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The role of PBL in air quality modelling: experience of SILAM

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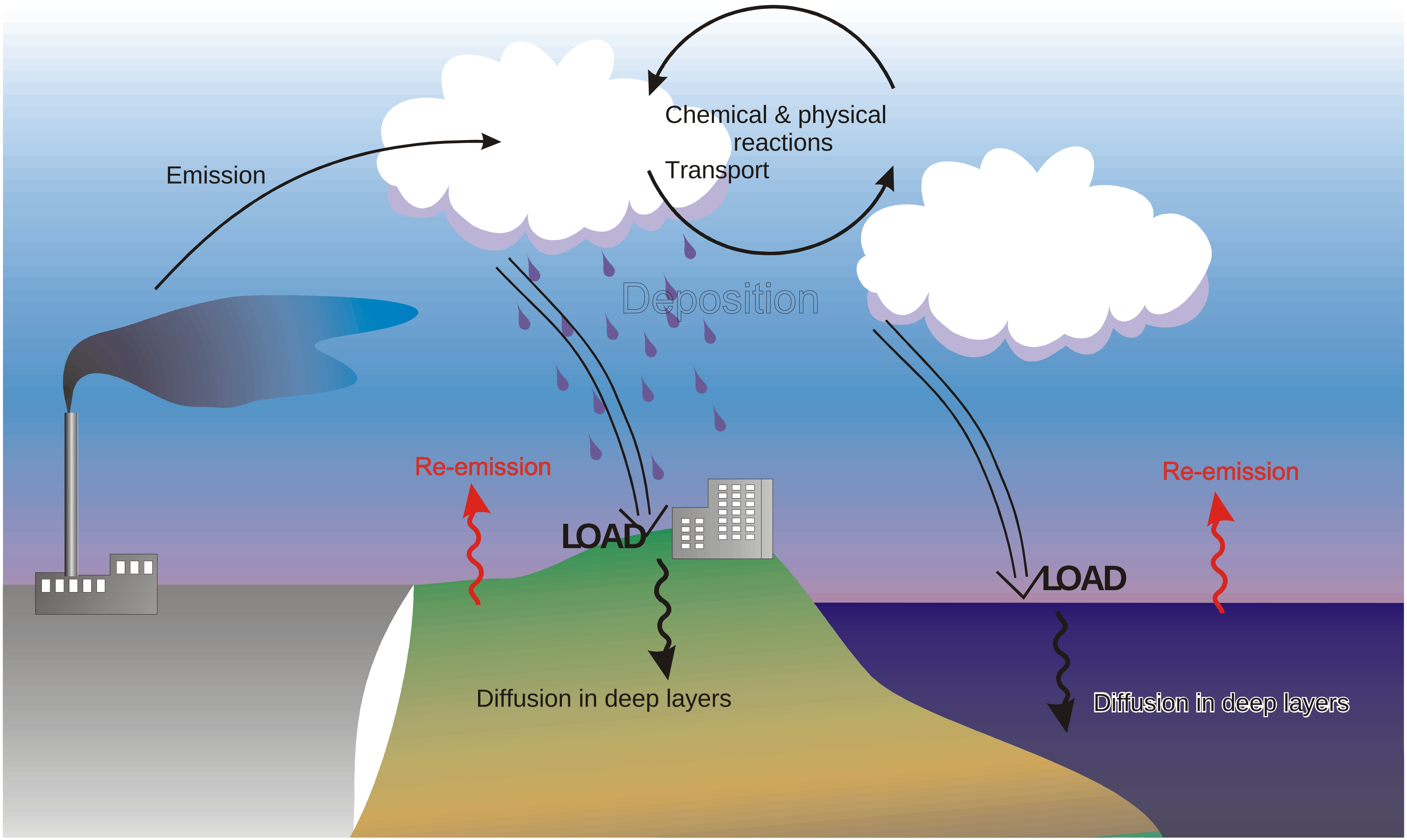
Content

- What is the air quality (AQ) modelling?
  - sources, species, tasks
  - chemical composition modelling
  - PBL: the main environment for Chemical Transport Models (CTMs)
- CTM as specific user of meteorological (or numerical weather prediction, NWP) models
- Coupling NWP and CTM models: towards Chemical Weather models
- Examples
- Summary

Air pollution due to anthropogenic emission



Air quality vs chemical composition modelling

- Air quality regards to atmospheric chemical composition near the surface and reaction of people and ecosystems onto it
- Chemical composition regards to the whole atmosphere and does not have an object of impact (such as human being)
- AQ is a relative characteristic related to thresholds, target levels, and guidelines set by users – public, health authorities, etc.
- Conclusion: AQ modelling is a specific application of a Chemical Transport Model (CTM) for the needs of public health protection

Chemical composition: areas of interest

- Anthropogenic species are mostly confined within the boundary layer but:
  - long-living species (toxic metals, persistent organic compounds, etc.) – generally up to tropopause
  - buoyant sources – wild-land fires (natural / man-made), major technogenic disasters, … – up to tropopause
  - aviation: a major contributor of anthropogenic species in the upper troposphere
- Natural sources: a rich zoo
  - near-surface: biogenic organic compounds, sea salt, pollen, dust, …
  - lightning as the main NO_2 producer in tropics in the upper troposphere
  - stratospheric ozone
- Spatial and temporal scales vary widely depending on the problem
  - determine the main chemistry mechanism and impact
- A “single-atmosphere” principle: all-in-one.
  - interactions
  - in extremes, brain-free implementation

Chemical composition vs meteorological modelling

- Chemical Transport Modelling (CTM) is often considered (with reasons) as a downstream to meteorological modelling
  - 4-D meteorological fields are the main part of the CTM input, being largely independent from chemical composition
- Feedback to meteorology exists and can be significant
  - direct: radiation propagation through aerosol layers
  - semi-direct: cloud properties through altered radiation
  - indirect: cloud processes affected by aerosols through microphysics
  - playing by mass: e.g. Saharan dust storms strongly affect nearly all tropospheric features in the region

Focus of the talk: meso-to-regional CTM

- Meso- and regional spatial scales (many definitions)
  - spatial horizontal resolution from 1km to 50km
  - horizontal coverage up to Europe and surroundings
- Other parameters follow
  - vertical coverage: troposphere
  - vertical resolution: stress to PBL
  - time scale: hours to months (years/decades for long-term trends)
  - species
    - basic acid and nutrient chemistry (SO_x, NO_x, NH_x)
    - aerosols and related physics and chemistry
    - allergenic species (pollen)
    - tropospheric ozone O_3 and hydrocarbon chemistry

Content

- What is the air quality (AQ) modelling?
- CTM as specific user of meteorological (or numerical weather prediction, NWP) models
  - basic formulations
  - driving parameters
  - information flow from NWP
    - atmospheric features through prism of NWP model
- Coupling NWP and CTM models: towards Chemical Weather models
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Textbook: dispersion equation

$$Lj \equiv \frac{\partial j}{\partial t} + \frac{\partial}{\partial x_i}(u_i j) - \frac{\partial}{\partial x_i} m_{ii} \frac{\partial j}{\partial x_i} + s(j) = f$$

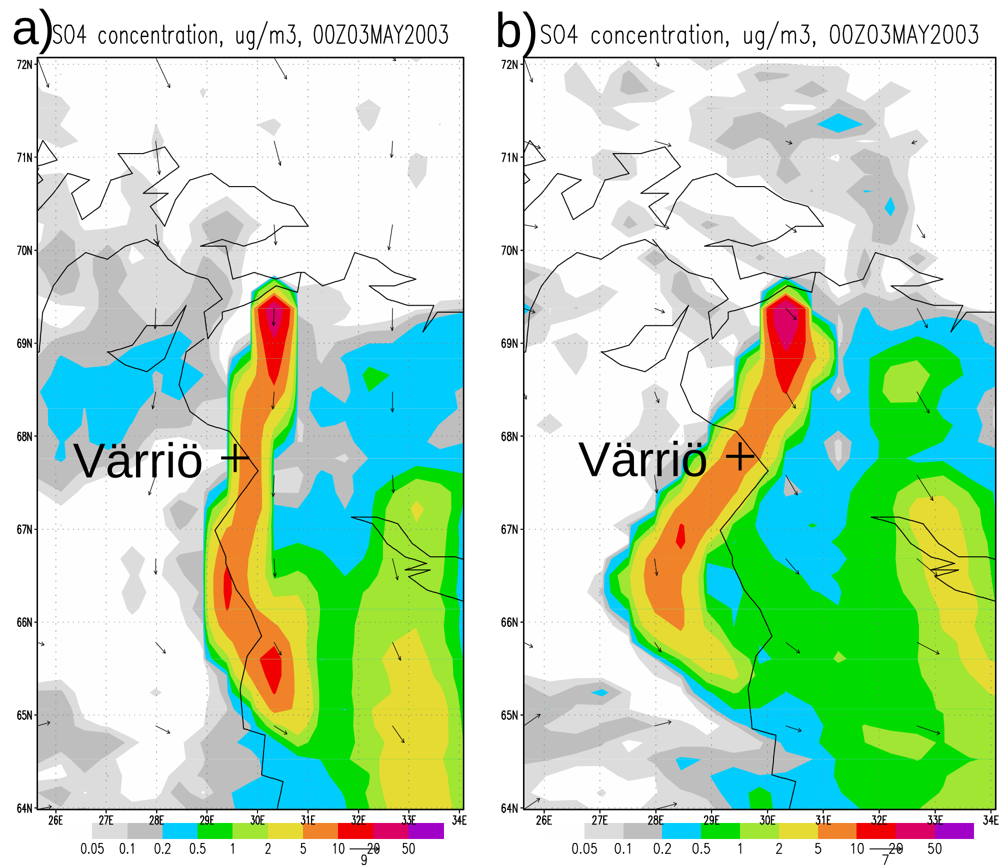
advect. *diffusion* *sink* *source*

$$j(t=0) = j_0(\vec{x}); \quad j(\vec{x} = \partial\Omega) = j_b(\vec{x}, t)$$

- Just one equation!
  - devil in details: it is multi-dimensional (φ is vector), “sink” term is non-linear and can result in mass transfer between the φ components (chemistry)
- Meteorology drives all terms
  - list of input variables depends on task
  - sensitivity to meteo variables is different
  - CTM can be sensitive to “unimportant” NWP variable
    - “unimportant” ≈ “non-verified”

A crucial parameter: 3D wind

- Drives the always dominating advection term
- Subject to divergence problem (see next section)
- Fairly well verified on a routine basis
  - speed verification is probably more strict
  - direction is much more important for CTM

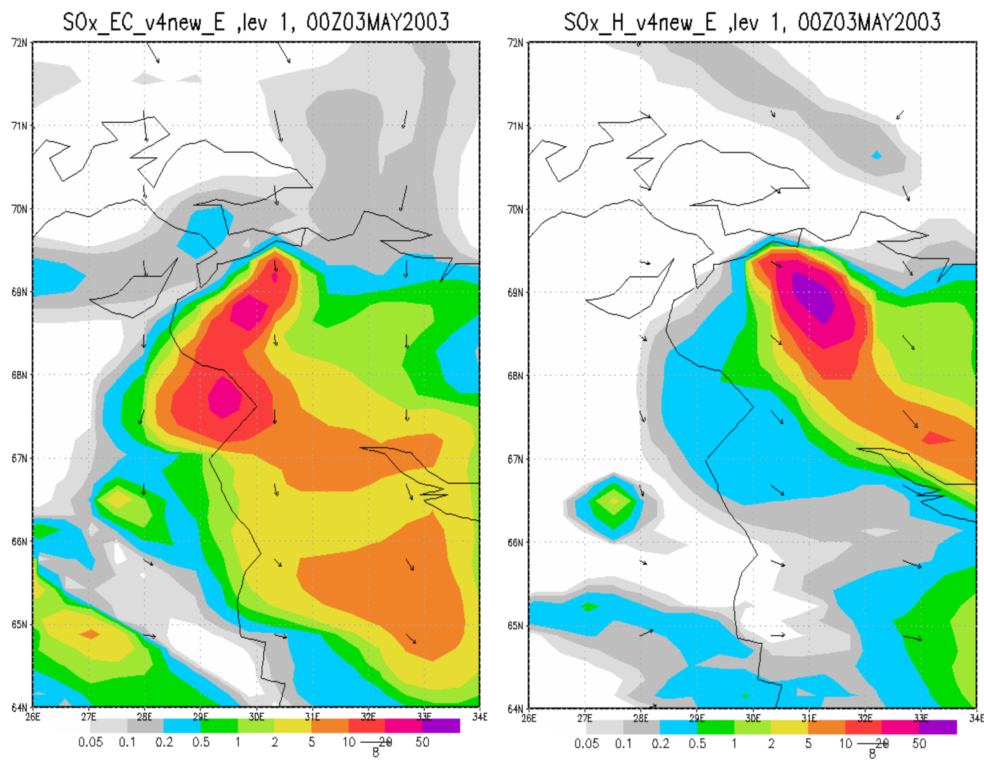


ECMWF input HIRLAM input

SILAM, Lagrangian dynamics, SO_4 in air, ug S /m3, 00:00 3.5.2003

A crucial parameter: 3D wind (2)

- Vertical wind component: drives the all-dominating advection term
- Very sensitive to divergence problem (see next section) and interfacing methodology
- Poorly verified



ECMWF input HIRLAM input

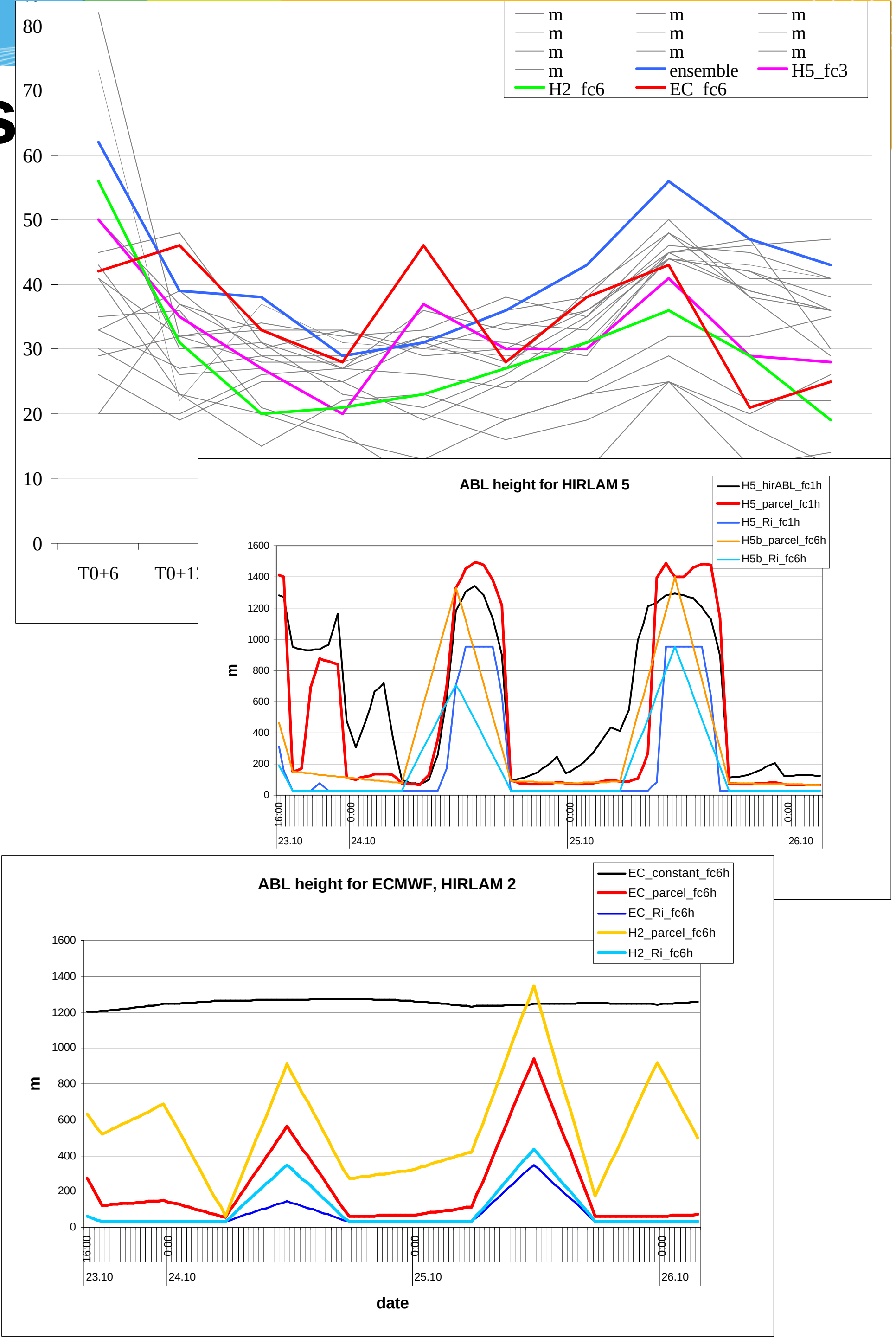
SILAM, Eulerian dynamics, SO_4 in air, ug S /m3, 00:00 3.5.2003

Mixing characteristics

- Drive the diffusion term
  - ➢ spread of the plume
    - – vertical diffusion – also via wind turn with height
  - ➢ deposition characteristics
  - ➢ moderate sensitivity of CTM
- Diagnostic set of variables, practically non-verified in NWP routine
  - ➢ participates in generation of diagnosed screen-level variables
  - ➢ otherwise is not interesting for “normal” users of weather forecast
    - – rarely available from archives
- Most of CTMs (re-)create the whole set using basic profiles and own methodologies (see next section)

Mixing characteristics

- European Tracer experiment
  - actual release of passive tracer, 23.10.1994, western France
  - careful monitoring of the cloud in its way over Europe
- SILAM played with 3 NWP datasets:
  - HIRLAM v2, 0.25^0, 1 hr
  - HIRLAM v5, 0.5^0, 6 hr
  - ECMWF from archive, 0.75^0, 6 hr
- No major difference, EC-run is the best up to +30 hr
  - wrong ABL during release night in HIRLAM: contributed?



NWP for source term: pollen

- Pollen is released from vegetation during flowering and constitutes the main part of spring allergenic outbreaks
- In many cases, acceptable accuracy for flowering prediction is obtained from thermal-sum models

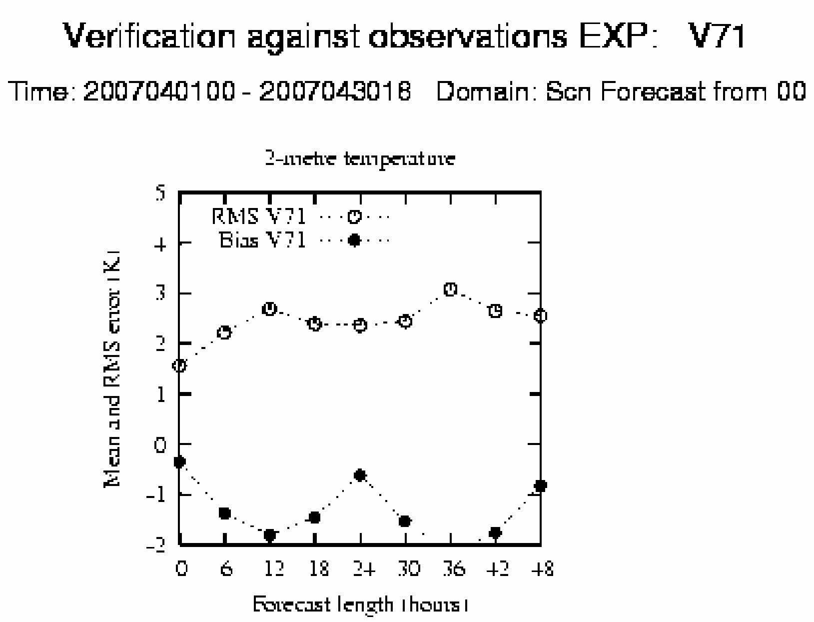
$$HS = \int_{t=t_0}^{t_{flowering}} (T(t) - T_{cutoff})\, 1(T(t) - T_{cutoff})\, dt$$

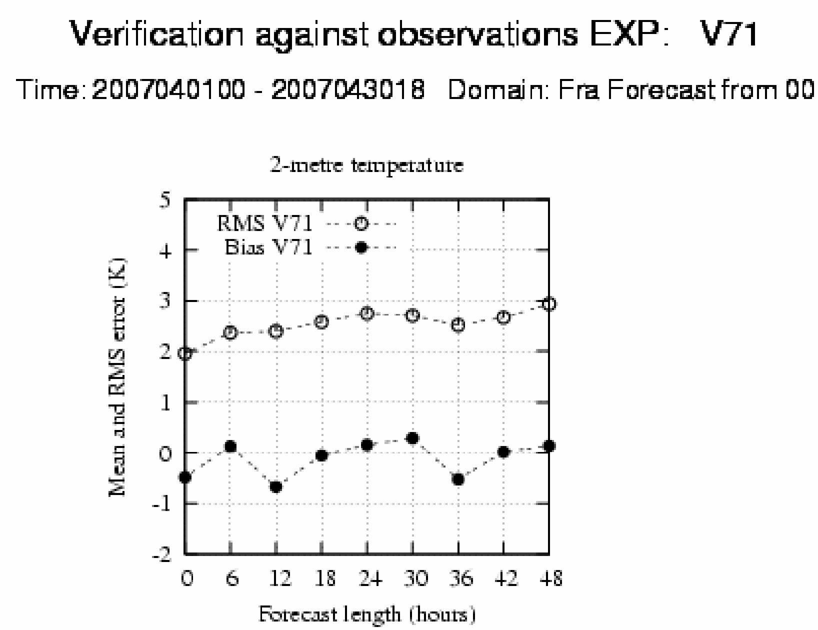
$$flowering: \; HS \geq HS_{threshold}(x, y)$$

- Integration (or summation of daily/hourly means) of temperature starts early in spring and continues until the flowering starts
  - ➢ prone to huge errors in case of temperature bias

NWP for source term: pollen (2)

- Spring 2007
  - FMI pollen forecasts: OK in most of Europe, hopelessly late in northern parts
  - Reason: bug in new HIRLAM v.7.1, combined with general HIRLAM feature of cold bias in spring





T2m comparison:

Scandinavia

France

NWP for source: wind-induced emission

- Two main components are wind-induced
  - sea salt

$$E_{sea\_salt}(U_{10m}, T_w, S_w, d_{part}, \Delta d) = W(U_{10m})\ F_1(T_w, S_w, d_{part}, \Delta d)$$

$$W = 3.84 * 10^{-6} U_{10m}^{3.41}$$ (Monahan et al, 1986)

  - dust (Gillette et al, 1988)

$$E_{dust} = C\ u_*^4\ (1 - u_{*cutoff} / u_*)\ 1(u_* - u_{*cutoff})$$

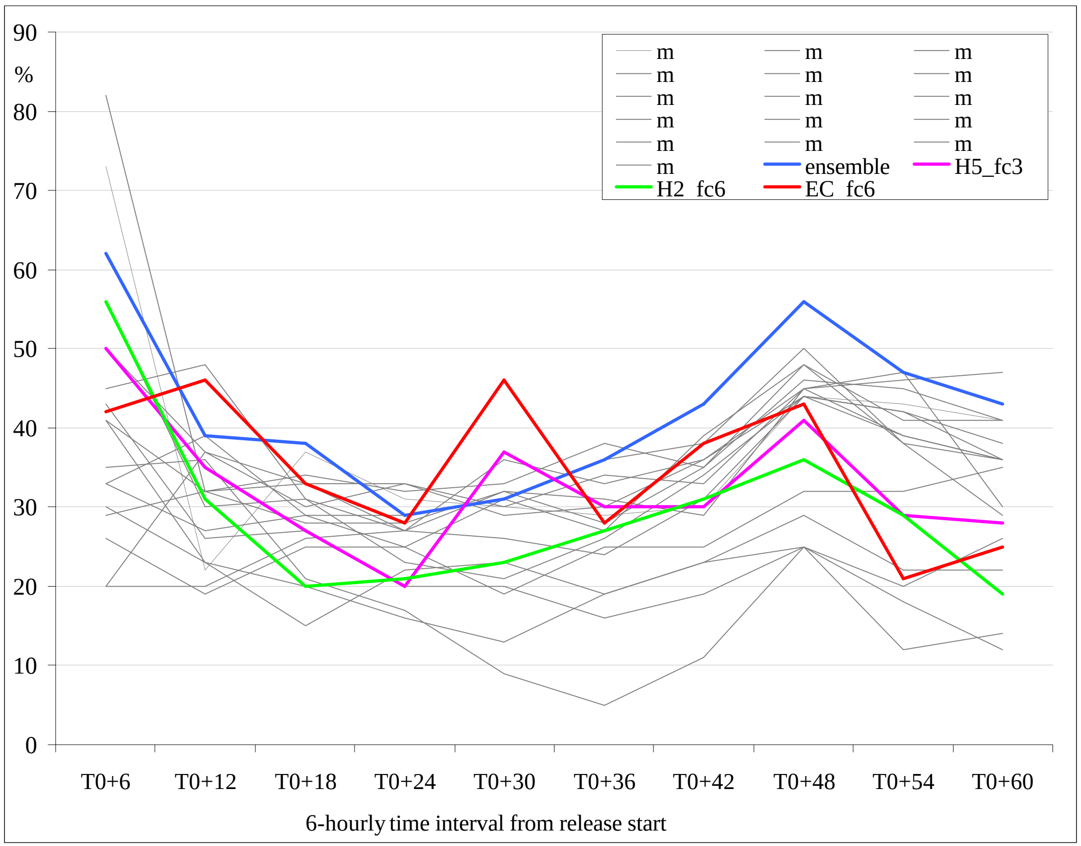
- Enormous sensitivity to low-level wind

NWP-CTM: ensemble as a tool

- In operational conditions problems with NWP and CTM model(s) may cost too much
- Model specifics mix-up with limited atmospheric predictability
- No data/time for verification
- Possible solution: convert bugs to features
- A set of “generally good” NWPs and CTMs is considered an ensemble
  - Forecast is then computed as a “common ground”, if any
- Statistically, all existing ensembles are not significant but they work
  - providing “moral support” for the forecaster if all models converge
  - highlighting outliers, if any
  - ringing alarm bell if forecasts diverge

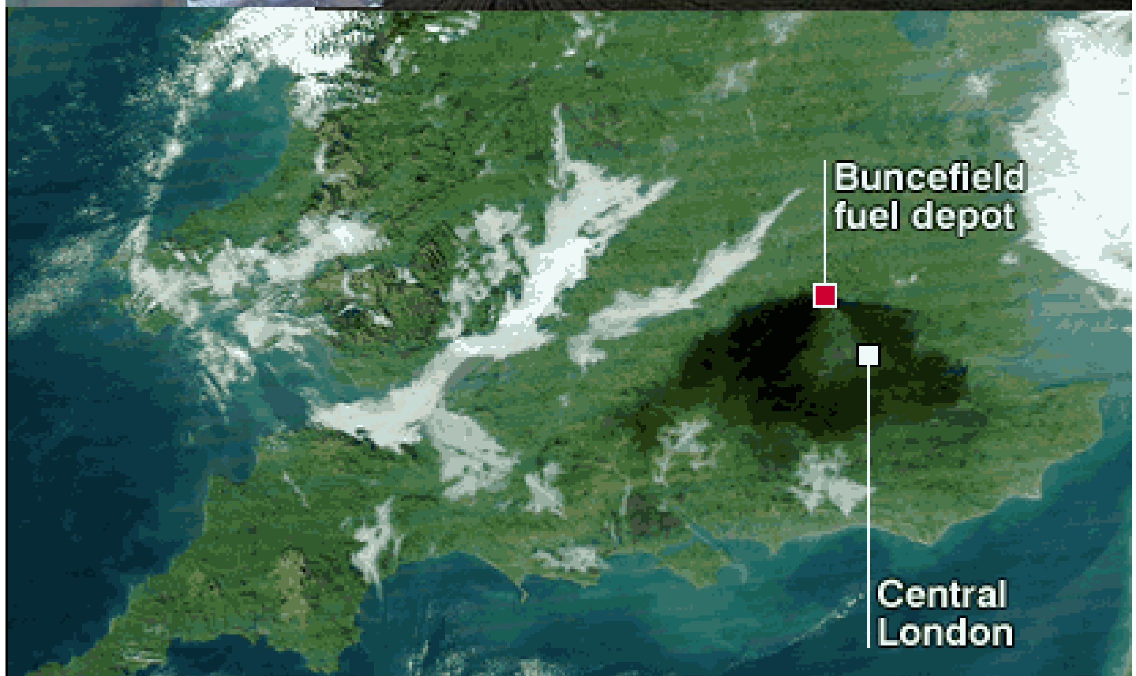
Ensemble as a tool (2): ETEX case

- ETEX simulations: ensemble (thick blue line) is nearly always superior to ALL individual models it consists of (Galmarini et al, 2004, Sofiev et al, 2006)



Ensemble as a tool (3): Buncefield fire

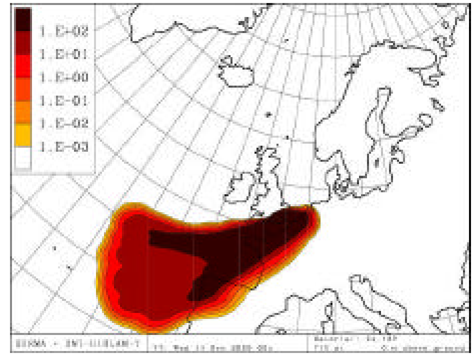
- Major explosion at Buncefield oil depot
- 2005-12-11 06:00 UTC
- several days of duration – until the fuel expired
- Meteorological conditions: UK winter, stable BL, significant wind shear with height
- Source: huge buoyancy, blows rise up to 3km through inversions (also a fraction confined within 300m of BL)

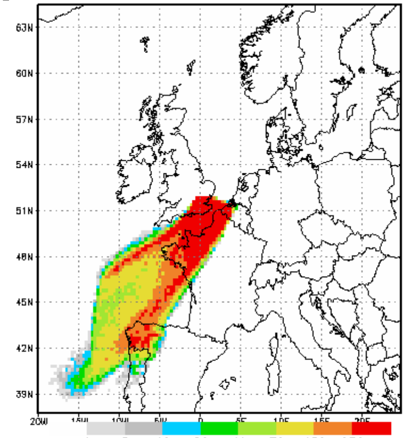


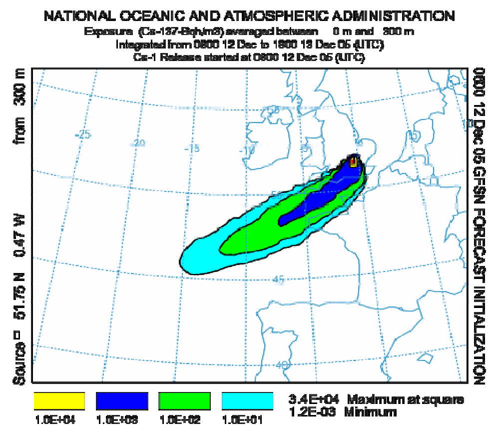
photos: *http://www.buncefield-oil-fire-hemel-hempstead.wingedfeet.co.uk/*

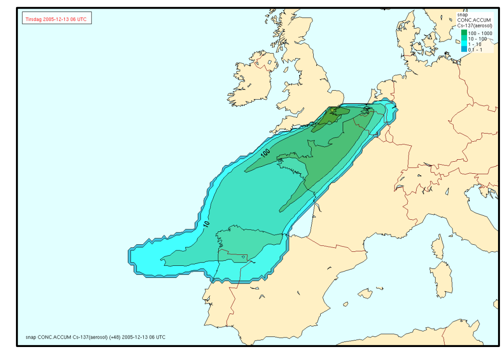
CTM-NWP, ensemble as a tool: NKS MetNet

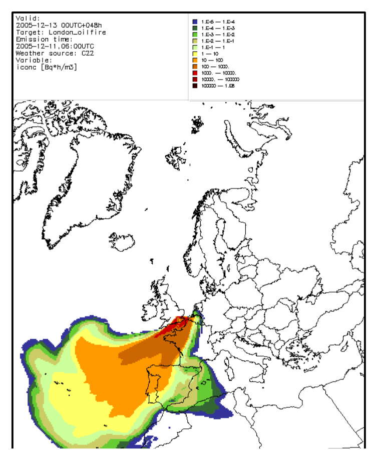
- MetNet: Nordic Network of Met Services engaged in emergency preparedness
  - mutual backup, both in meteorology and transport models
  - several exercises per year – dry runs and actual cases
- Buncefield fire has been simulated same day, with source height up to 300m











MetNet final report,
Christer et al, 2007

Content

- What is the air quality (AQ) modelling?
- CTM as specific user of meteorological (or numerical weather prediction, NWP) models
- Coupling NWP and CTM models: towards Chemical Weather models
  - NWP + CTM: a single modelling couple
  - means of coupling
  - example of NWP->CTM interface tasks
    - consistency issues
    - re-stating ABL
- Examples
- Summary

NWP + CTM: a single modelling couple

- Historically, each CTM is made downstream of some specific NWP
  - possibility to use in-full its strengths and adjust to “tricks”
  - lack of both technical compatibility across different systems
- Recently, improvements in both sides allowed further flexibility, so many CTMs are now linked to more than one NWP – and vise versa
  - still, sensitive parameters must be cross-verified and, possibly, internal adjustments to “tricks” introduced
    - technical, e.g. ECMWF reports precipitation in [m] instead of [kg/m2]=[mm]
    - methodological, e.g. scale dependence
- Features of NWP+CTM couple vary strongly if any of components is changed
  - The couple constitutes a Chemical Weather (CW) model

Coupling NWP and CTM

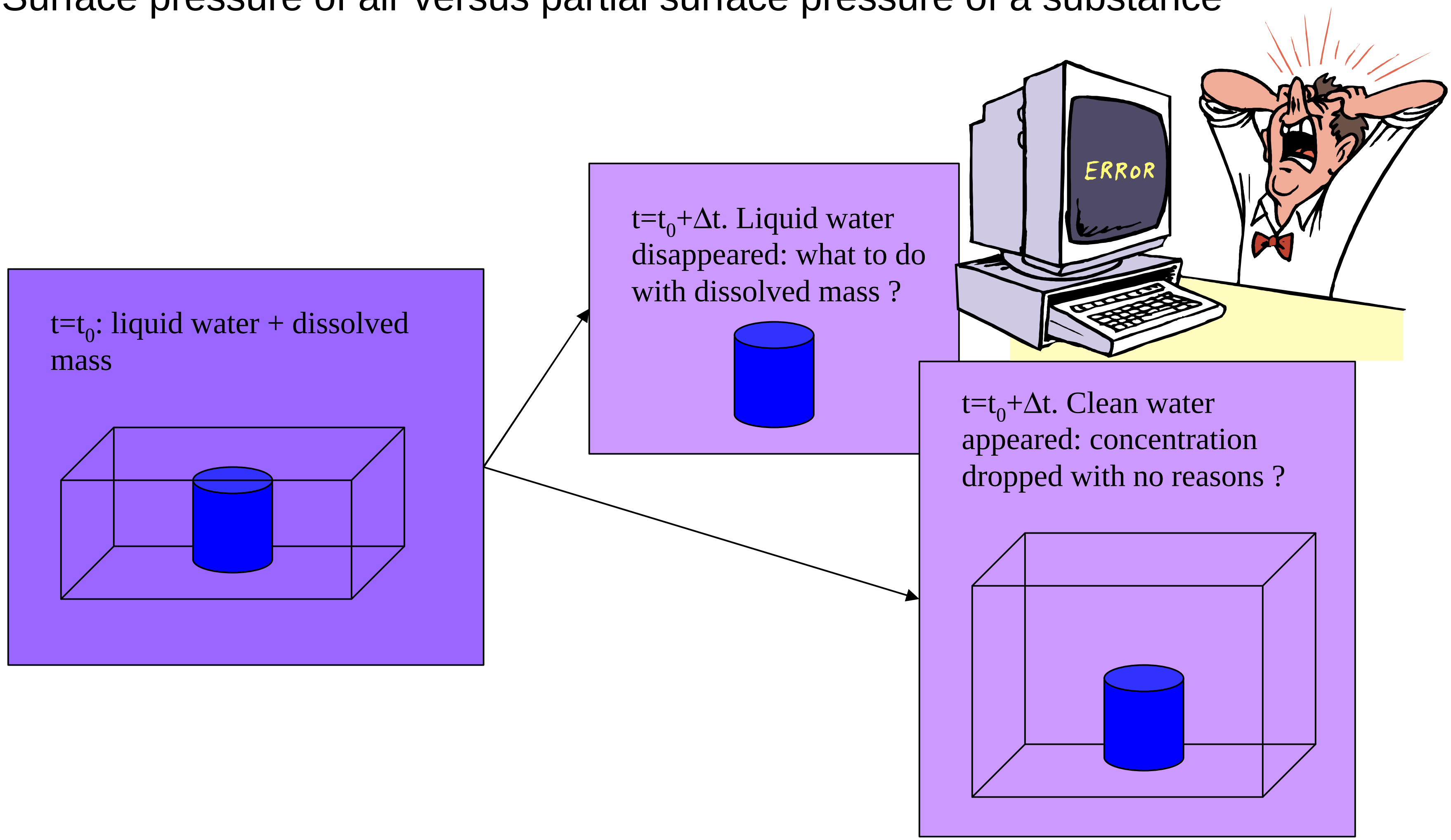
- Two main streams: online and offline coupling
- Online: a single model
  - Atmospheric chemistry is a subroutine of the CW model – similar to atmospheric dynamics or physics
  - Outstanding internal harmony
  - Easy information exchange between all modules
  - Heavy system, difficult to develop and modify
  - Convenient in some, unnecessary in other applications
  - …

Coupling NWP and CTM (2)

- Offline: two models + interface
  - Models are separate, interface ensures information transfer
  - No redundancy in computations
  - Easy development of all parts
  - Multiple NWP+CTM combinations are possible
  - Consistency issues
  - Feedback CTM -> NWP is somewhat trickier
  - …
- Conclusion: all animals have equal rights, each suits to own niche

NWP -> CTM interface: consistency

- Liquid water versus water-solved species
- Surface pressure of air versus partial surface pressure of a substance



NWP -> CTM interface: consistency (2)

- NWP models tend to limit their accuracy just fitting their own needs
- E.g. numerical differentiation is difficult to implement

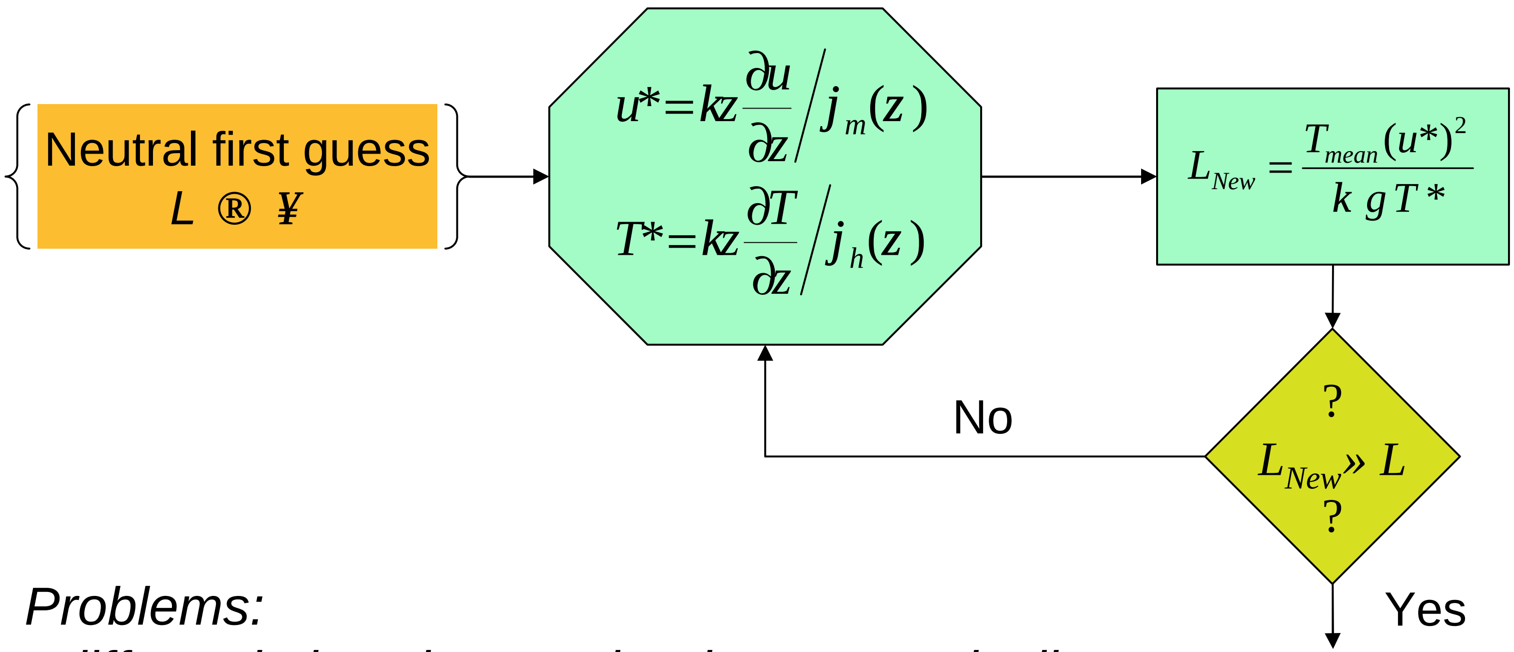
$$\frac{\partial T}{\partial z} \approx \frac{\Delta T}{\Delta z} \sim \frac{4^0}{1km} \sim \frac{0.04\deg}{10m}$$

- GRIB (WMO standard for NWP information storage) accuracy ~ $0.01^0 \Rightarrow$ for *Dz~10m* signal = noise
- The better resolution – the worse the signal–to–noise ratio
- The stronger mixing – the worse the s-to-n ratio

NWP->CTM: ABL re-stating

- Problem: the above-mentioned need to re-state (or create) the parameters driving mixing in the ABL and above
- Input: standard well-verified profiles of wind, temperature and humidity
  - e.g. heat fluxes, even if available, are dangerous due to no verification
- Output: standard set of scaling variables
- Extra requirements
  - limit numerical differentiation
  - stability of the scheme
  - efficiency

Problem discussion: iterative solution



Problems:

- differentiations have to be done numerically

- convergence of the iterations is not proven

SILAM ABL diagnostic

$$K_z(z_K) = \left[\int_0^{z_K} \frac{\left(\left(\partial U / \partial z\right)^2 - s b \, \partial T / \partial z \right)^{5/4}}{\left(\partial U / \partial z\right)^2 - 0.5 s b \, \partial T / \partial z} dz \right]^2$$

$$u^* = \sqrt{K_z(z_K) \frac{\partial U}{\partial z}(z_K)}$$

$$H_s = -\frac{c_p r}{\Pr} K_z(z_K) \frac{\partial T}{\partial z}(z_K)$$

$$T^* = -\frac{H_s}{c_p r \; u^*}$$

$$L = -\frac{(u^*)^3 c_p r}{kb \; H}$$

$$H_l = -\frac{E r}{\Pr} K_z(z_K) \frac{\partial q}{\partial z}(z_K)$$

Here all derivatives are NOT computed numerically but rather taken from the analytical approximations of profiles.

Since z_k*~1m*, these profiles can be taken purely logarithmic. Non-logarithmic corrections start to play a strong role at *|z/L|~0.5*

Assuming the logarithmic shape, it is enough to have 2 values – at the screening and the 1st model levels – to determine the profile.

All fluctuating and not well-defined parameters are inside the integral, thus their effect is smoothed out

Problem solution(1)

- Closure equation obtained from M-O similarity consideration (Berlyand & Genikhovich, 1971):

$$\sqrt{TKE}\frac{d}{dz}\left(\frac{K_z}{TKE}\right)=k\,c_e^{0.25}\Phi(z)$$

- For practical applications, $\Phi = 1$; it corresponds to a differential expression combining the eddy diffusivity and TKE
- Using this closure expression together with equations governing the surface layer, one can obtain the following formula:

$$K_z = \left\{ \frac{k}{2}\int_0^z \frac{\left[\left(dU/dz\right)^2 - sb\,dq/dz\right]^{5/4}}{\left(dU/dz\right)^2 - 0.5sb\,dq/dz}\,dz \right\}^2$$

Problem solution (3)

Logarithmic profile assumption near the surface (*z*<<|*L*|)

$$T(z) = T_g + T^* \Pr \ln \frac{z}{z_{0T}} \quad \Rightarrow \quad \frac{\partial T}{\partial z}(z) = T^* \Pr \frac{1}{z}$$

Having temperature values at two levels, obtain:

$$T(z_2) - T(z_1) = T^* \Pr \ln \frac{z_2}{z_1} \quad \Rightarrow \quad T^* \Pr = \frac{T(z_2) - T(z_1)}{\ln \frac{z_2}{z_1}} \quad \Rightarrow \quad \frac{\partial T}{\partial z} = \frac{T(z_2) - T(z_1)}{z \ln \frac{z_2}{z_1}}$$

Analogously, for velocity scale:

$$\frac{\partial U}{\partial z} = \frac{U(z_2) - U(z_1)}{z \ln \frac{z_2}{z_1}}$$

These dependencies are substituted into K_z formula, where the integral is tabulated

SILAM ABL: non-classical additions

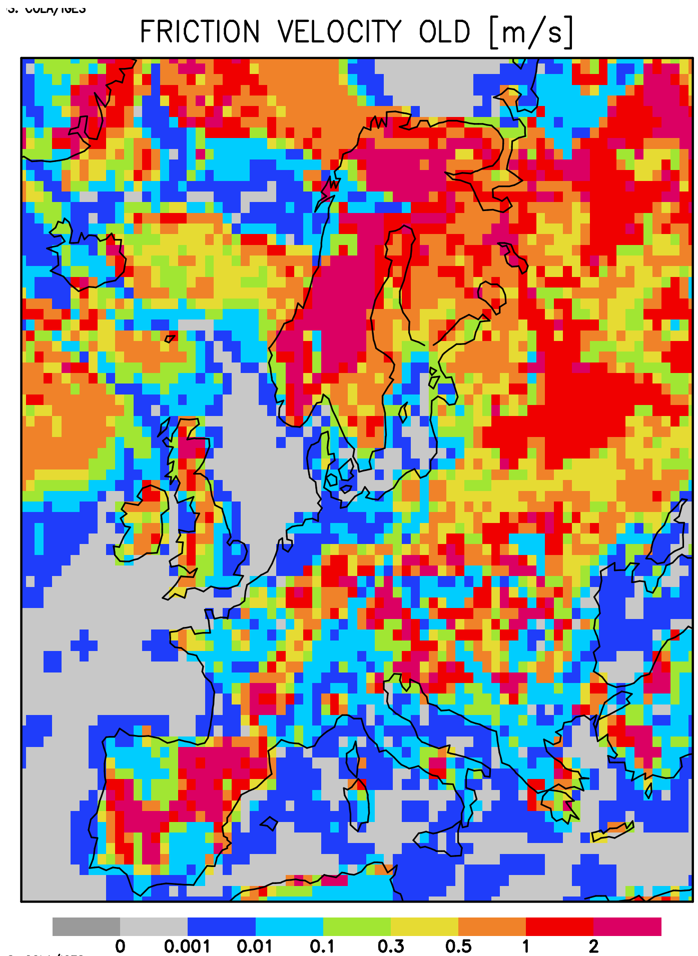
- Pr = Pr(Ri) for stable and Pr(z/L) for unstable conditions
  - dependence is just a fit of experimental data

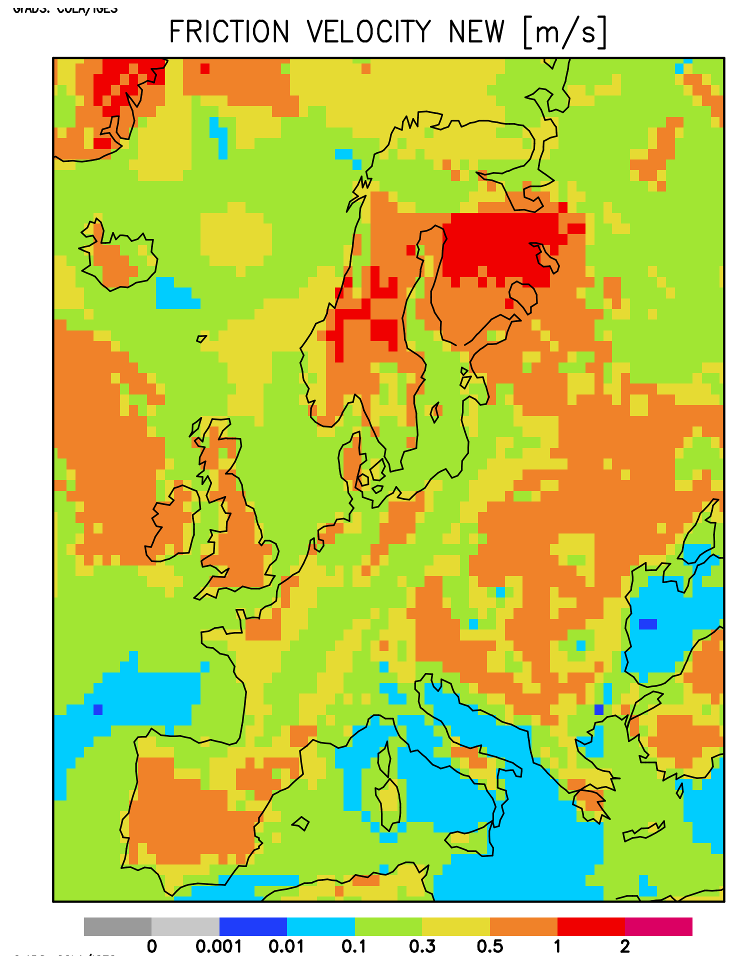
$$\Pr = \Pr_{neutral}(1 + Ri^{1.078})$$

    - note: after new theory of S.Zilitinkevich et al, must be 1+Ri for large Ri

- in principle, the second iteration is allowed with non-logarithmic profiles (not used)

Comparison of solutions





Friction velocity, iterative solution

Friction velocity, K_z-based solution

Evaluation of SILAM ABL diagnostic

- Elements
  - Cabauw mast: classical case
  - Hyytiela mast: displacement height is to be introduced to deal with forest canopy, low inversions during winter make the constant-flux assumption above the roughness elements doubtful/invalid
  - HIRLAM sensible / latent heat fluxes
- Conclusions
  - Cabauw mast: as good as one can expect or hope
  - Hyytiela: robust enough as long as constant-flux assumption holds
  - HIRLAM: qualitatively OK, quantitatively agreement is worse than that with the masts

Evaluation of SILAM ABL diagnostic

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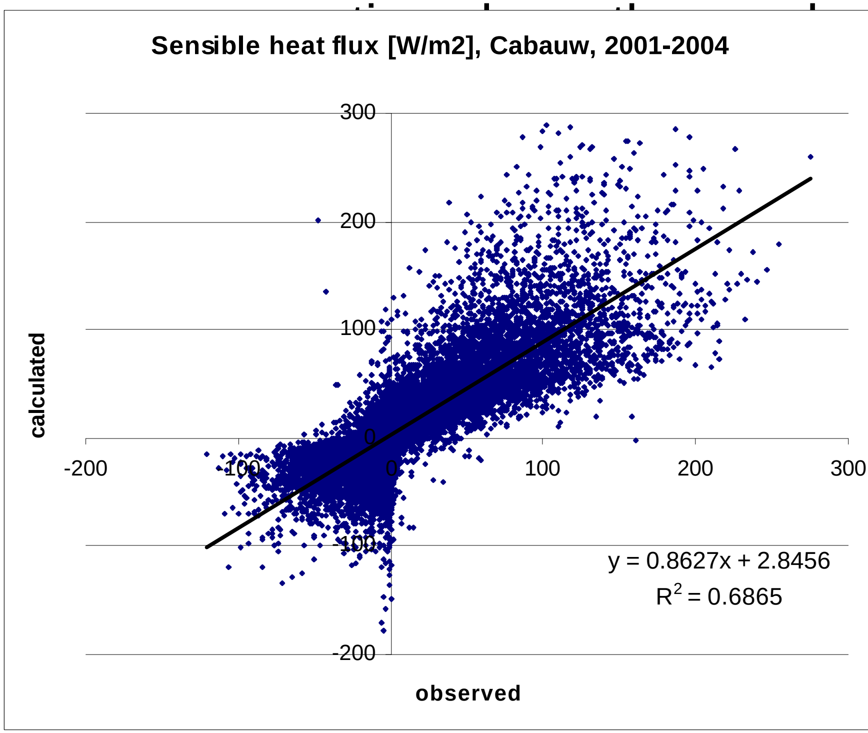

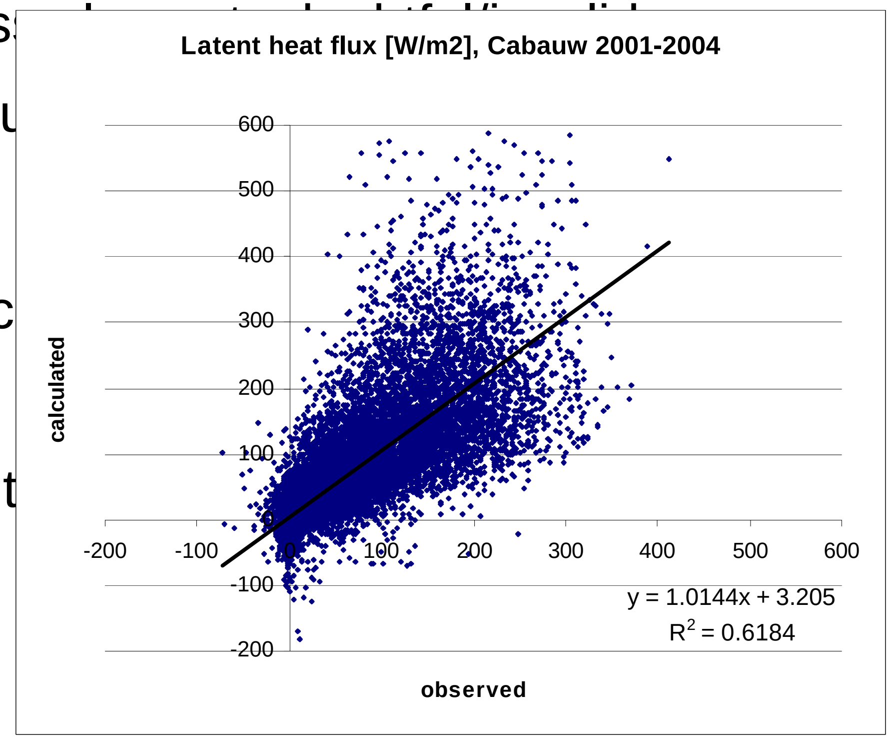

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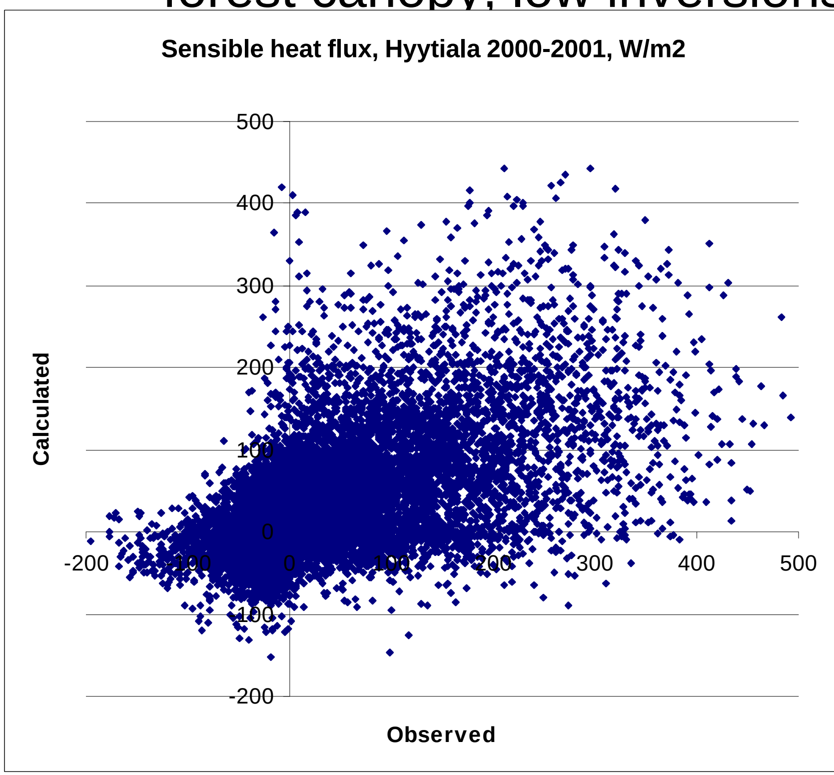

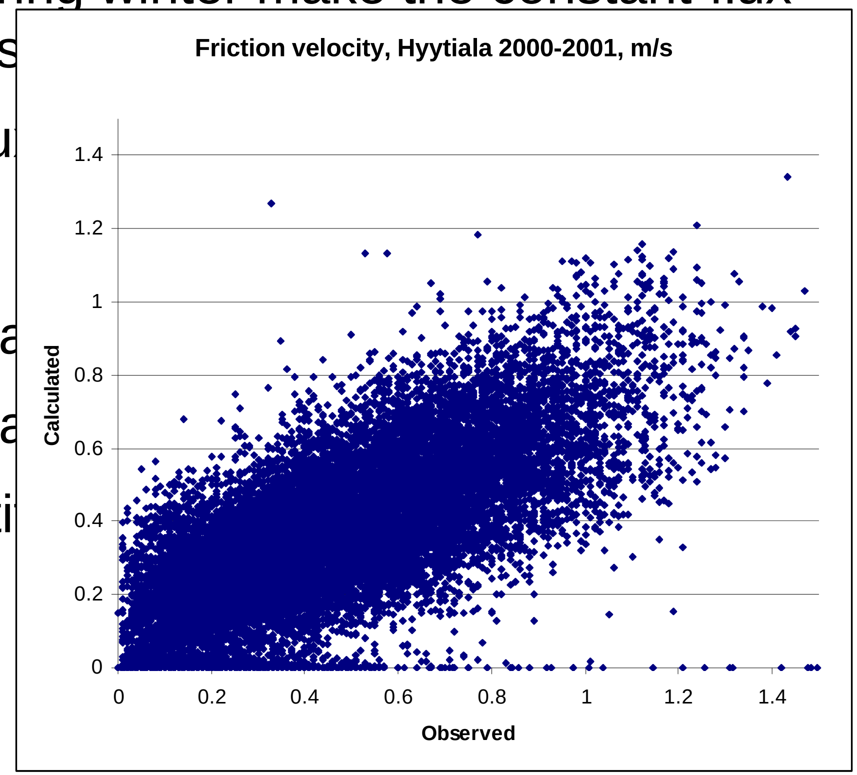

Evaluation of SILAM ABL diagnostic

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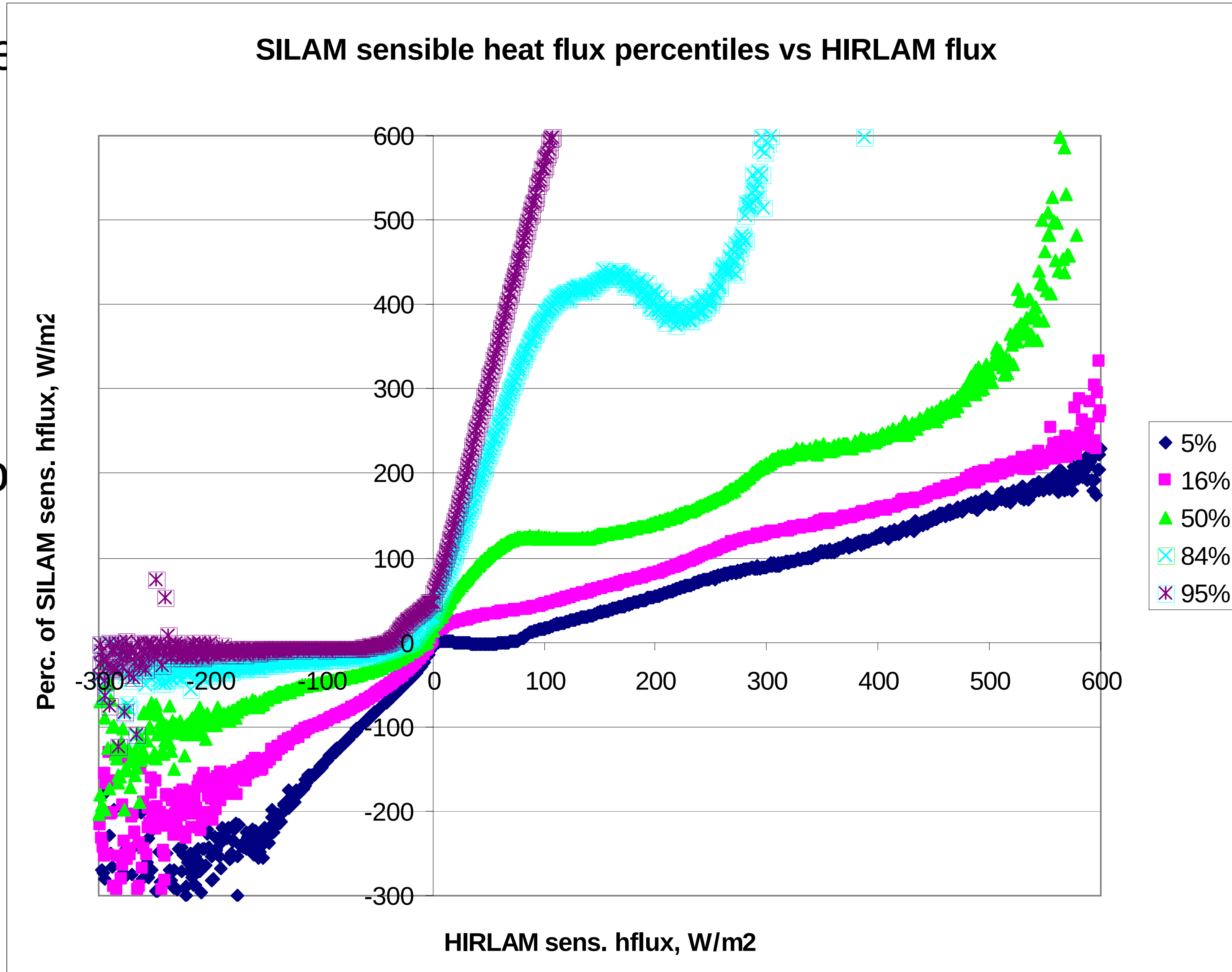

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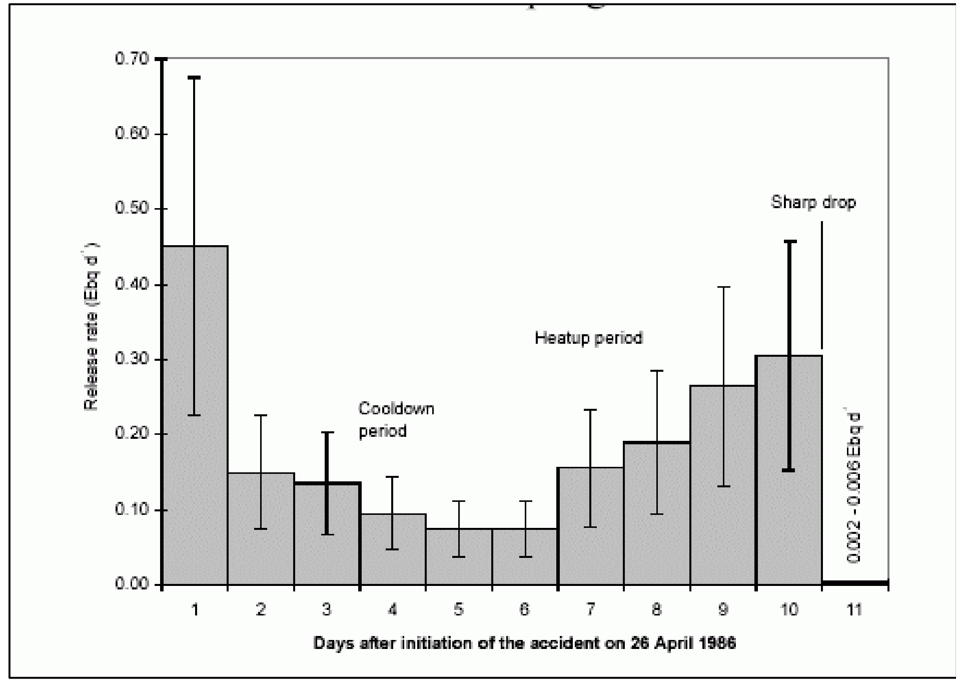
  - synoptic-scale dissipation of information
  - air quality forecasting
- Summary

Synoptic-scale information dissipation

- Dissipation of the information happens not only due to sub-grid turbulence, with growing time scale the synoptic motions start to act just the same
- Example: Chernobyl accident
  - Information on the catastrophe and release characteristics were hidden for a few days, thus posing a need for source apportionment
- Modelling assessment with SILAM+HIRLAM/ECMWF
  - straightforward simulations do not pose major problems
  - inverse problem (source apportionment) proved to be impossible with that-time monitoring network (and, to a large extent, with today’s one too)

SILAM setup for the simulations

- General setup
  - Meteorological fields: HIRLAM-6 (operational in 2006, re-run for 1986); ECMWF (operational in 1986); HIRLAM-2 (operational in 1986)
  - Resolution of the dispersion output: 1 hr, 30 km
- Forward runs
  - Emission: 23 nuclides covering >99% of the estimated release, daily values for release intensity and vertical distribution
  - Computed period: 25.04 – 20.05.1986
- Inverse runs
  - Observations: up to 94 stations (depending on nuclide) in Western Europe; up to hourly resolution (mainly daily or lower)
  - Modified 4D-VAR data assimilation approach
  - Analysed period: 20.04 – 15.05.1986



Results of the forward simulations

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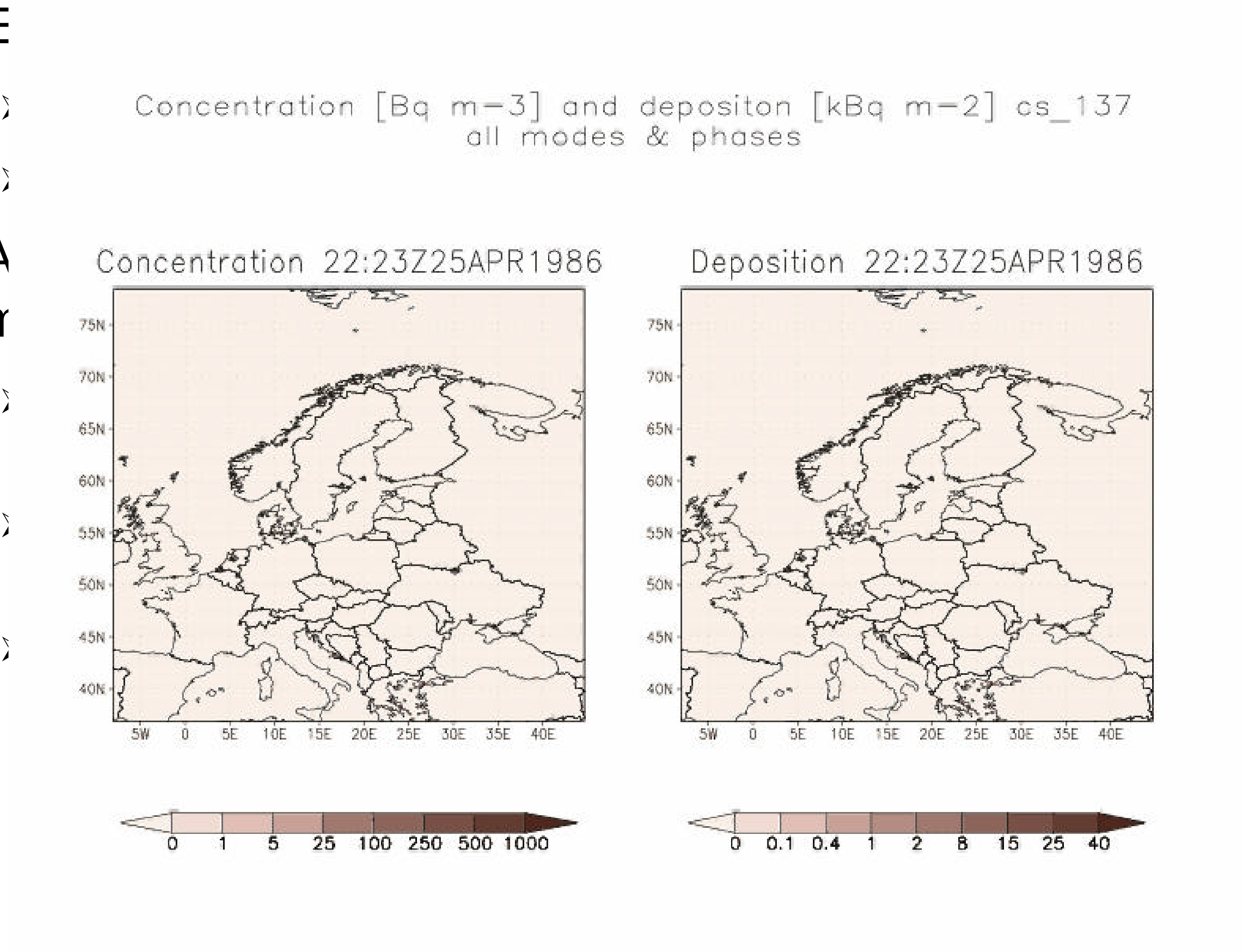
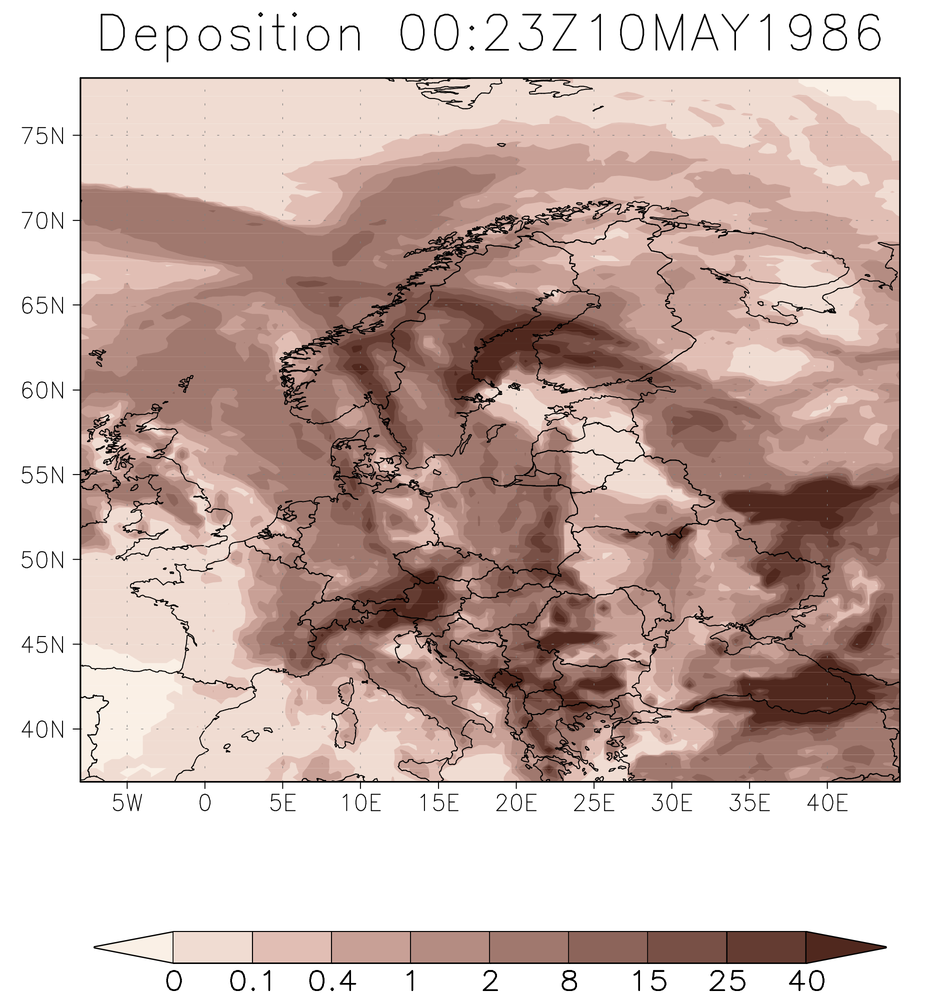
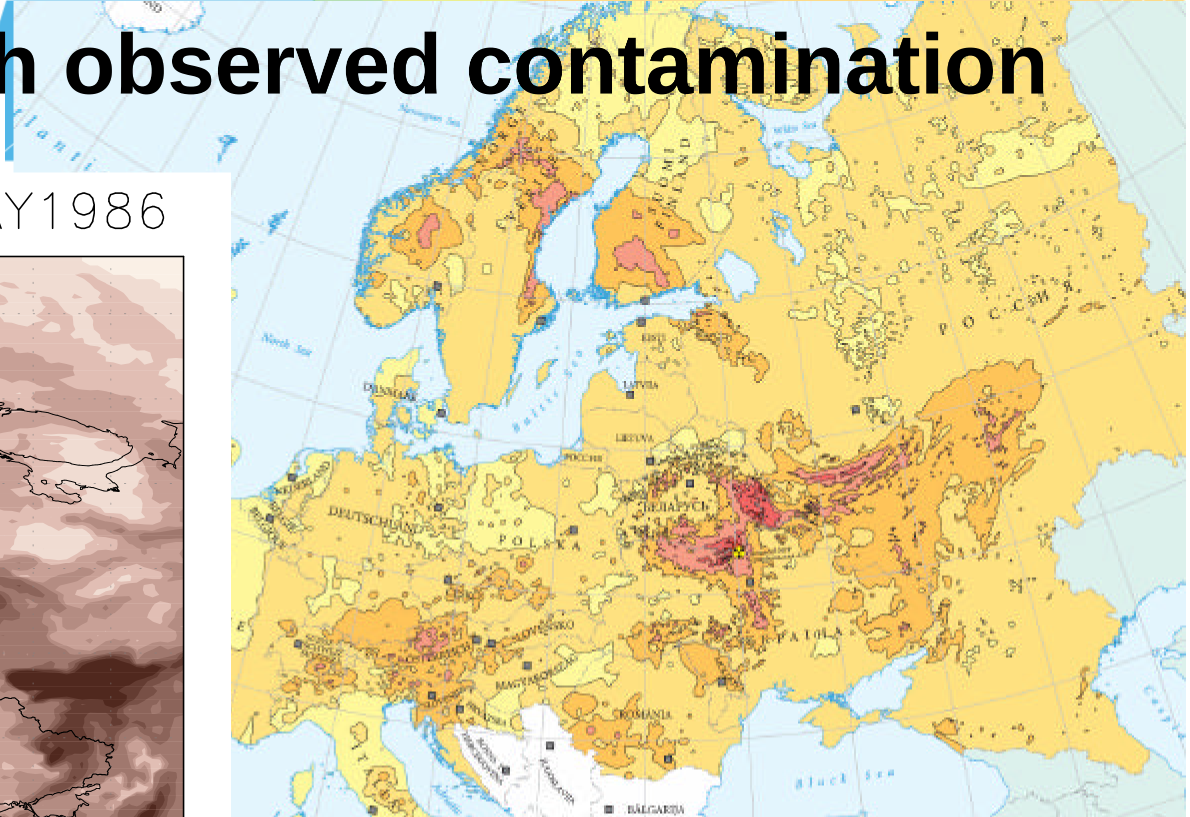


Comparison with observed contamination

CS-137, kBq m^{-2} cumulative





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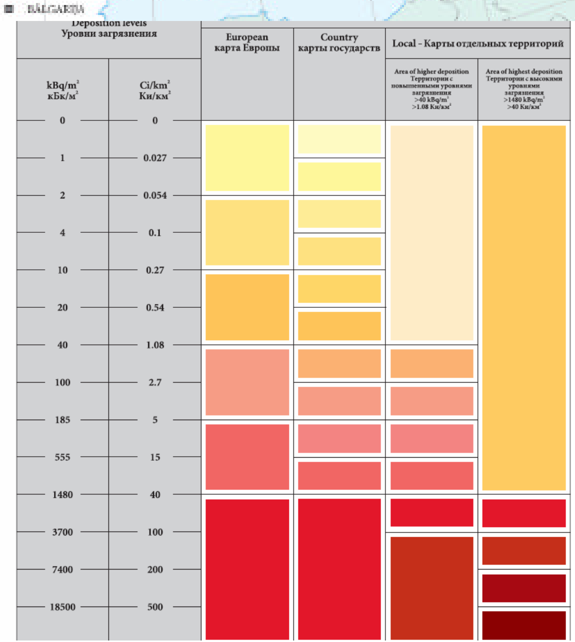

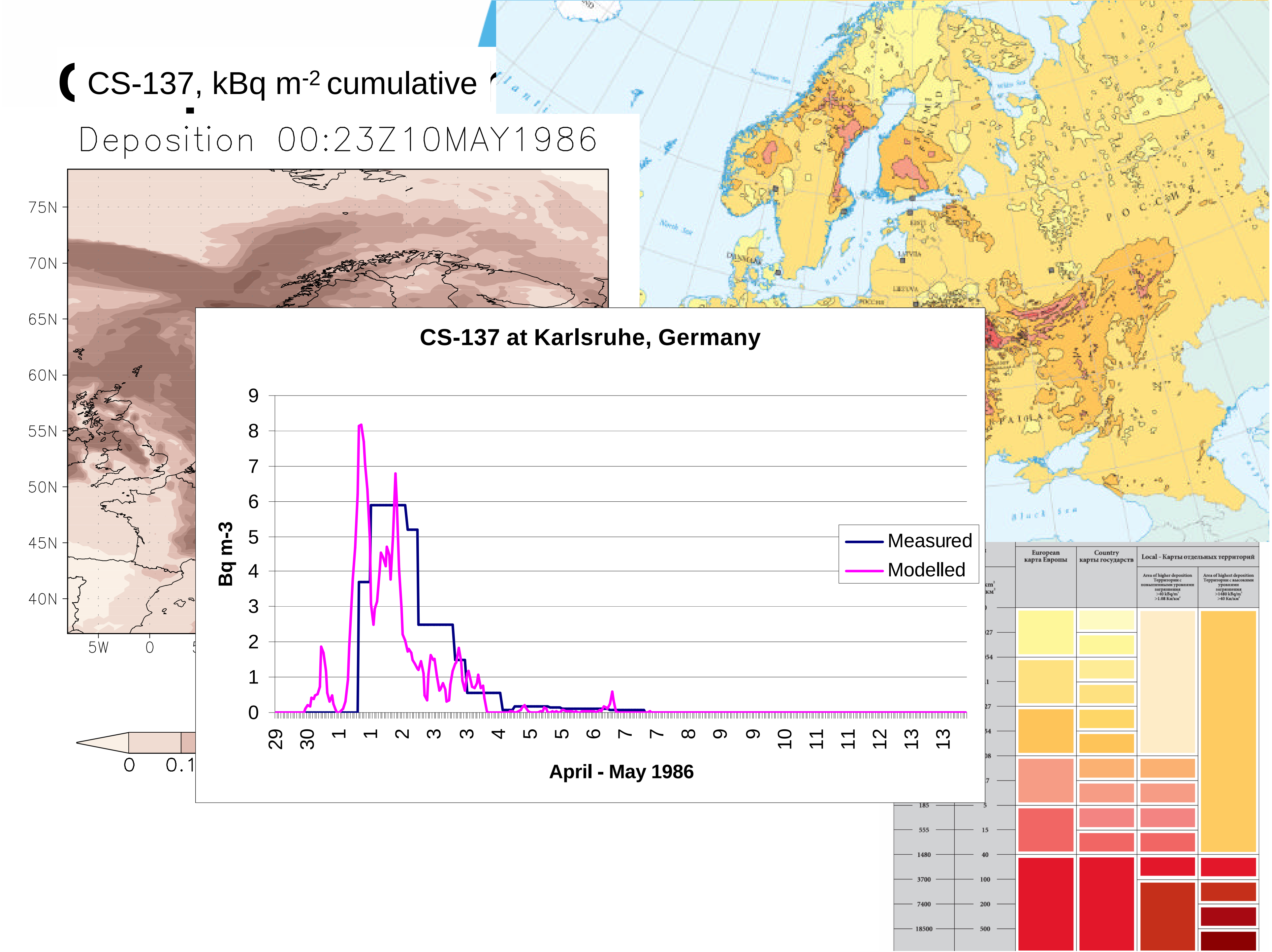

CS-137, kBq m-2 cumulative
Deposition 00:23Z10MAY1986
75N
70N
65N
60N
55N
50N
45N
40N
5W
0
0
0.1
CS-137 at Karlsruhe, Germany
Bq m-3
0
1
2
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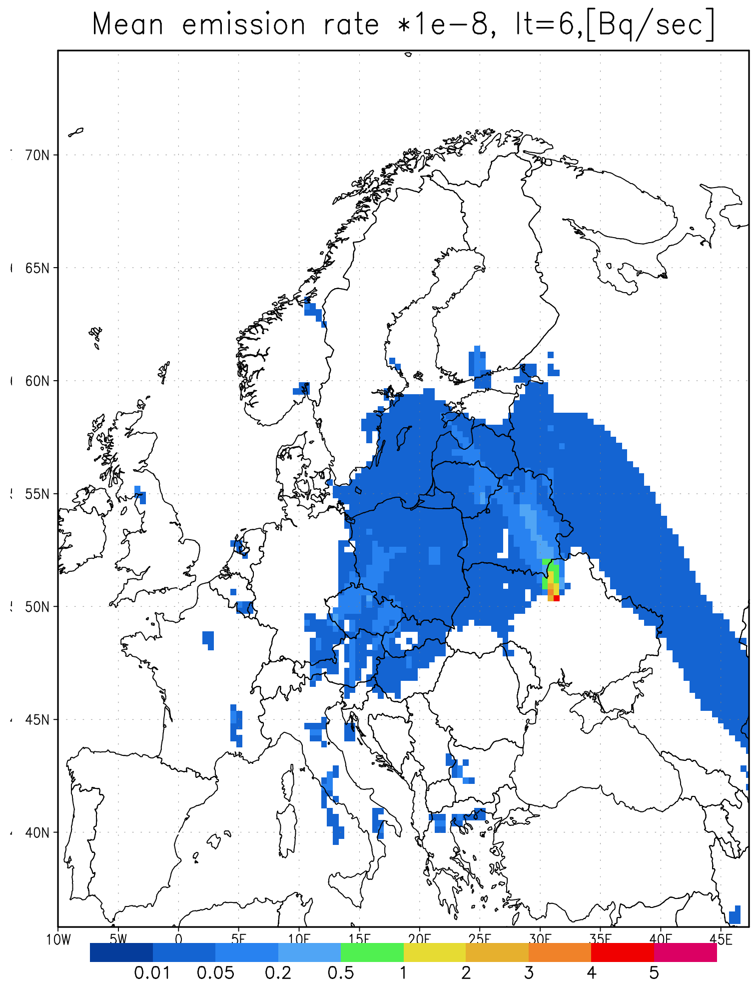
April - May 1986
Measured
Modelled
European карта Европы
Country карты государств
Local - Карты отдельных территорий

Comparison with observed contamination

- Comparison specifics
  - ➢ time-resolved concentration measurements are compared with dynamic fields using MMAS software
    - – low time resolution of most of data
  - ➢ cumulated deposition measurements are compared with the final totals
  - ➢ large fraction of observations is still not available in numerical format
- General results
  - ➢ deposition pattern is reproduced surprisingly well, while absolute levels strongly depend on emission specification and can be right of wrong depending on nuclide composition and total release estimates
  - ➢ concentration evolution: mean time correlation >0.7, absolute levels depend on emission specification
  - ➢ low time resolution “helps” to reach very high time correlation (>0.9 for 30% of stations) but hides details of the development

4D-VAR iterations: time-integrated emission fields

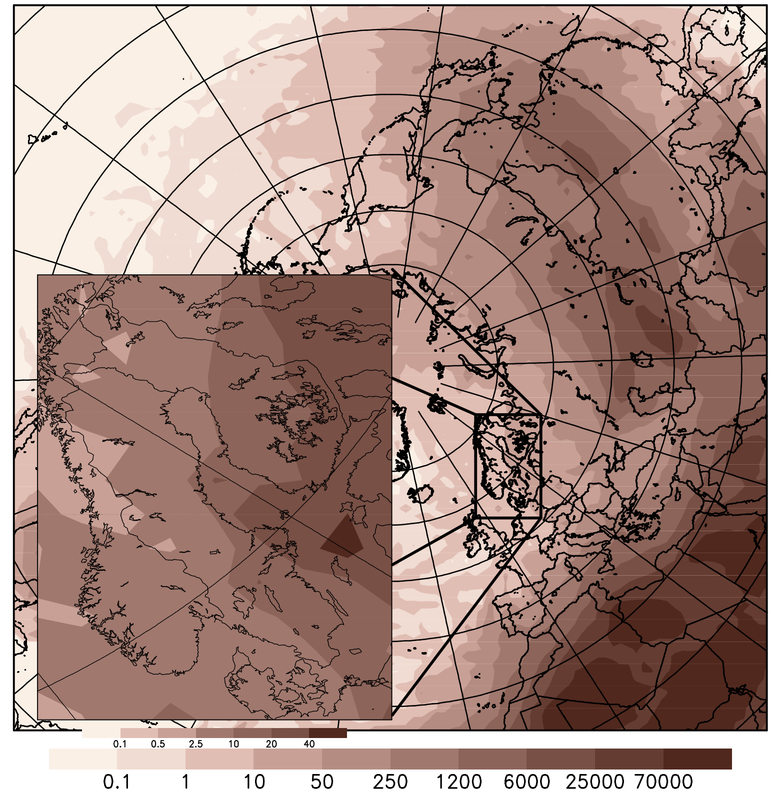


Results of the 4D-VAR for Chernobyl

- Formally, the inverse problem is solved
  - the site location is disclosed and time variation is reasonable
  - further time adjustment is possible with a site location constraint
- However, the run showed severe lack of input information
  - Most of observational sites are located at large distances from the source,
  - Actual site place was disclosed by just one neighbouring site
- Very complicated meteorological pattern: synoptic-scale mixing
  - Pollution was cycling over central and eastern Europe for a few days
  - The origin of these clouds cannot be resolved without observational information from these regions
  - The model did not learn new info from 4D-VAR iterations (contrary to ETEX source apportionment)
  - Reason: limited “memory” over time: the nearly-well-mixed plume cannot be inverted

Example 2: desert dust re-analysis

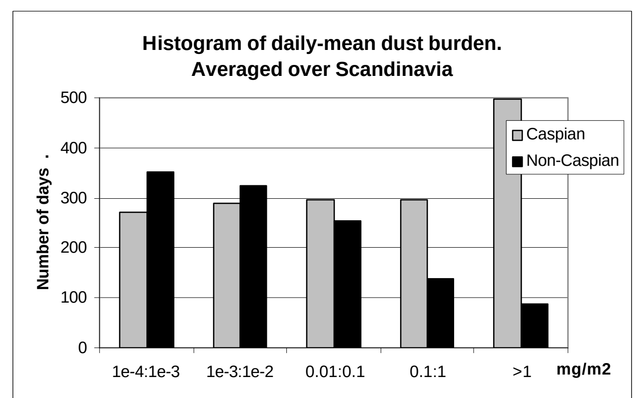
- Deserts are not too common in Europe, especially in Northern Europe
- However, the impact of dust storms can be substantial – episodically
- To get some long-term statistics, a hemispheric model DMAT has been run over 22 years with NCEP re-analysis as NWP forcing



Map: dust load, mg PM m^{-2}, mean 1967-1988

Chart: Nbr of episodes with specific dust load

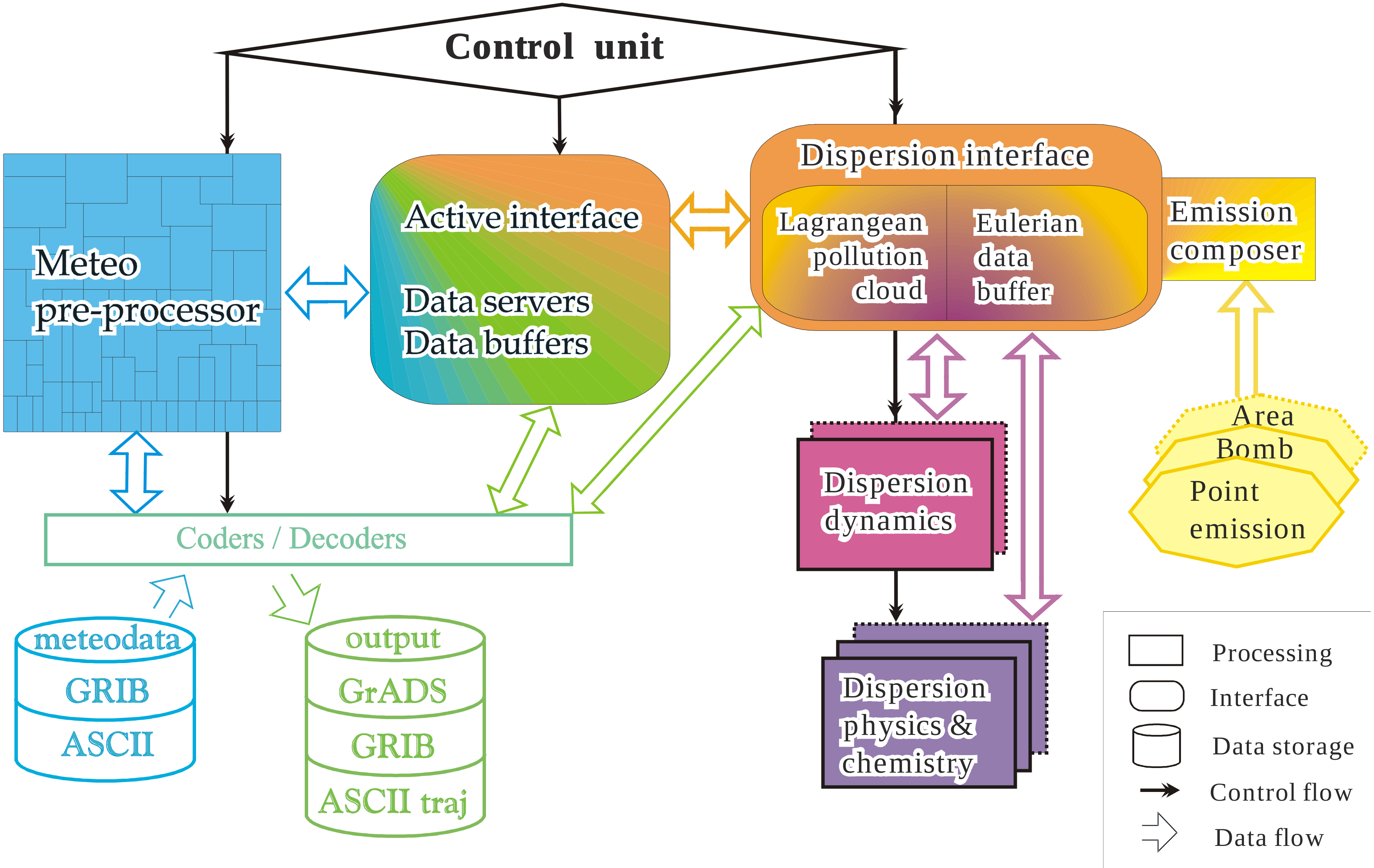
(Hongisto & Sofiev, 2004)



Example 3: air quality forecasting

- Main practical interest in Finland: atmospheric aerosols
  - ozone problem is not that pressing (yet)
- A large variety of sources
  - anthropogenic emissions
    - direct anthropogenic emission of particles
    - anthropogenic emission of aerosol pre-cursors
  - natural or seemingly natural
    - biogenic emission of aerosol precursors
    - sea salt
    - wind-blown dust
  - wild-land fires (whatever the origin is)
- Target is hourly resolution
  - strong influence of hour-by-hour emission time variations, which are entirely unknown (only climatologic variation coefficients are available)
  - meteorology-driven emission

SILAM modelling system

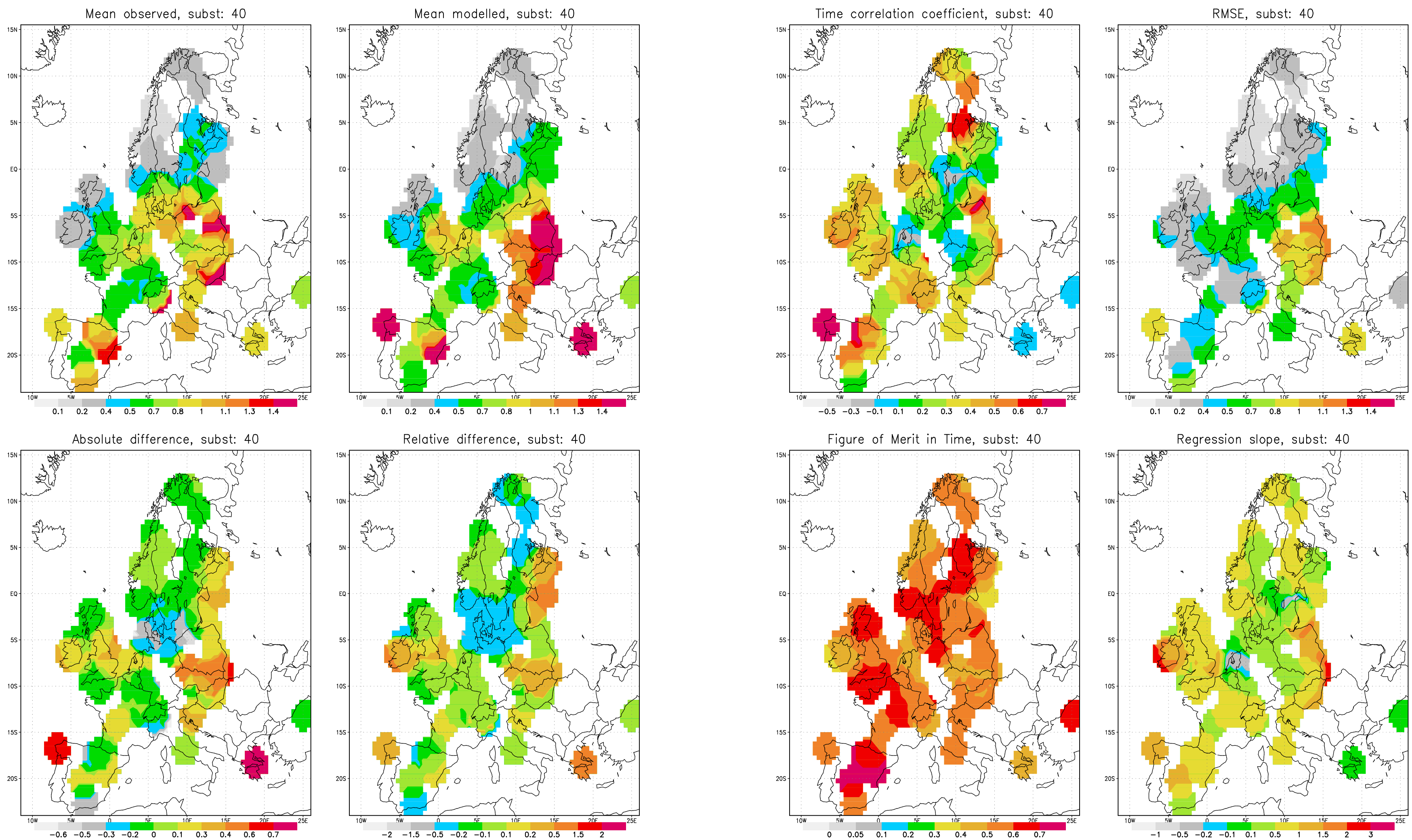


Evaluation of the re-analysis results

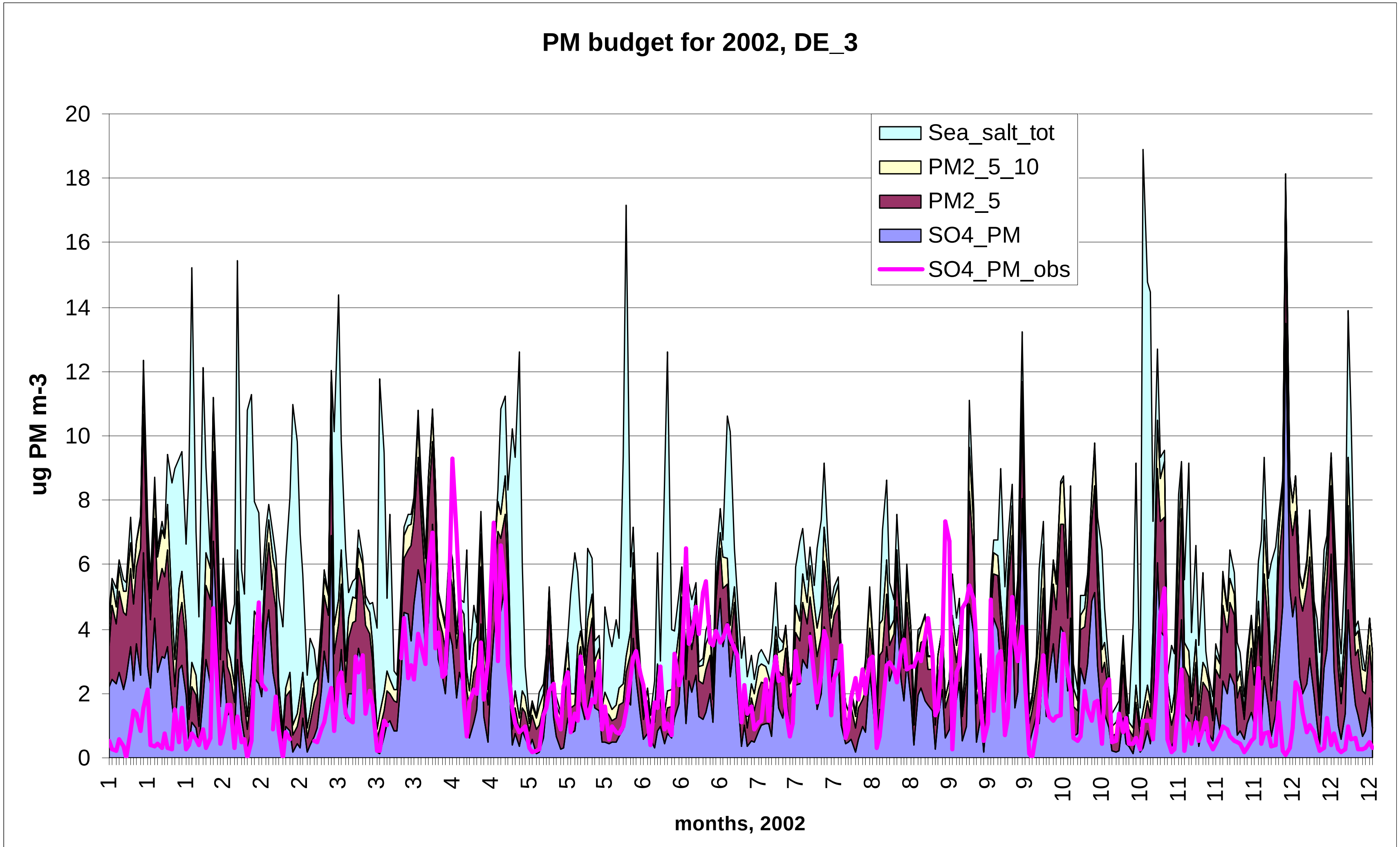
- Comparison with EMEP data
  - SO_x as the main dataset: SO_2 in air, SO_4 in aerosol, SO_4 wet deposition
  - aerosol observations are scarce and do not include speciation; however, work is on-going to compare the bulk concentrations (PPM 2.5 / PPM 10 + SO_4 + SeaSalt $\Rightarrow$ ~80% of PM)
  - Mean values are good and quality is homogeneous in space
  - Temporal correlation is somewhat low for monthly level (seasonality of emission is 15 years old)
  - Specific parameters – FMT, RMSE, RelDiff – are within fair-to-good limits
- Comparison with some campaign results: on-going (Biofor-1999, Varrio-2003, etc…)

Examples of the comparison

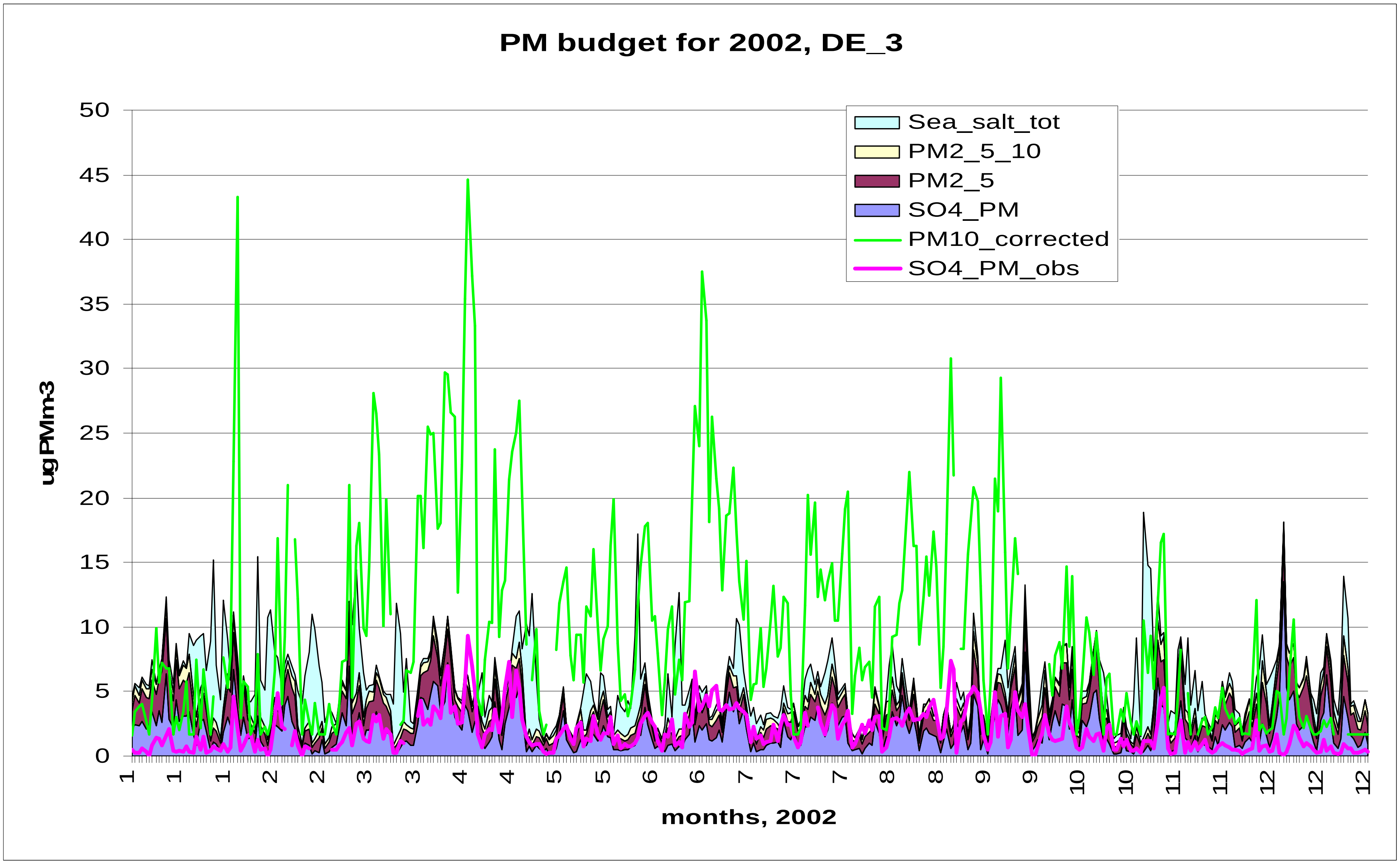
- SO_4 concentrations, µg S m^{-3}



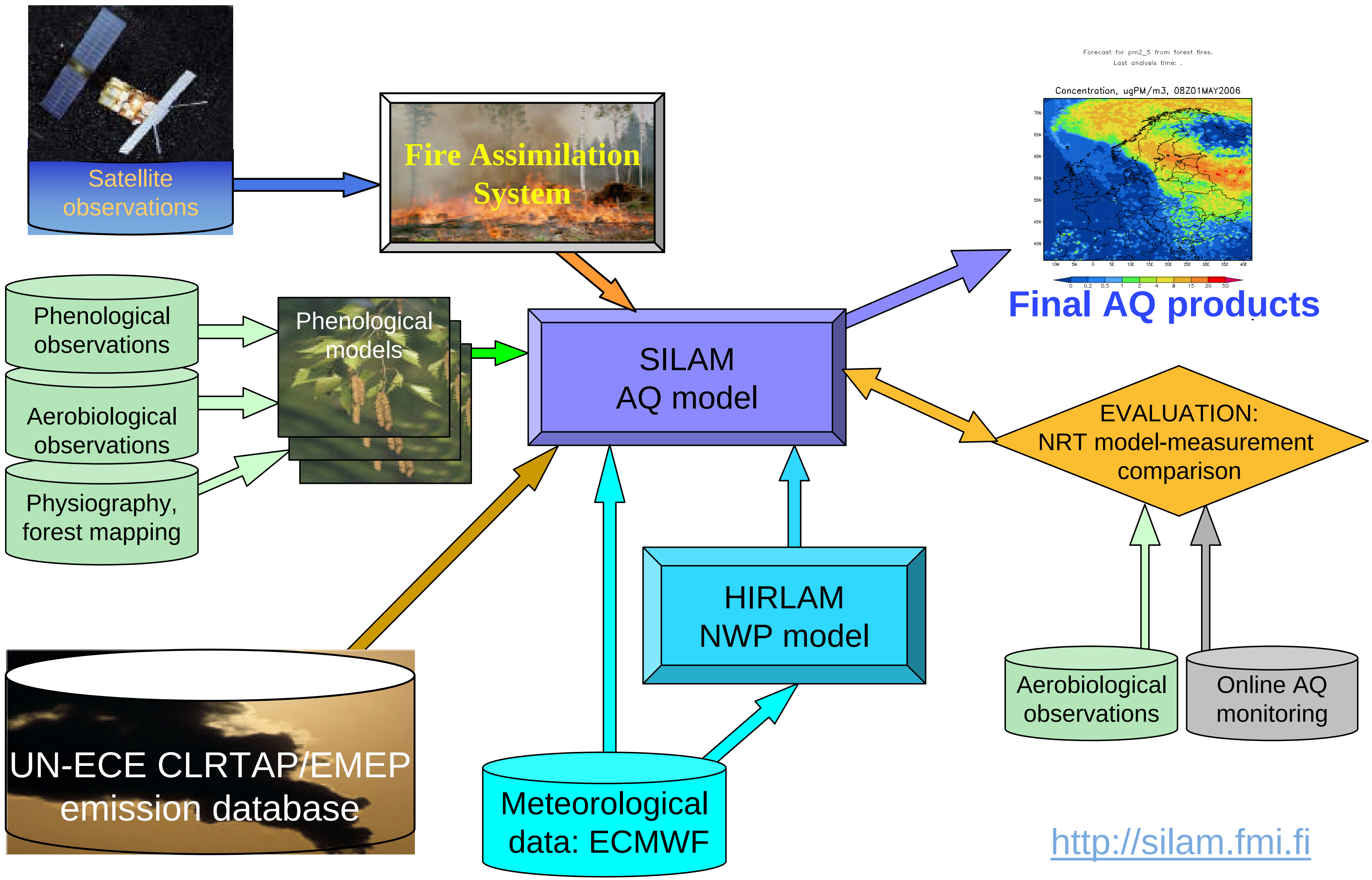
Example of central-Germany EMEP station GE-3



Example of central-Germany EMEP station GE-3



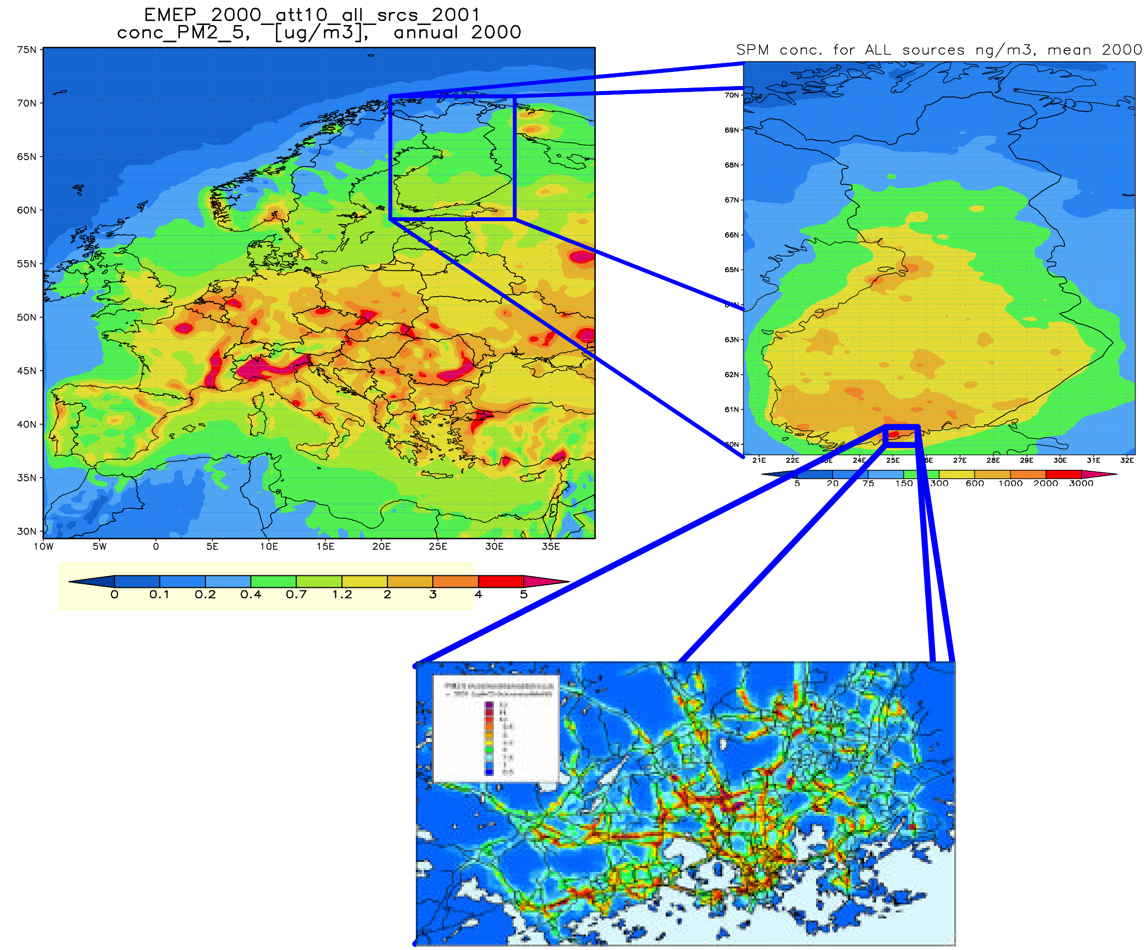
Regional CTM system at FMI for AQ forecasting



http://silam.fmi.fi

Forecast: target configuration

- Maps: PM 2.5 mean-2001 concentrations, ug PM /m3
  - European
  - Finnish source contribution (obs different scale)
  - Helsinki city-scale



Summary

- Chemical transport models, born as downstream applications of meteorological models, are growing (has grown??) up to become the other side of the coin called “Chemical Weather Modelling System”
  - CTM is the most demanding user – and unique supplier of data – for NWP
  - needs and possibilities of joint complex verification
- Means of creating CW system from NWP and CTM couple are twofold: online and offline coupling
  - each has own strong points and weaknesses, as well as application areas
- Systematic research of CW systems and their features is just getting the steam

Instead of conclusion

- **Mechanitis**: occupational decease of one who believes that a mathematical problem, which he can neither solve nor even formulate, can readily be answered, once he has access to a sufficiently expensive machine.

Bernard Koopman (**1956**) *Operations research,* **4**, 422-430