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# Data assimilation and inverse problems

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# Introduction

- **“How to combine observations and model fields into an estimate of the atmospheric state?”**
  - Chemical data assimilation for forecasting and reanalysis
- **“Where is the source of the toxic pollutant that we measured?” or “How much SO2 was emitted in this volcanic eruption”**
  - Inverse problems related to individual sources
- **“What is the geographic distribution of emission fluxes of CH4?” or “How can we refine emission inventories using observations”**
  - Flux inversion studies. A priori emission estimate usually required.

# Outline

- **Some data assimilation methods**
- **Examples**
  - Chemical data assimilation: 3D-Var analyses of ozone
  - Chemical data assimilation with emission adjustment: 4D-Var assimilation of SO2
  - Variational inversion to determine SO2 emission flux in a volcanic eruption

# Data assimilation and inverse problems: definition and methods

- **Inverse problem: use indirect measurements to estimate quantities not directly observed**
  - example: determine shape of a drum from the sound of drum (this one was shown to be unsolvable, though!)
- **Data assimilation in meteorology:**
  - combine observations and the previous model forecast
  - use the state estimate for initializing the next forecast
- **Data assimilation may form an inverse problem**
  - indirect measurements
  - past state may be adjusted using current observations
  - data assimilation may be extended to the source term

# Basic data assimilation concepts

- **Control variable $\xi$: the parameter being adjusted**
- **The background $\xi_b$: the a priori value for control variable**
- **The analysis $\xi_a$: the adjusted value for the control variable**
- **Model operator maps the control variable to model state:**

$$M\colon \xi \mapsto M(\xi) = x$$

- **Observation operator maps the model state to an observed quantity**

$$H\colon x \mapsto H(x) = y$$

- **Cost function measures the difference between simulated and real measurements, and from the background value**

$$J(\xi) = \| \xi - \xi_b \|^2 + \| y - H(M(\xi)) \|^2$$

# Ozone analyses

- **Surface O3 measurements assimilated every hour**
- **Method: 3D-Var**
  - every hour, minimize

$$J(x) = \| x - x_b \|^2 + \| H(x) - y \|^2$$

  - $x_b$ is the concentration forecasted from previous analysis
  - $y = Hx$ is the observations at stations
  - B is the background error covariance matrix, defines the shape of the increment $x_a$ - $x_b$

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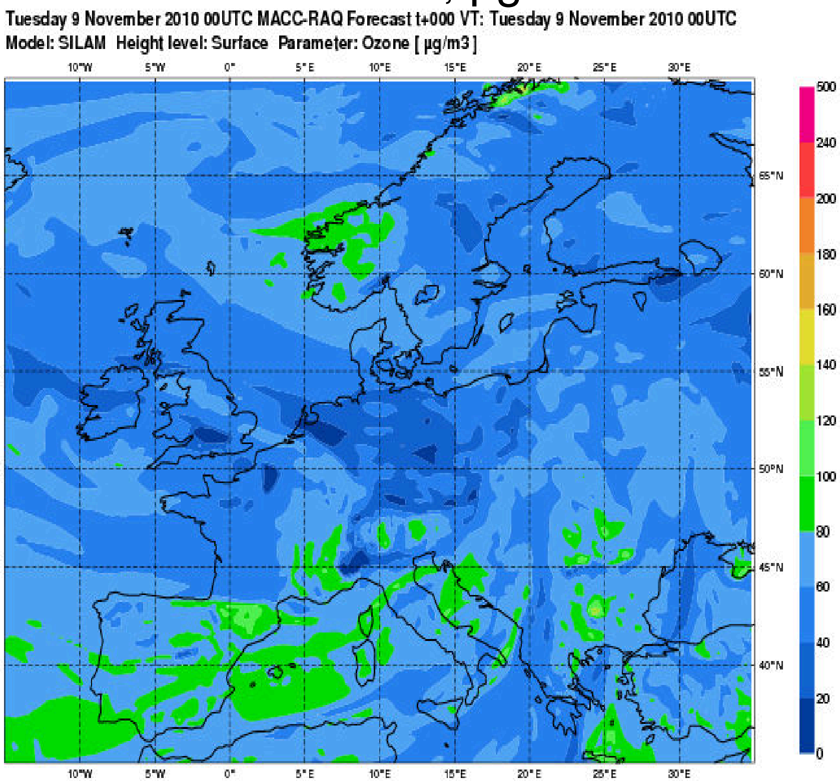
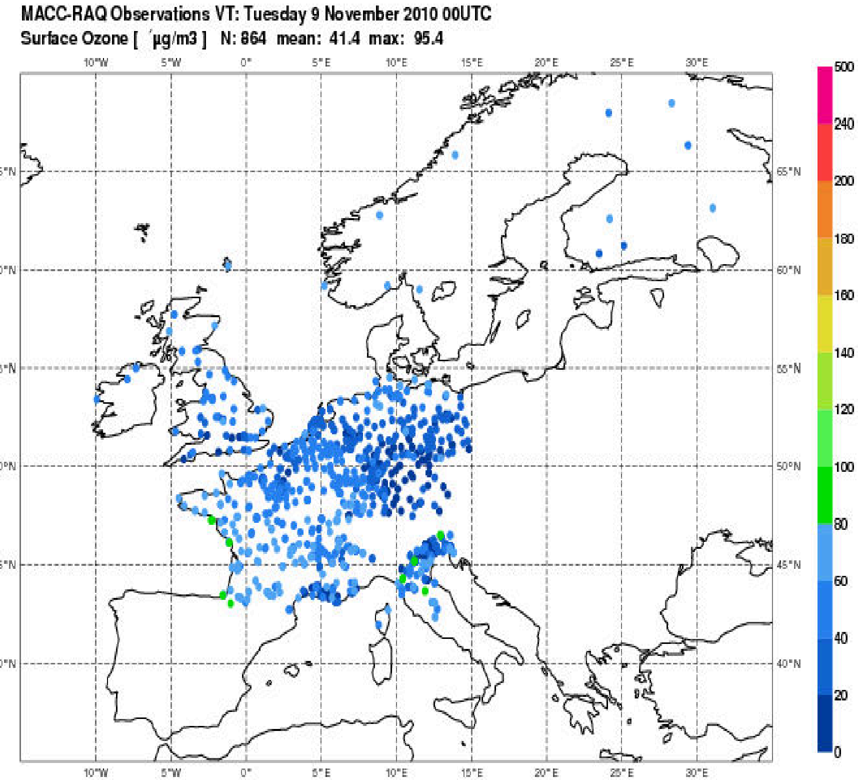
# Example: SILAM $O_3$ forecast and observations in MACC for 9 November, 2010 00UTC

Concentration of O3, µg/m$^3$



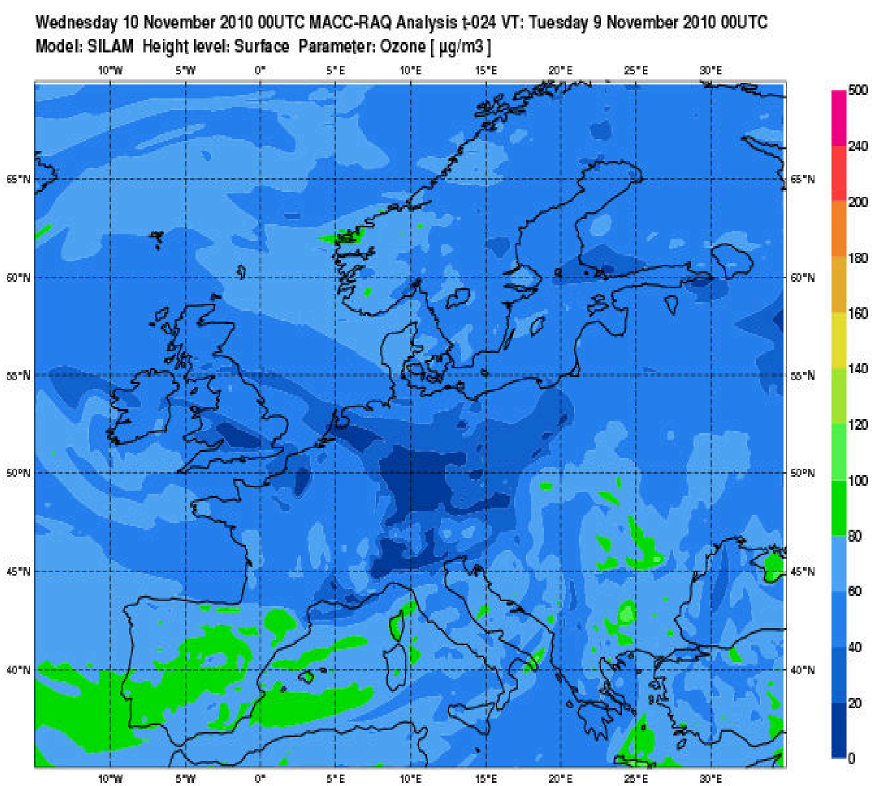

Forecast



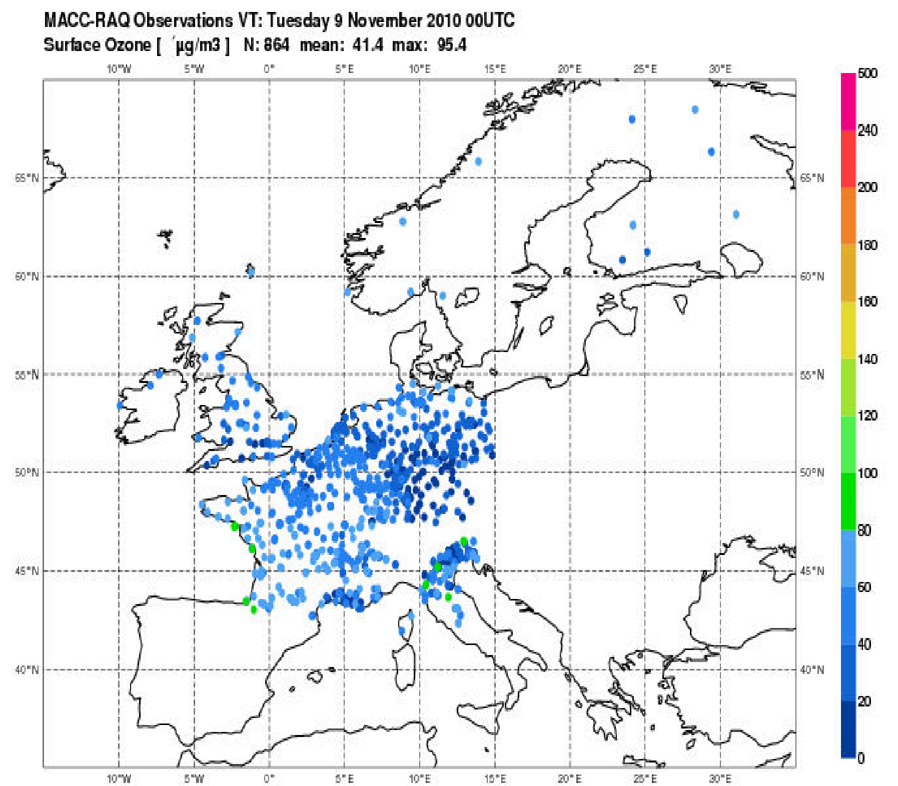

Observations

# Example: SILAM $O_3$ analysis and observations in MACC, for 9 November, 2010 00UTC

Concentration of O3, µg/m$^3$




Analysis




Observations

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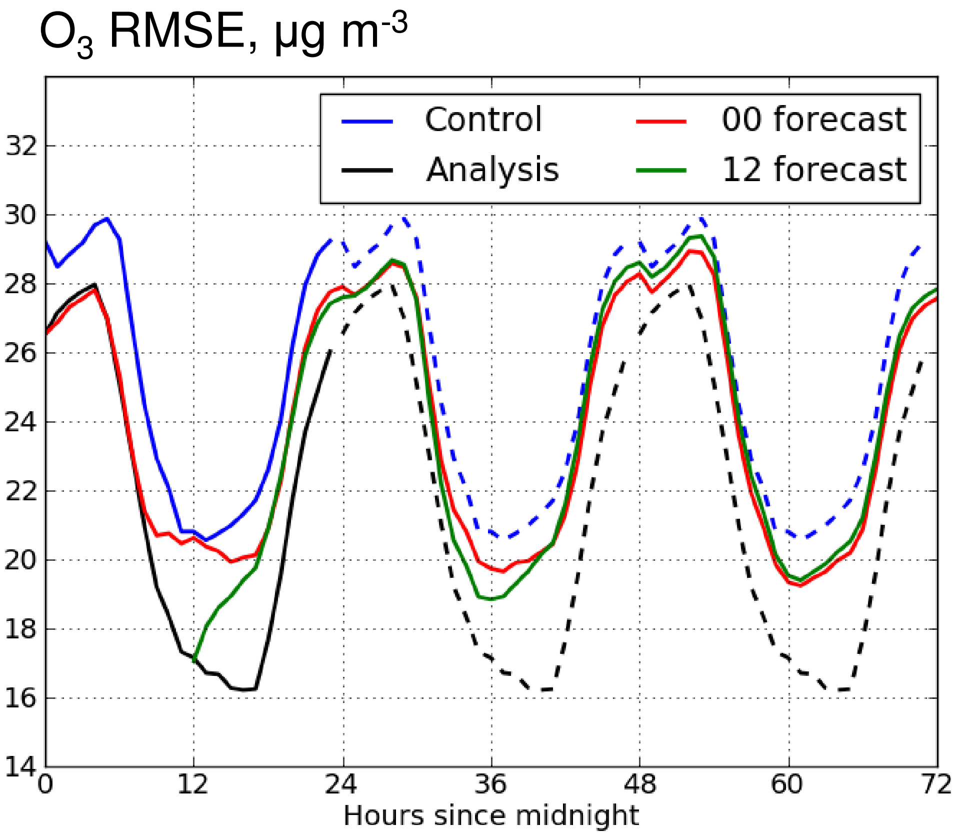
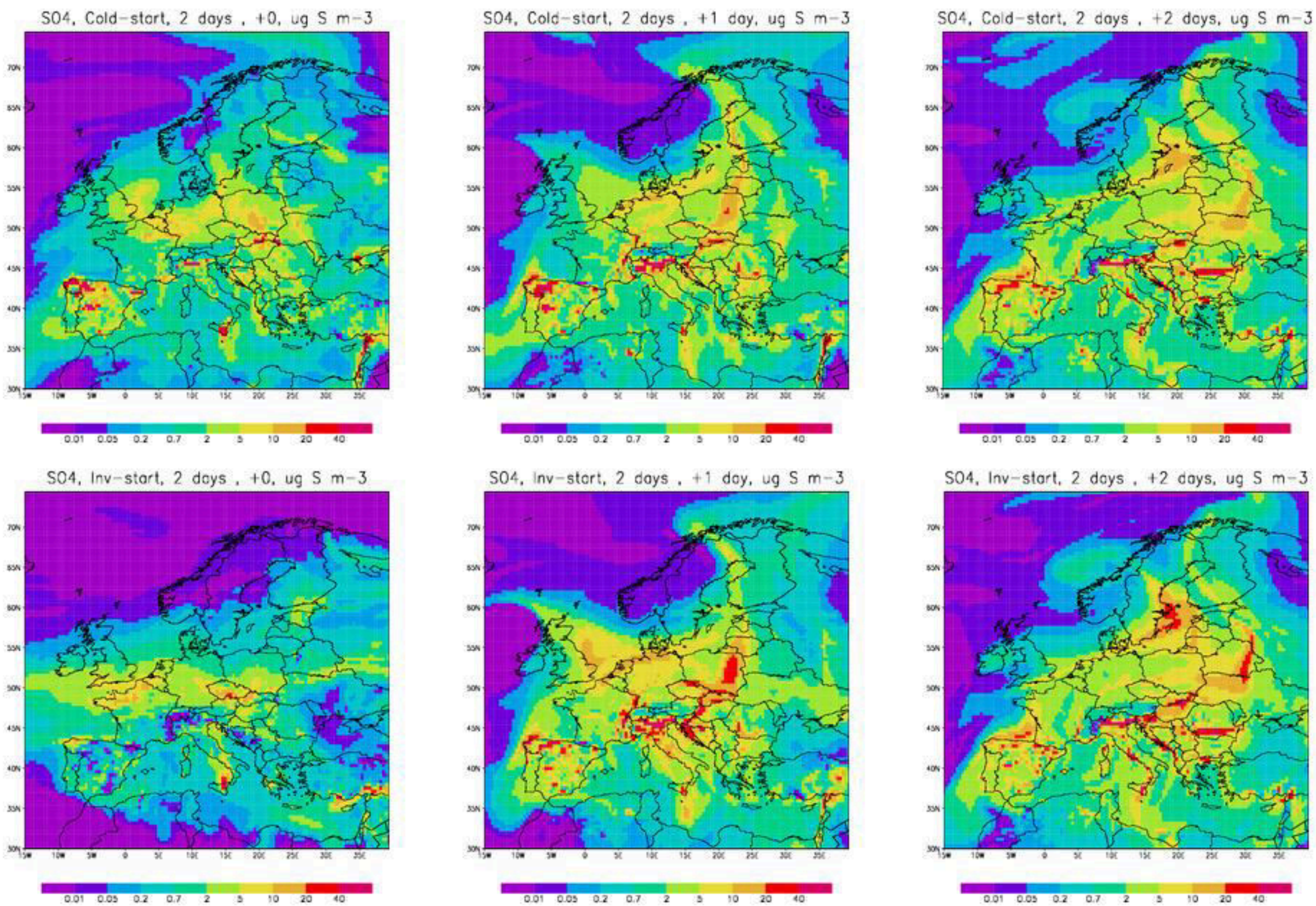
# Assimilation of $O_3$, 3 weeks in July 2009

- **Assimilation experiment with the 3D-Var setup**
- **72 h forecast started every 00 and 12 UTC**
- **RMSE calculated for 132 not assimilated stations**
- **Control run with no assimilation**



# The effect of initial condition on the forecast

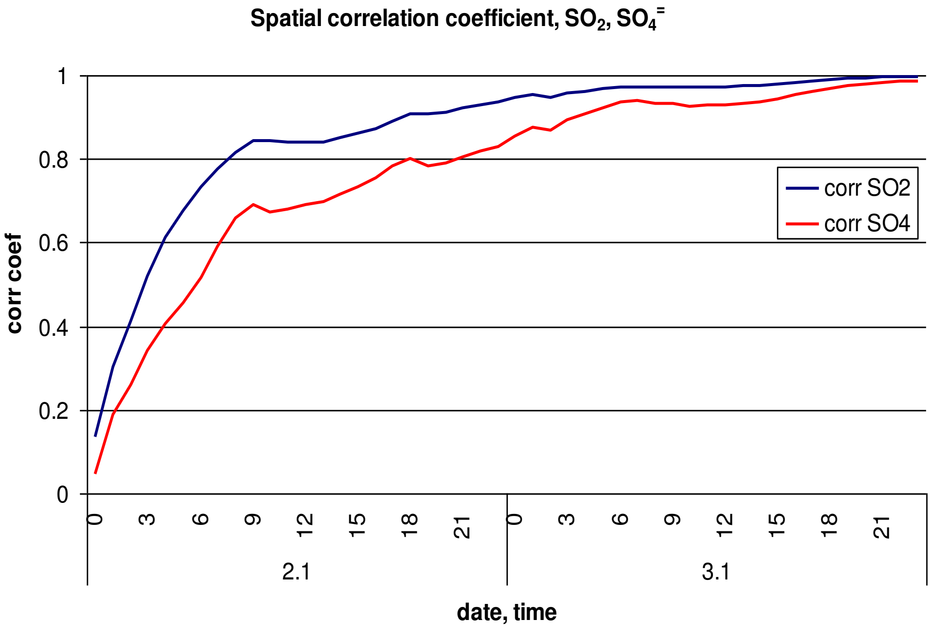
- Contrasting initial condition created with inverted wind field
- Identical meteorological and emission forcing for the next 48 hours
- Aerosol sulfate shown, HIRLAM meteorology for January 2000




+ 0 h | + 24 h | + 48 h

# Chemical DA beyond the “initial state” approach

- **The evolution of atmospheric composition weakly affected by the initial state**
- **Effect likely to vary by chemical compound**
  - Best chances with pollutants with a dense observation network and moderate or long lifetime (ozone!)

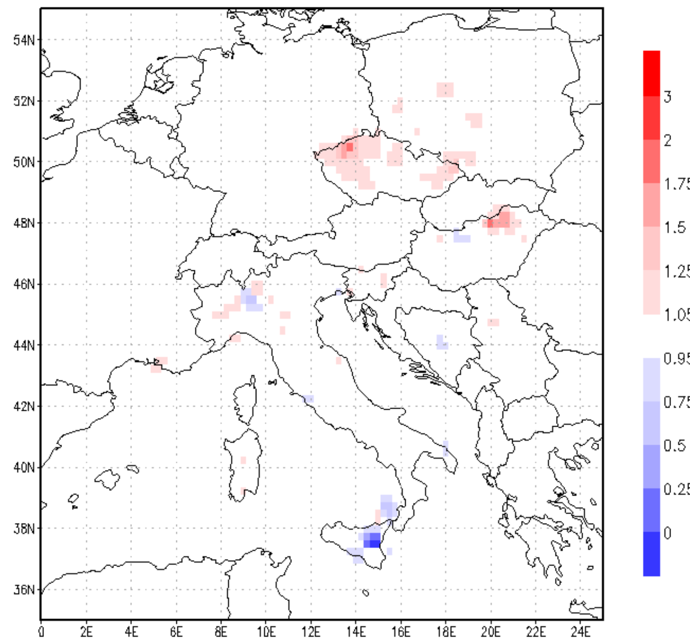



- **Chemical composition is strongly driven by pollutant emissions**
  - Can the emissions be adjusted with data assimilation?

# Assimilation experiment with emission adjustment

- **Assimilation experiment for Southern Europe covering 2006/2/8 … 2006/2/22**
- **Data assimilation: 4D-VAR, in-situ observations**
  - ➢ Both initial condition field and emission correction fluxes are influenced by observations
  - ➢ 24 h assimilation windows + 24 h forecasts
- **Consistent emission corrections on some areas:**
  - ➢ Mt. Etna: up to 70% decrease in total emission
  - ➢ Smaller adjustments in Hungary, Czech and northern Italy
- **Significant day-to-day variation**

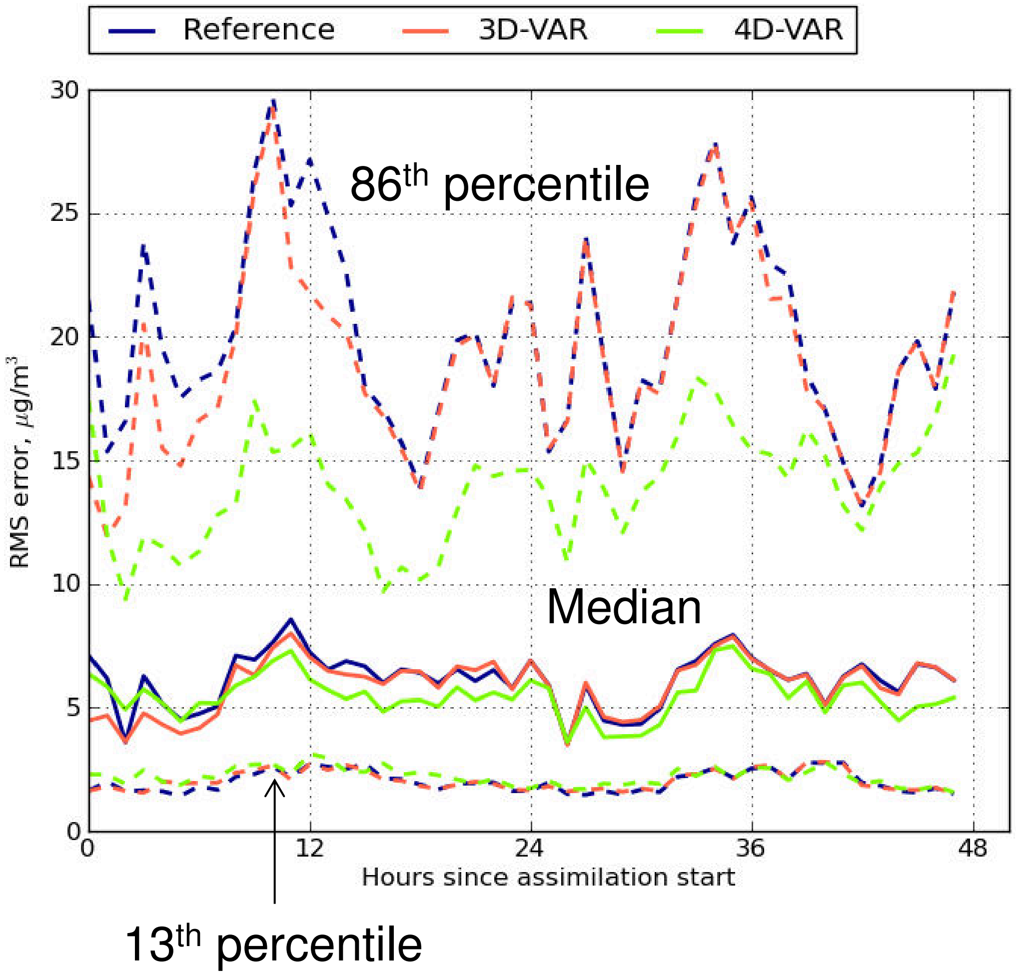
Average emission correction, days 1…14




Ref.: Vira & Sofiev (2012), Atmos. Env.

# Adjusting the emission or initial condition?

- **$SO_2$ assimilated at 260 stations**
- **RMSE for $SO_2$ compared at 50 control stations**
- **4D-Var: observations assimilated for the first 24 hours**
- **3D-Var: observations used only at *t* = 0h**
- **Reference: no assimilation**



# Comments on chemical data assimilation in air quality forecasting

- **For short and medium lived species, emission rate is potentially powerful control parameter**
  - how to avoid attributing model errors to emission?
  - how to forecast emission rates?
- **3D-Var type methods useful for reanalysis and sometimes forecasting, however chemical coupling may cause surprises**
  - example: photostationary equilibrium $[O_3] = \frac{j}{k}\frac{[NO_2]}{[NO]}$
  - Our experience: assimilation of $NO_2$ not beneficial for $O_3$

# Estimating SO2 emission in the Grimsvötn eruption

- **SO2 emitted massively in volcanic eruptions and observable with satellite instruments**
- **Use the data from the OMI instrument to determine amount, timing and vertical profile of SO2 emission during the Grimsvötn eruption in May 2011**
- **120 h simulation, emission rate adjusted every 24 h**
- **4D-Var based inversion method, control variable $E_i^k$ where $i = 1 \ldots N_{levels}$ and $k = 1 \ldots 5$ for each 24 h slot**
- **Total column observations – vertical structure not observed**
- **work in progress!**

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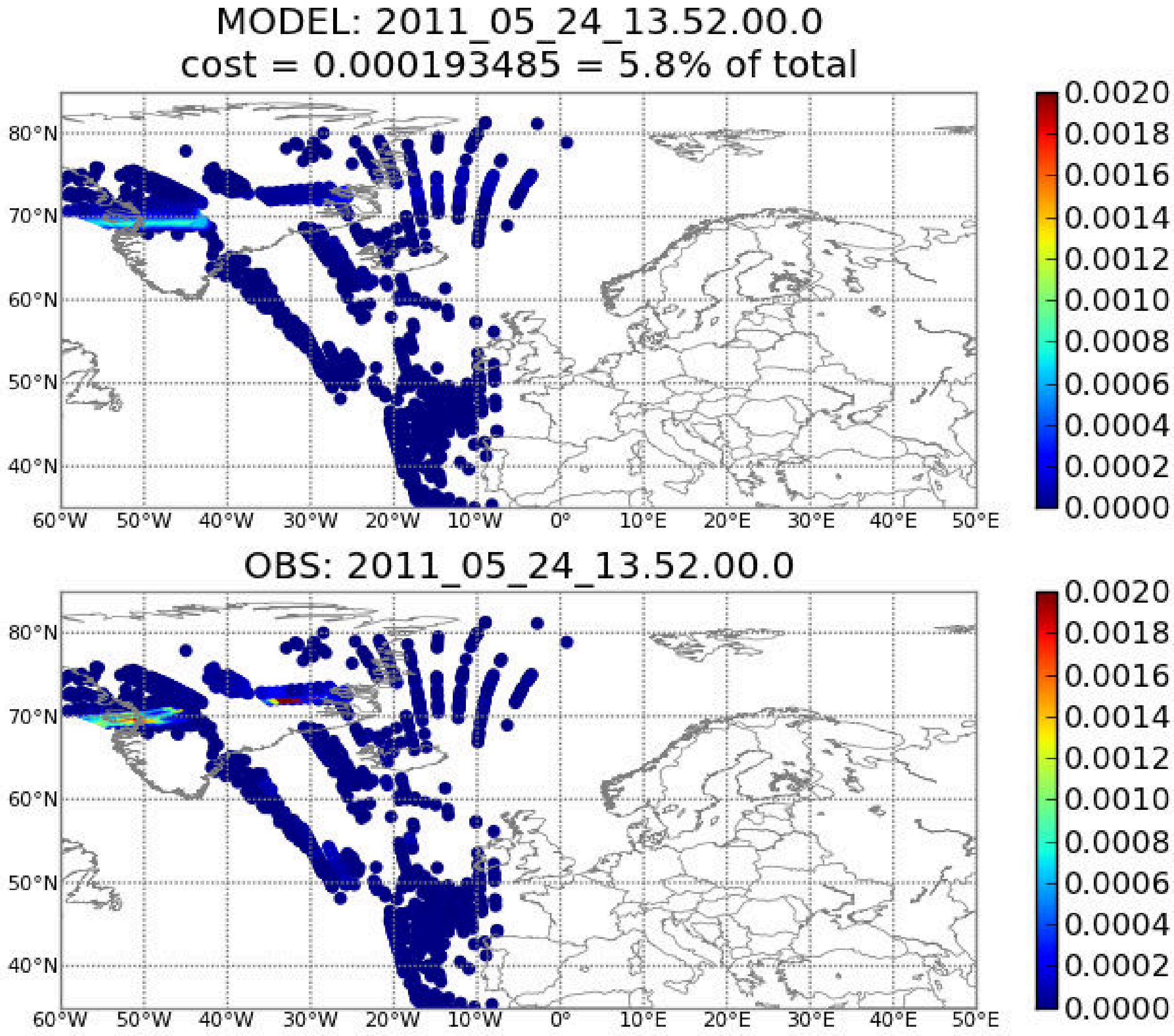
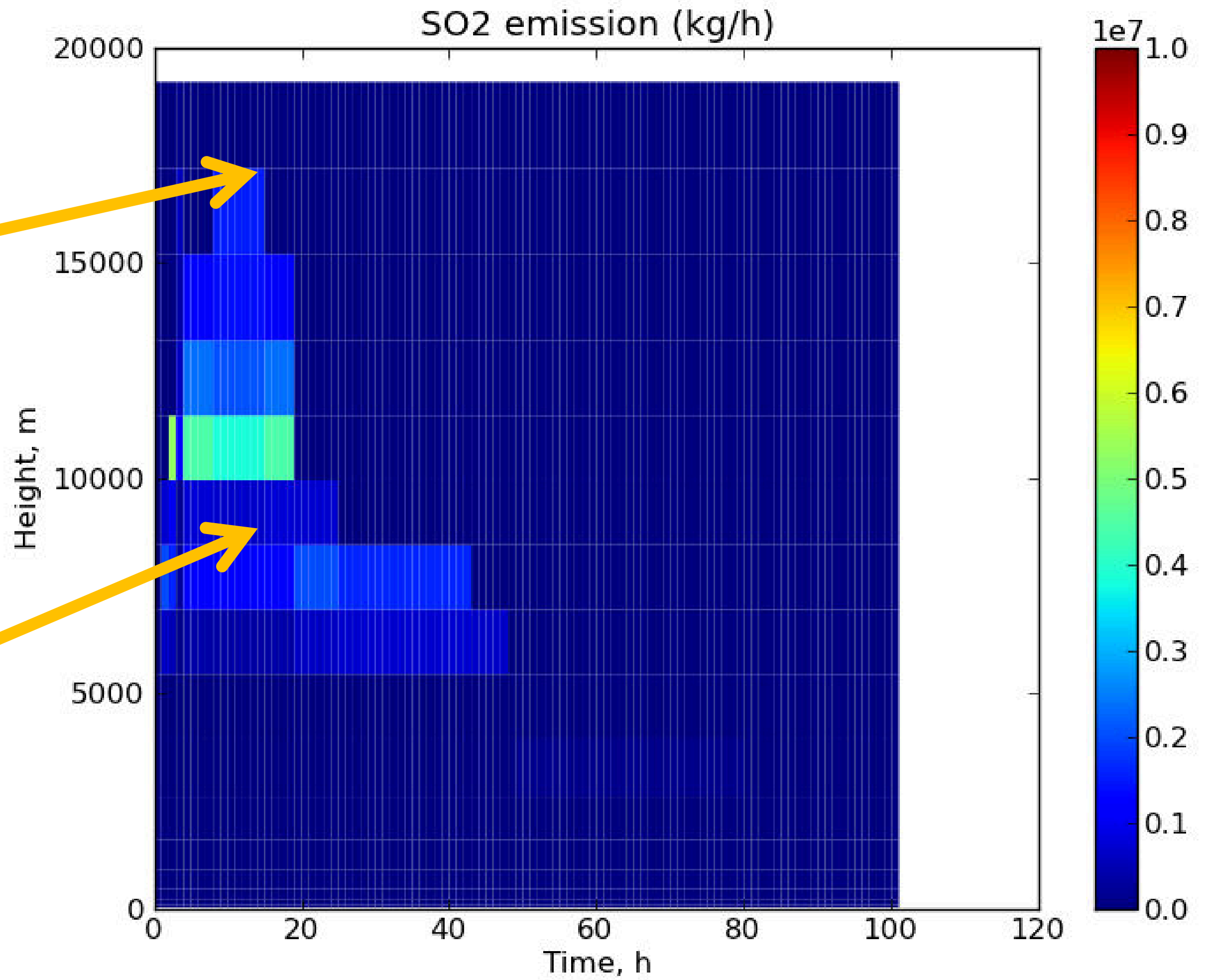
# Ob



# Emission flux after inversion

Plume top determined a priori

Other vertical structure determined in inversion



# Conclusions

- **A number of inverse problems in atmospheric composition modeling are studied in connection to data assimilation**
  - among them, chemical data assimilation analogous to data assimilation in weather forecasting
- **Hot Topic #1: satellite data usage**
  - potentially good coverage with good representativeness
  - often not vertically resolving
- **Hot Topic #2: emission assessments**
  - volcanoes and other natural sources
  - anthropogenic sources: especially in developing countries