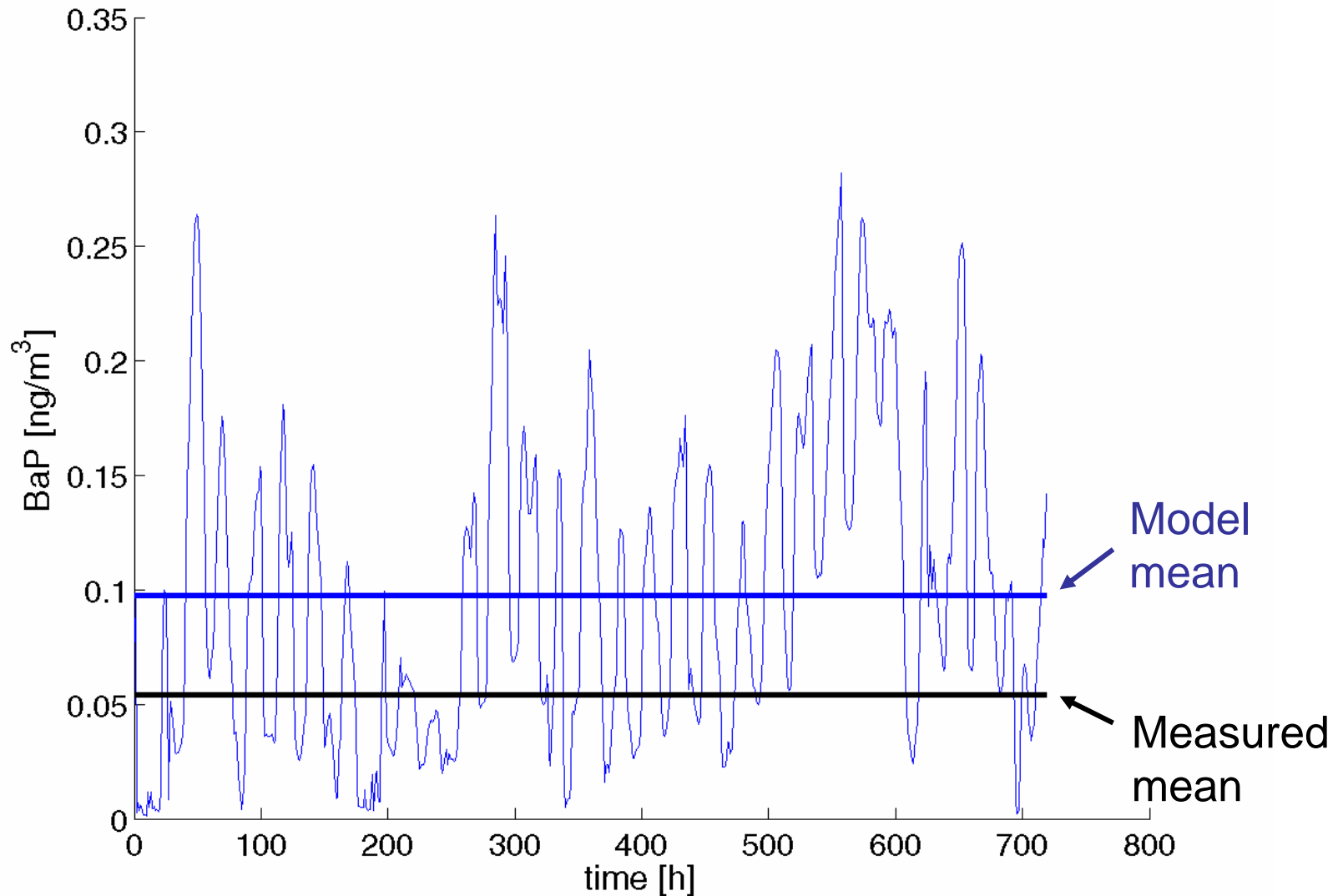Armin Aulinger

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Simulations vs. ground measurements

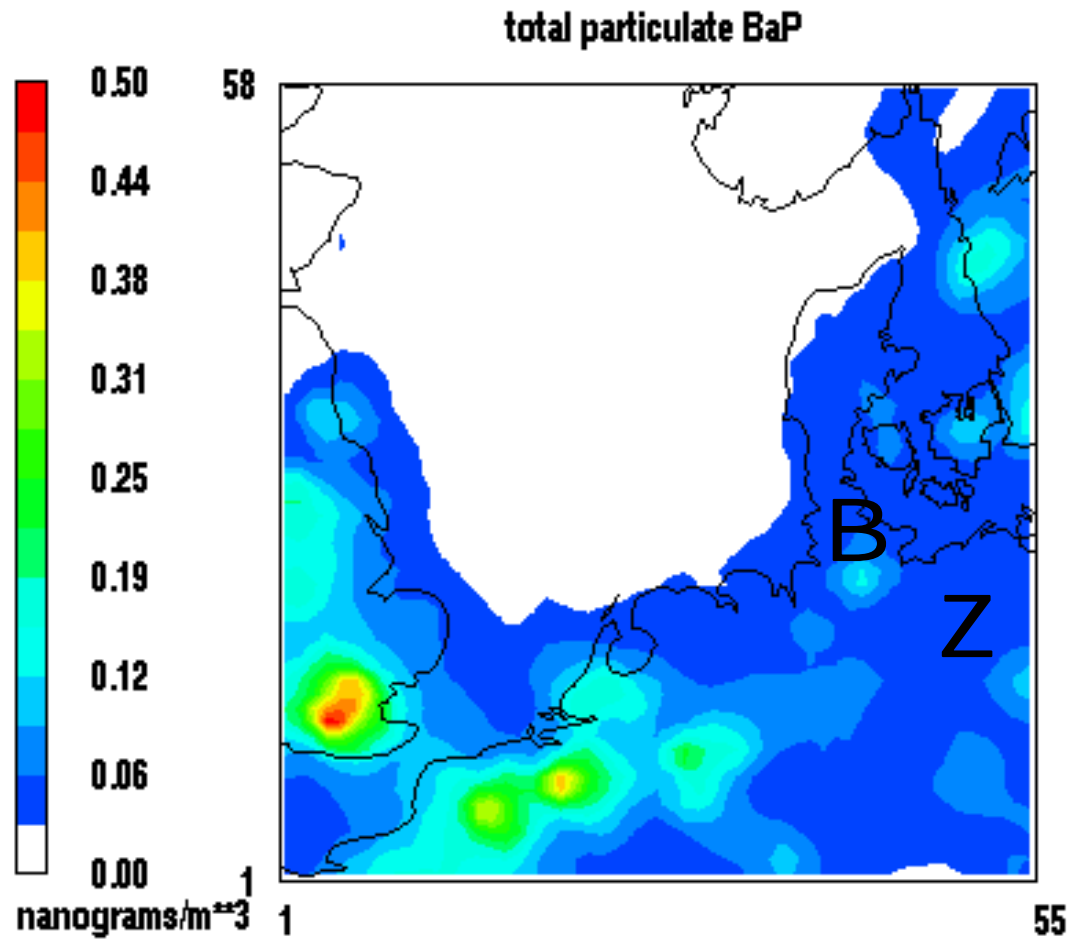
Air concentrations at Aspvreten (rural) in Sept 2001
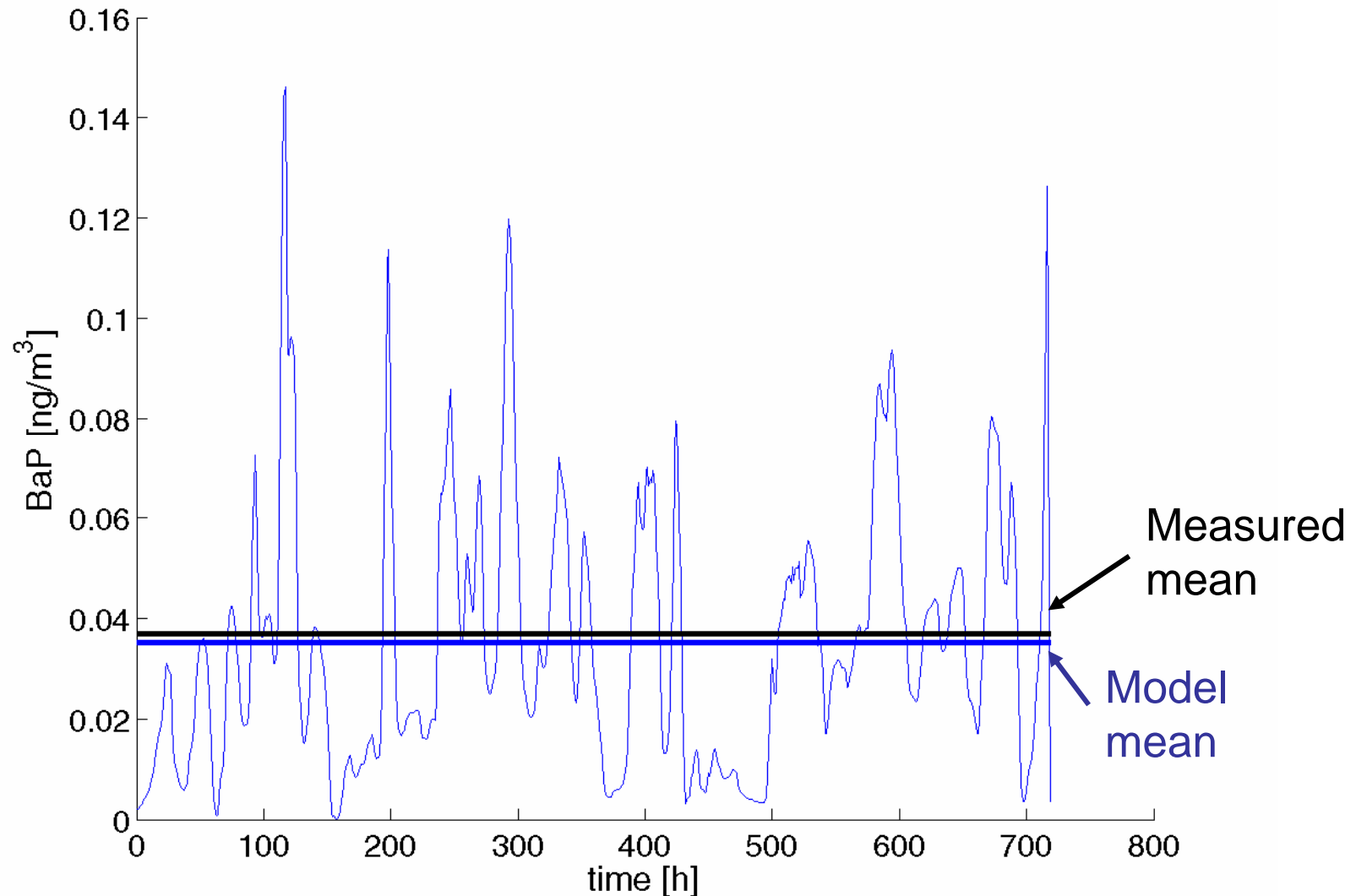
Simulations vs. ground measurements

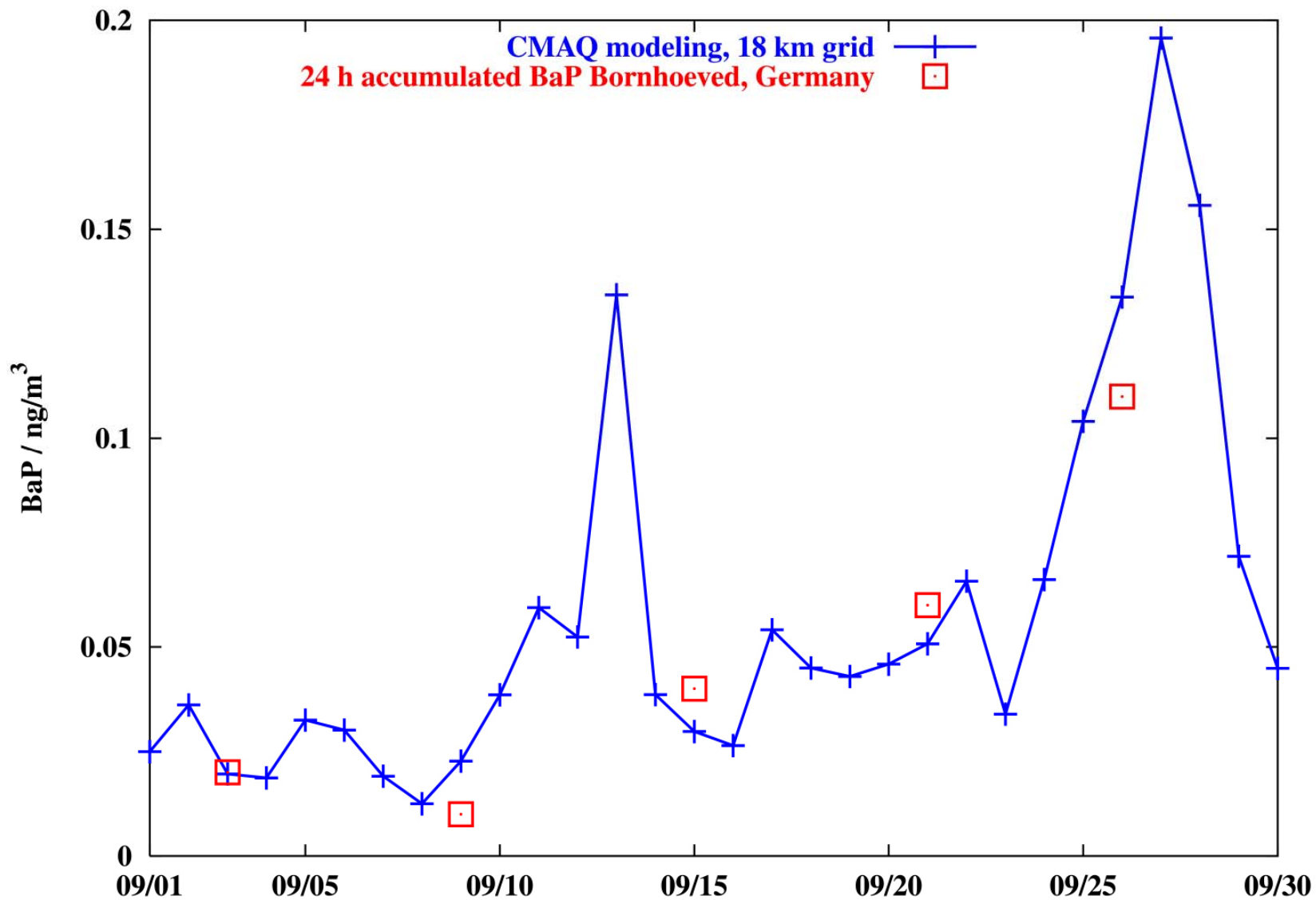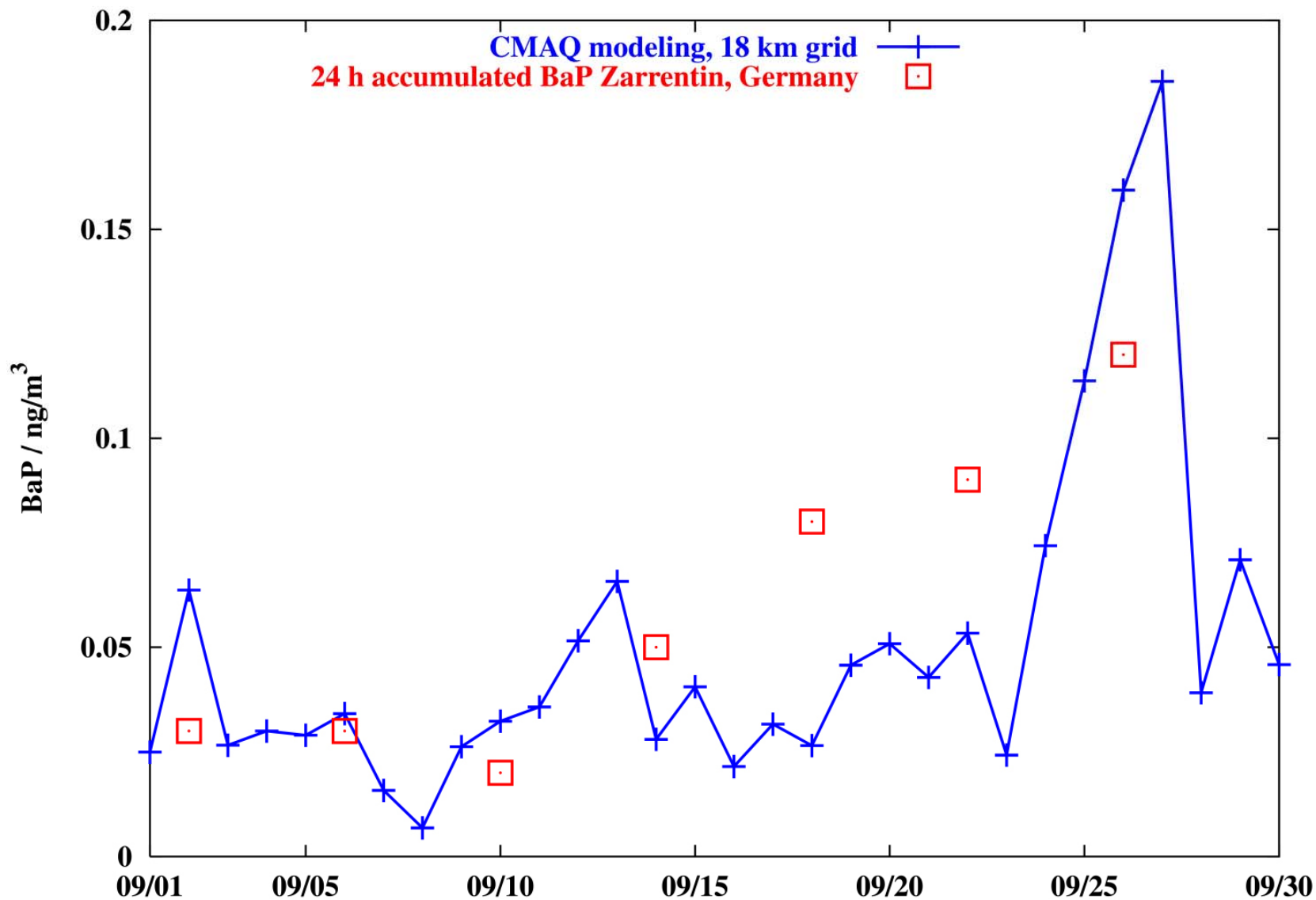Air concentrations at Kosetice (urban) in Sept 2001

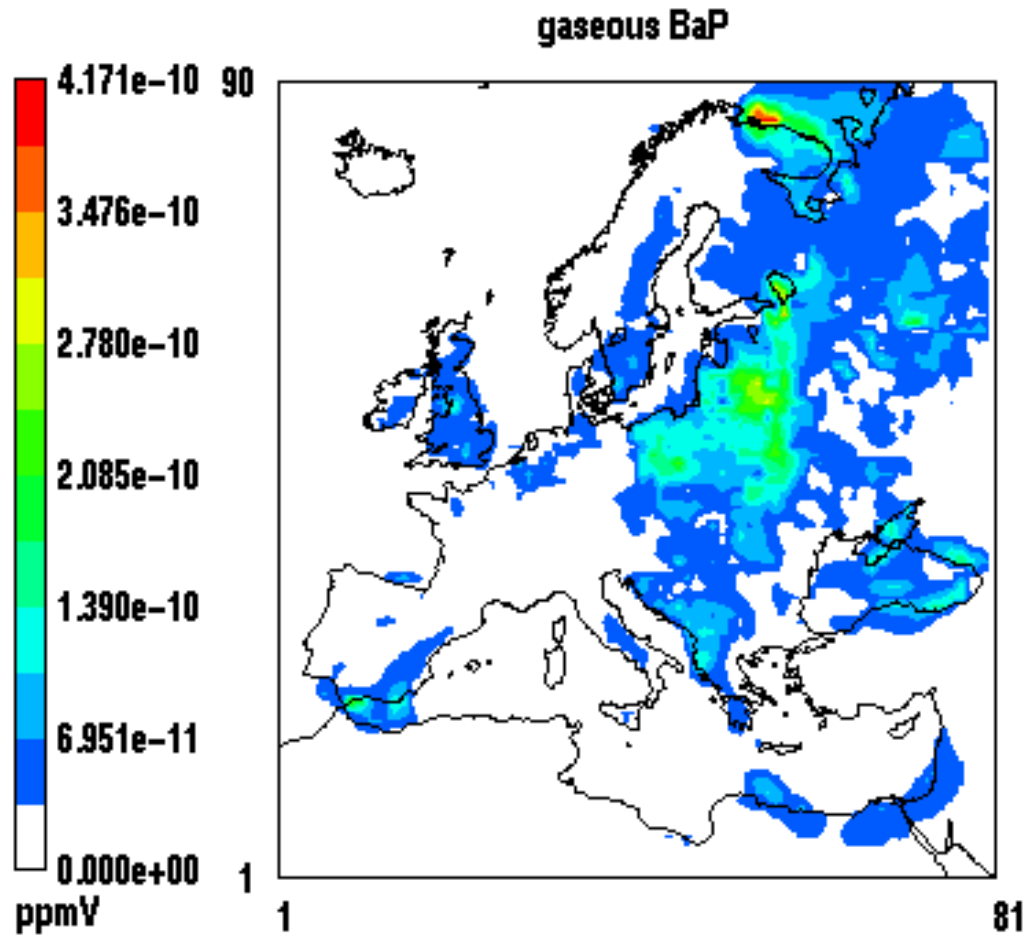# Simulated particulate BaP concentrations in September 2001

total particulate BaP

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Simulations vs. ground measurements

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Simulations vs. ground measurements

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Simulated gaseous BaP concentrations in September 2001

gaseous BaP

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Total simulated BaP depositions in September 2001

total deposition in sept. 2001
total particulate BaP

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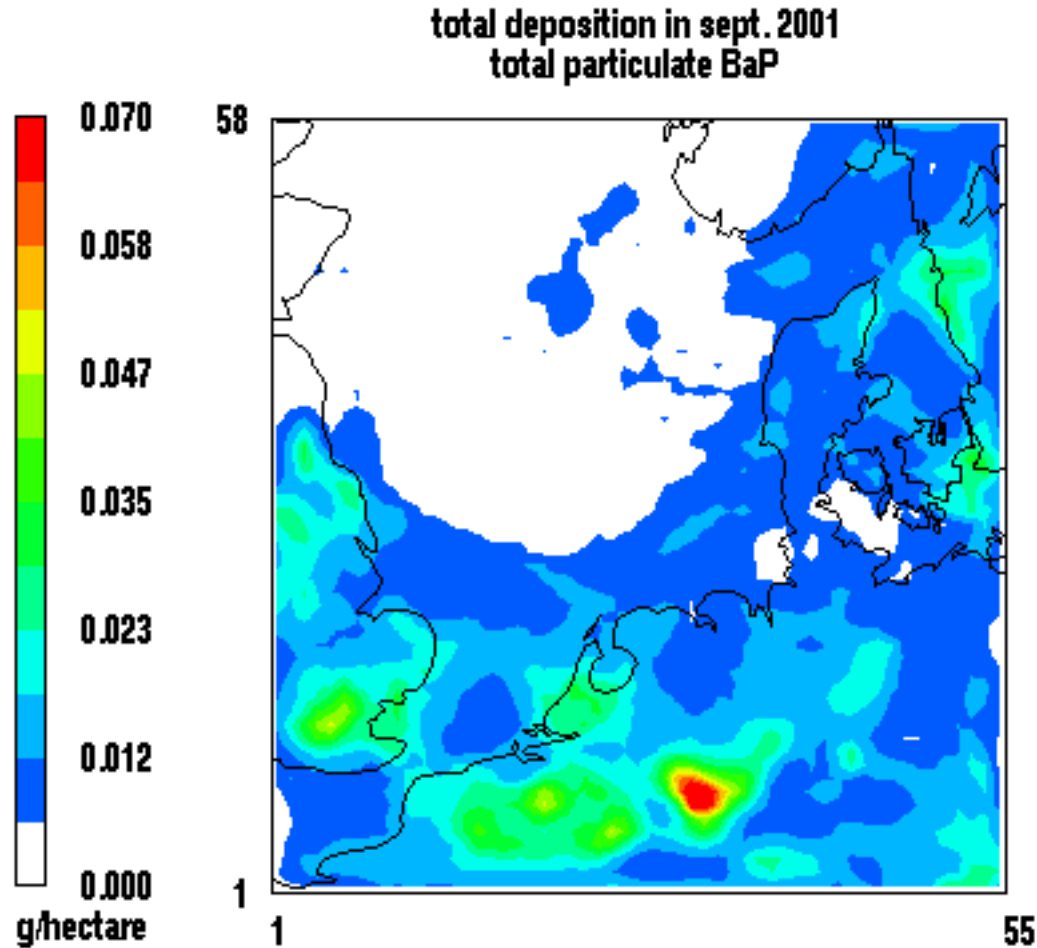
Outlook

- More realistic emissions (incl. ship emissions) and boundary conditions

- Include chemical mechanisms

- Include other POPs (eg. PAHs, PCBs, PFOS)

- Implement a second nest (German Wadden Sea)

- Long-term simulations

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