ILMATIETEEN LAITOS
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Examples of forward and inverse simulations

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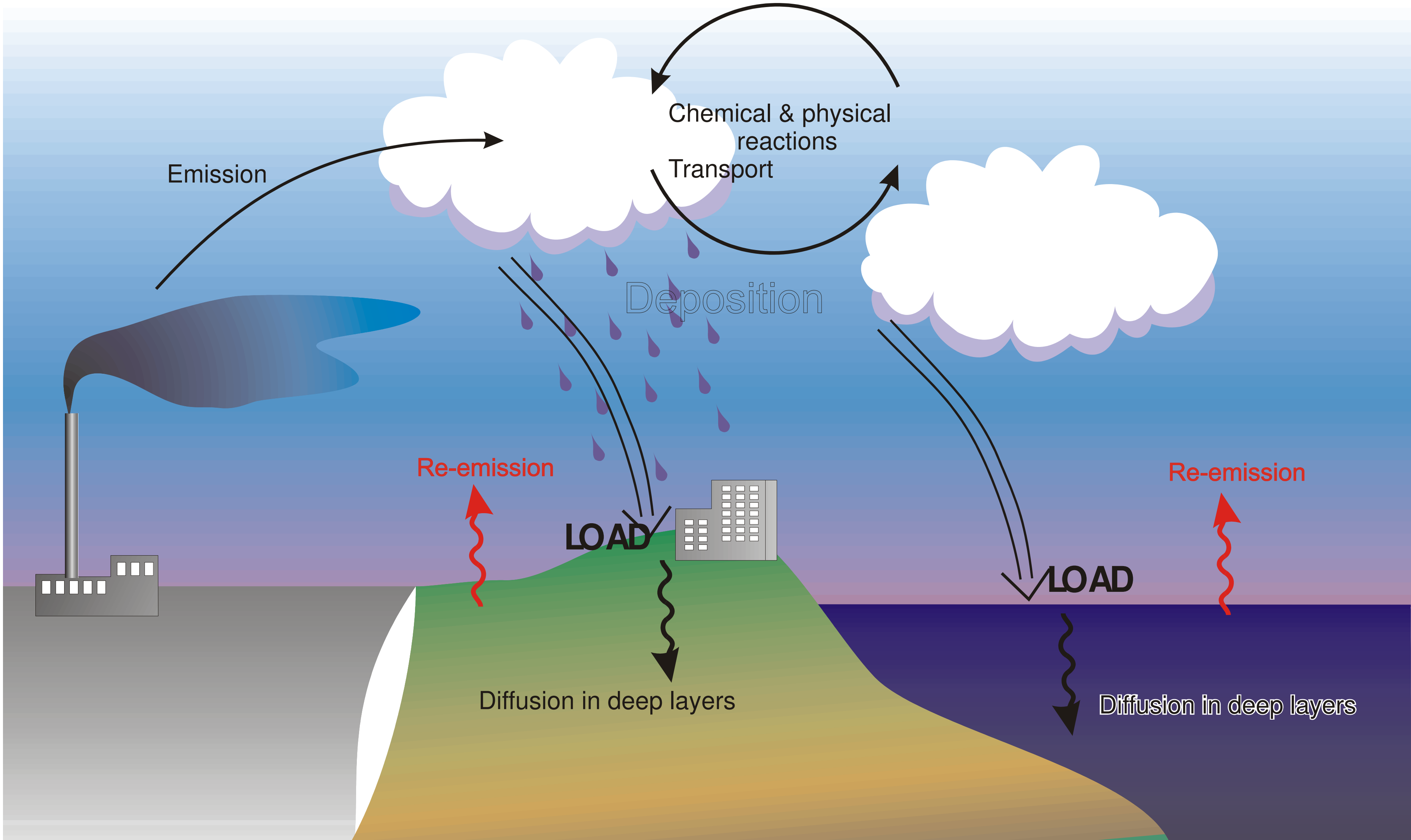
  - Data assimilation in atmospheric modelling
- Basic equations
  - Forward and adjoint diffusion equations
  - An optimization problem of data assimilation
- Materials and methods
  - Overview of SILAM dispersion model
  - Outline of the European Tracer Experiment ETEX
- Inverse problem solution for ETEX
  - Generation of the first guess with adjoint dispersion simulation
  - Iterative minimization of the cost function
  - Post-processing of emission fields
- Summary

Forward dispersion problem



Inverse dispersion problem

Forward diffusion equation

$$LC \equiv \frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i}(U_i C) - \frac{\partial}{\partial x_i}\rho K_{ii}\frac{\partial (C/\rho)}{\partial x_i} + R(C) = E$$

advect. diffusion sink source

$$C(t=0) = C_0(\vec{x}); \quad C(\vec{x} = \partial\Omega) = C_b(\vec{x}, t)$$

Forward diffusion equation: an exposure (load) functional

$$\varphi \in H - \text{Hilbert space}, \; (g,h) = \int_0^T dt \int_{-\infty}^{\infty} gh\, dx$$

$$M = \int_0^T dt \int_{-\infty}^{\infty} C\, p\, dx = (C, p) - \text{load functional}$$

p is a weight (sensitivity) function of the load:

- Population exposure $p(x,t) = \delta(\vec{x} - \vec{x}_{city})$
- Ecosystem damage $p(x,t) = p(t)\, \Theta(A_{ecosystem})$
- Model-measurement comparison for *K* stations

$$p(x,t) = \sum_{k=1}^{K} \alpha_k \delta(\vec{x} - \vec{x}_k)$$

Adjoint diffusion equation

$$(C^*, f) = (C^*, LC) = (L^*C^*, C) = (p, C)$$

$$L^*C^* = p \quad - \quad \text{adjoint diffusion equation}$$

$$L^* = -\frac{\partial}{\partial t} - \frac{\partial}{\partial x_i}(U_i) - \frac{\partial}{\partial x_i} K_{ii} \frac{\partial}{\partial x_i} + R$$

$$C, C^* \xrightarrow{x \to \infty} 0$$

$$C^*(t = T) = 0$$

Load functional:

$$M = (p, C) = (C^*, f)$$

Dual features of atmospheric dispersion problem

Forward problem:

$$L = \frac{\partial}{\partial t} + \frac{\partial}{\partial x_i}(U_i) - \frac{\partial}{\partial x_i}\rho K_{ii}\frac{\partial(1/\rho)}{\partial x_i} + R; \qquad LC = E; \;\; M = (p, C)$$

Adjoint problem

$$L^* = -\frac{\partial}{\partial t} - \frac{\partial}{\partial x_i}(U_i) - \frac{\partial}{\partial x_i}K_{ii}\frac{\partial}{\partial x_i} + R; \qquad L^* C^* = p; \;\; M = (E, C^*)$$

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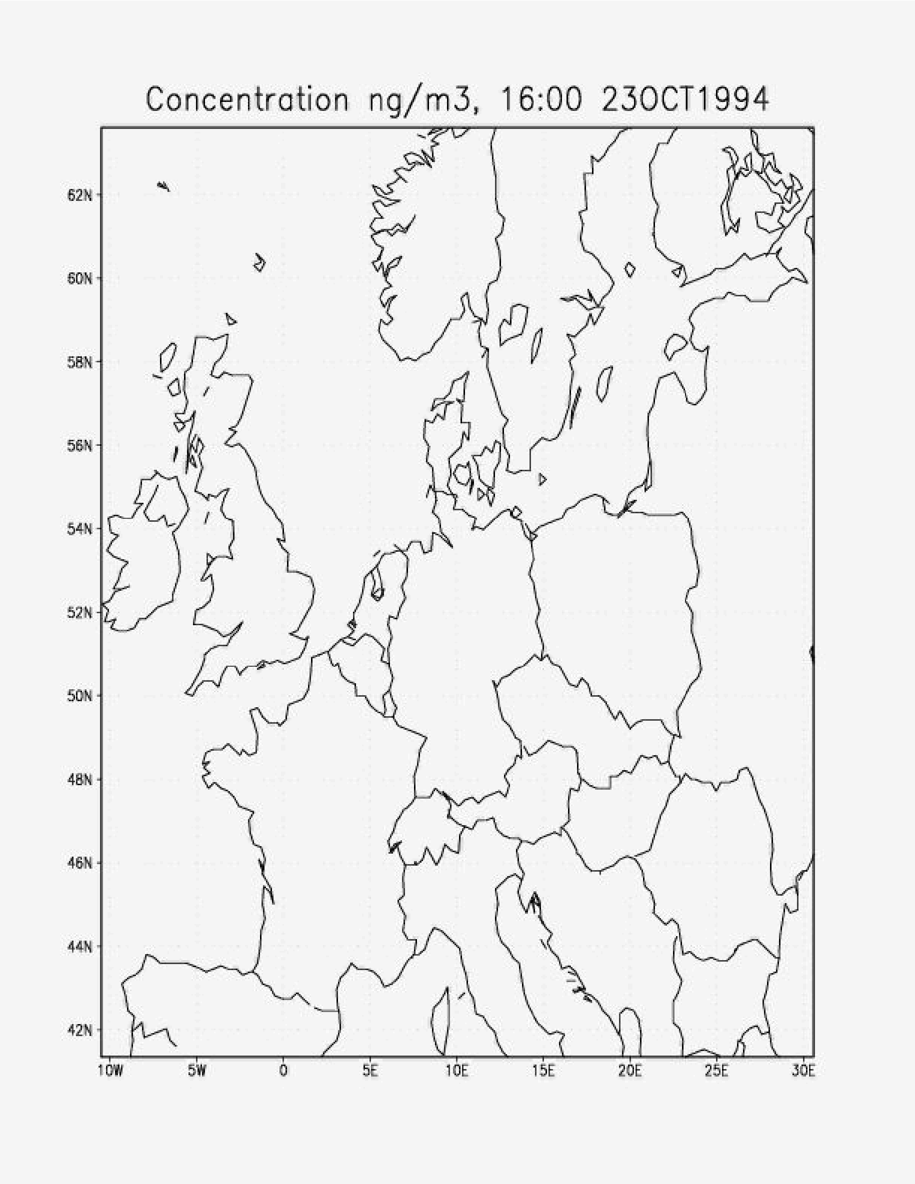
European Tracer Experiment ETEX

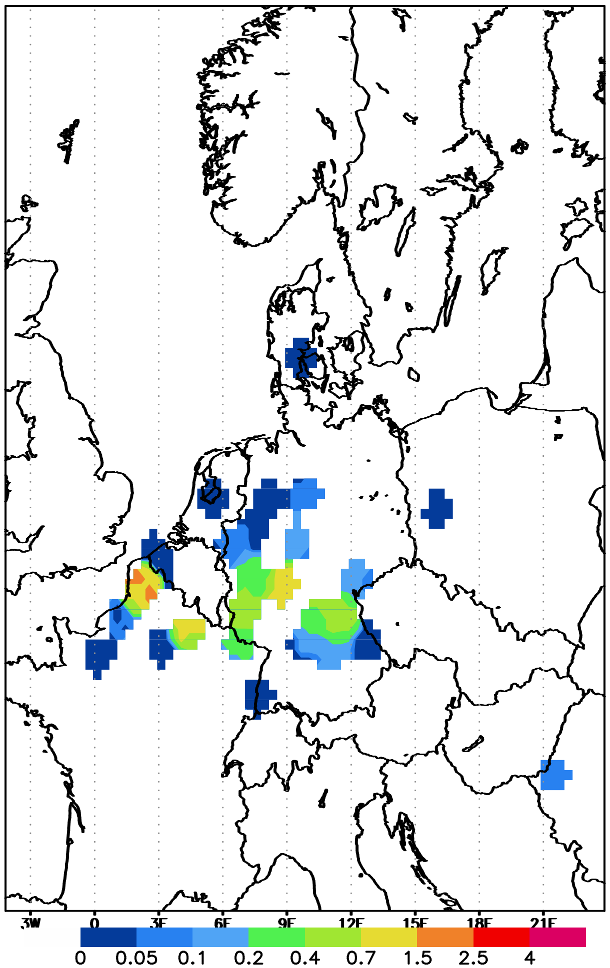
- Inert tracer release: 23-24.10.1994, north-western France
- ~160 observation stations over Europe
  - ~90 hours sampling period
  - 3-hour mean data
- ~30 numerical models, 6 sets of meteo data
- Over 20 statistical measures of model quality

Plume evolution (SILAM)

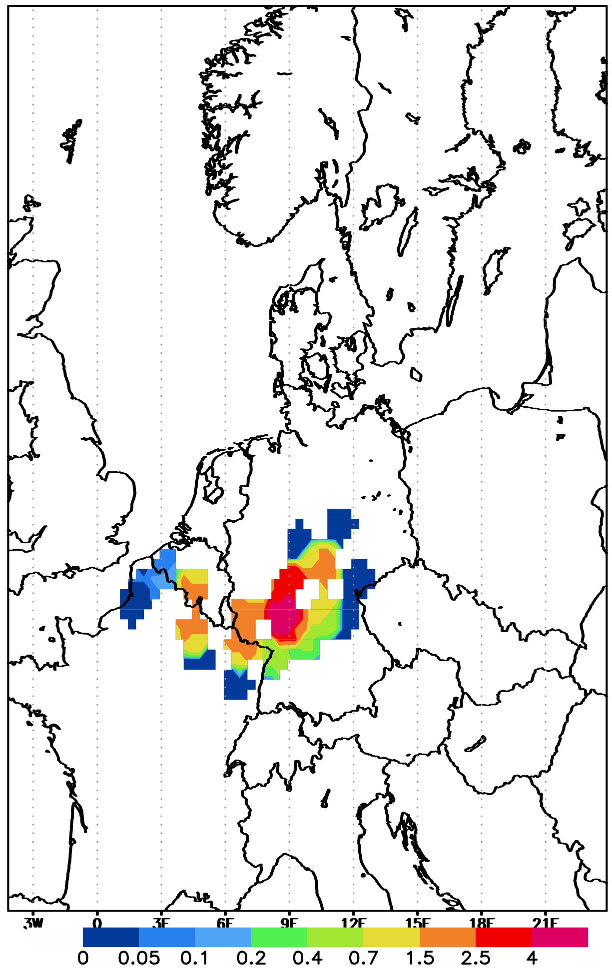


Concentrations at T+1 day

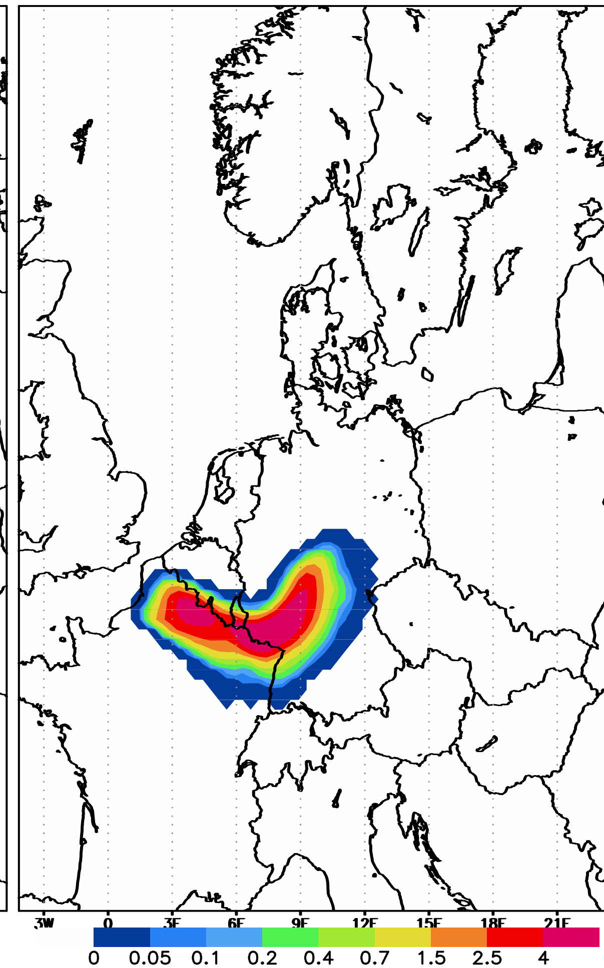
Conc.observed ng/m3,
18:00 24OCT1994



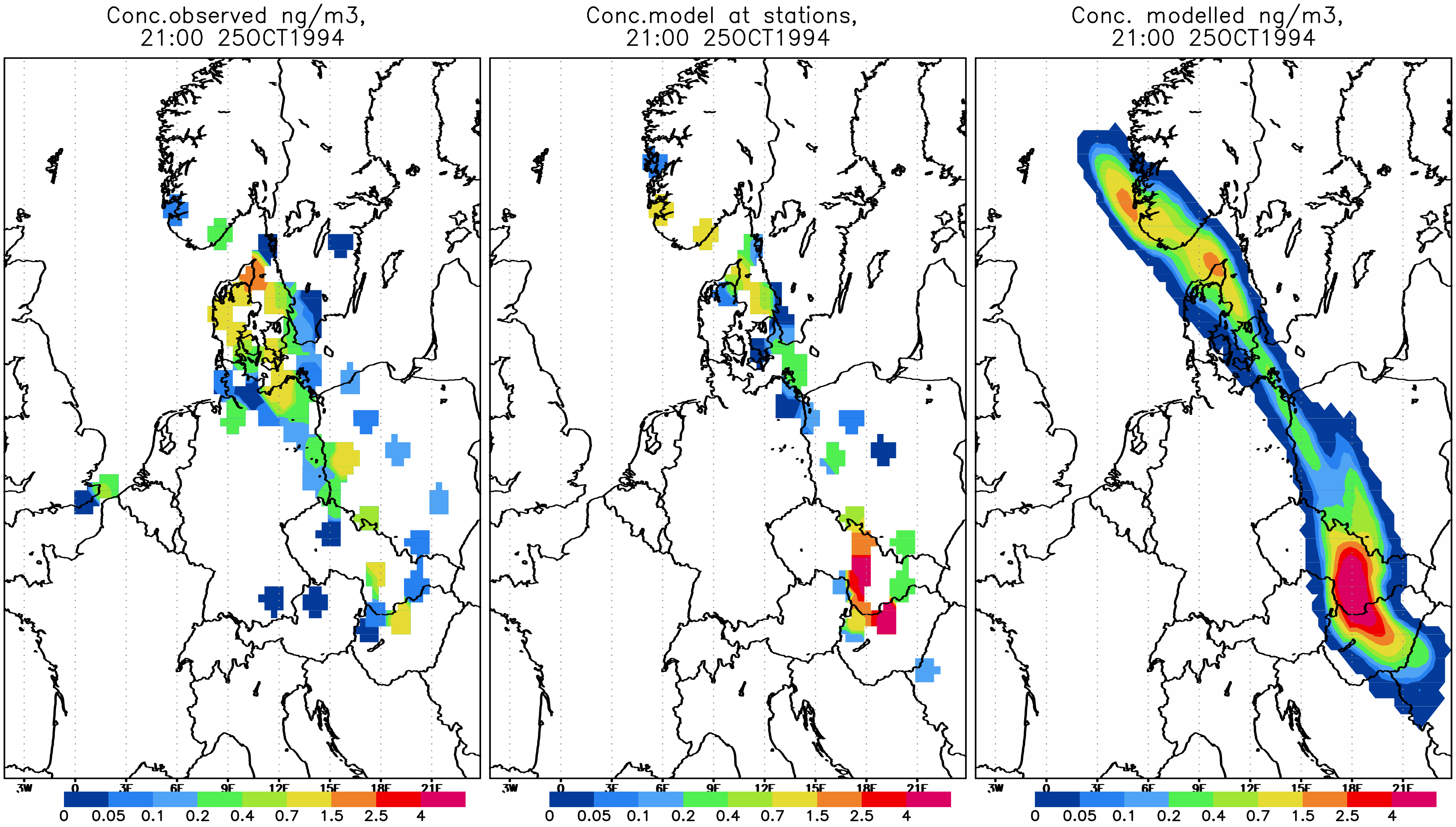
Conc.model at stations,
18:00 24OCT1994



Conc. modelled ng/m3,
18:00 24OCT1994



Concentrations at T+2 days



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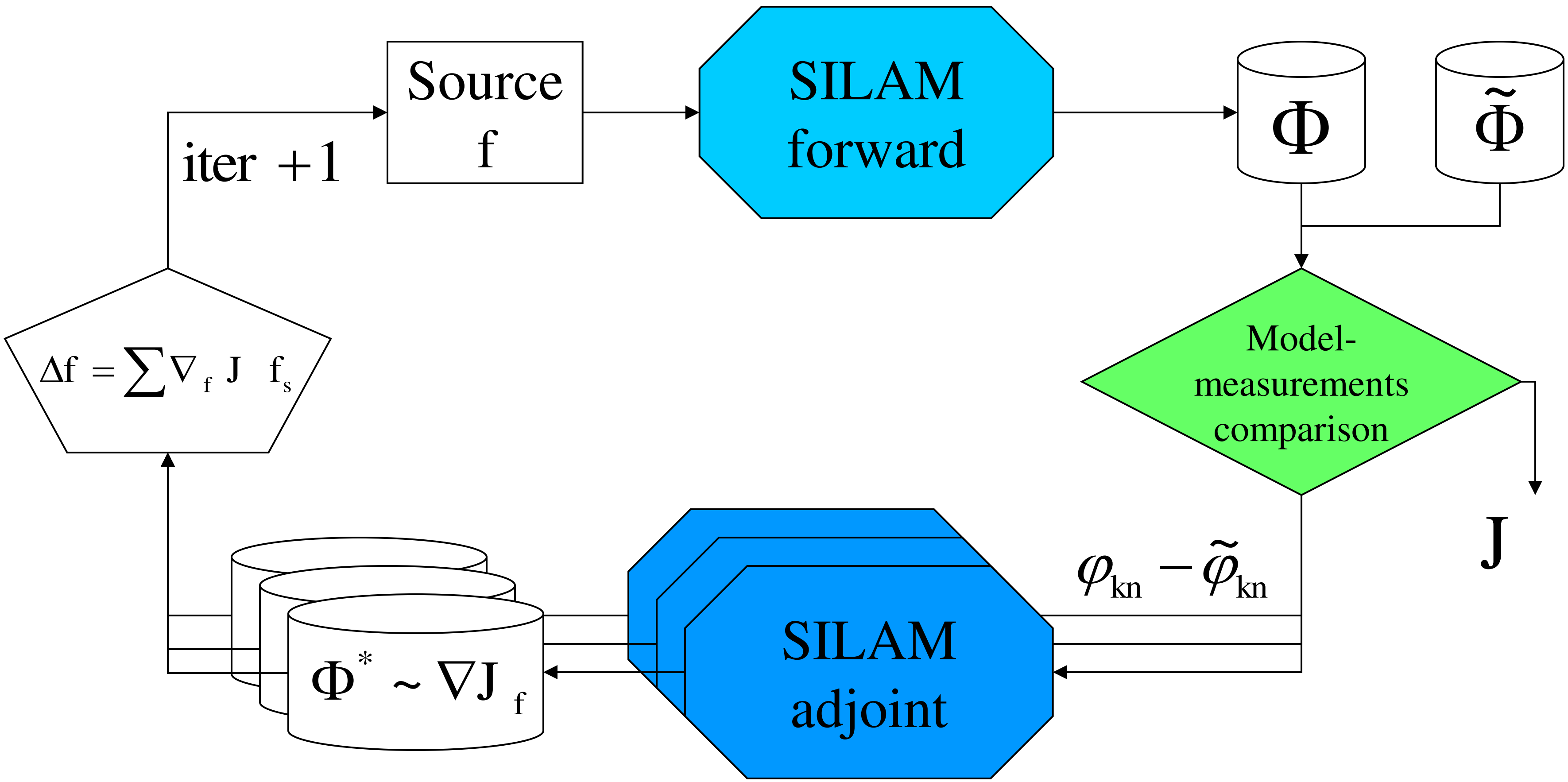
Input and output of adjoint runs

- First-guess generation
  - ➢ Zero-source first guess $\Rightarrow$ modelled concentrations $\equiv 0$
  - ➢ Two kinds of measurements as input for adjoint runs
    - – Non-zero value => sensitivity distribution covers possible source area
    - – Zero value => sensitivity distribution covers “no-source” area
- Iterations
  - ➢ Three kinds of model-measurement relations in input to adjoint runs
    - – Model – measurement > 0 – over-estimation
    - – Model – measurement < 0 – under-estimation (equal to above non-zero case)
    - – Model = measurement = 0 – all-zero case, (equal to above zero case)
- A way to combine in the adjoint runs output:
  - ➢ make two / three adjoint SILAM runs, one for each case;
  - ➢ subtract C^* for zeroes and C^* for over-estimation cases from C^* for under-estimation cases

Iterative cost function minimization



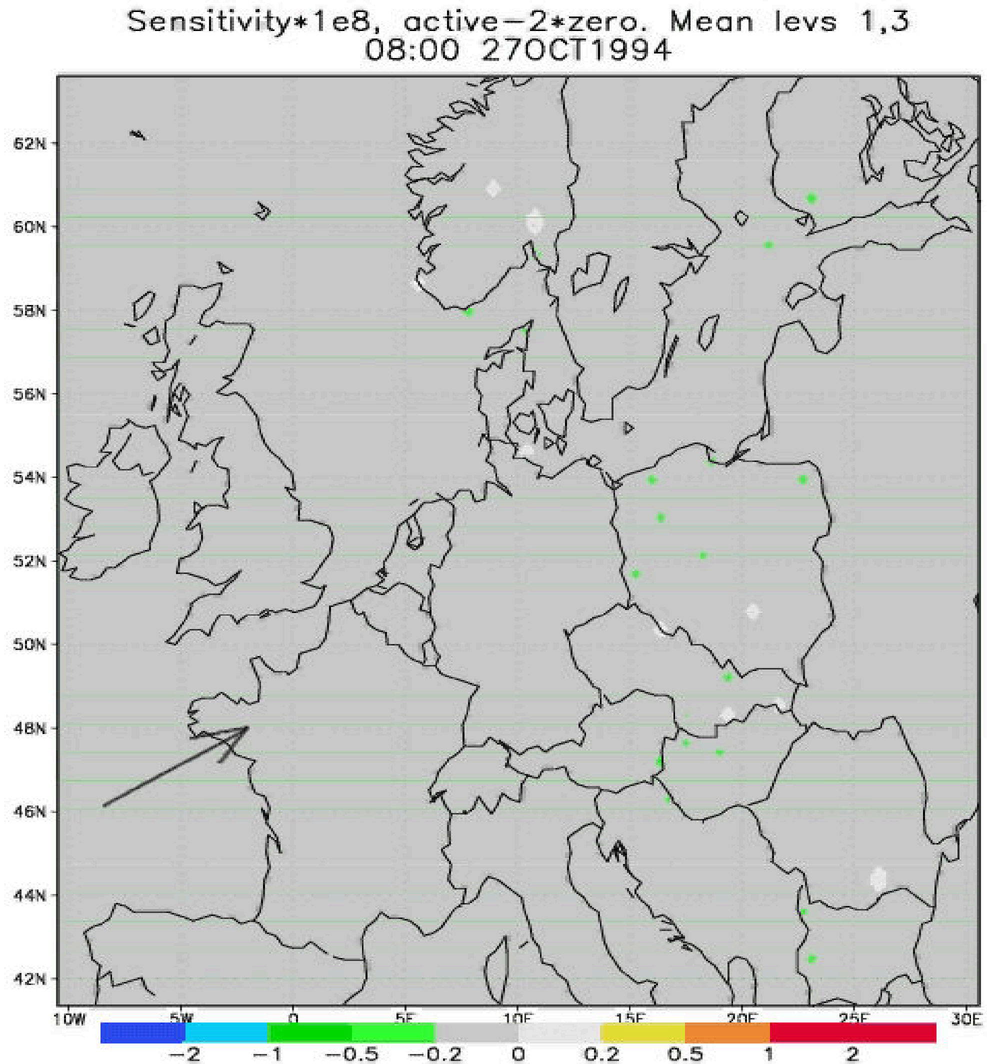
Evolution of sensitivity distribution (1st guess)

True source:

(2^0 W, 48.05^0 N)

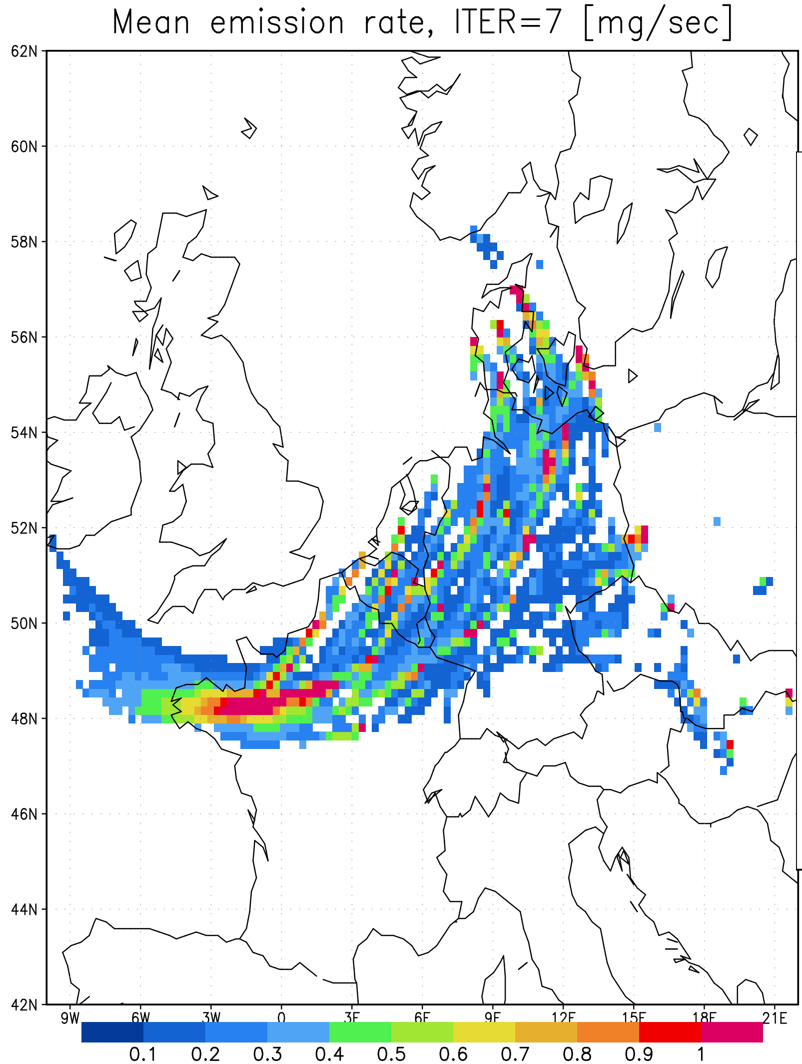
Release time:
23.10.1994 16:00 ->

24.10.1994 3:50
(duration ~12 hours)



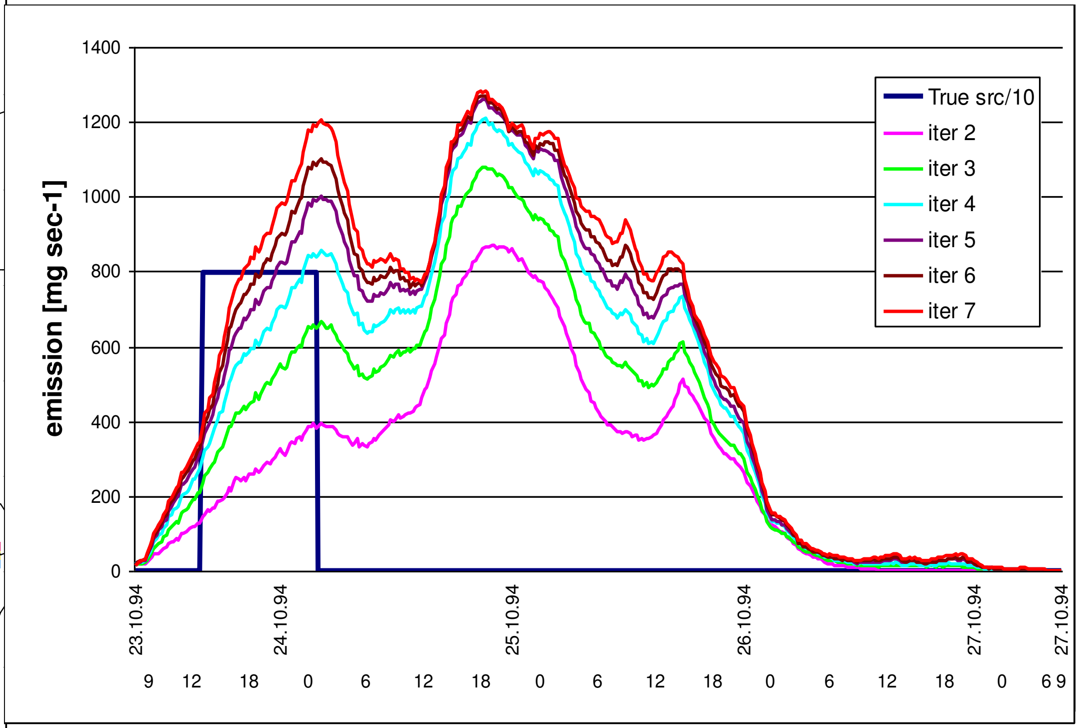
Emission from assimilation cycle 7 (before post-processing)

Map

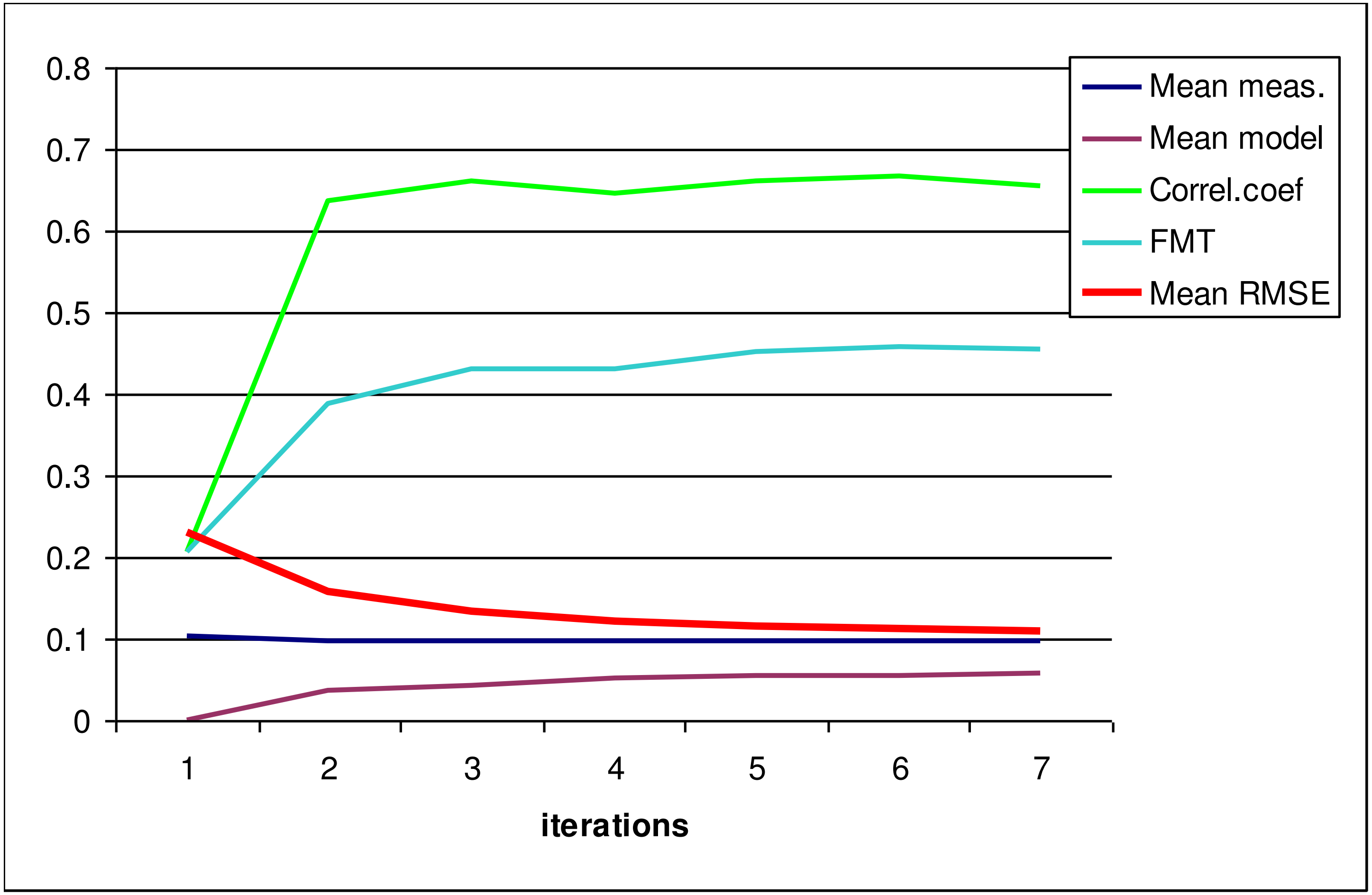


7

Time evolution

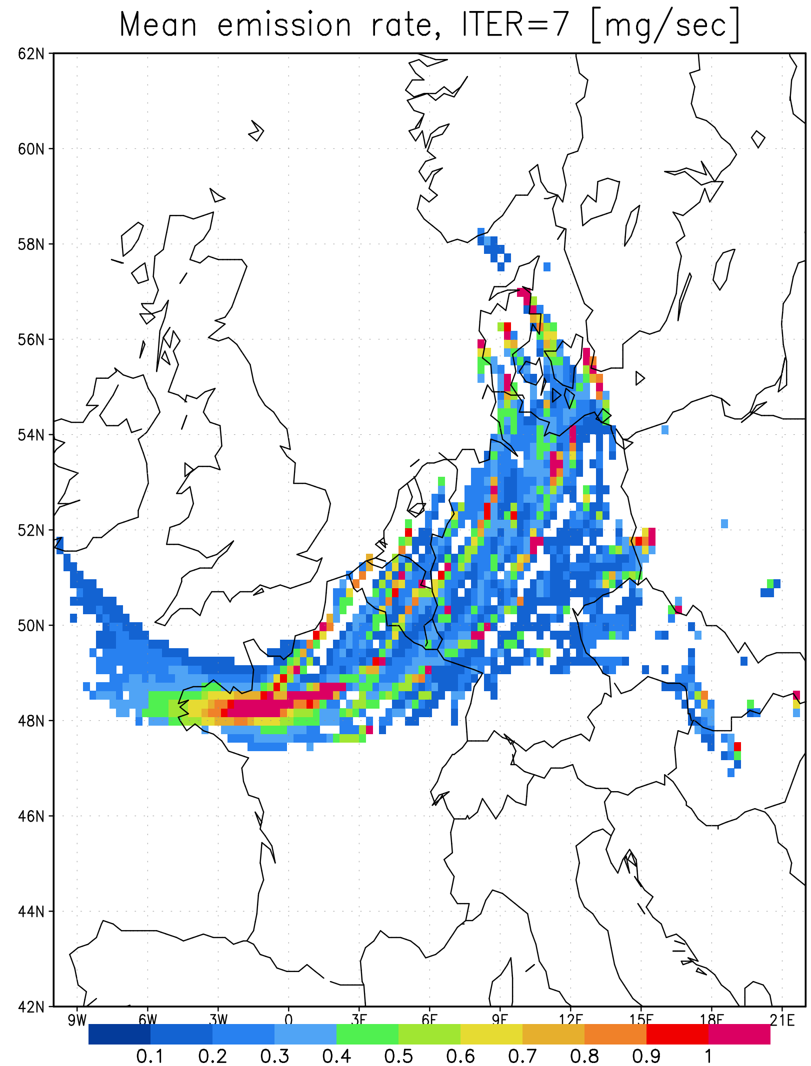


Comparison with observations. Cost function



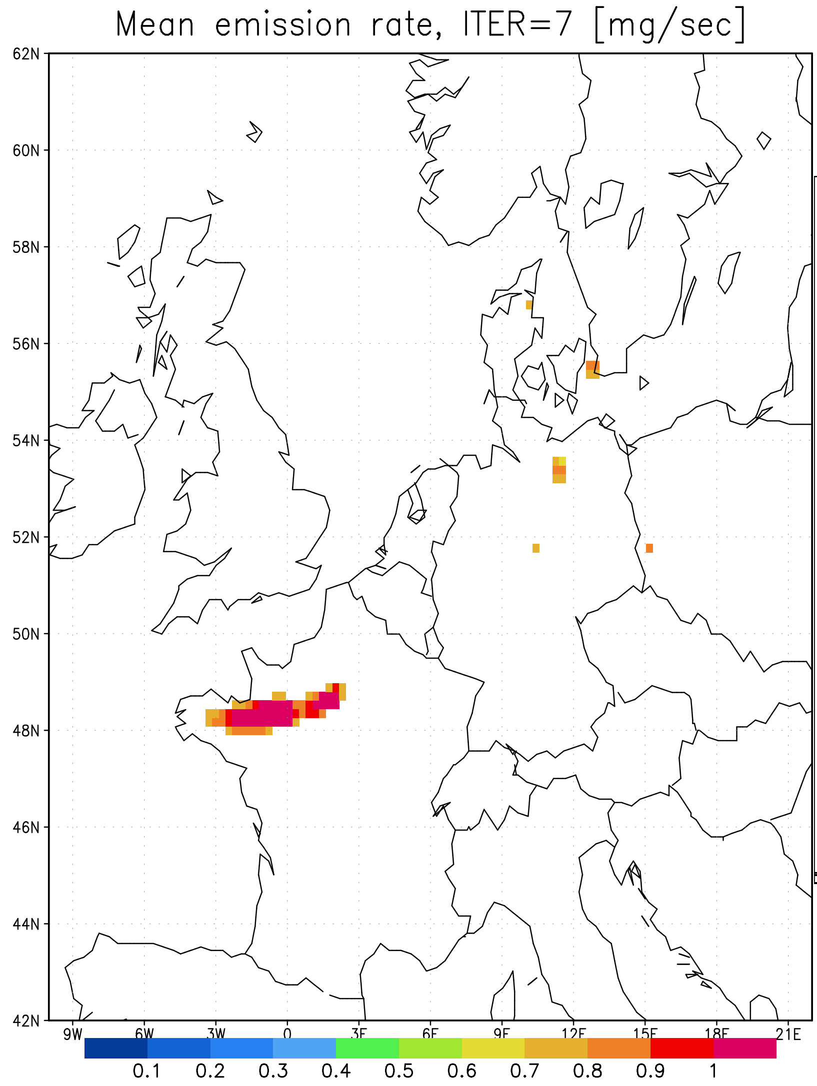
Emission from assimilation cycle 7 (before post-processing)

Post-processing the emission map (no feedback to assimilation iterations!):
- low-pass filtering of high-frequency noise
- cutting out the background level of emission

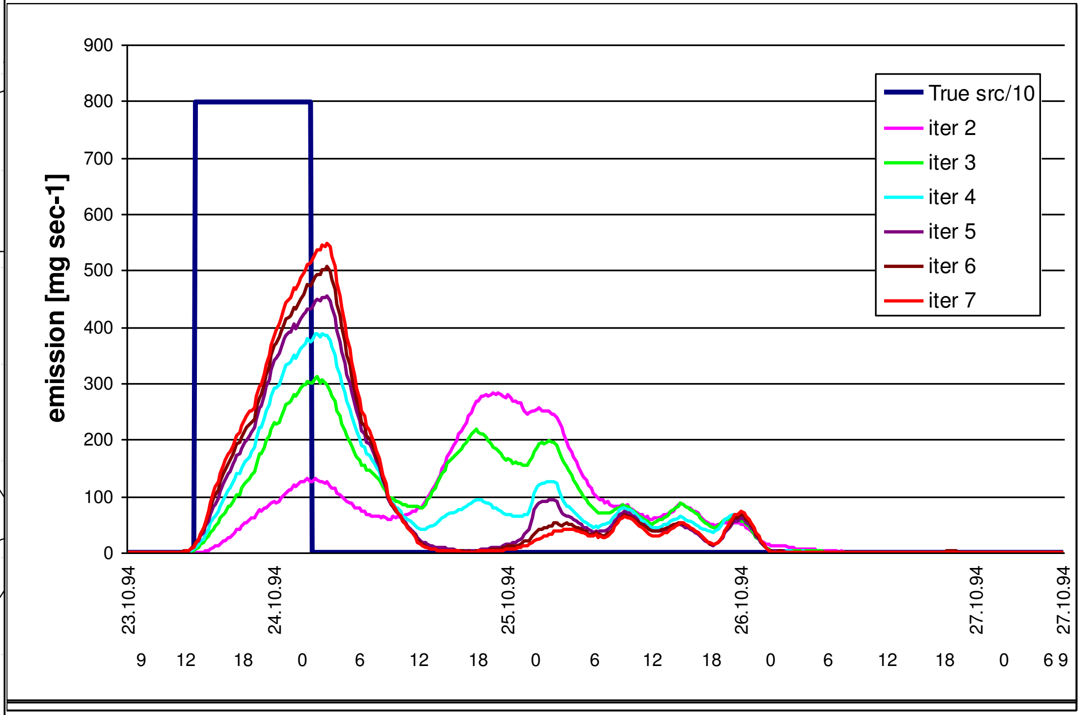


Final emission distribution

Map iteration: 7



Time evolution



Summary

- Adjoint formalism and data assimilation can be used for solving inverse dispersion problem
  - The constraint and resolving differential operator are linear
  - There exist convenient observation operator and cost function
  - Measurements are comparably easy and plentiful
- Probabilistic interpretation of footprint allows for inclusion of zero-reporting measurements into the simulations
- ETEX application confirmed the method strengths and highlighted necessity for a proper assessment of observation quality and representativeness
- A problem of the absolute emission rate is to be addressed

Acknowledgements

- SILAM programming team
  - M.Salonoja (FMI, 1995-1999)
  - M.Ilvonen (VTT)
  - P.Siljamo (FMI)
  - I.Valkama (FMI)