Numerical models of atmospheric composition

M.Sofiev, E.Genikhovich

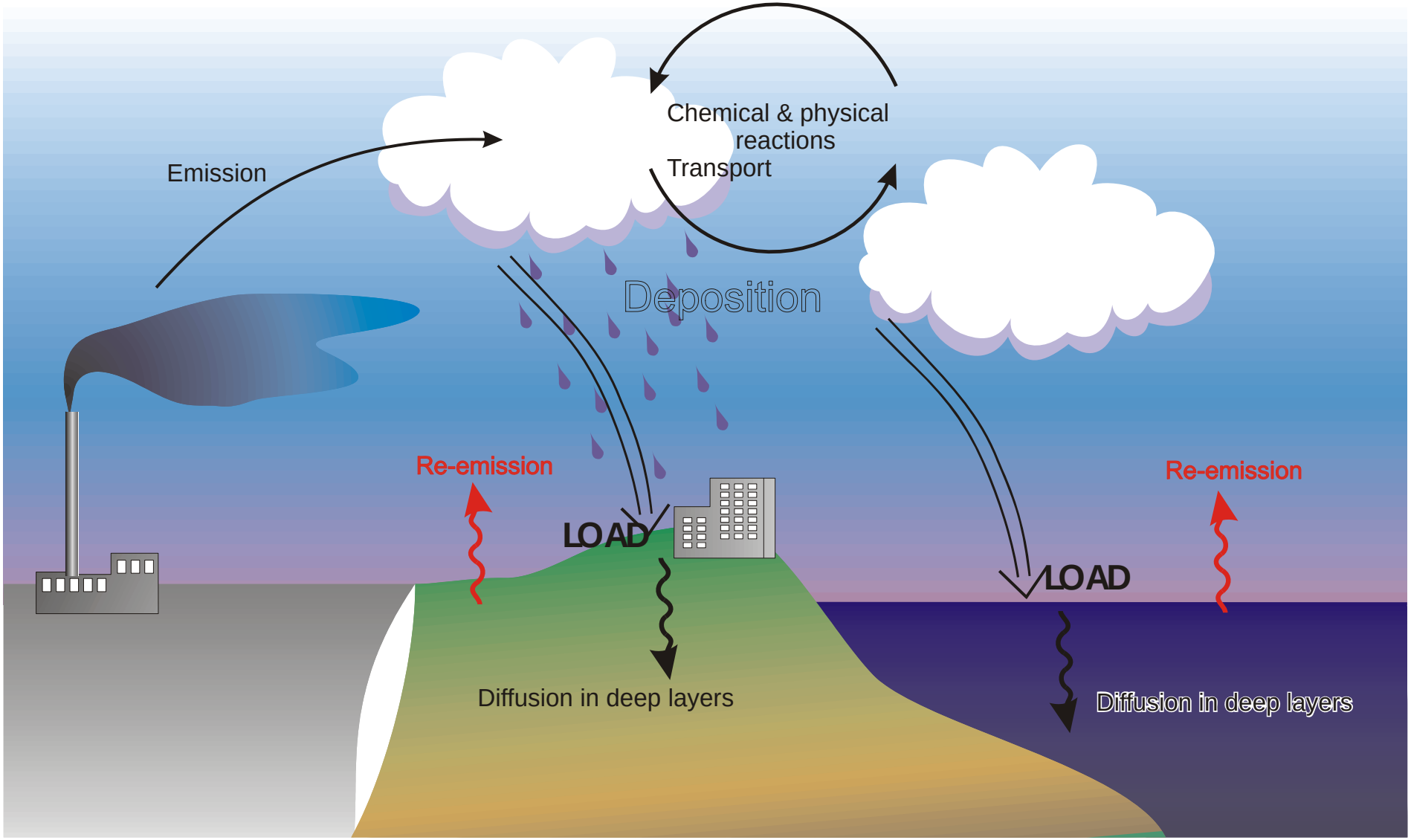
Finnish Meteorological Institute

Main Geophysical Observatory

Content

- Introduction
- Mathematical background
- Structure of a chemical transport model (CTM)
- Could we cope with atmospheric stochasticity?
- Examples of the model constructions
- Examples of the model applications
- Summary
- References

Pollution cycle in the troposphere

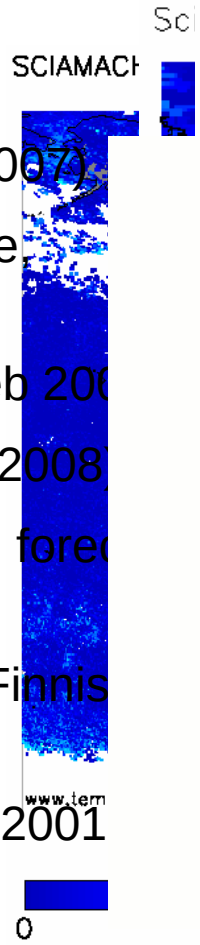


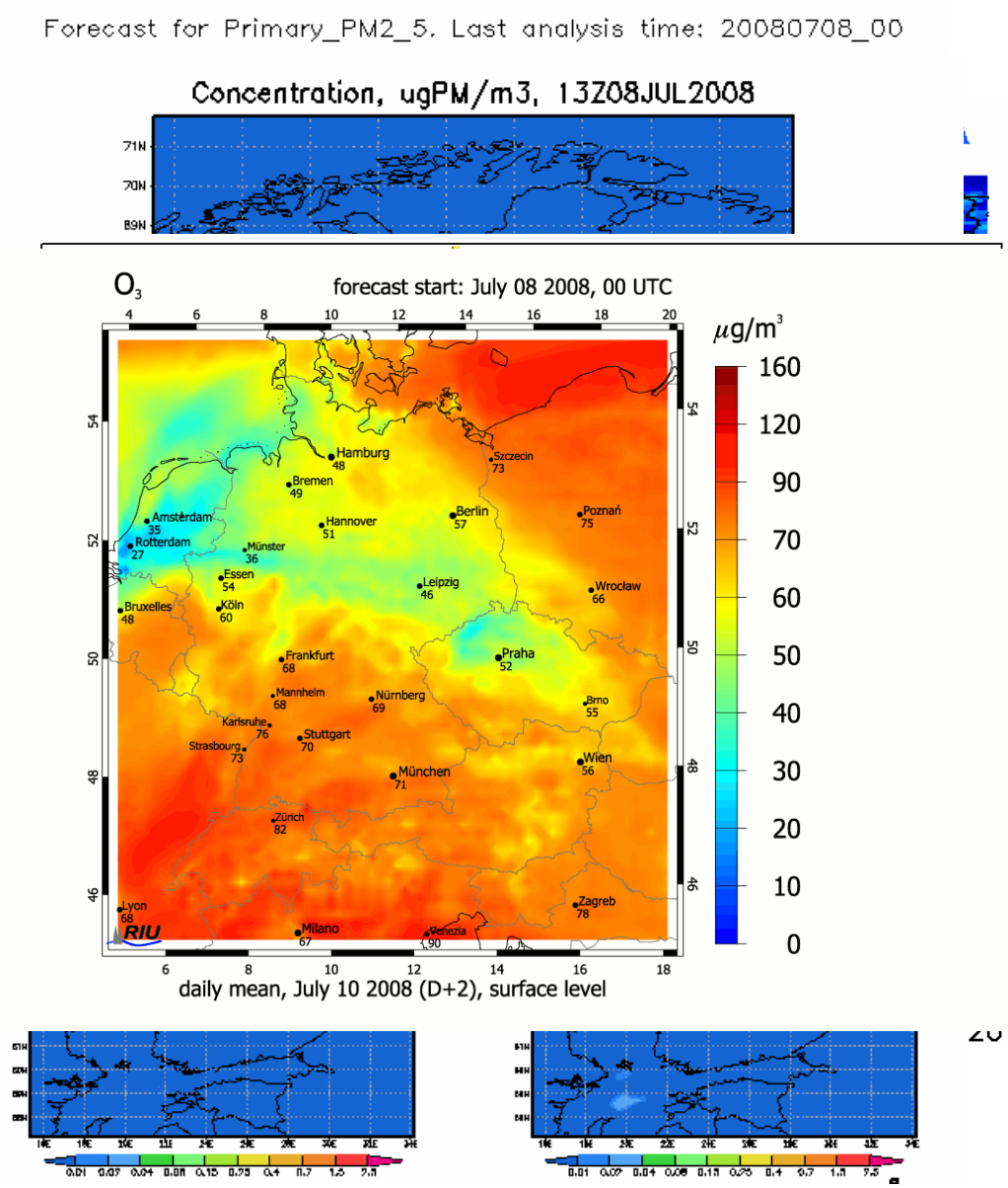
Scales of atmospheric composition

- A specific feature of the atmospheric composition problem is a very wide range of scales, both temporal and spatial combined with very sharp gradients of the species
  - scales are largely dictated by chemical and removal lifetimes
  - gradients are largely dictated by sources
- Gradients tend to reproduce themselves at every spatial scale, from street-canyon to global
  - consequence: at every resolution the model has to be able to deal with highly irregular field
- Non-linearities in the governing equations make averaging problematic and further complicate the scale interaction problem

Scales of atmospheric composition.2

- Global NO2 in column observed from space (SCHIAMACHY, mean July 2007)
- NO2 column over Europe (SCIAMACHY, mean July 2007)
- PM 2.5 observed from space, Northern Italy (June 2004)
- Global CO, modelled (17 Feb 20
- NO_2 forecast, Europe (10.7.2008
- Ozone over Central Europe, forec (8.7.2008)
- Ex.2: Primary PM 2.5 from Finnis sources, forecast (8.7.2008)
- Ex.4 NO2 for Lisbon (mean 2001 2002)





Basic equations

- Eulerian approach

advection diffusion chemistry removal emission

$$L\overline{\varphi} \equiv \frac{\partial \overline{\varphi}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{u}_i \overline{\varphi}) + \frac{\partial}{\partial x_i}(\overline{u_i' \varphi'}) + \sigma(\overline{\varphi}) = \overline{f}$$

$$u_i = \overline{u}_i + u_i' \; : \; turbulent \; wind = mean + \; fluctuation$$

$$\varphi = \overline{\varphi} + \varphi'$$

$$\frac{\partial u_i}{\partial x_i} = 0 \; : \; continuity \; equation$$

Basic equations.2

K-theory:

$$\overline{u_i' \varphi'} \approx -\mu_{ij} \frac{\partial \overline{\varphi}}{\partial x_j}$$

$$L\varphi \equiv \frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x_i}(u_i \varphi) - \frac{\partial}{\partial x_i} \mu_i \frac{\partial \varphi}{\partial x_i} + \sigma\varphi = f$$

Boundary & initial conditions:

$$\varphi(t = 0) = \varphi_0$$

$$\varphi(\vec{r} \in S) = \varphi_S$$

Basic equations.3

Forward problem:

$$L = \frac{\partial}{\partial t} + \frac{\partial}{\partial x_i}(u_i) - \frac{\partial}{\partial x_i}\mu_i \frac{\partial}{\partial x_i} + \sigma; \qquad L\varphi = f;\ M = (p, \varphi)$$

Inverse (adjoint) problem

$$L^* = -\frac{\partial}{\partial t} - \frac{\partial}{\partial x_i}(u_i) - \frac{\partial}{\partial x_i}\mu_i \frac{\partial}{\partial x_i} + \sigma; \qquad L^*\varphi^* = p;\ M = (f, \varphi^*)$$

advection diffusion chemistry removal receptor sensitivity emission

Numerical algorithms: split

- Why not to discretise and solve directly ?
- Formal operator split

$$\frac{\partial \varphi}{\partial t} + L\varphi = 0; \quad L = L_1 + L_2$$

- Physical processes -based split

$$\frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x_i}(u_i \varphi) = 0 \quad transport,\ mass-concervative$$

$$\frac{\partial \varphi}{\partial t} = \frac{\partial}{\partial x_i}\mu_i \frac{\partial \varphi}{\partial x_i} - \sigma\varphi - f \quad diffusion,\ sink,\ emission$$

Numerical algorithms: split.2

- Physical processes split
  - **LOCALLY** independent, additive processes
  - Symmetrization of the algorithms within a single time step τ

$$\tau/2 \text{ advection} \rightarrow \tau/2 \text{ diffusion} \rightarrow \tau/2 \text{ diffusion} \rightarrow \tau/2 \text{ advection}$$

Numerical algorithms: discretization

1D case: $\frac{\partial \varphi}{\partial t} + u \frac{\partial \varphi}{\partial x} = 0; \quad let \quad \varphi_k^j = \varphi(x_k, t_j)$

- Explicit scheme

$$\frac{\varphi_k^{j+1} - \varphi_k^j}{\tau} + u \frac{\varphi_k^j - \varphi_{k-1}^j}{\Delta x} = 0$$

- Implicit scheme

$$\frac{\varphi_k^{j+1} - \varphi_k^j}{\tau} + u \frac{\varphi_k^{j+1} - \varphi_{k-1}^{j+1}}{\Delta x} = 0$$

Structure of a dispersion model

- Input data pre-processors
  - emission
  - meteorology
  - physiography (domain properties)
- Dynamic emission (simulated vs imported)
- Advection scheme
- Diffusion module
- Chemical transformation module
- Aerosol dynamics module
- Dry and wet deposition module
- Diagnostic quantities
- Output post-processing

Input data pre-processors

- Emission
  - various source types (point, area, stack…)
  - time variation (diurnal, weekly, seasonal)
  - chemical content (time-dependent)
- Meteorology
  - create extra variables (e.g. ABL parameters)
  - interpolation to the model grid
  - time interpolation

Advection scheme

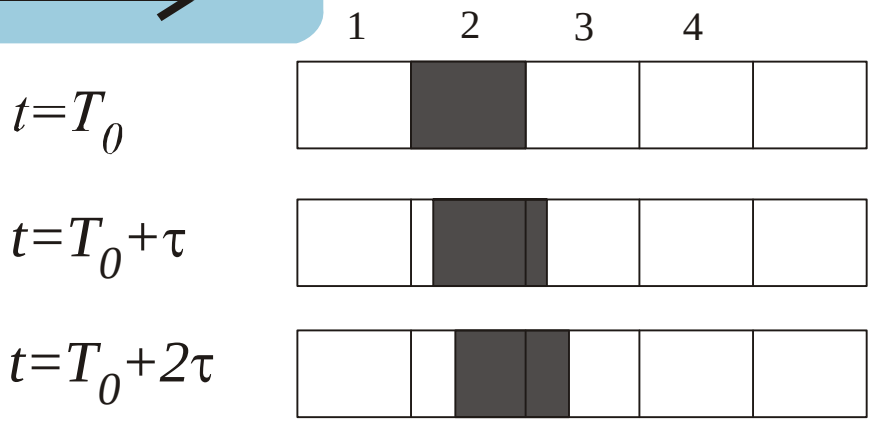
- There is no ideal scheme
- Scheme type depends on particular task
  - Eulerian schemes are the only ones applicable to non-linear case
    - often suffer from numerical viscosity
  - Large point sources are easier to treat by Lagrangian schemes
    - Problem of representativeness of a single Lagrangian particle

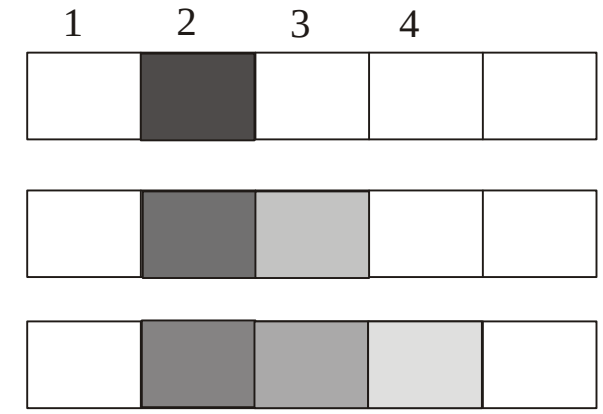
Advection scheme: numerical viscosity

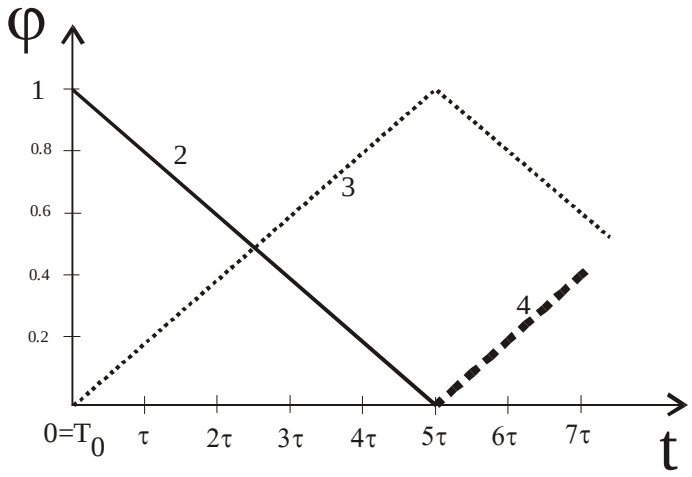
$u=0.2\,\Delta x\,\tau^{-1}$ →

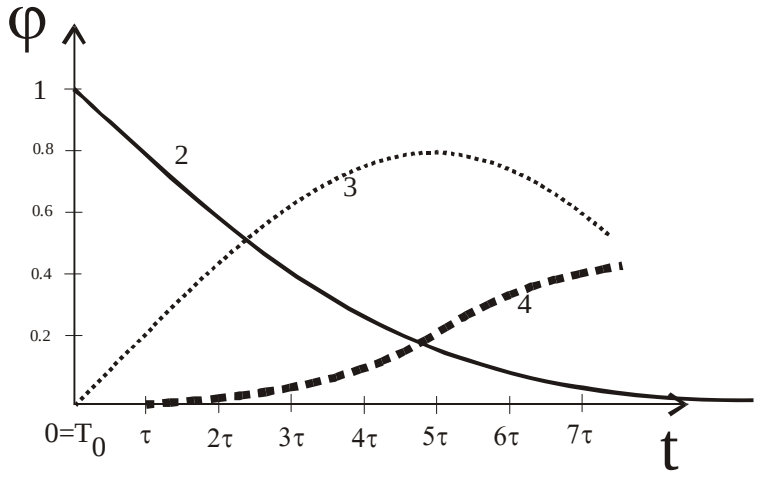
In "reality"

In idealized grid scheme







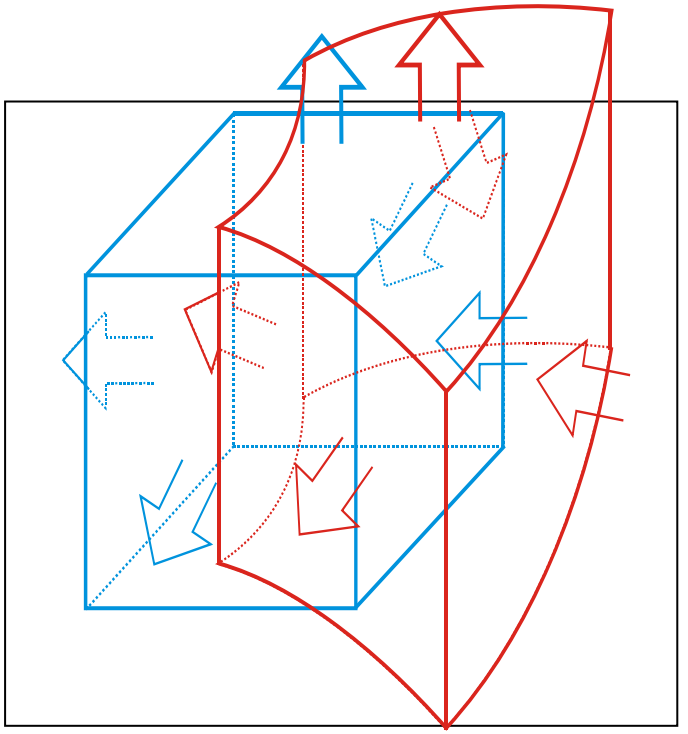


Mass conservation

- Mass conservation is ensured by the continuity equation
- Meteorological and dispersion models may have different:
  - grids
  - vertical structures
  - advection schemes
  - time dimension
- Any non-linear grid transformation destroys the continuity equation

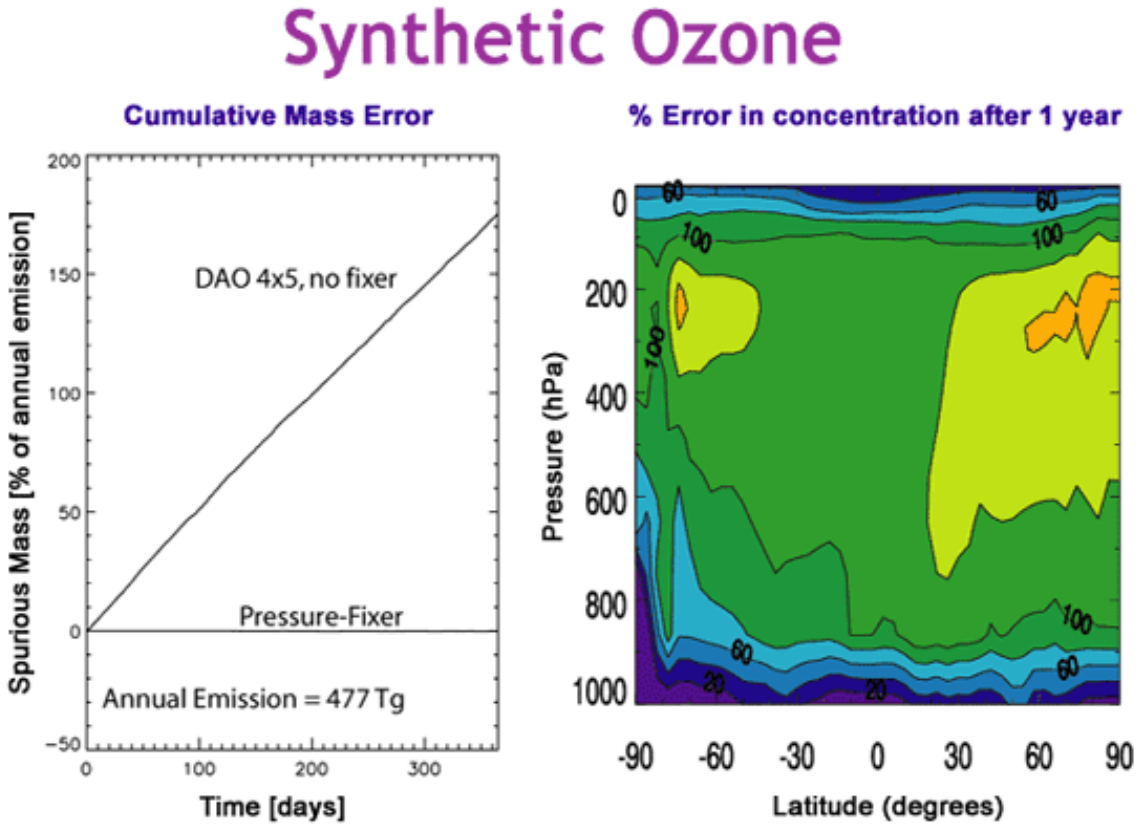
  $\Rightarrow$ interpolated fields are divergent

  $\Rightarrow$ dispersion model does not conserve mass



Mass conservation (3)

- Mass conservation problem: meteorological models often use non-conservative schemes
  - local mass conservation: continuity equation
  - global mass conservation: globally integrated continuity equation



Advection scheme: numerical viscosity.2

1D case. $\frac{\partial \varphi}{\partial t} + u\frac{\partial \varphi}{\partial x} = K\frac{\partial^2 \varphi}{dx^2}; \quad let \quad \varphi_k^j = \varphi(x_k, t_j)$

Tailor series for $\varphi(x,t)$ near $x=x_k$, $t=t_j$:

$$\varphi(x,t) = \varphi_k^j + (\varphi_t)_k^j (t - t_j) + (\varphi_x)_k^j (x - x_k) + ...$$

substituting discrete equation, we get:

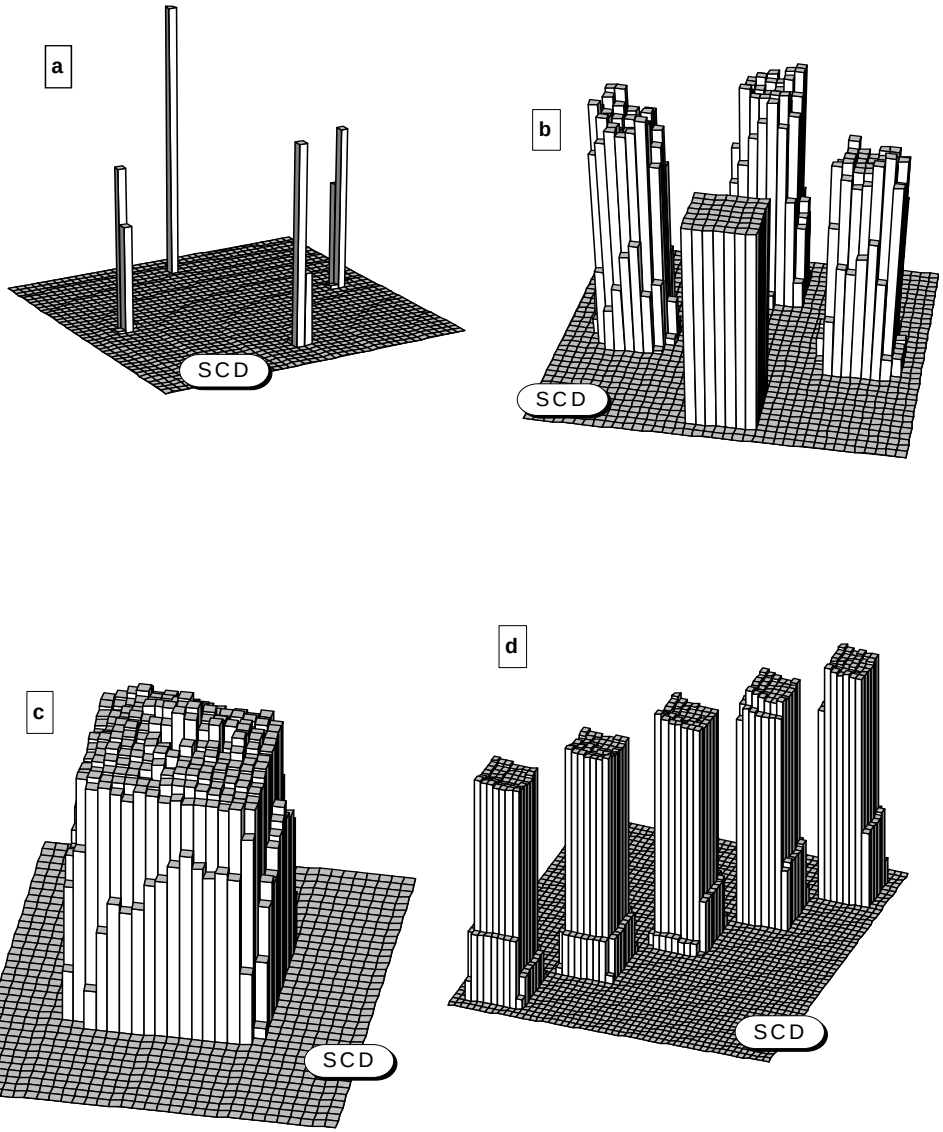
$$\frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x}(u_x \varphi) = (K - 0.5u\Delta x)\frac{\partial^2 \varphi}{\partial x^2} \quad at \quad x = x_k, \; t = t_j$$

$u < K/\Delta x$ – *stable with numerical viscosity*

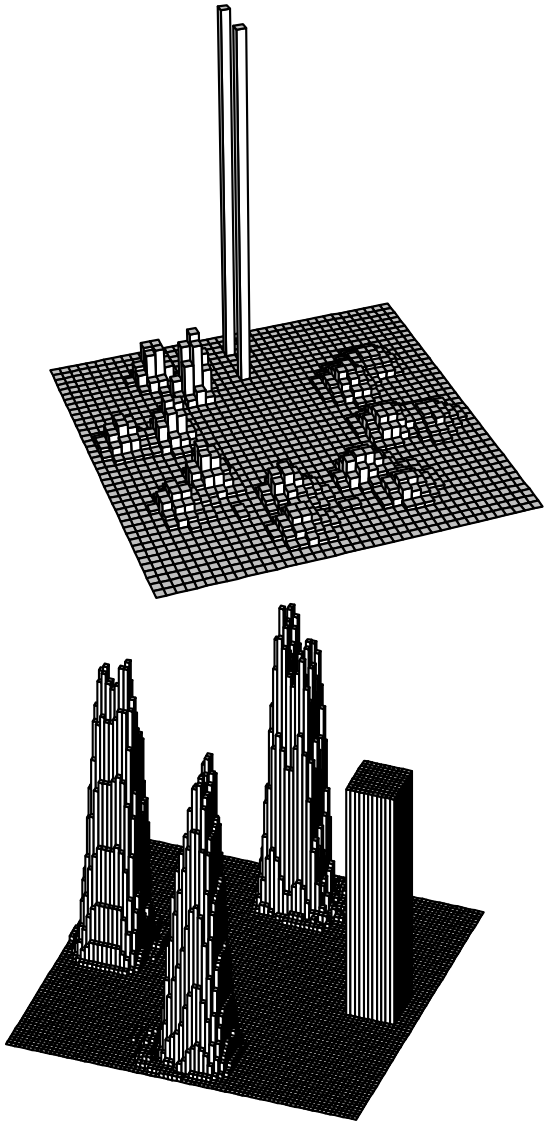
$u > K/\Delta x$ – *unstable (implicit scheme!)*

SCD advection: some examples

SCD scheme:



Bott scheme:



Diffusion module

- Straightforward discretization of 1D diffusion equation with e.g. Crank-Nicolson semi-implicit 2d-order accuracy scheme
  - suitable for both vertical and horizontal diffusion
- 2.5-D with well-mixed boundary layer (somewhat old-fashioned)
  - Additional equation for the mixing height
- Semi-analytic vertical profile of concentrations (2.5-D as well)

Chemical scheme

- One of the most time-consuming modules
- Contains of the most severe non-linearities, also the stiffest sub-system (several orders of magnitude of reaction time scales)
- Chemical kinetics

$$A + B \rightarrow C: \quad \frac{d[C]}{dt} = K[A][B]$$

Aerosol dynamics

- Based on solution of integro-differential equation describing at least
  - Nucleation
  - Condensation
  - Coagulation
- New dimension !!
  - particle size
- The most time-consuming module

Dry and wet deposition

- Dry deposition
  - linear (well, sometimes)
  - surface process
  - moderate intensity
  - can be bi-directional (evaporation $\Rightarrow$ re-emission)
  - approached via e.g. resistive analogy (Wessely, 1989)
    - aerodynamic resistance
    - laminar-layer resistance
    - surface resistances: soil, canopy, water surface, …
    - sedimentation
  - detailed landuse needed

- Wet deposition
  - can be non-linear volume process
  - high intensity
  - high complexity and dependence on precipitation and species features =>
    - usually treated via “empirical” 1st-order equation:

$$\frac{\partial \varphi}{\partial t} = \Lambda(I,...,\varphi)\varphi$$

where *I* is a precipitation intensity

Diagnostic and output post-processing

- Computation of diagnostic variables
  - e.g. optical features of the atmosphere from concentrations
  - proxies for health impact and risk assessment
- Transformation from model-convenient variables to user-friendly ones
  - generation of integrated / averaged variables
- Conversion to convenient file formats
- Grid interpolation (if needed)

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

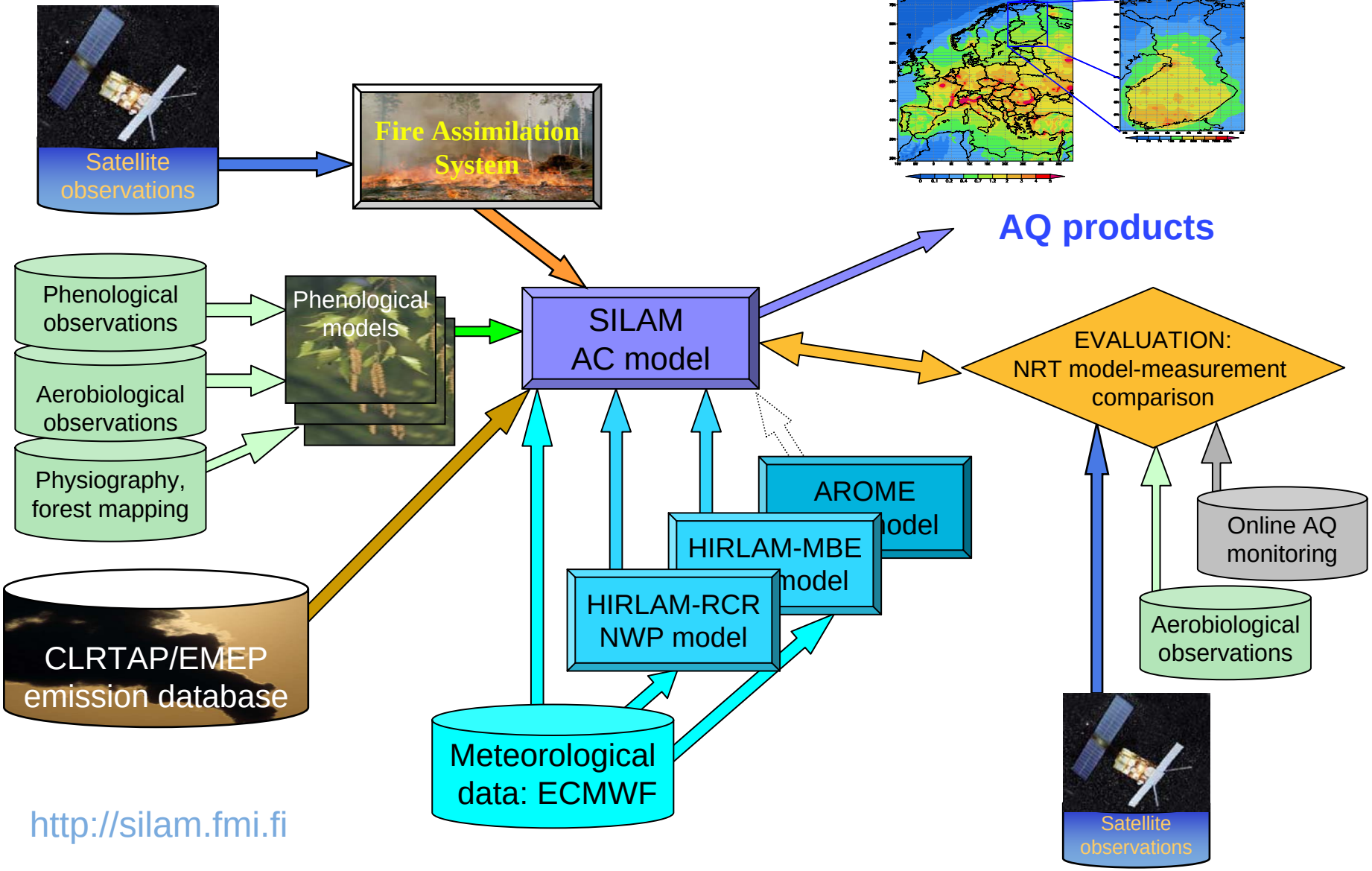
Can we cope with the stochasticity of the atmosphere?

Microsoft
erPoint Presenta

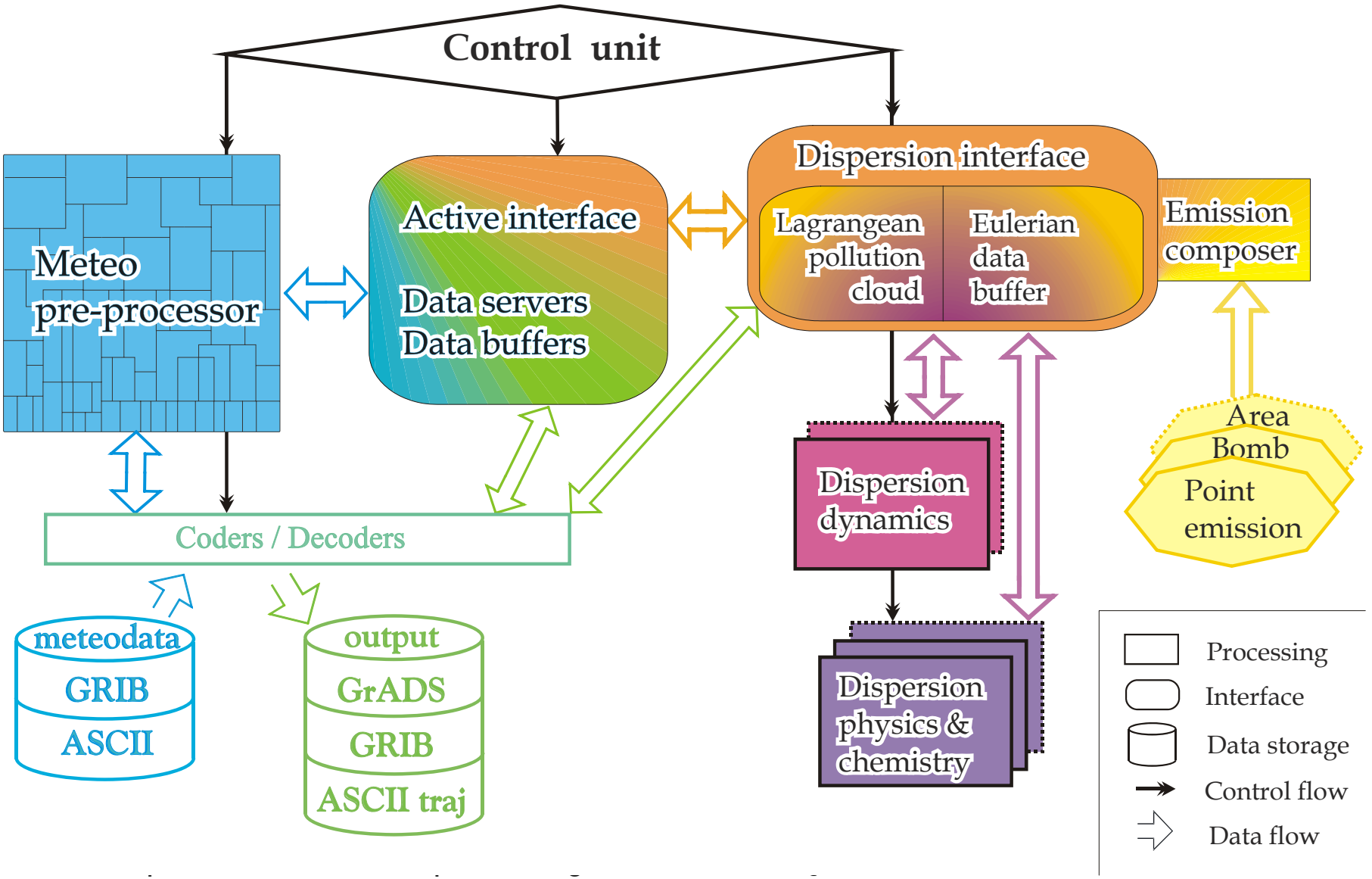
ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

An example of the SILAM CTM and its applications

Regional AQ forecasting platform (example)



SILAM modelling system: main parts

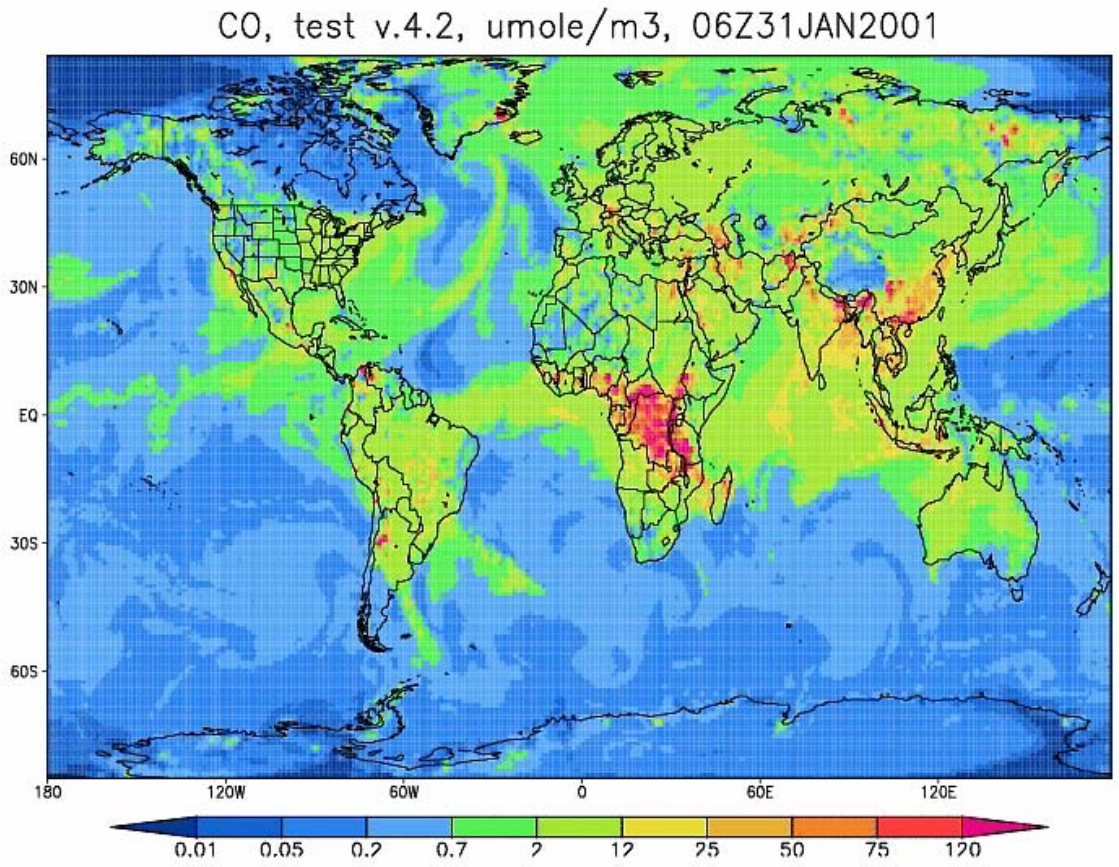


Current model functionality

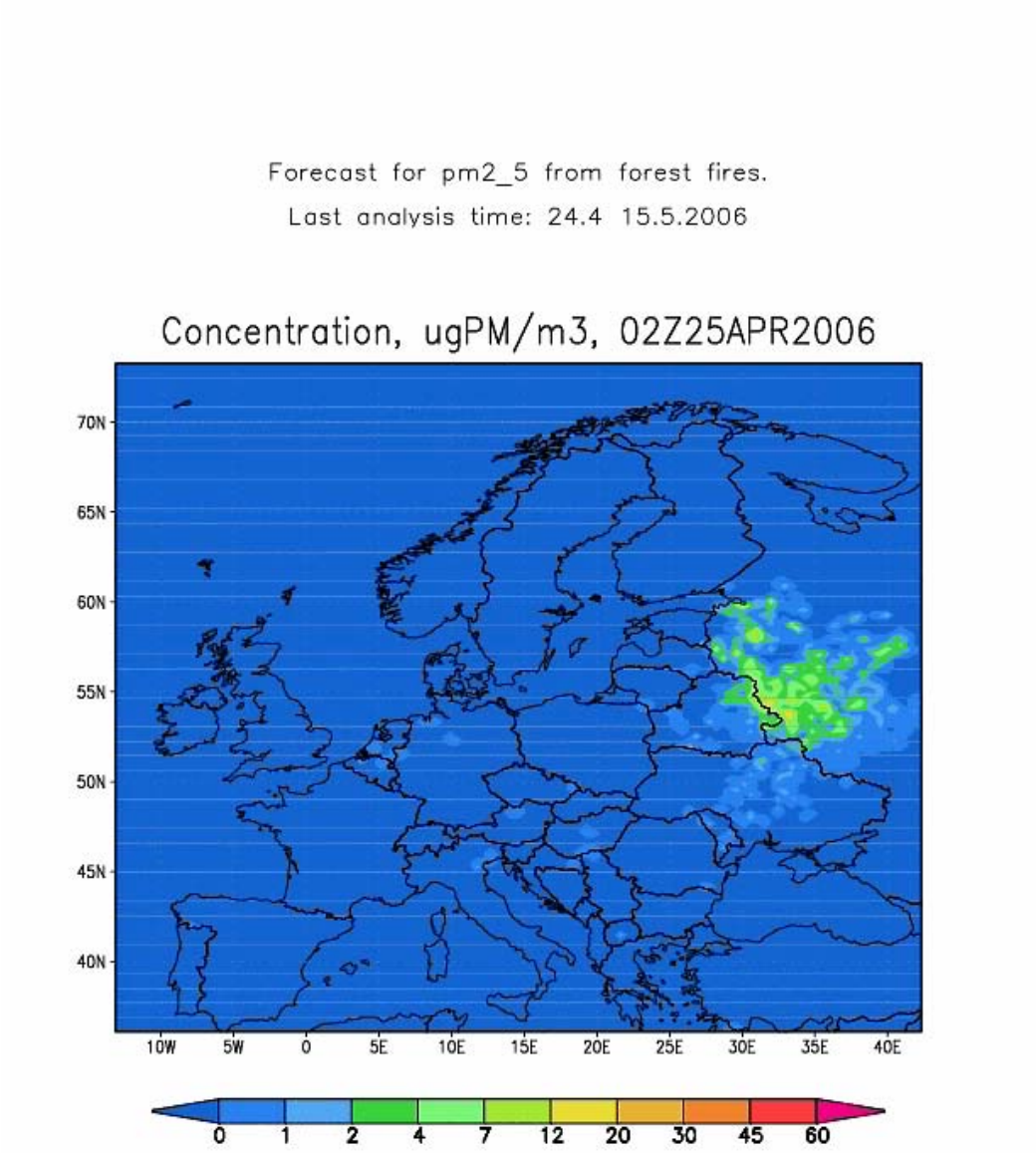
- Dispersion
  - forward (compute concentrations from given emission sources)
  - inverse (find sources of observed concentrations: source apportionment)
  - Lagrangian and Eulerian advection schemes
- Chemistry and physics
  - SOx-NOx-NHx-O3 chemistry
  - Linear SOx transformations
  - Radioactive decay for up to ~500 nuclides
  - Natural bioaerosols (pollen)
  - Sea salt production and dispersion
  - Inert aerosol (for general particulates of given size distribution)
  - Toxic persistent pollutants (generalised)
  - Passive tracer (probabilistic computations)
- Aerosol representation: sections or modes, arbitrary number and characteristics of size classes

Example of global run

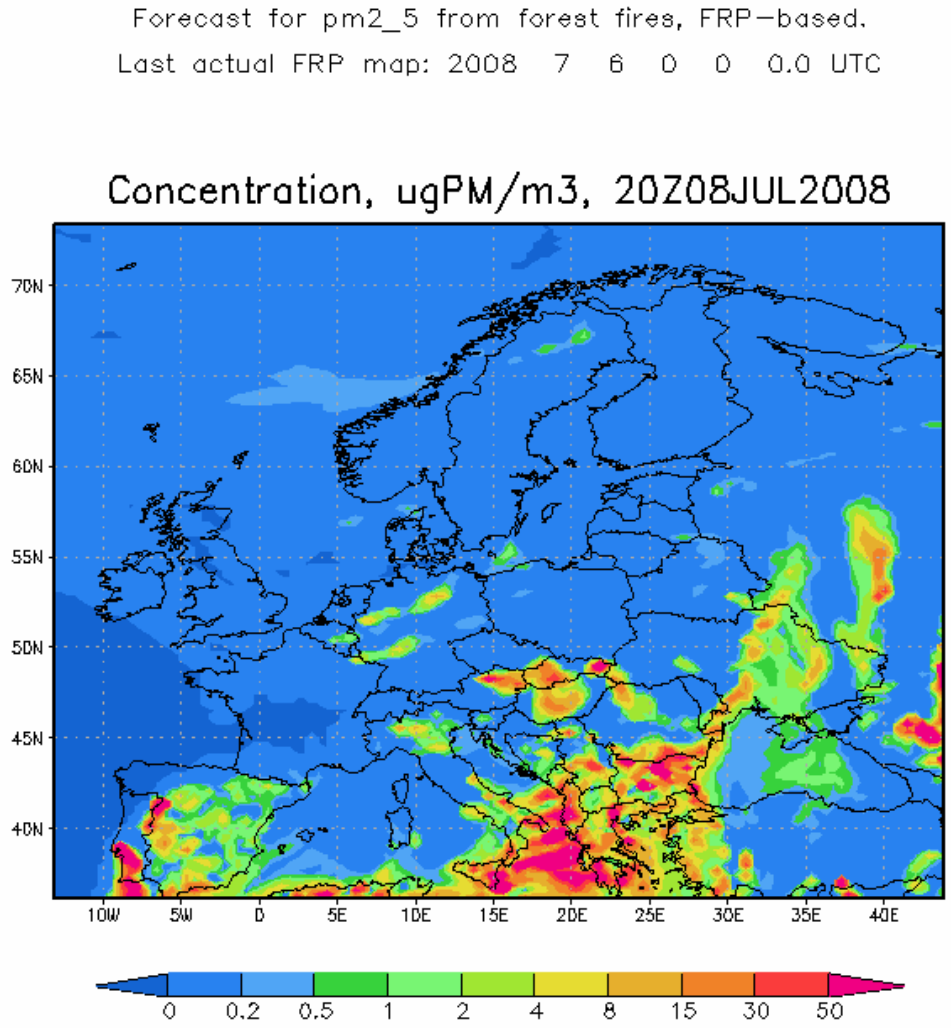
- CO concentrations, February 2001
  - (experimental SILAM application)



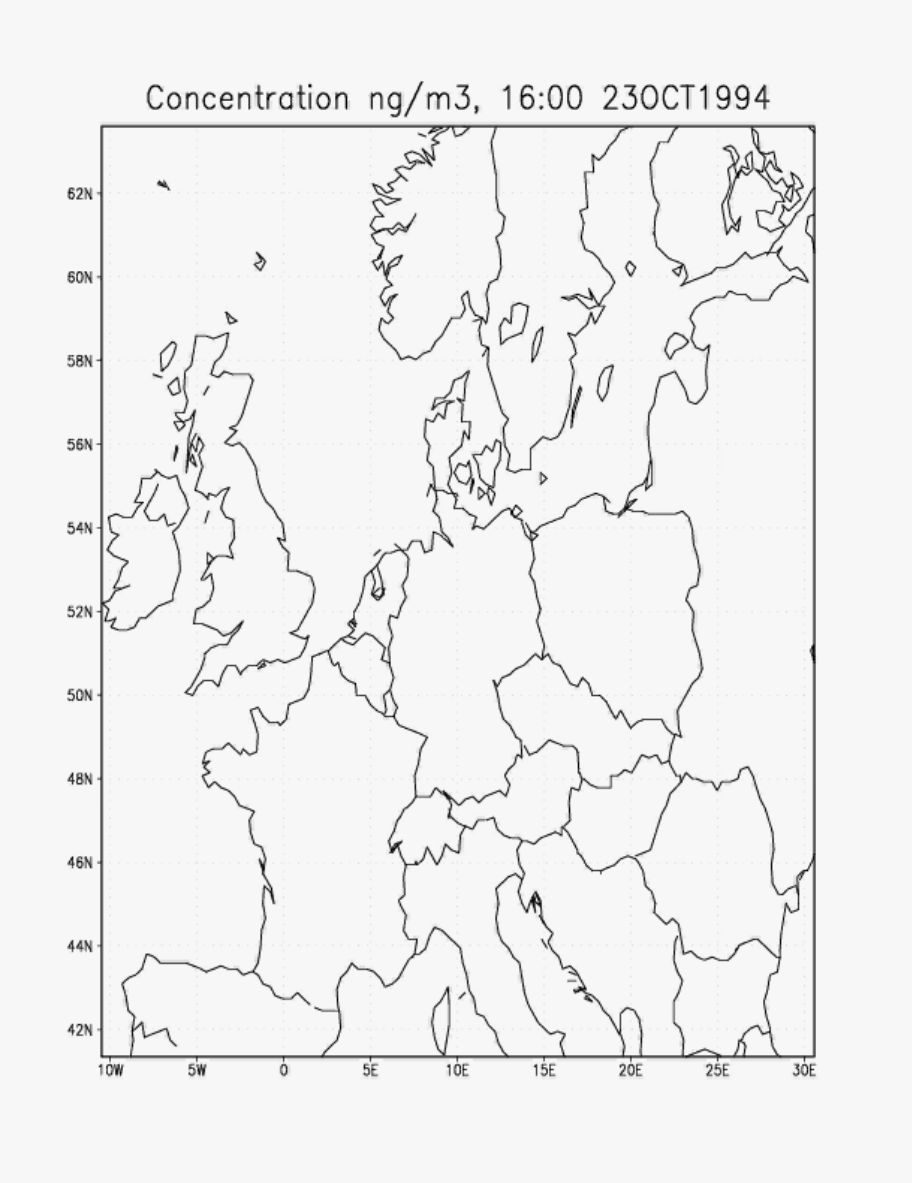
PM2.5 from wild-land fires, Apr-May 2006



Fire plumes operational forecast (PM 2.5)



ETEX-1 plume evolution (forward problem)



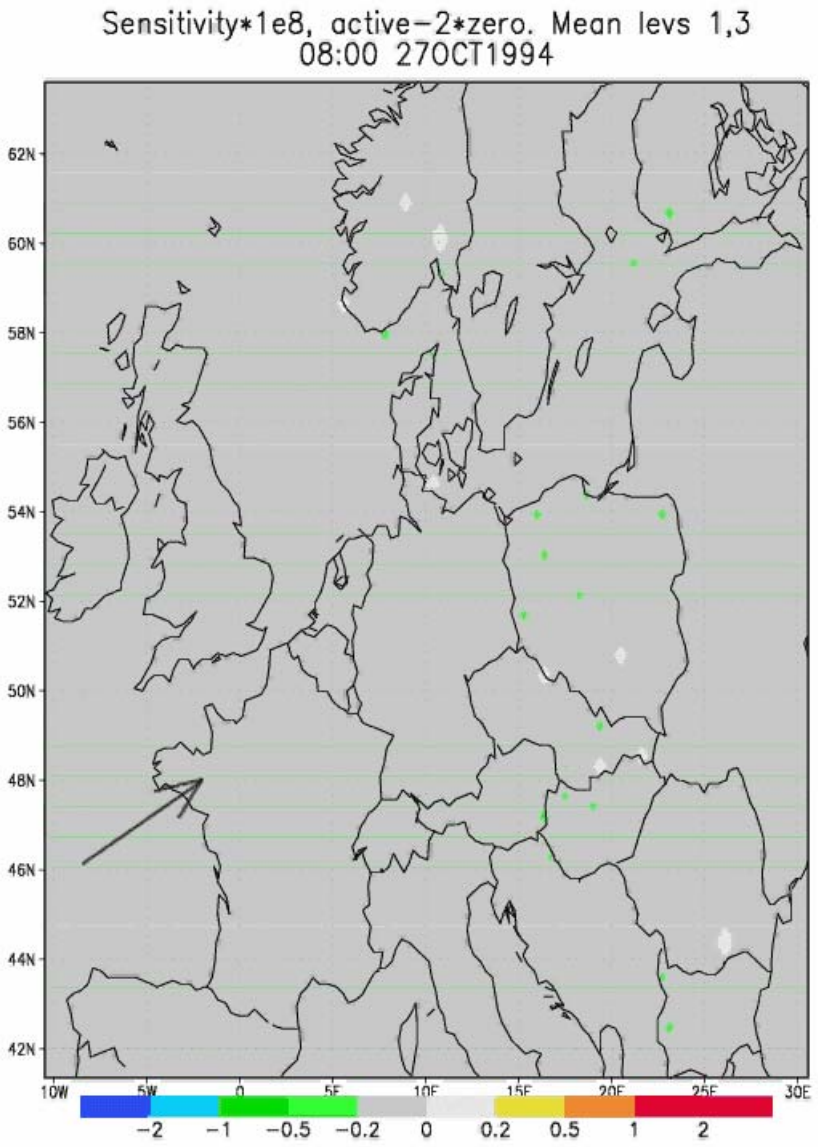
ETEX-1 inverse problem via adjoint simulation (4

True source:

(2^0 W, 48.05^0 N)

Release time:
23.10.1994 16:00 ->

24.10.1994 3:50
(duration ~12 hours)



Summary

- Modelling of distribution of atmospheric trace components is based on solving the turbulent diffusion equation
- Particular realization and corresponding simplifications depend on specific task and available resources
- The technology of computation and corresponding results should be "adequate" to the problem under consideration
- Model quality assurance should cover ALL stages of the model development
- When carrying out CTM, one should be aware of the stochastic nature of the modeled atmospheric processes, expected magnitude of fluctuation of concentration etc
  - To obtain smart answer one has to ask smart question…

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

Thank you for your attention