Training Programme

Air Quality Monitoring, Emission Inventory and Source Apportionment Studies

Source Dispersion Modelling

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Overview

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- **General Introduction**
  - Statistical Models,
  - Deterministic Models

- **Chemistry Transport Models**
  - Theoretical aspects
  - Input data
  - Validation

Overview

- **Application of Chemistry Transport Models**
  - Emission Scenarios,
  - Source Apportionment
  - Process Analysis

General Aspects

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- **Statistical approach**
  - **Receptor Models**
    - Based on **measured** pollutant concentrations
    - Valid for **non-reactive** (or slowly reactive) species
  - Chemical Mass Balance (CMB)
    - for source apportionments
  - Principal Component Analysis (PCA)
    - for source identification
  - Empirical Orthogonal Functions (EOF)
    - for location and strength of emittors.

General Aspects

- **Statistical approach**
  - **Receptor Models**
    - Based on **measured** pollutant concentrations
    - Valid for **non-reactive** (or slowly reactive) species

  - Air parcel trajectory analysis

Statistical approach

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- **CMB**

$$c_i = \sum_{j=1}^{m} a_{ij} s_j \qquad i = 1, \ldots, n$$

a_{ij} source emission signature (composition)
s_j source contribution
m = number of sources

- Constant source emission composition
- Non-reactive species
- Sources contribute to concentration
- Uncertainties are un-related
- Number of sources ≤ number of species
- Measurement errors random

Statistical approach

- **PCA**

$$A = \begin{pmatrix} 1 & \dots & r_{ij} \\ \dots & \dots & \dots \\ r_{ji} & \dots & 1 \end{pmatrix} \qquad r_{ij} = \frac{1}{k-1} \sum_{l=1}^{k} \frac{\left(c_{li} - \overline{c_i}\right)}{\sigma_i} \frac{\left(c_{lj} - \overline{c_j}\right)}{\sigma_j}$$

$$Ax = \lambda x$$

$$\left(A - \lambda I\right)x = 0$$

A = correlation matrix between species c_i and c_j (over range k)

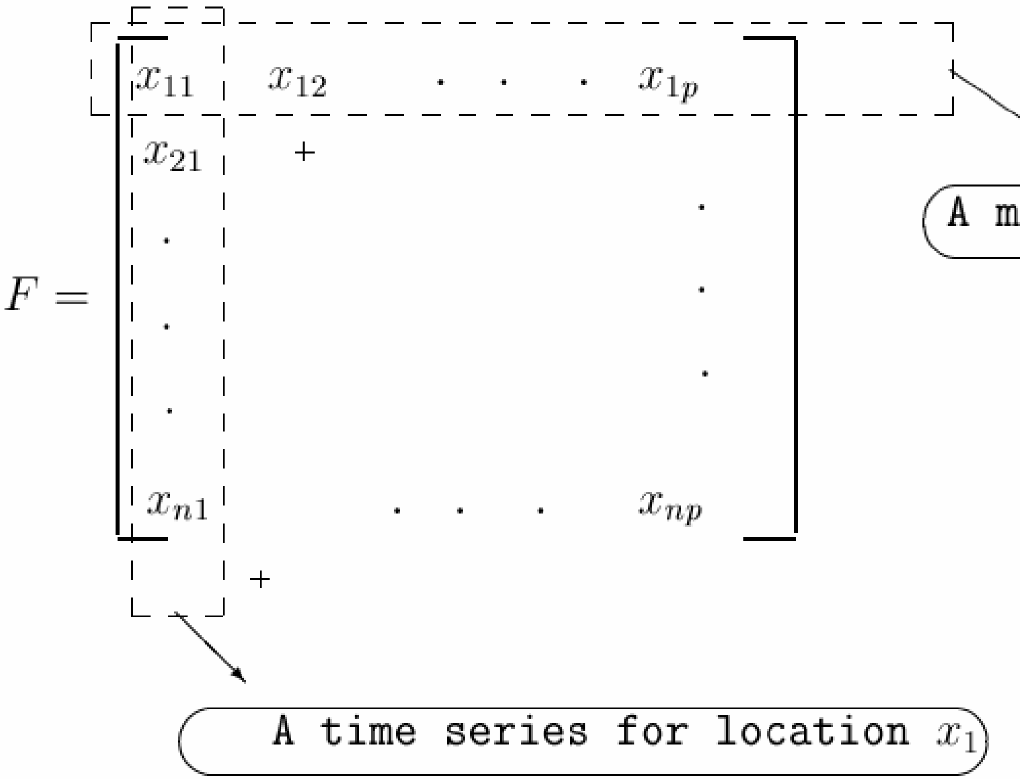
x = Eigenvectors

λ = Eigenvalues

I = unity

Statistical approach

- EOF



form the *covariance matrix*

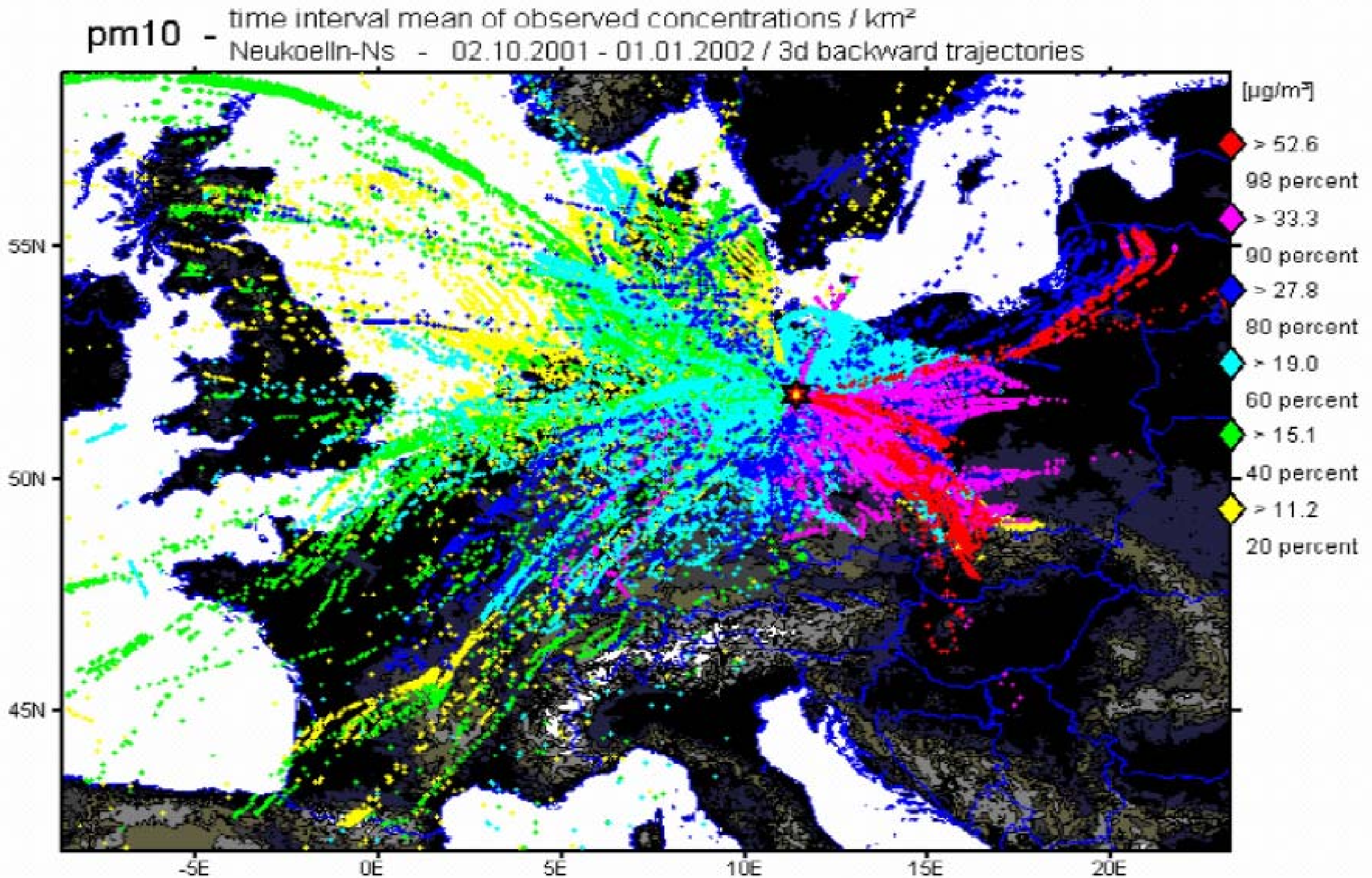
$$RC = C\Lambda.$$

$$F = \sum_{j=1}^{p} \vec{a}_j (EOF_j)$$

Figure 1.1: The matrix F. Each row is one map, and each column is a time series of observations for a given location..

Statistical approach

- **Air Parcel Trajectories**



Statistical approach

- **Probability Distribution**
  - Based on **measured** pollutant concentrations
  - Log-Normal Distribution
    - for source apportionments
  - Weibull Distribution

- Quantiles, Moments
- Extreme values
- Exceedances of critical levels

Deterministic Models

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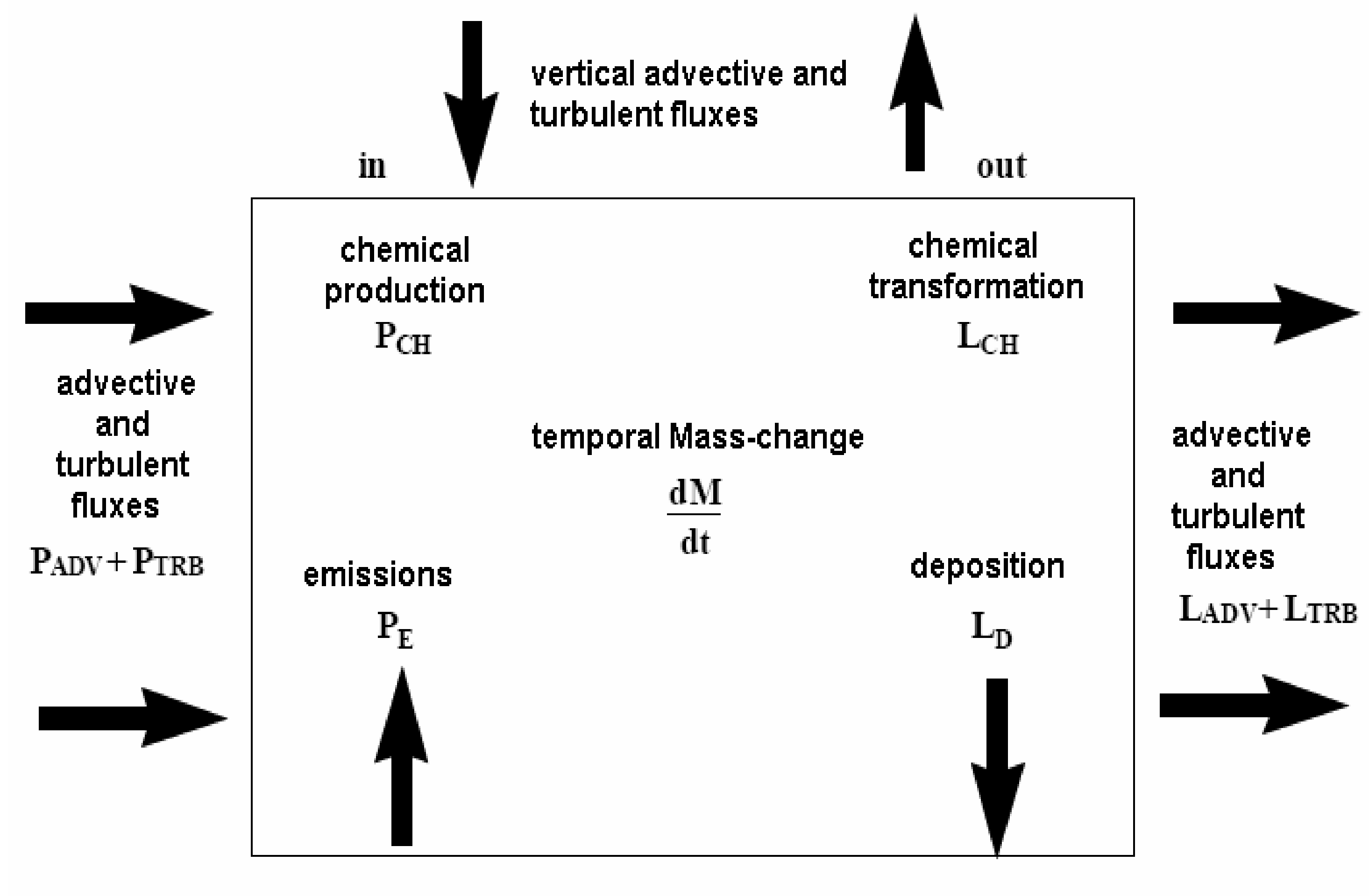
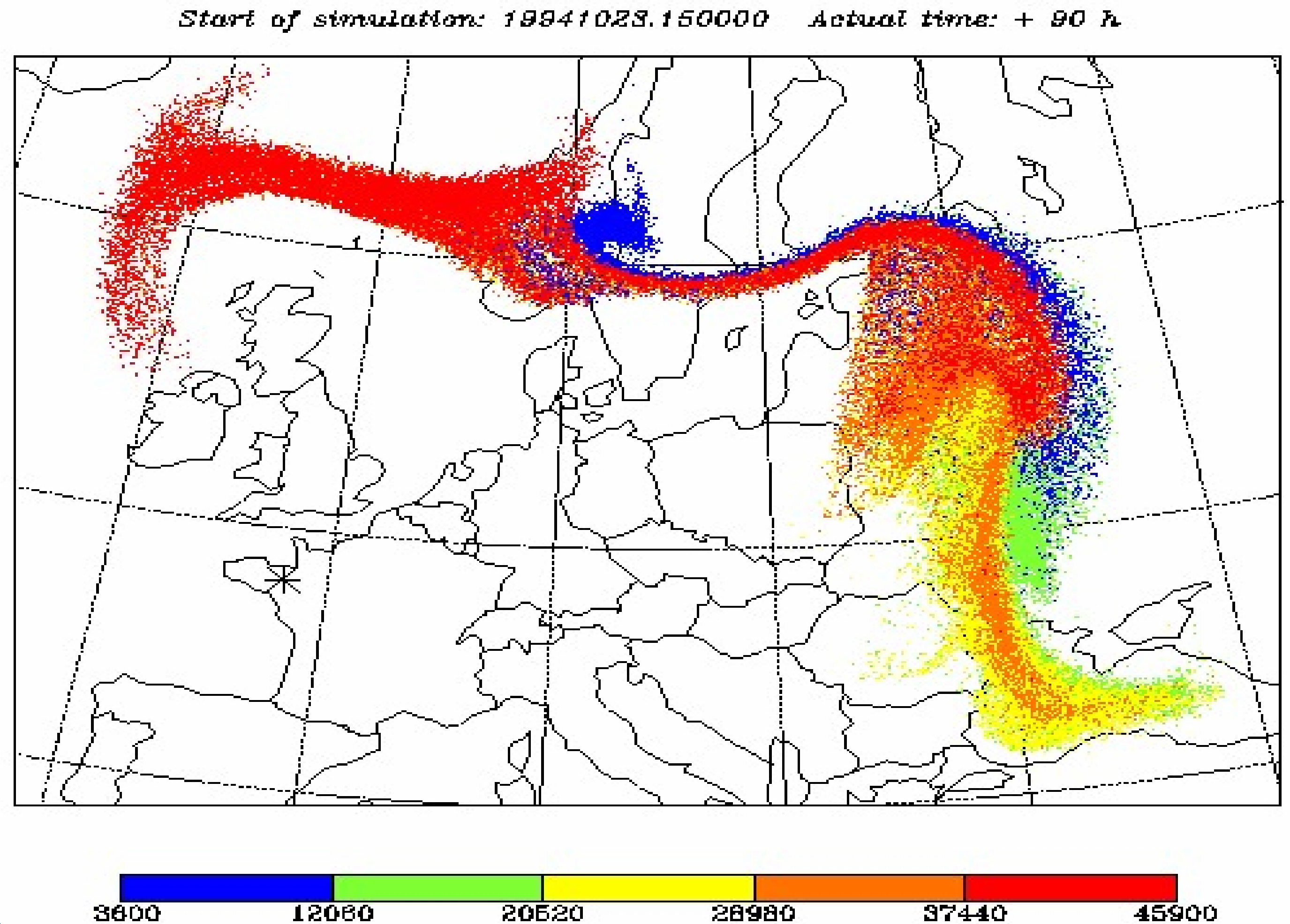
Box model



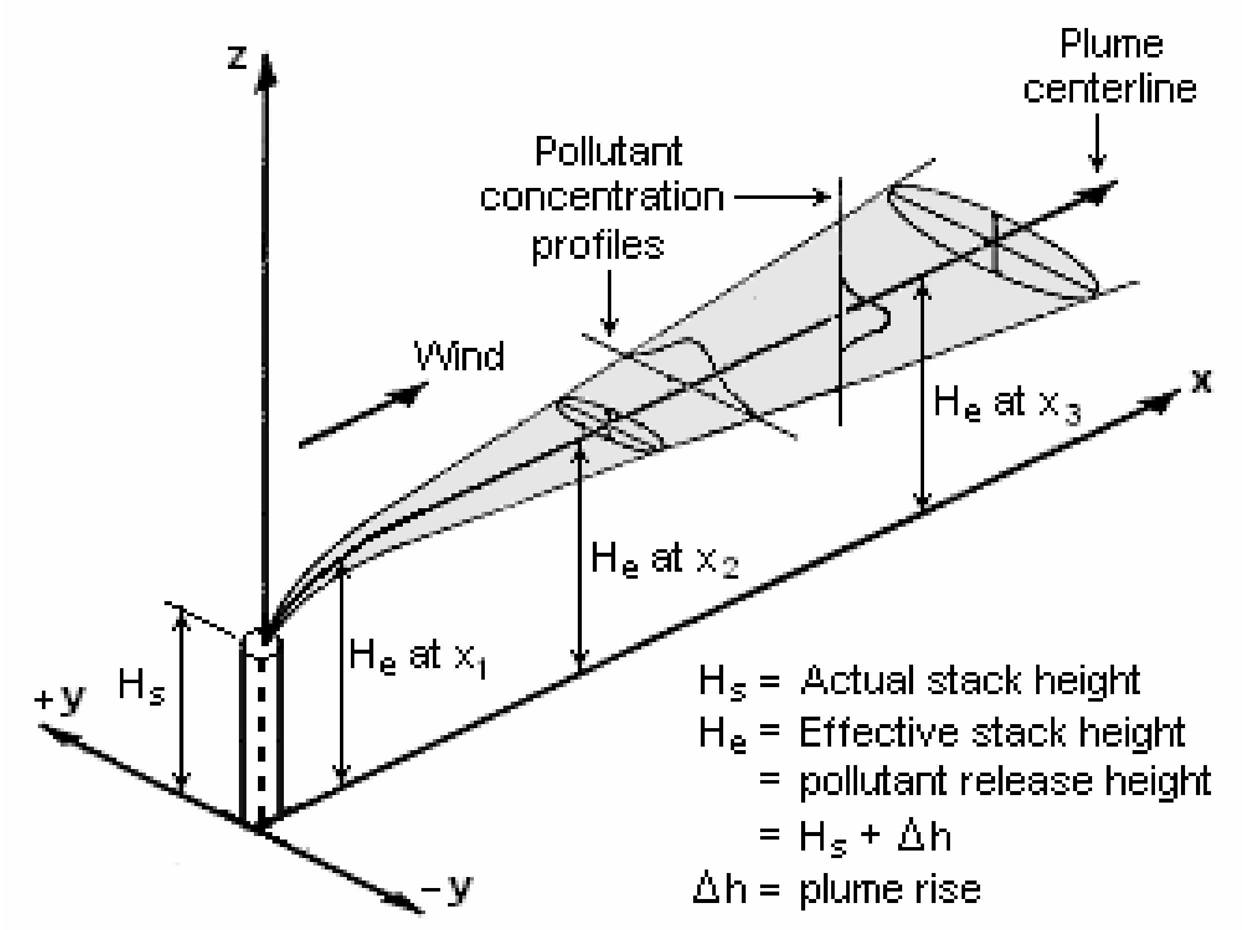
Deterministic Models

Lagrange model



Deterministic Models

Gaussian models



Deterministic Models

Gaussian models

$$\left\langle C(x,y,z,t)\right\rangle = \frac{Q}{2\pi \bar{u}\sigma_y\sigma_z}\exp\left(-\frac{y^2}{2{\sigma_y}^2}\right)\left[\exp\left(-\frac{(z-h)^2}{2{\sigma_z}^2}\right)+\exp\left(-\frac{(z+h)^2}{2{\sigma_z}^2}\right)\right]$$

where

C(x, y, z) : pollutant concentration at point (x, y, z);

U: wind speed (in the x "downwind" direction, m/s)

σ: standard deviation of the concentration in the x and y direction, i.e., in the wind direction and cross-wind, in meters;

Q is the emission strength (g/s)

h is the emission release height,

Deterministic Models

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CHEMISTRY-TRANSPORT-MODELS

The basis of atmospheric transport-chemistry modelling

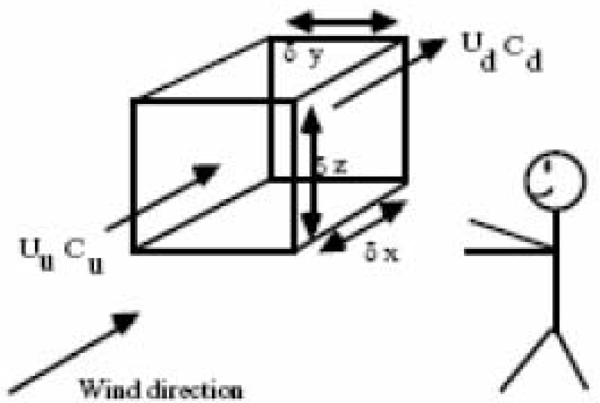
$$\frac{\partial C_i}{\partial t} + u\frac{\partial C_i}{\partial x} + v\frac{\partial C_i}{\partial y} + w\frac{\partial C_i}{\partial z} = \frac{\partial}{\partial x}\left(K_h \frac{\partial C_i}{\partial x}\right) +$$

$$\frac{\partial}{\partial y}\left(K_h \frac{\partial C_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial C_i}{\partial z}\right) +$$

chemistry + emissions – dry deposition – wet deposition

Chem. Transport Model

3-D Grid Modelling



- An observer standing at a fixed point in space measures changing concentrations. The observer must account for the chemical sources and sinks as well as for the motion of the air. This is called an Eulerian measurement since it is at a point.

3-D Grid Modelling

Global scale, continental scale, urban scale.

Model system at TRUMF : REM/CALGRID (continental)
+ urban version

Model system at TNO : LOTOS (continental)
and LOTOS –zoom (urban)

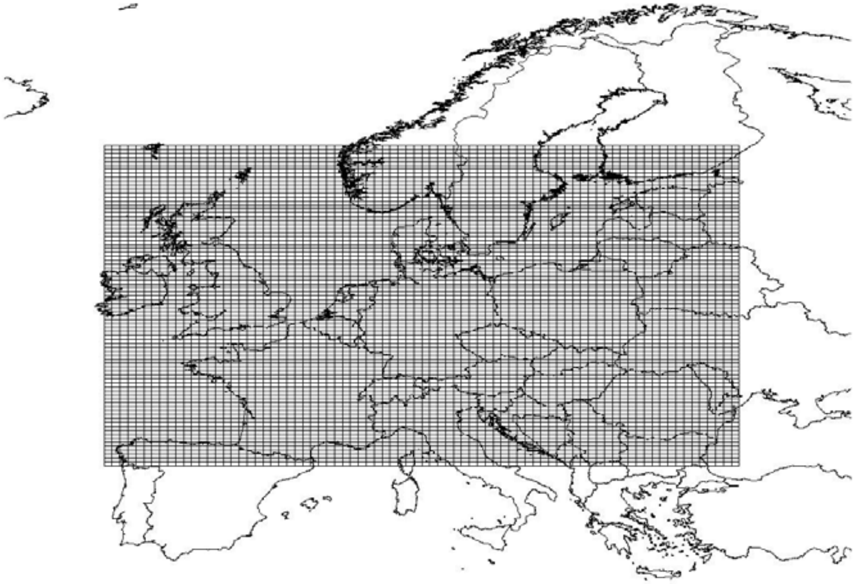
Characteristics of the model –systems:

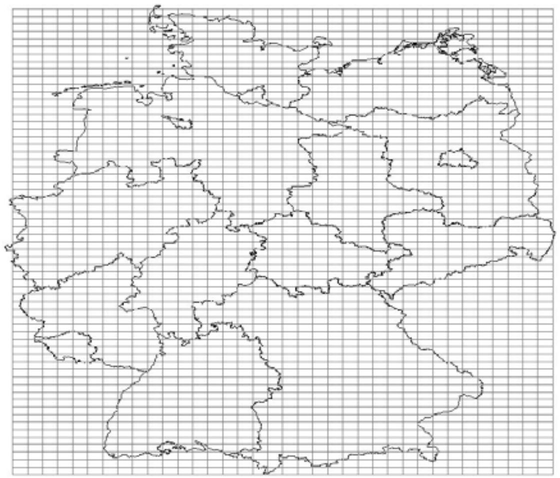
Horizontal grid resolution 0.25 x 0.5 latlong, with nesting down to about 4 x 4 km^2

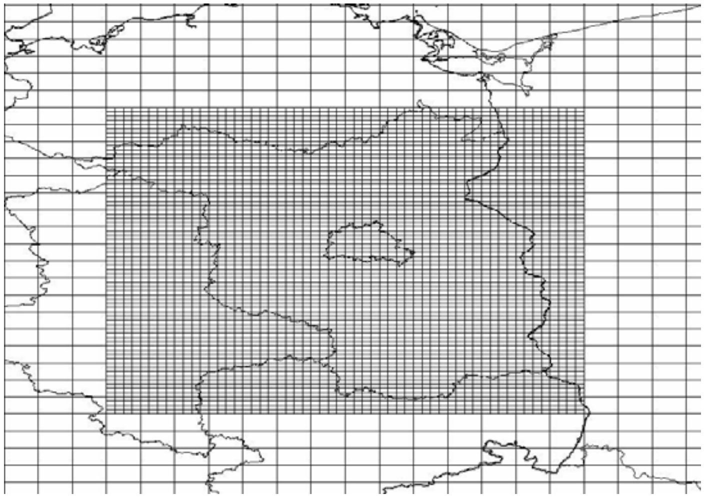
Vertical layers: 5-10 upto about 3-5 km

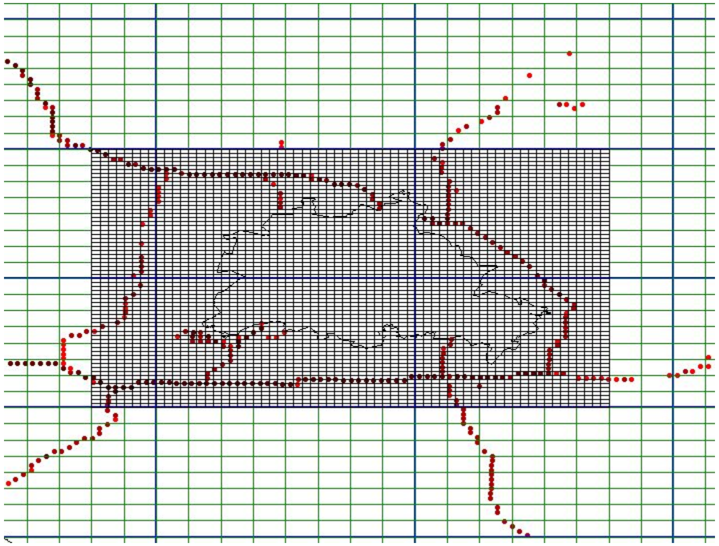
Gasphase chemistry (O_3) and aerosol physics and chemistry

Chem. Transport Model







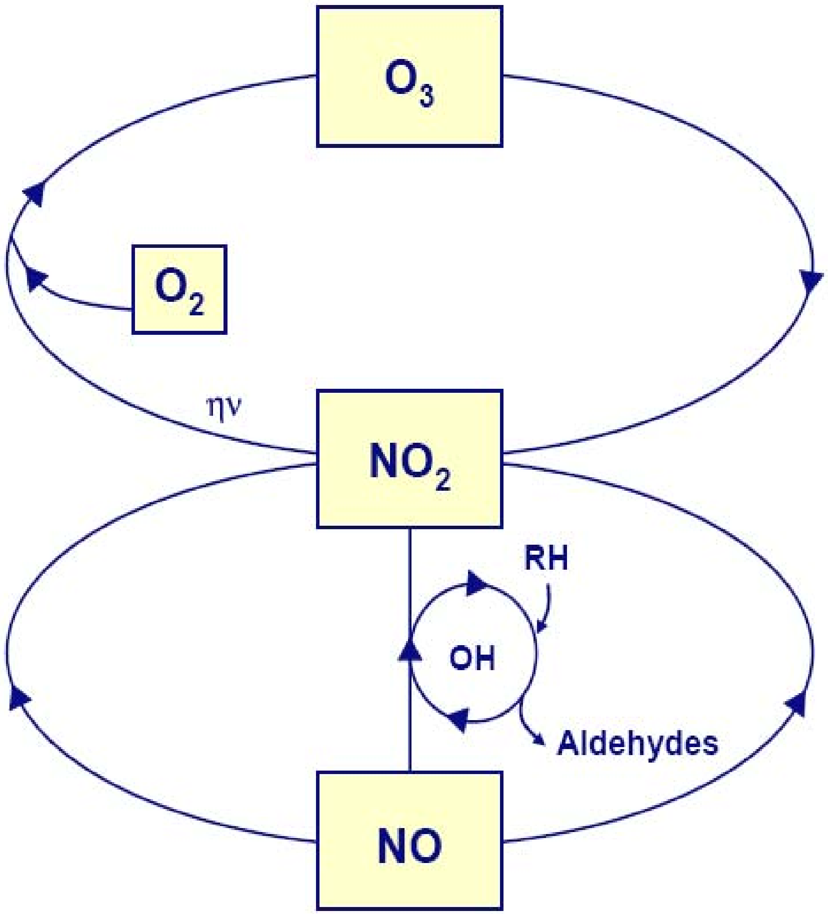


Chem. Transport Model

Required input data

- Boundary conditions from observations, or global modelling (TM-3)
- Anthropogenic and biogenic and natural emissions
- Land use data base
- Diagnostic meteorological fields (by Eberhard Reimer)
- Prognostic meteorological fields:
  - DWD-LM
  - NWP
  - MM5-reanalysis
  - ECMWF-ERA 40

Tropospheric chemistry



Policy for tropospheric O_3

RH versus NO_x abatement,

Non-lineair: $NO + O_3 \rightleftarrows NO_2 + O_2$

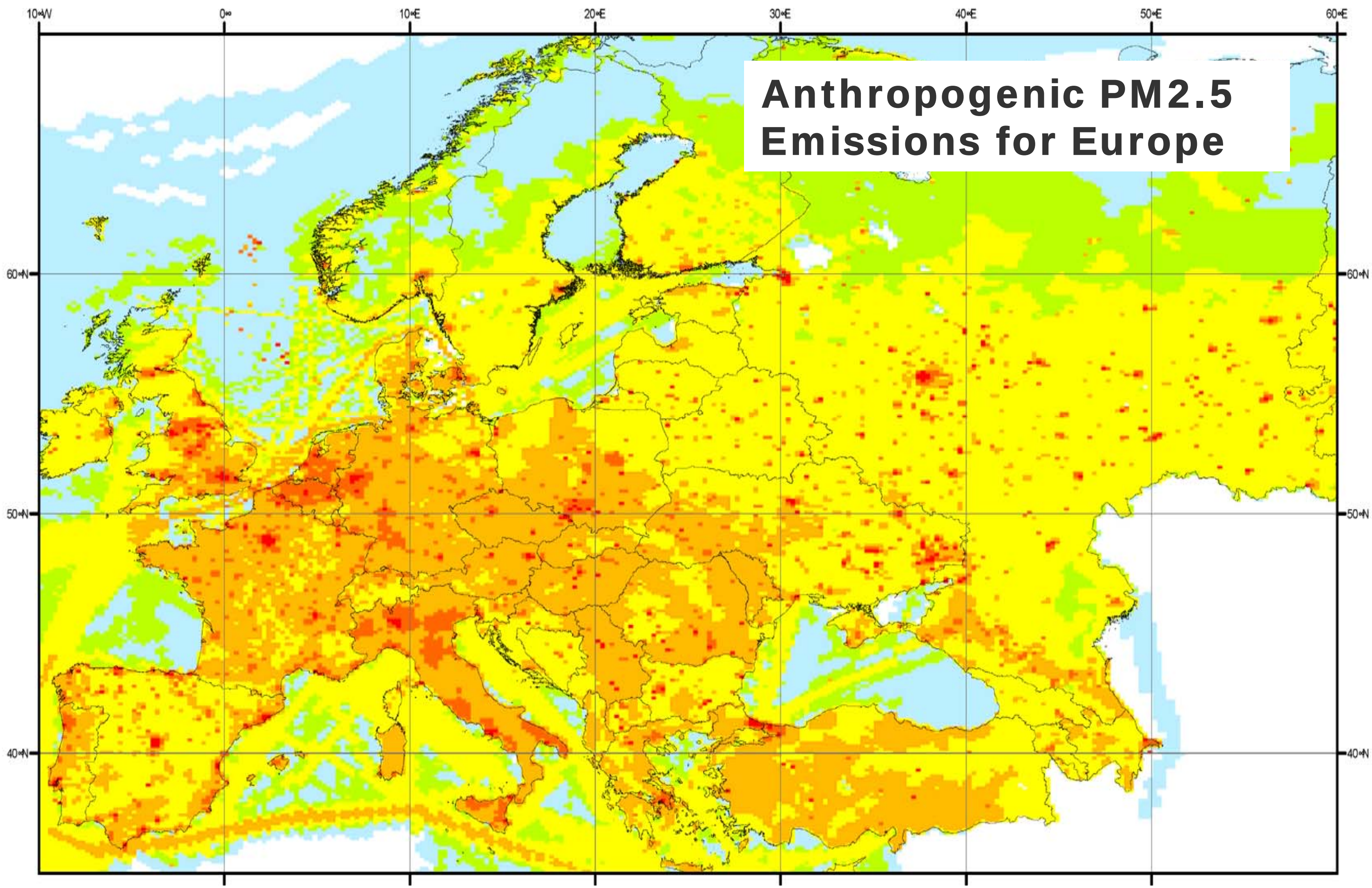
lowering of NO leads to increase in O_3

high RH/NO_x-ratio: NO_x-strategy

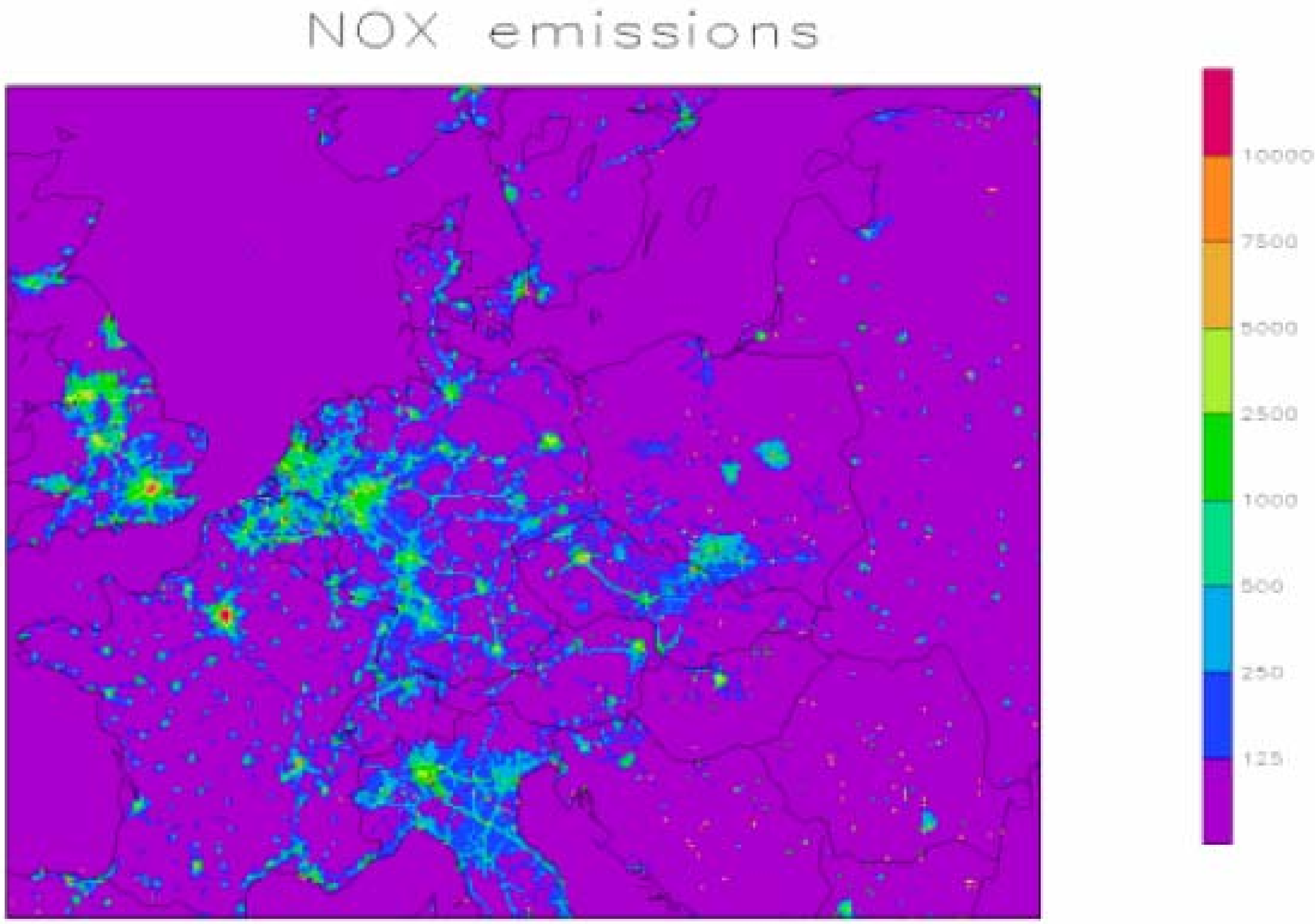
low RH/NO_x-ratio: RH-strategy

Biogenic RH-emissions

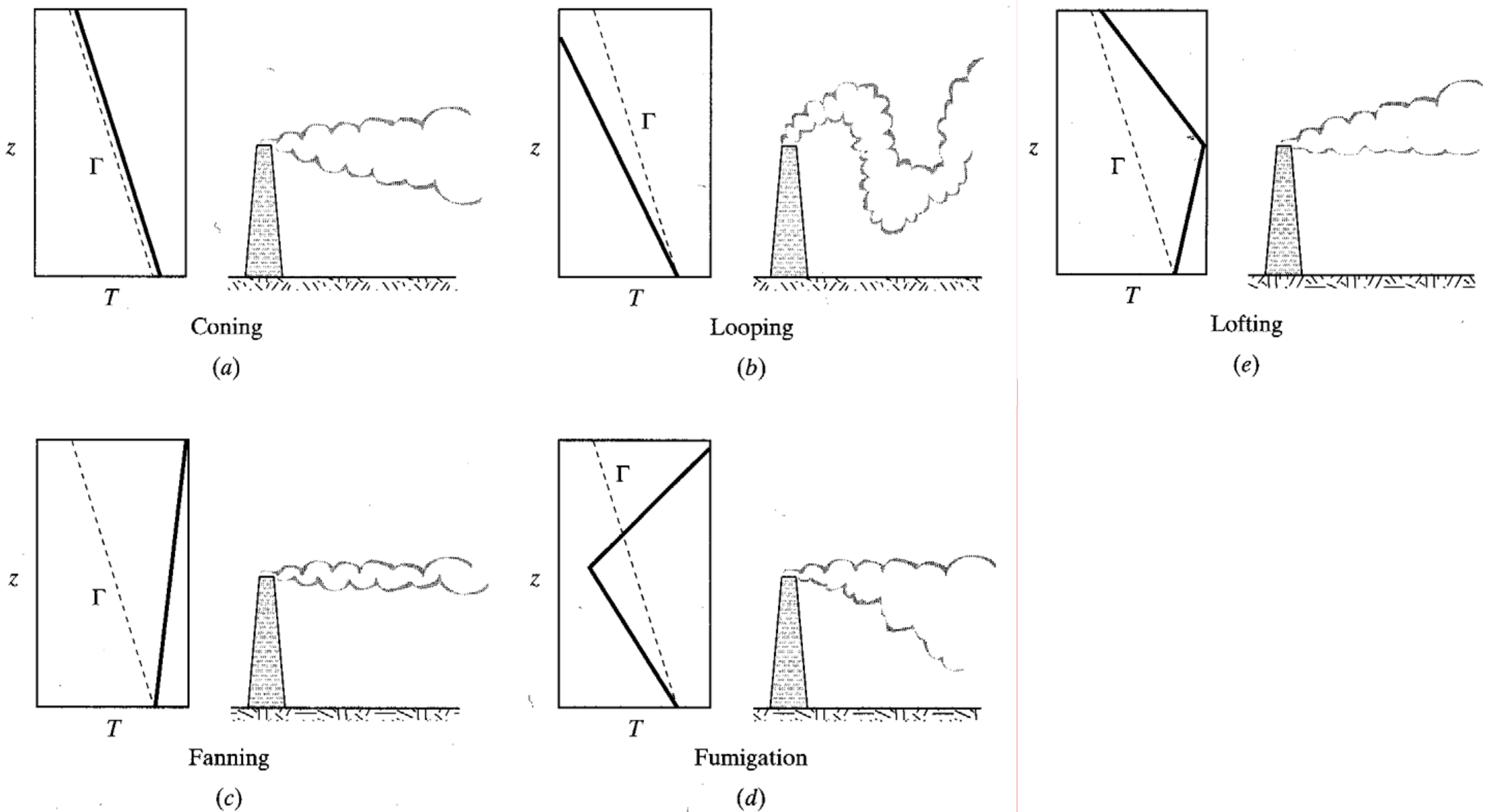
Emissions


Anthropogenic PM2.5
Emissions for Europe
10°W
0°
10°E
20°E
30°E
40°E
50°E
60°E
60°N
50°N
40°N

Emissions



Meteorology



Meteorology

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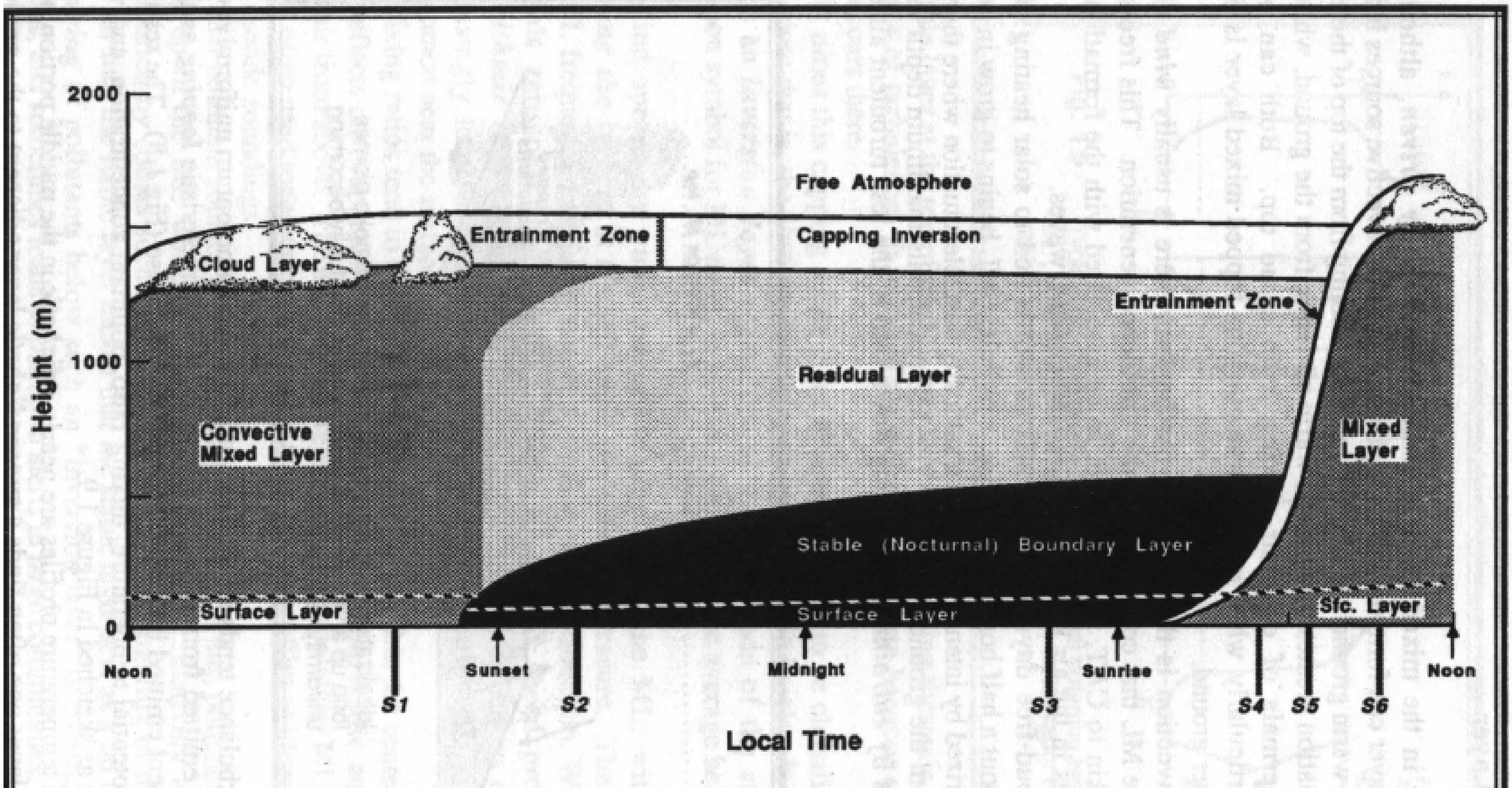
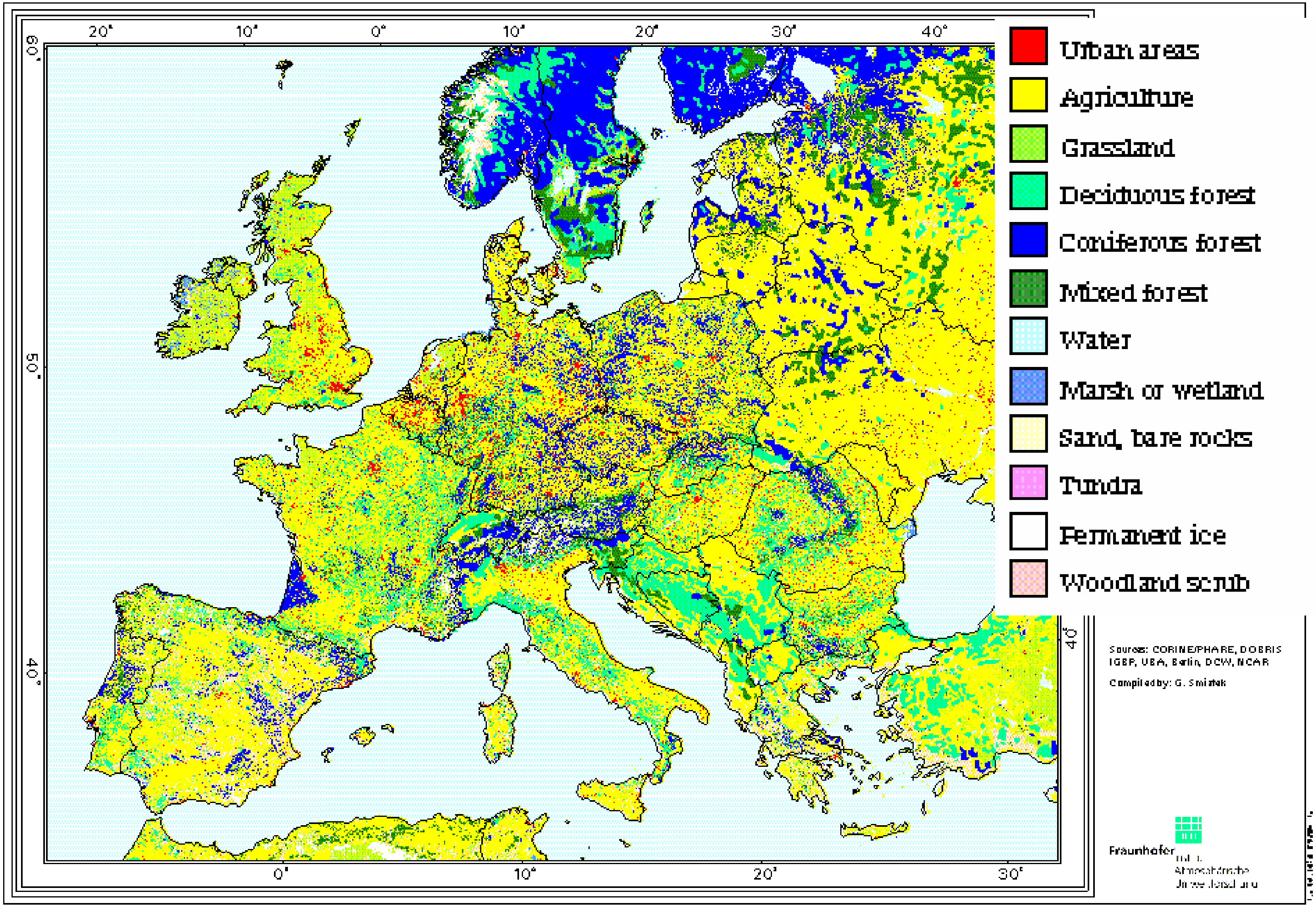


Fig. 1.7 The boundary layer in high pressure regions over land consists of three major parts: a very turbulent mixed layer; a less-turbulent residual layer containing former mixed-layer air; and a nocturnal stable boundary layer of sporadic turbulence. The mixed layer can be subdivided into a cloud layer and a subcloud layer. Time markers indicated by S1-S6 will be used in Fig. 1.12.

Landuse



Urban areas
Agriculture
Grassland
Deciduous forest
Coniferous forest
Mixed forest
Water
Marsh or wetland
Sand, bare rocks
Tundra
Permanent ice
Woodland scrub
Sources: CORINE/PHARE, DOBRIS
IGBP, UBA, Berlin, DCW, NCAR
Compiled by: G. Smiatek
Fraunhofer

Validation

Model evaluation:
How reliable present the model the ‘reality’

Aspects:

- Model calculates volume averaged concentrations, observations are at a specific point
- Observations (might) contain errors, and their spatial representativity is (often) not well known
- Uncertainty and errors in input data: emissions
- Weak parts of the model as description of vertical exchange processes and the treatment of clouds
- Chemistry is non-linear: Right for the wrong reasons

Validation

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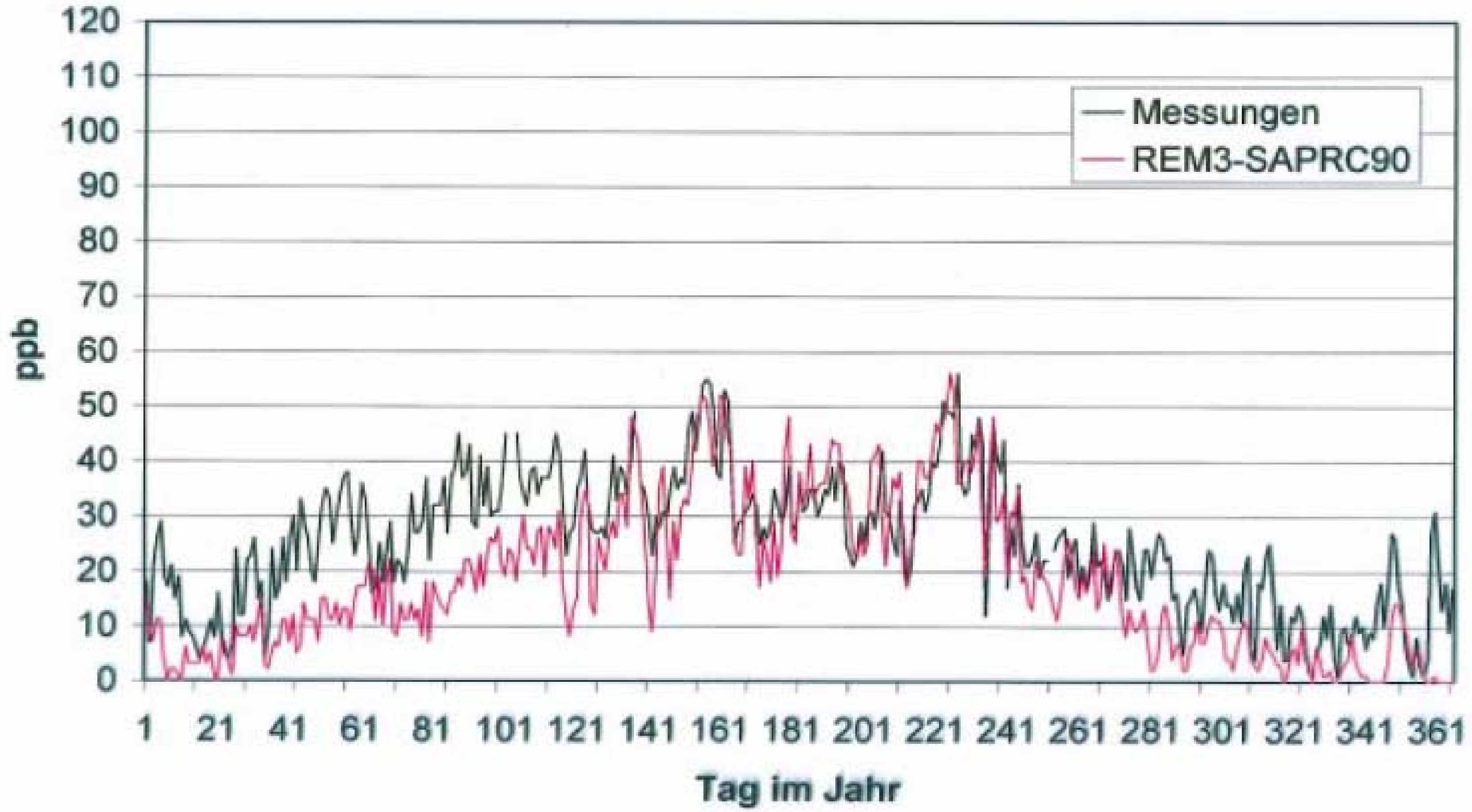
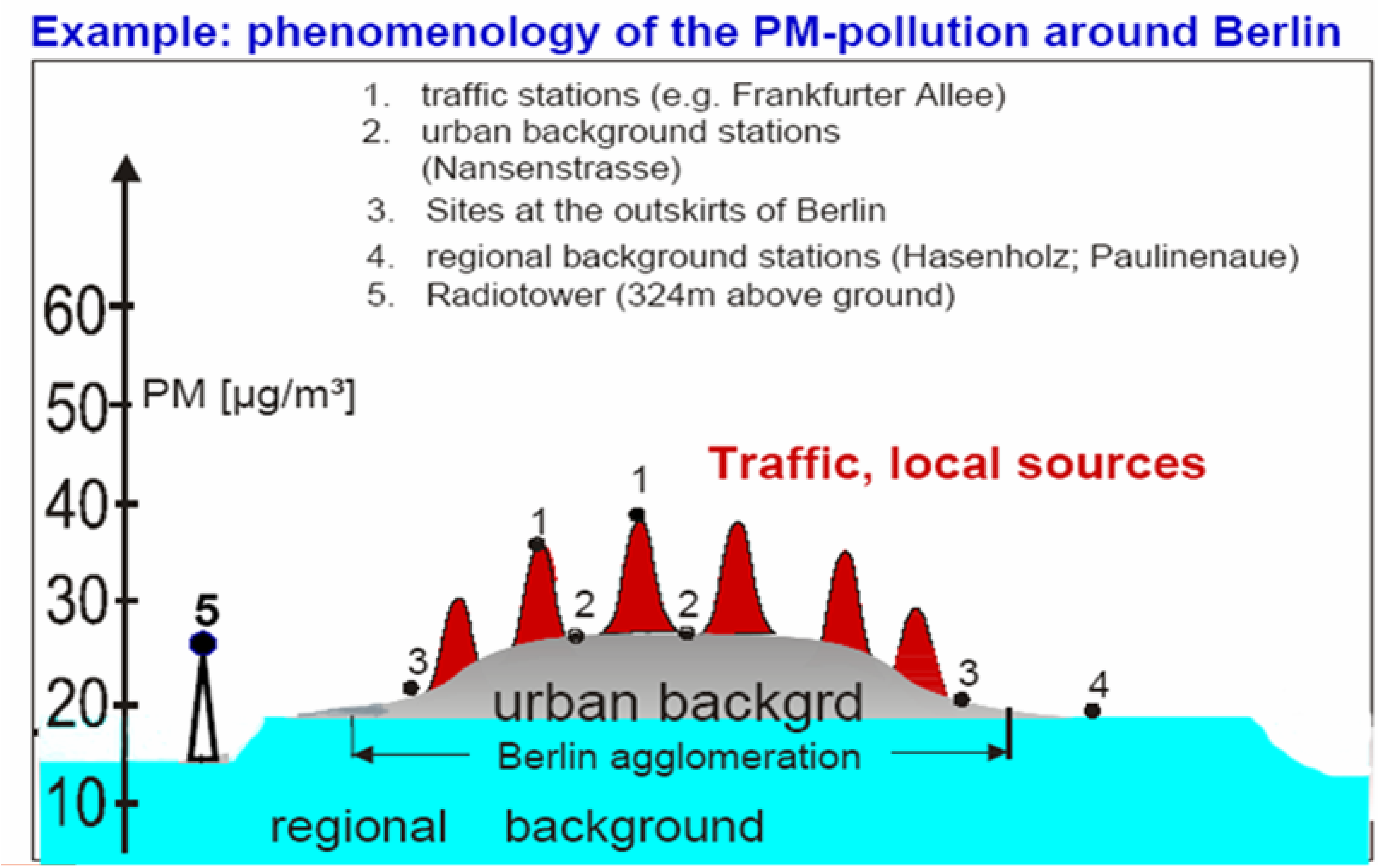
REM_Calgrid: Ozone Validation at rual background station 1997

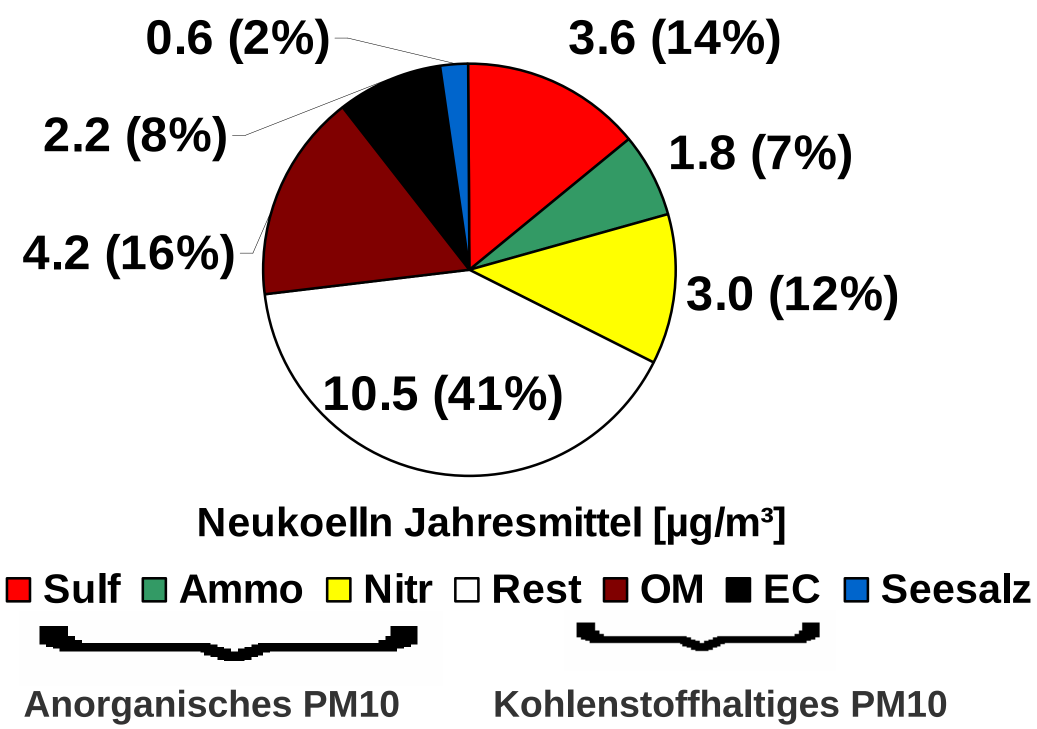


Validation



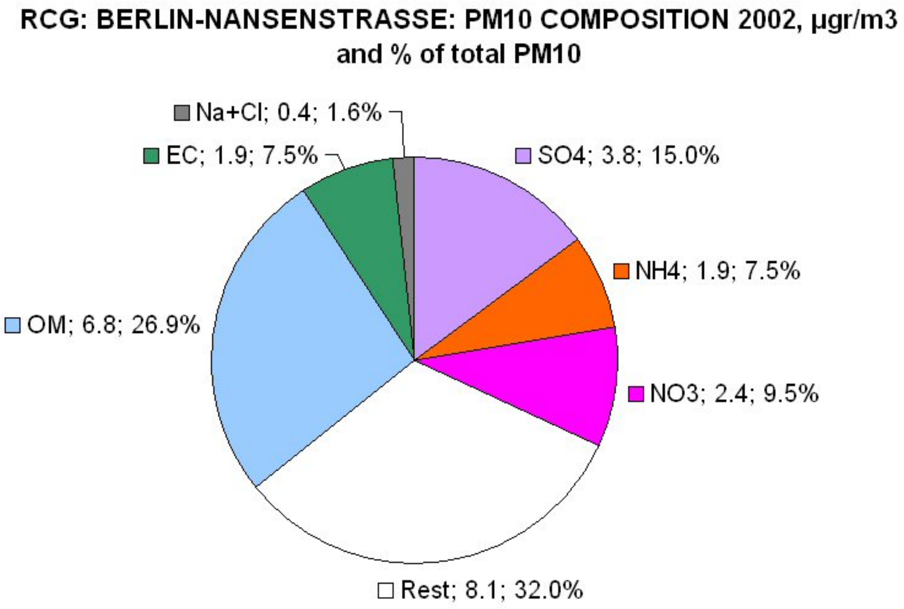
Example: phenomenology of the PM-pollution around Berlin
1. traffic stations (e.g. Frankfurter Allee)
2. urban background stations (Nansenstrasse)
3. Sites at the outskirts of Berlin
4. regional background stations (Hasenholz; Paulinenaue)
5. Radiotower (324m above ground)
60
50
40
30
20
10
PM [µg/m³]
Traffic, local sources
1
1
2
2
3
3
4
5
urban backgrd
Berlin agglomeration
regional background

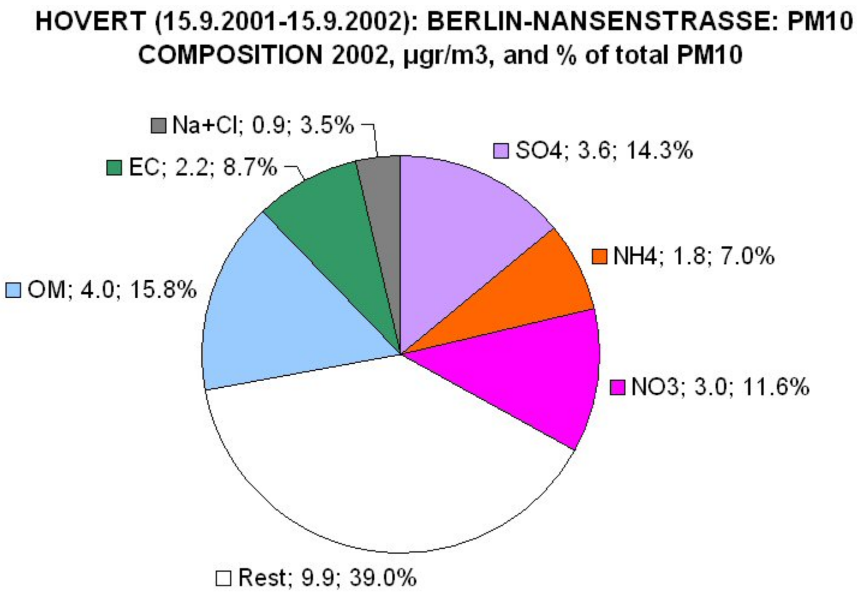
Validation


0.6 (2%)
3.6 (14%)
2.2 (8%)
1.8 (7%)
4.2 (16%)
3.0 (12%)
10.5 (41%)
Neukoelln Jahresmittel [µg/m³]
Sulf
Ammo
Nitr
Rest
OM
EC
Seesalz
Anorganisches PM10
Kohlenstoffhaltiges PM10


Paulinenaue
Frohnau T.
Buch
Beusselstr.
Hasenholz
Frankfurter A.
Neukoelln
Marienfelde

Validation


RCG: BERLIN-NANSENSTRASSE: PM10 COMPOSITION 2002, µgr/m3 and % of total PM10
Na+Cl; 0.4; 1.6%
EC; 1.9; 7.5%
SO4; 3.8; 15.0%
NH4; 1.9; 7.5%
OM; 6.8; 26.9%
NO3; 2.4; 9.5%
Rest; 8.1; 32.0%


HOVERT (15.9.2001-15.9.2002): BERLIN-NANSENSTRASSE: PM10 COMPOSITION 2002, µgr/m3, and % of total PM10
Na+Cl; 0.9; 3.5%
EC; 2.2; 8.7%
SO4; 3.6; 14.3%
NH4; 1.8; 7.0%
OM; 4.0; 15.8%
NO3; 3.0; 11.6%
Rest; 9.9; 39.0%

APPLICATIONS

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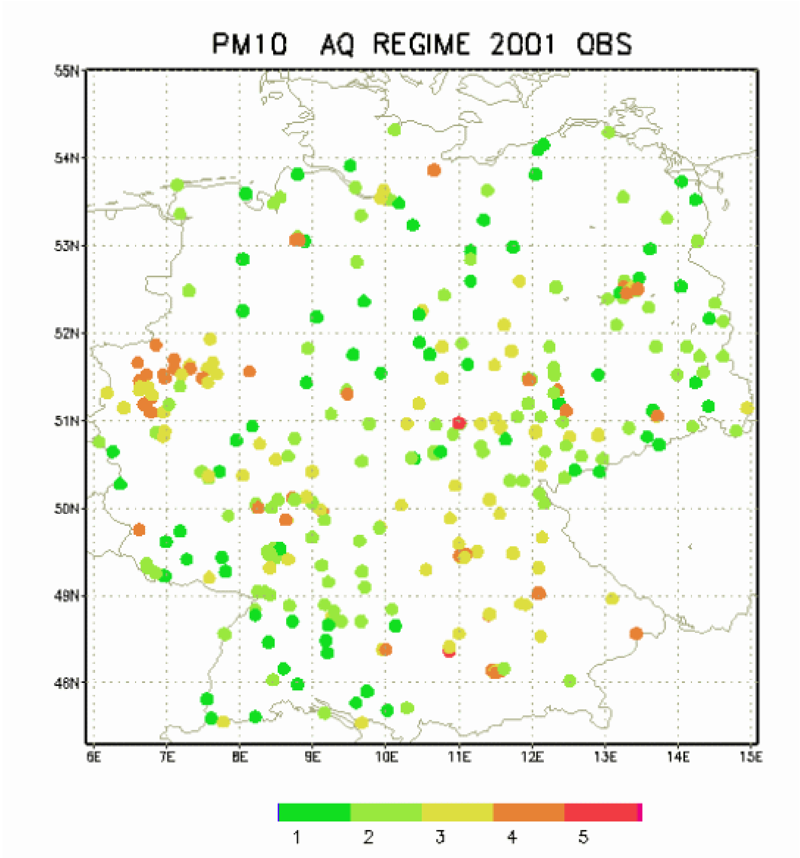
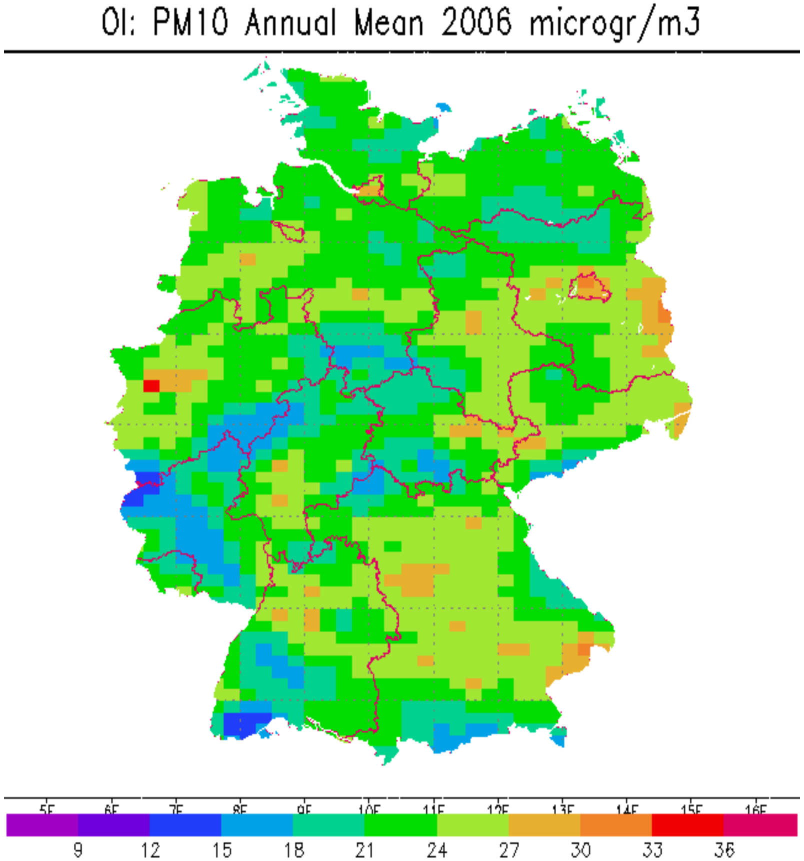
REPRESENTATION OF CURRENT STATE

- spatially homogenous





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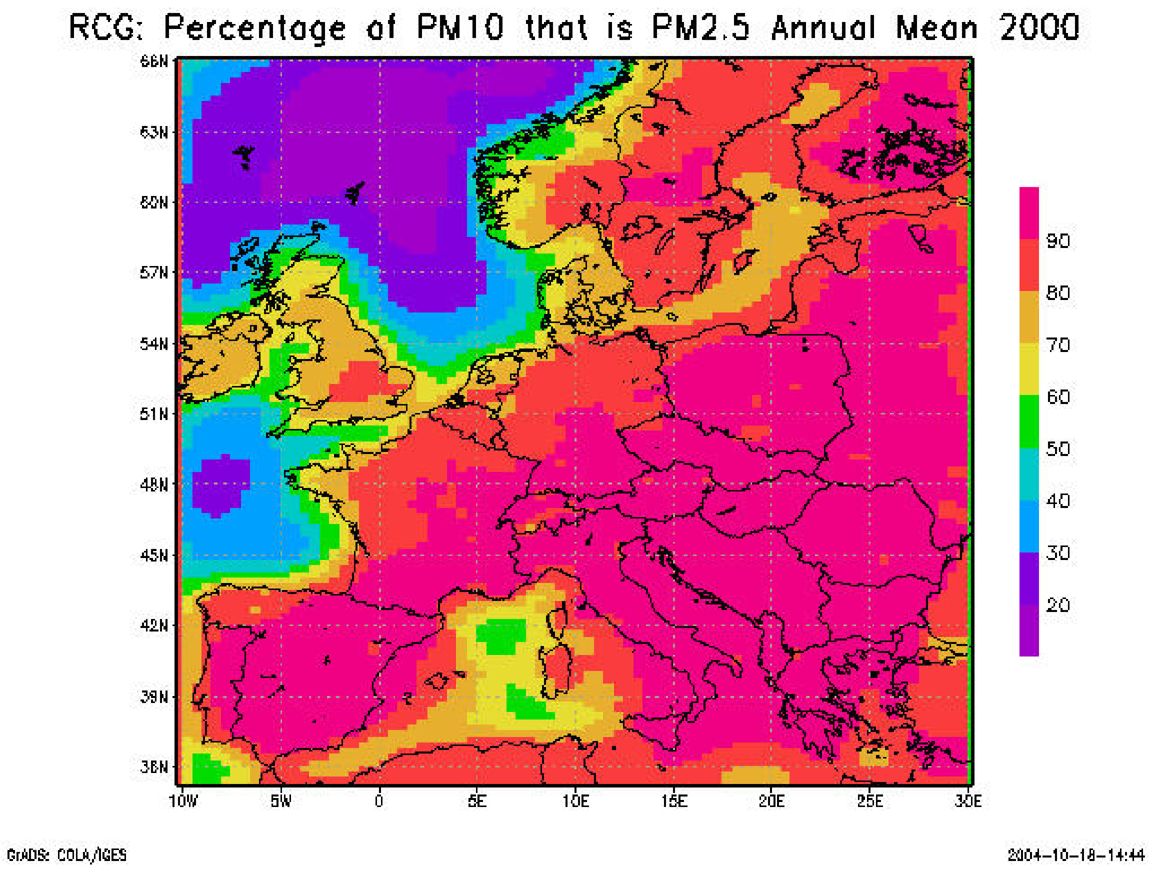
REPRESENTATION OF CURRENT STATE



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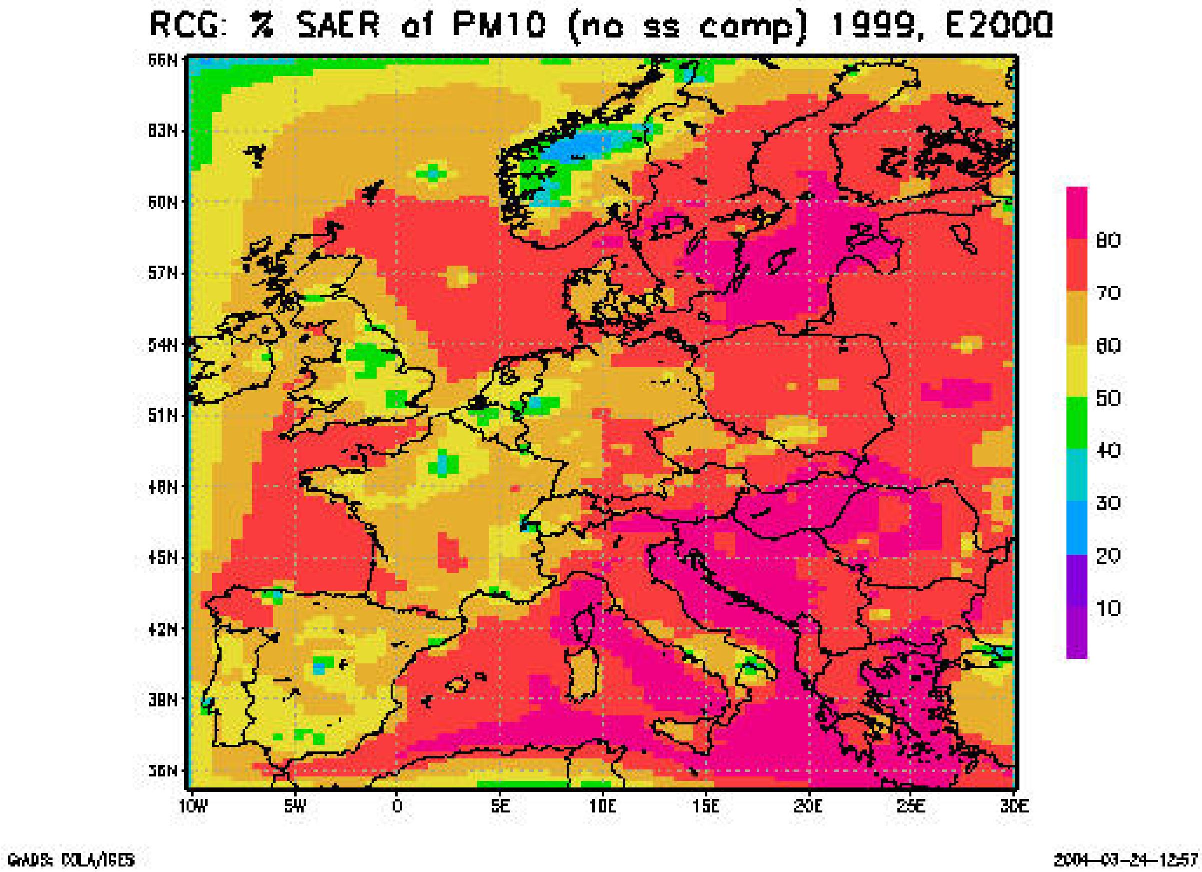
REPRESENTATION OF CURRENT STATE



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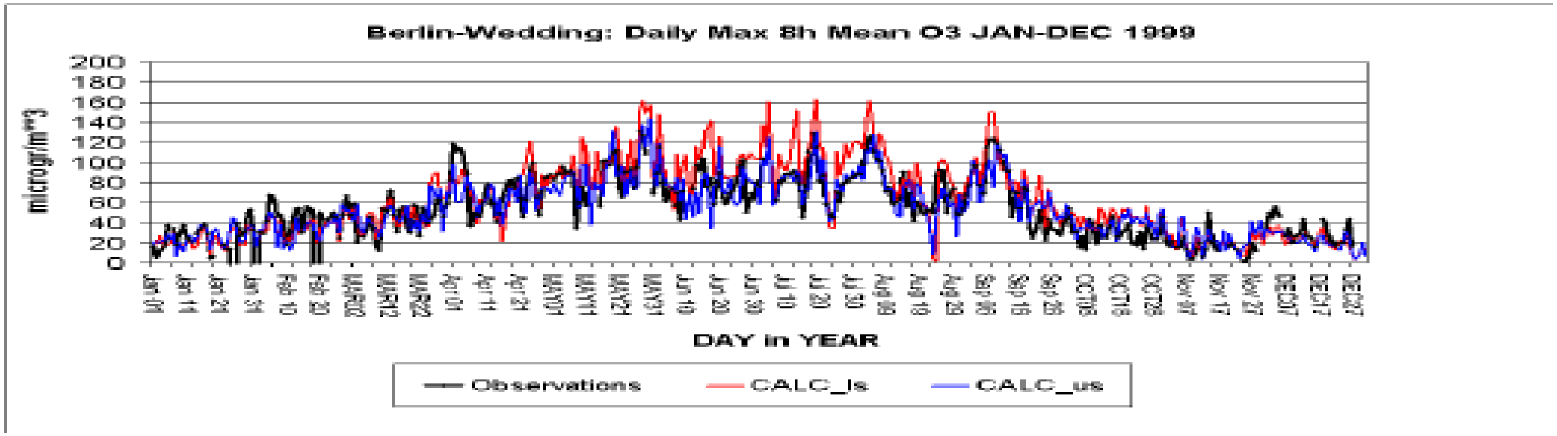
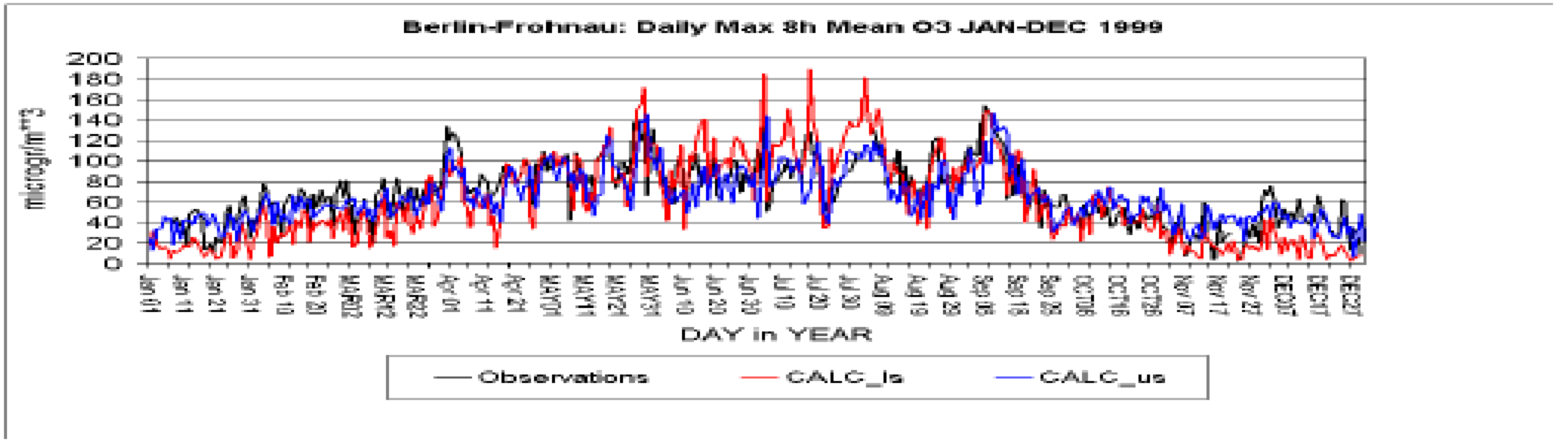
REPRESENTATION OF CURRENT STATE

- temporally continuous





APPLICATIONS

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Emission Scenarios

D2005 – MFR2020 [kt/yr]

SNAP	SO2	NOx	NMVOC	PM10	PM2.5	NH3
01 Combustion in energy and transformation industries	78	135	0	5	4	0
02 Non-industrial combustion plants	47	28	30	15	14	0
03 Combustion in manufacturing industry	3	46	-1	1	1	0
04 Production processes	42	38	7	11	5	1
05 Extraction and distribution of fossil fuels	2	0	13	1	0	0
06 Solvent and other product use	0	0	8	0	0	0
07 Road transport	0	544	73	17	18	3
08 Other mobil sources and machinery	0	68	25	8	8	0
09 Waste treatment and disposal	0	0	0	0	0	0
10 Agriculture	0	5	5	1	1	67
11 Other sources and sinks	0	0	0	2	0	0
Sum	172	864	160	61	51	71

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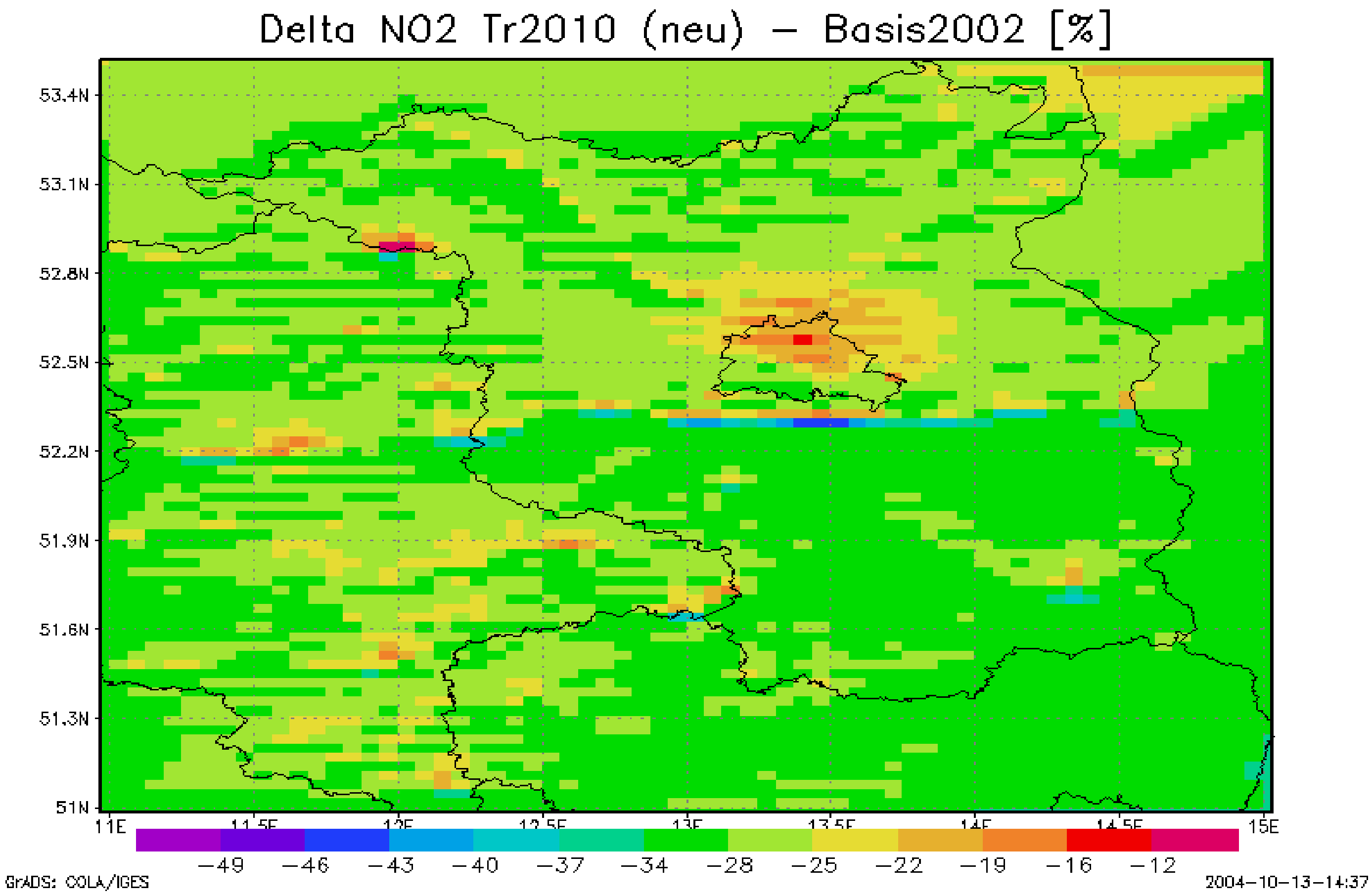
Emission Scenarios



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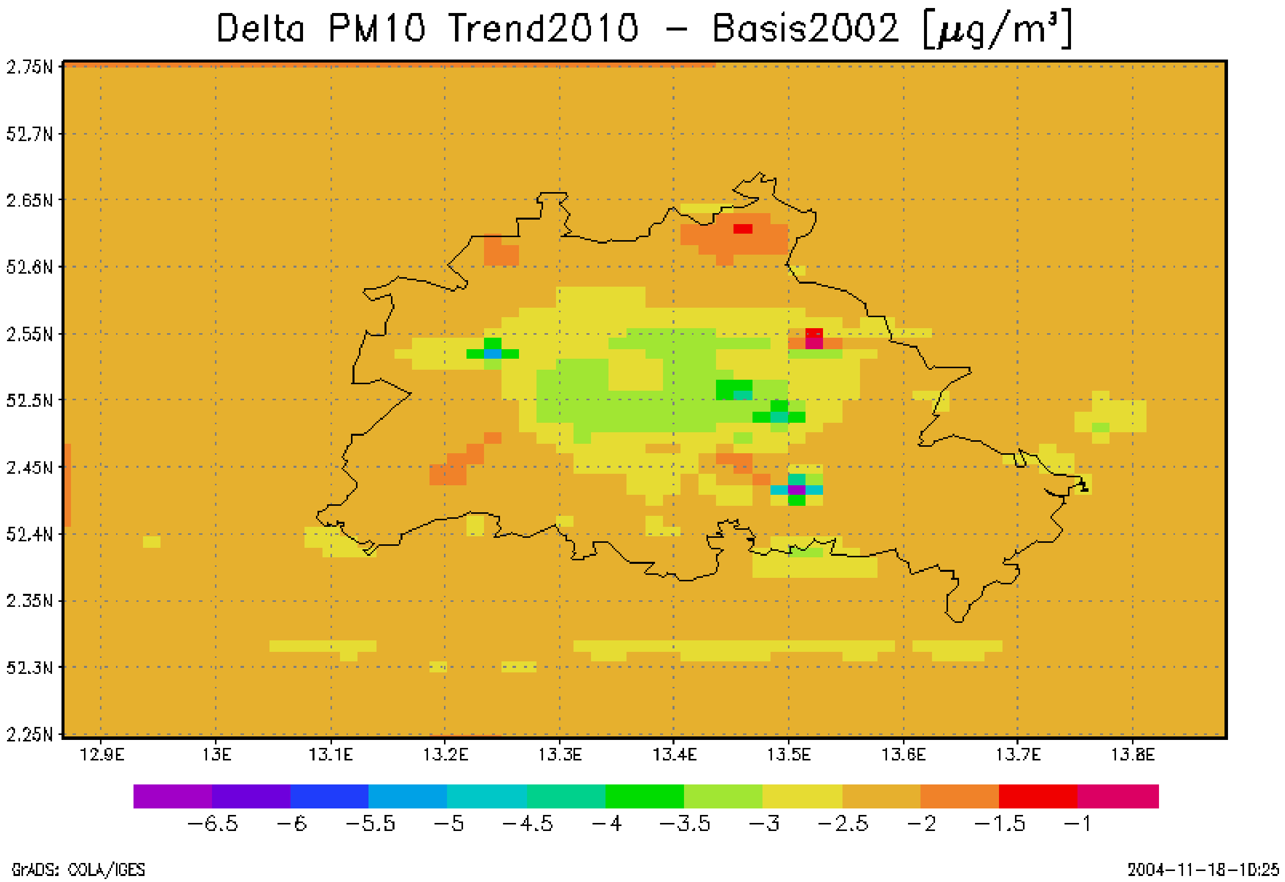
Emission Scenarios



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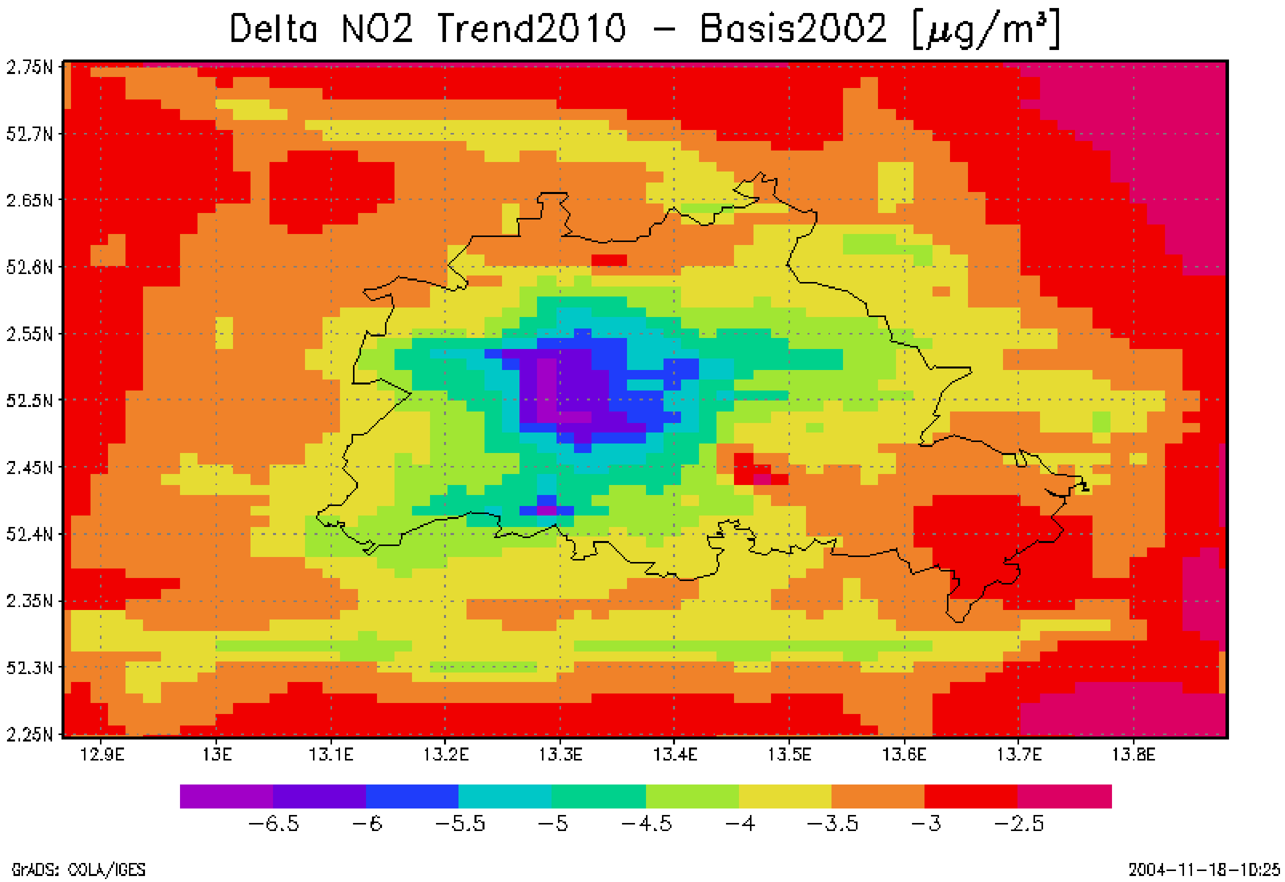
Emission Scenarios



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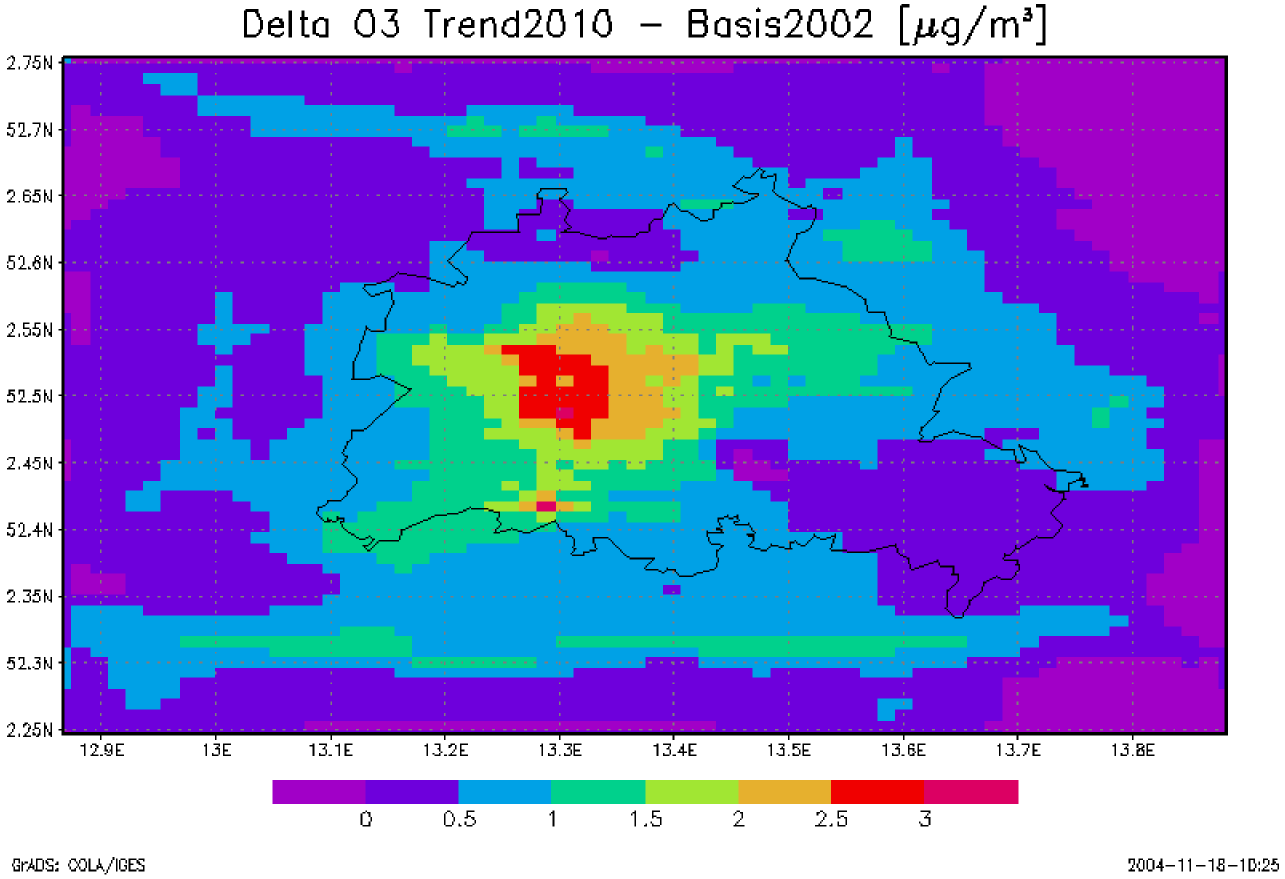
Emission Scenarios



Source Apportionment

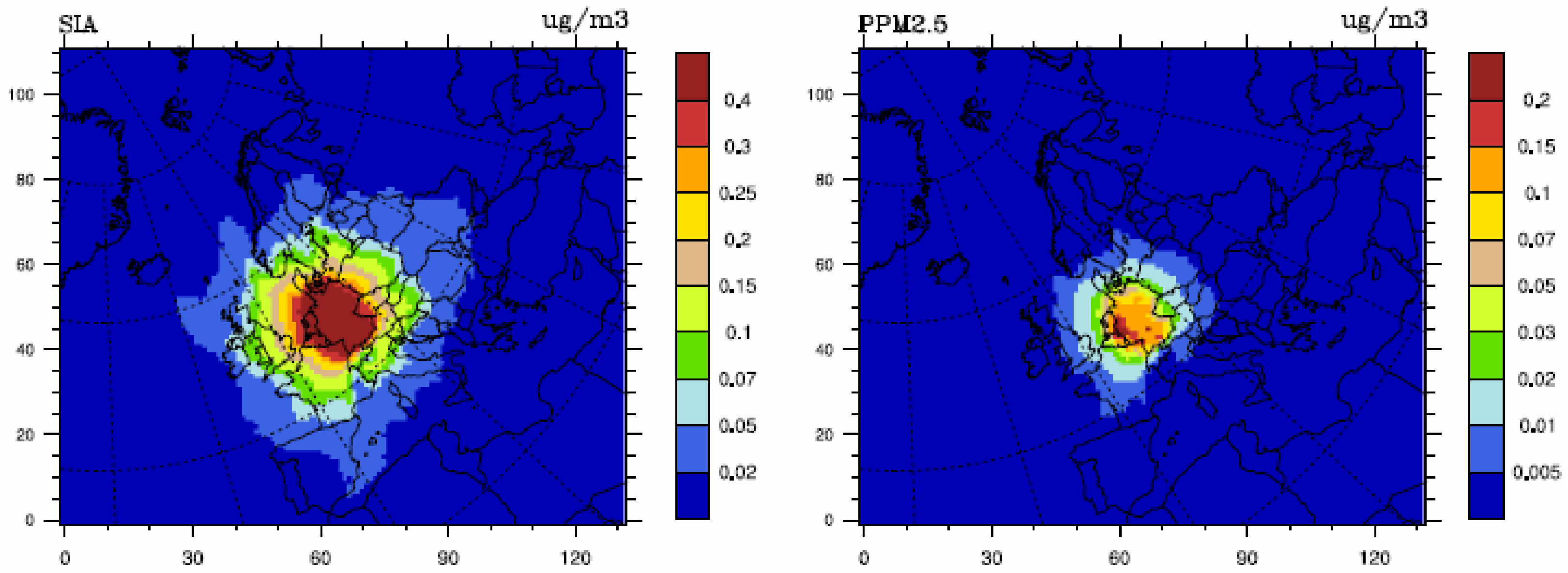


Figure 21: Reduction in SIA and PPM2.5 concentrations due to 15% emission reduction from Germany. Units: $\mu g/m^3$. Note the difference in scales.

from **EMEP**

APPLICATIONS

Source Apportionment

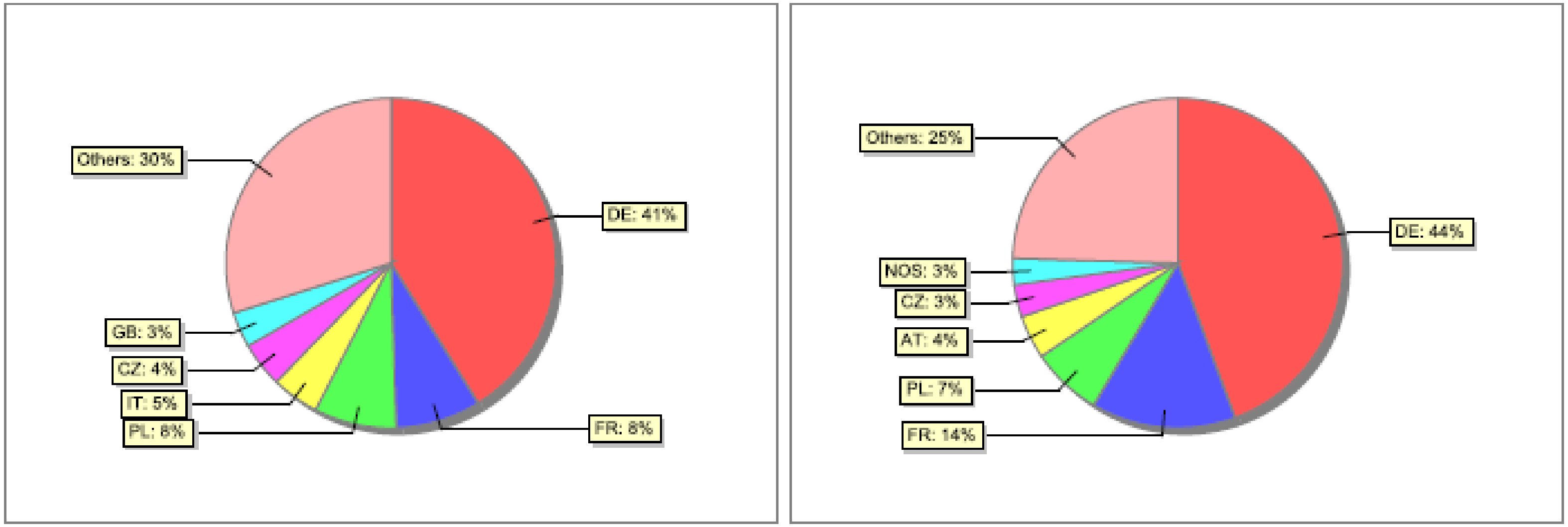
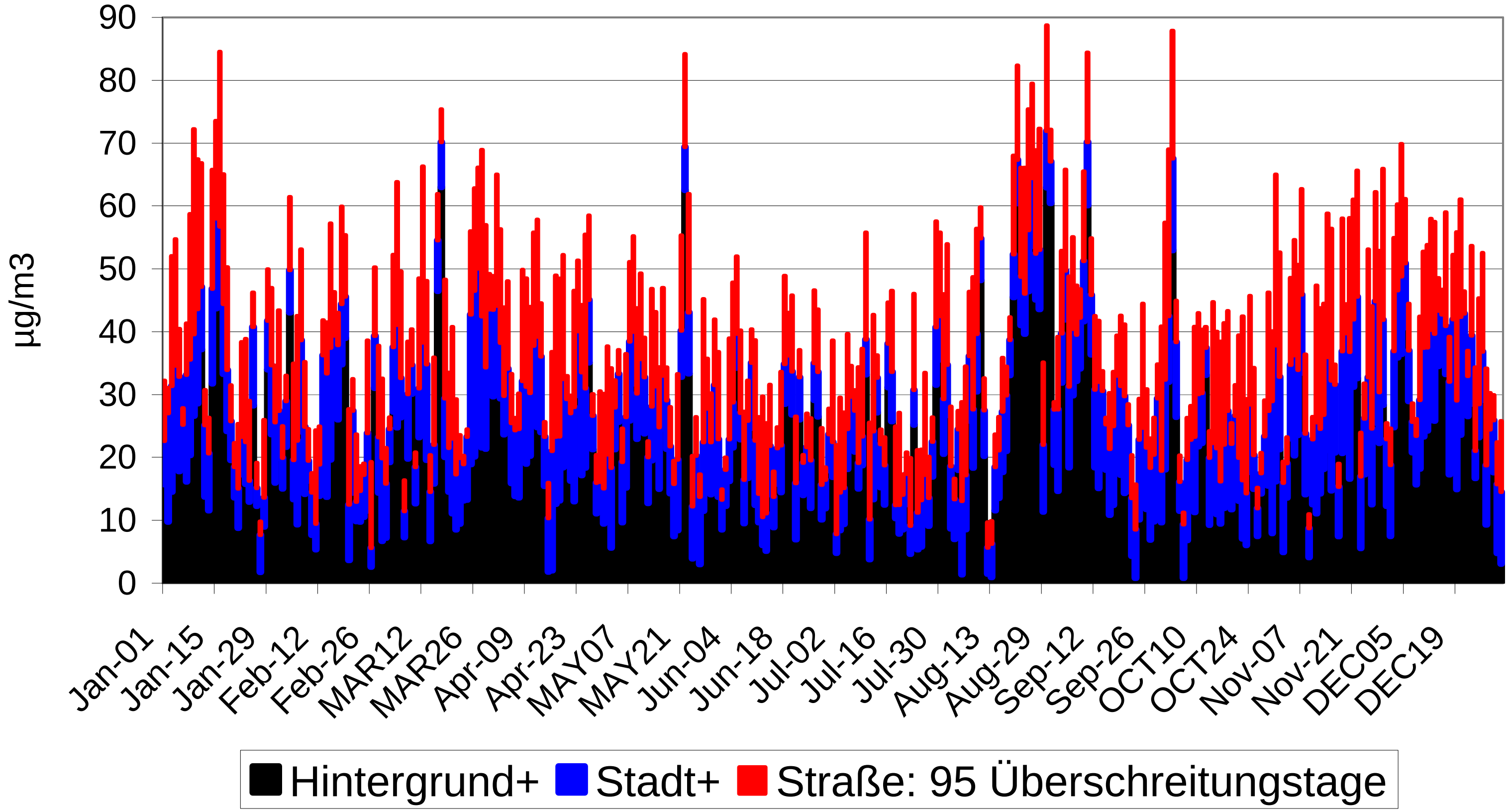


Figure 22: Main contributors to SIA (left) and PPM2.5 (right) concentrations in Germany. Units: (%)

from **EMEP**

Source Apportionment

Konzentrationsbeiträge zu den berechneten PM10-Tagesmittelwerten : Berlin-Silbersteinstr.



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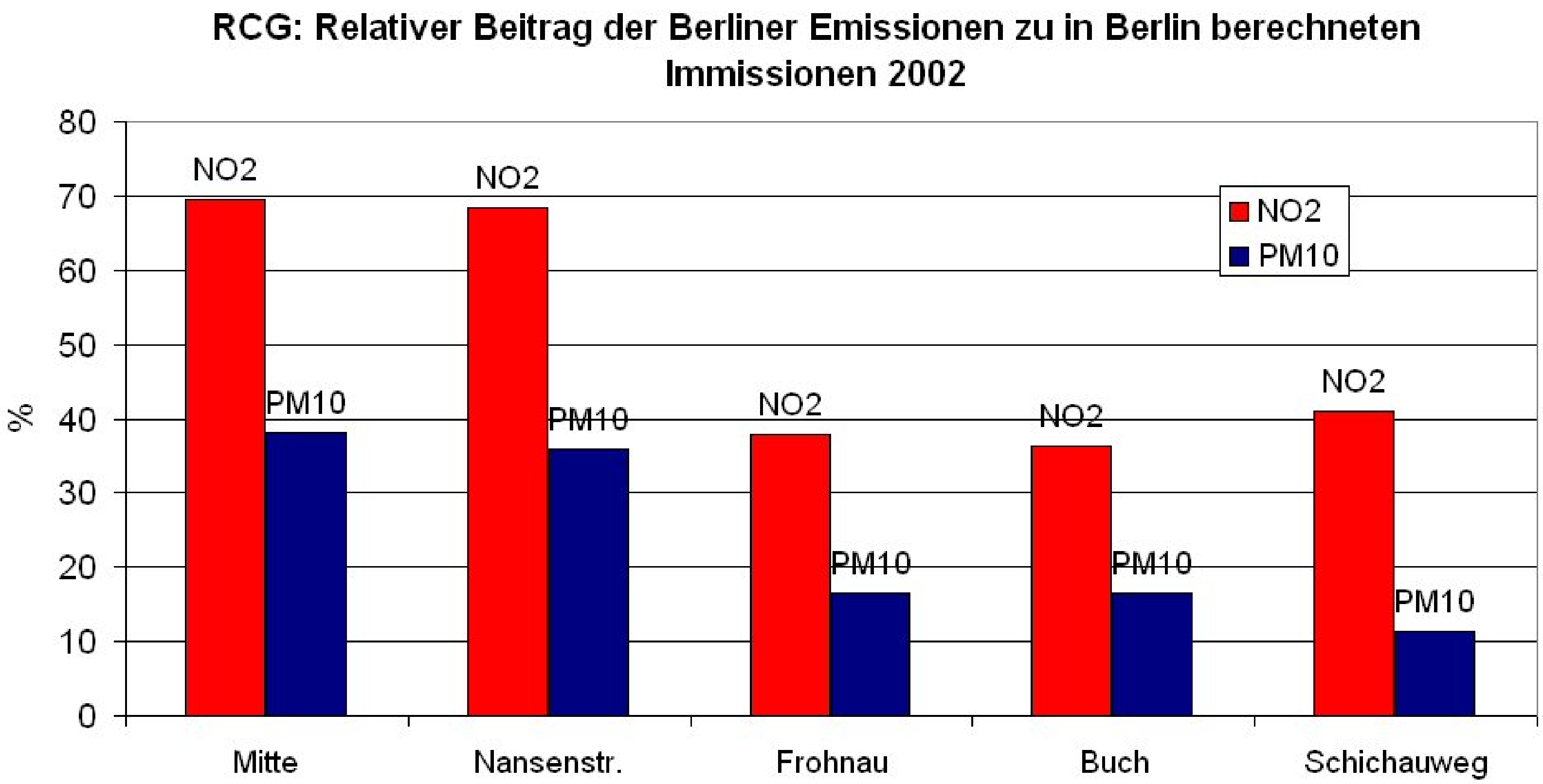
Source Apportionment



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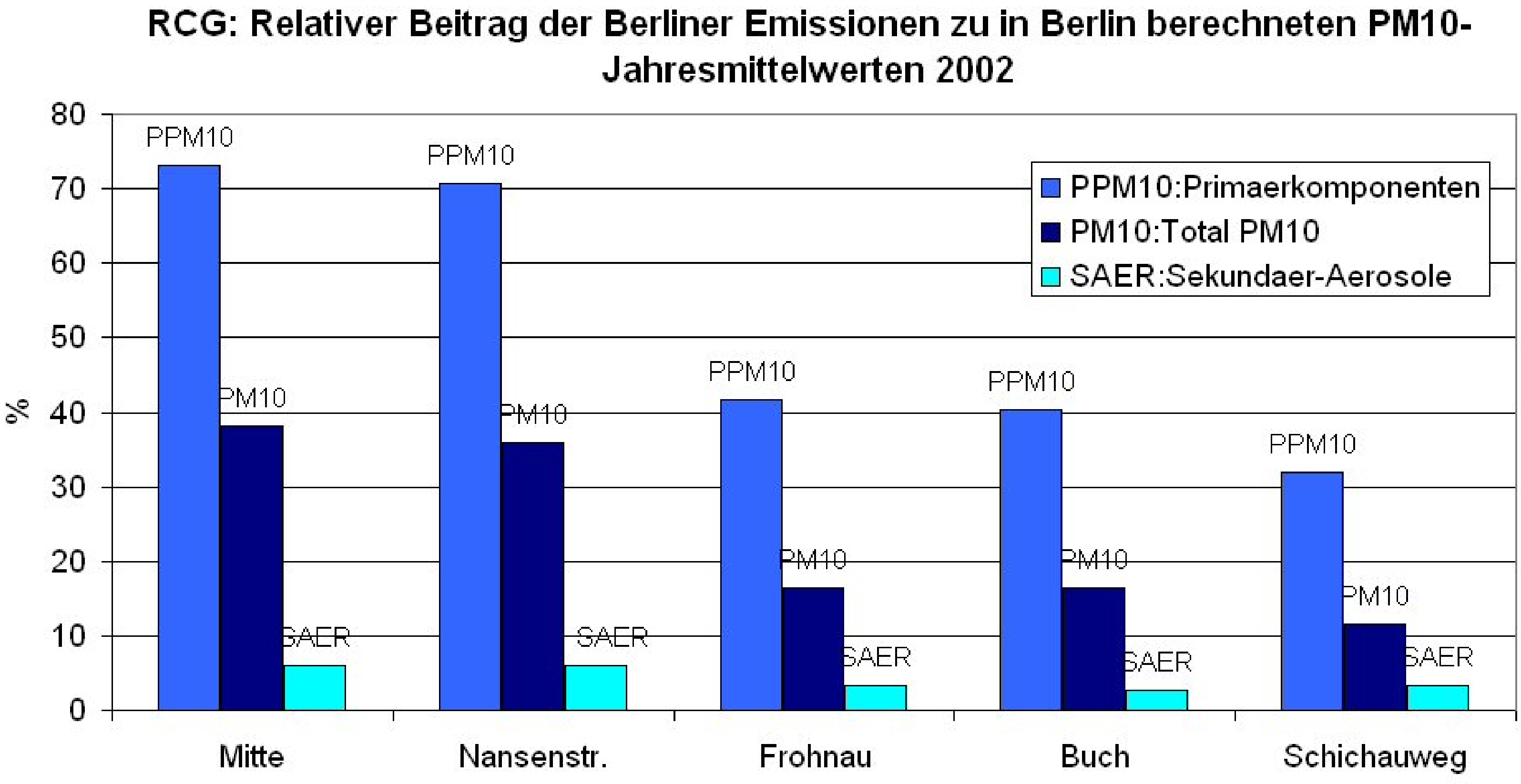
Source Apportionment



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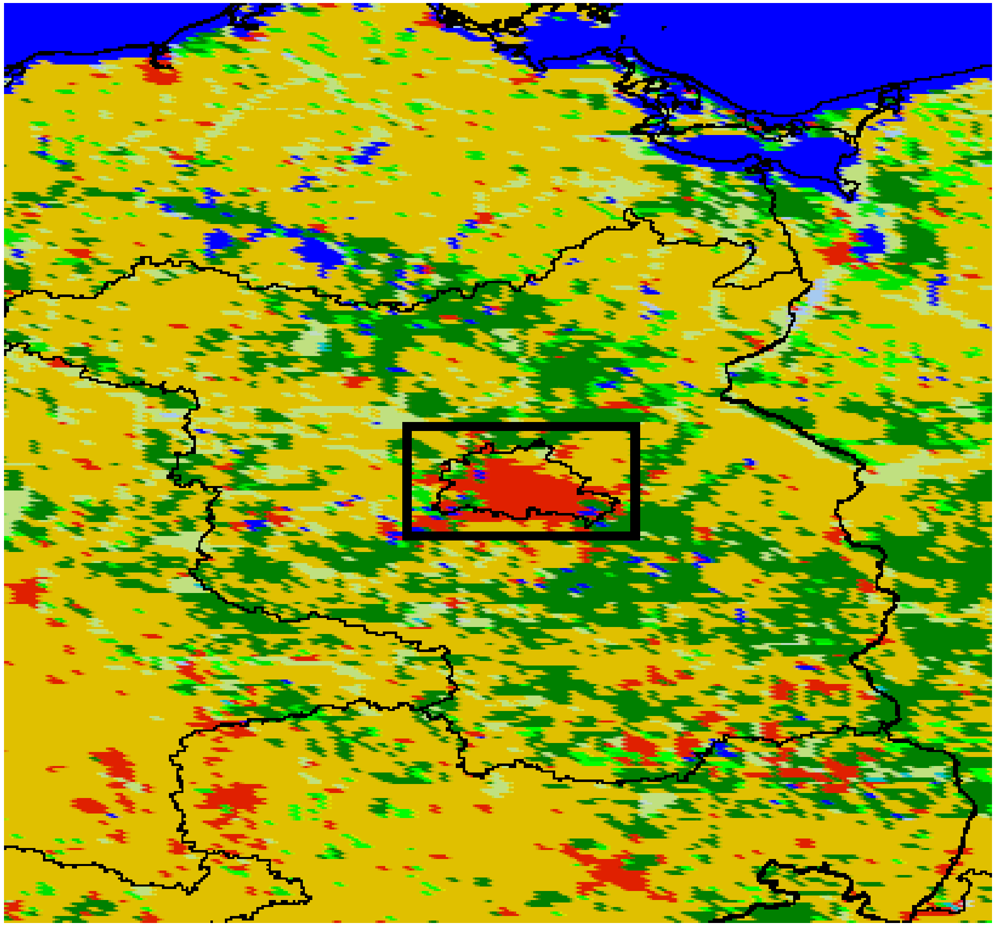
Process Analysis



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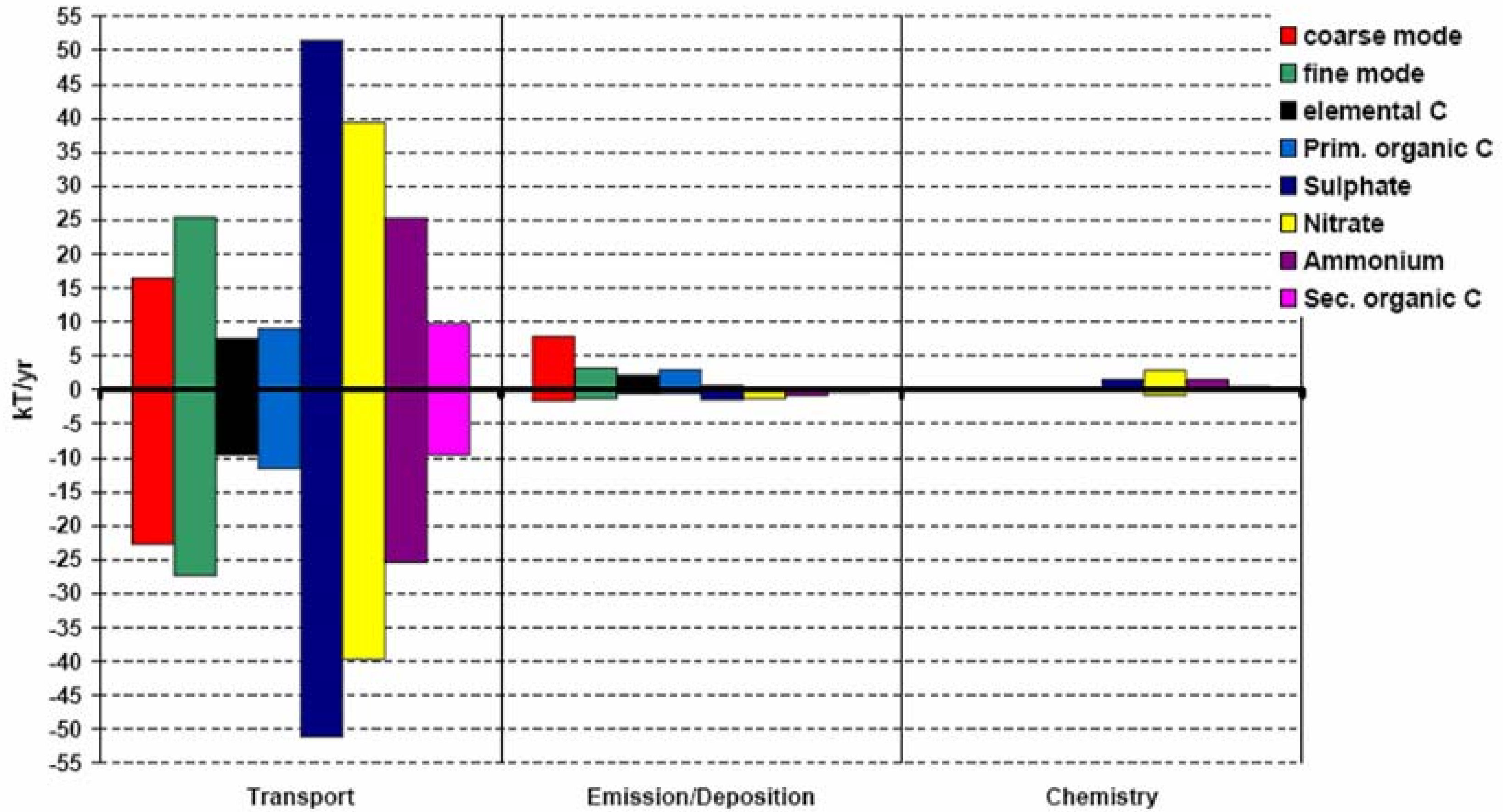
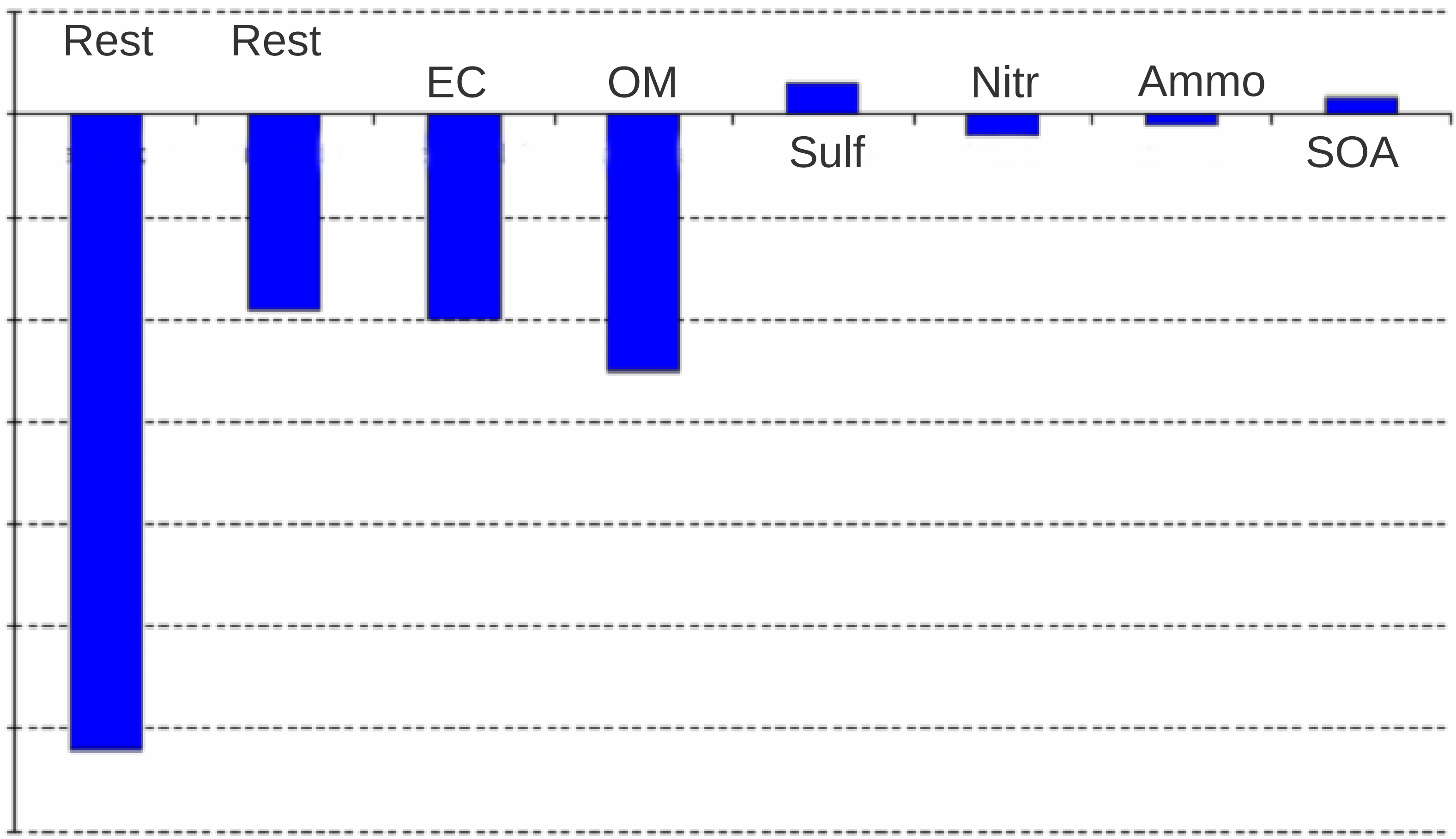
Process Analysis



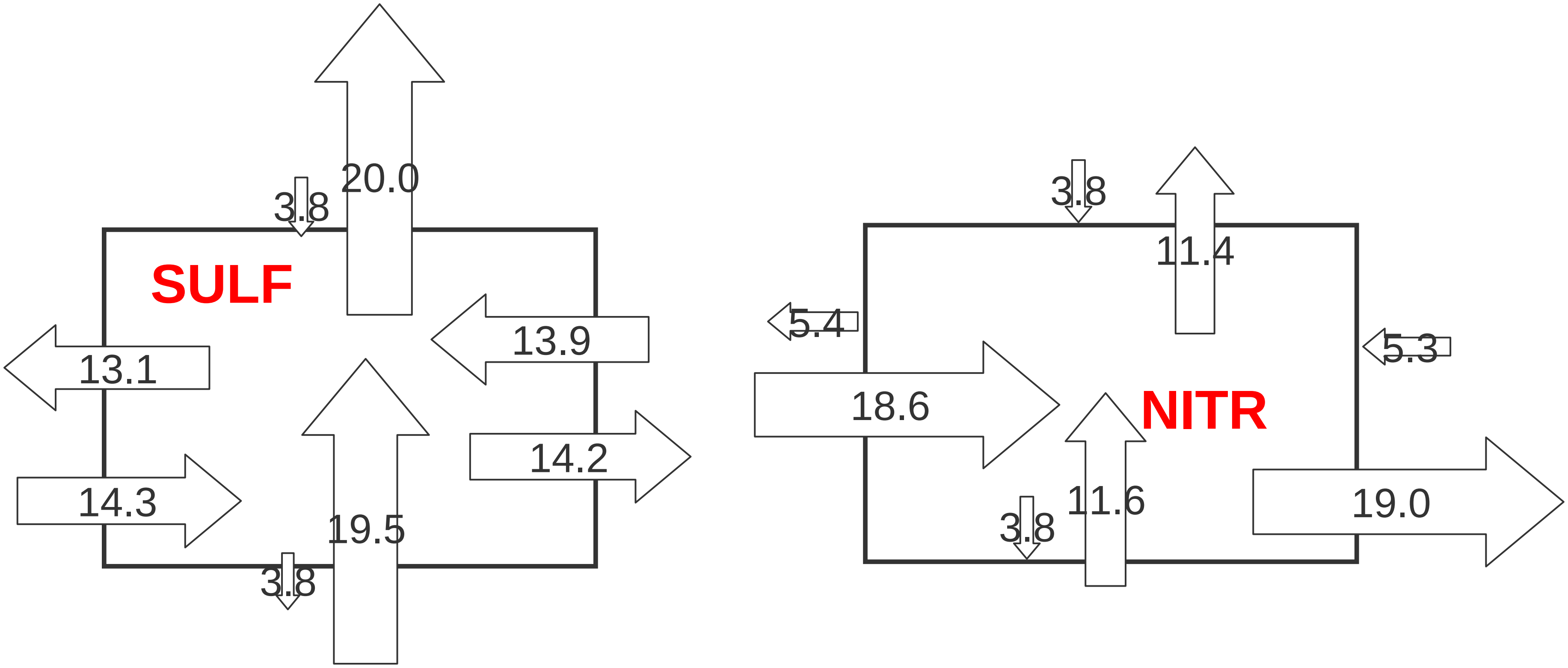
APPLICATIONS

Process Analysis net transport contribution



APPLICATIONS

Process Analysis **wind direction influence**



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