From global to regional inverse modelling of greenhouse gases

F Chevallier (LSCE, Gif-sur-Yvette, France)

This presentation discusses the potential introduction of surface fluxes (sources and sinks) in the control vector of the ECMWF 4D-Var . It starts from the example of the data assimilation systems set-up for methane (CH_4) in MACC-II, before highlighting the various molecules whose surface fluxes are estimated through inverse modelling in this project. In each case, the inverse modelling work is distinct from the IFS that estimates initial conditions within a much shorter observation window (hours rather than months, years or decades). Merging the two types of work is an ambitious objective, which is made particularly challenging by the high sophistication of the prior models and inventories of the surface fluxes: any inverted flux map needs to pass stringent realism tests that up to now have favoured dedicated inversion tools compared to all-in-one systems. The presentation discusses this issue from the point of view of the atmospheric observations (a small and ambiguous signal), of the observation operator (flawed by various biases that significantly degrade inversion results), of the prior error statistics (for CO_2, the error correlation scales are short, which makes the inversion problem intrinsically of very large dimension; the temporal correlation scales are large which hampers short assimilation windows). The conclusion emphasizes the importance of well characterizing the prior flux errors and the need of redundancy in the inversion systems to compensate for internal biases. A long inversion window is the most straight-forward way to achieve this redundancy.

From global to regional inverse modelling of greenhouse gases

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SEVENTH FRAMEWORK PROGRAMME

European Commission

Copernicus
The European Earth Observation Programme

Roadmap of the talk

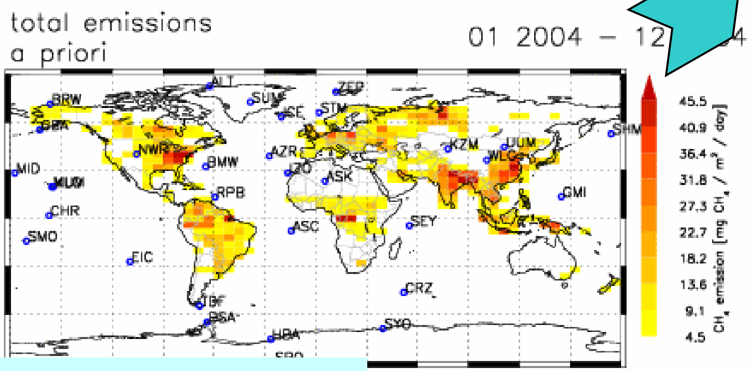
"The aim of the workshop is to see which existing methods could be used in the **ECMWF operational environment for atmospheric composition to improve the surface boundary conditions in terms of fluxes**, emissions, and point source releases. This could range from new on-line methods to better definitions of prescribed inventories.

I would therefore appreciate if you could discuss your work and ideas on greenhouse gas inversions within the above framework. Especially, **the potential use of flux increments in the 4D-Var control vector** would be of high relevance."

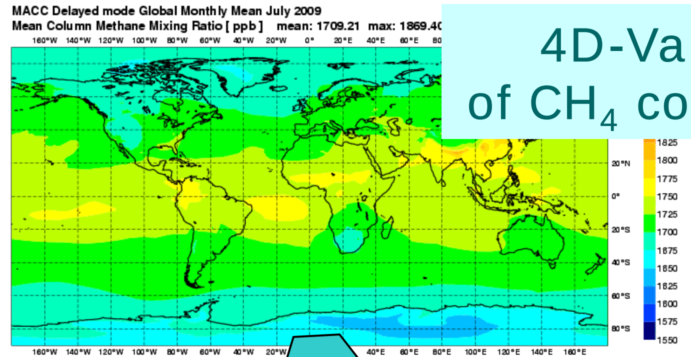
R. Engelen

LSCE

The MACC CH_4 system

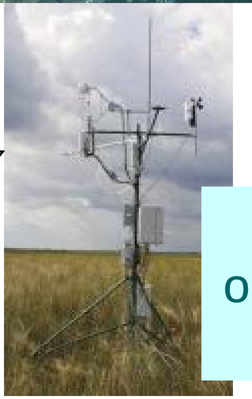


Prior information about CH_4 fluxes

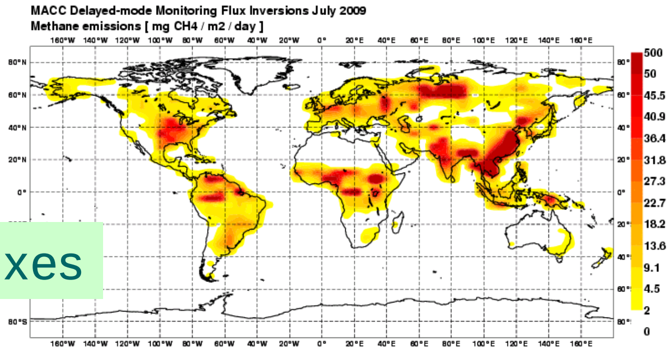


4D-Var analysis of CH_4 concentrations

Satellite observations of CH_4



Surface observations of CH_4



Optimized CH_4 fluxes

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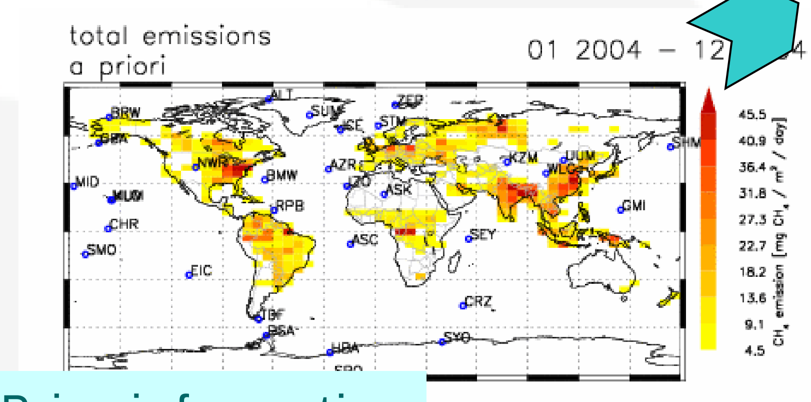
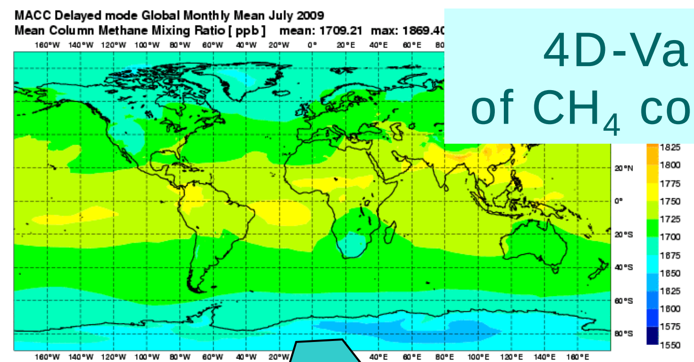
The MACC-II CH_4 system



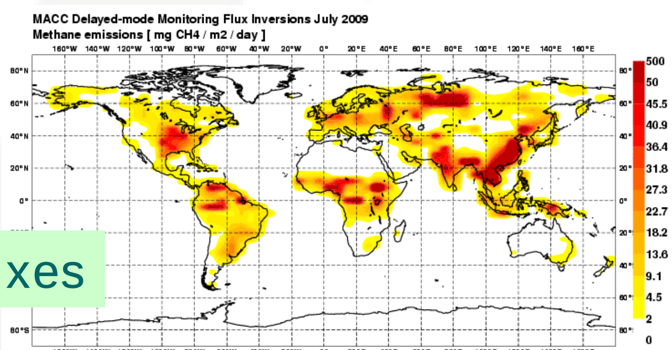
Prior information about CH_4 fluxes



4D-Var analysis of CH_4 concentrations

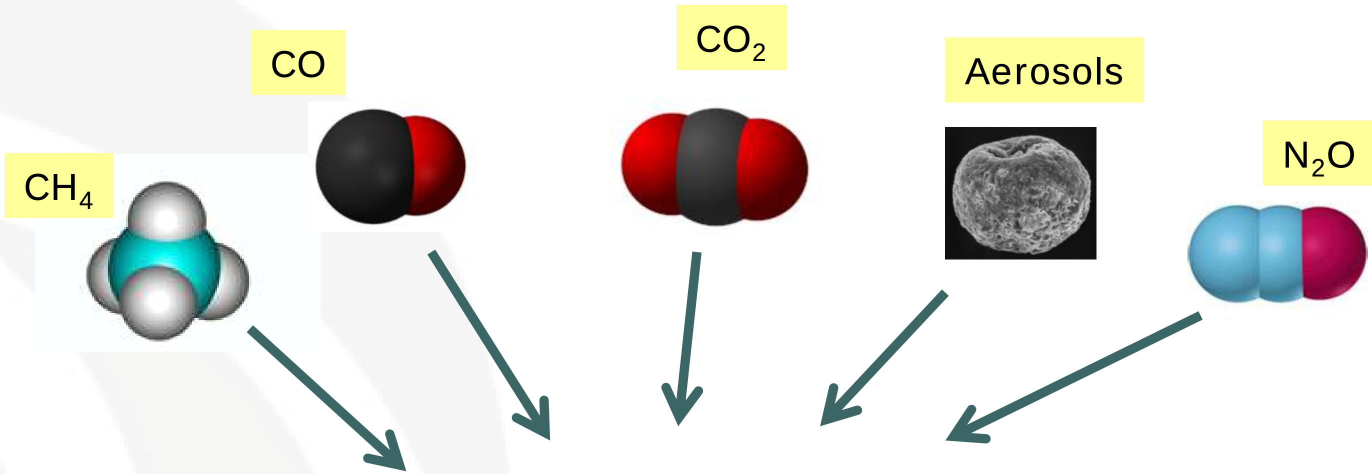
Satellite observations of CH_4

Surface observations of CH_4

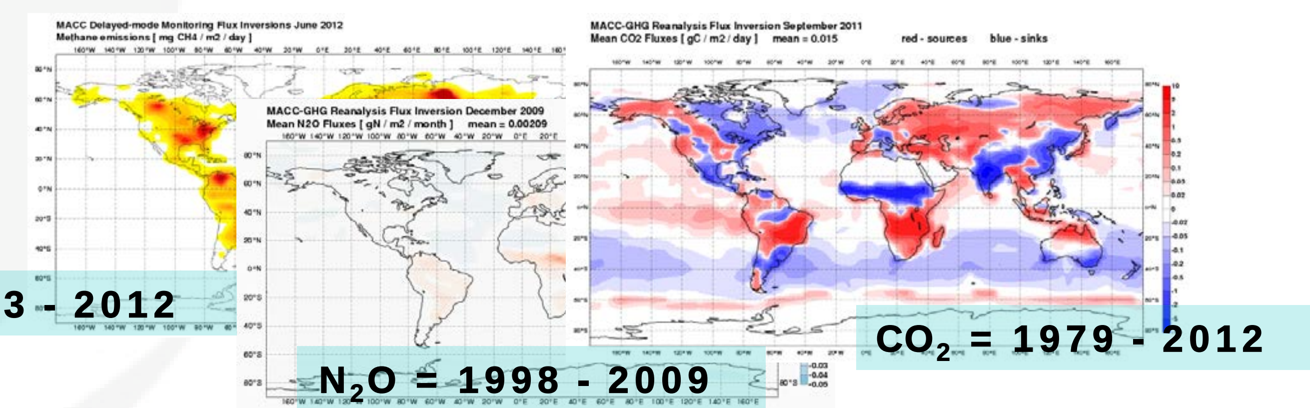


Optimized CH_4 fluxes

Atmospheric inversion in the MACC-II service



$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x})-\mathbf{y})$$



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Monitoring atmospheric composition & climate – II

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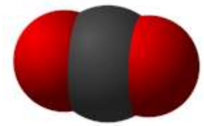
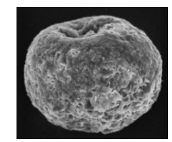
Atmospheric inversion in the MACC-II service

CO

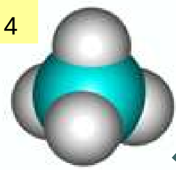
CO_2



Aerosols



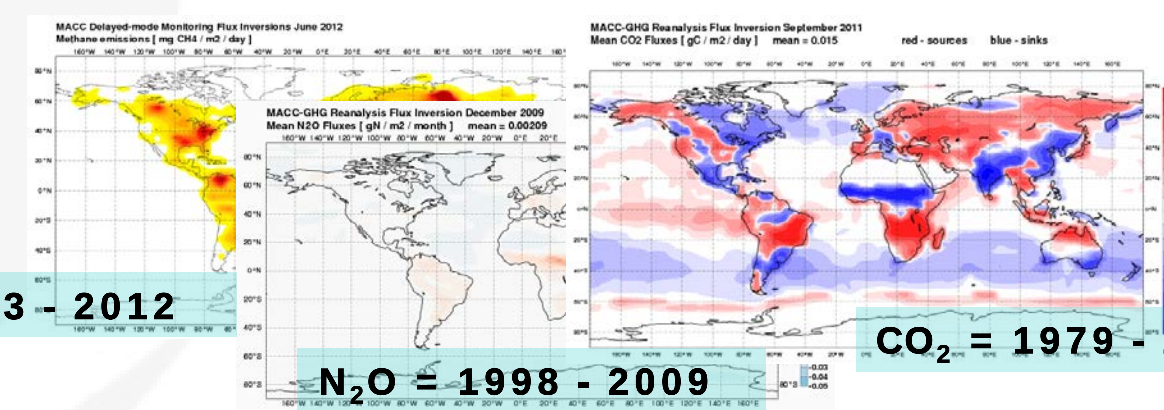
CH_4



N_2O

PYVAR,
TM5-4DVAR,
IFS?

$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}) - \mathbf{y})$$



CH_4 = 2003 - 2012

N_2O = 1998 - 2009

CO_2 = 1979 - 2012

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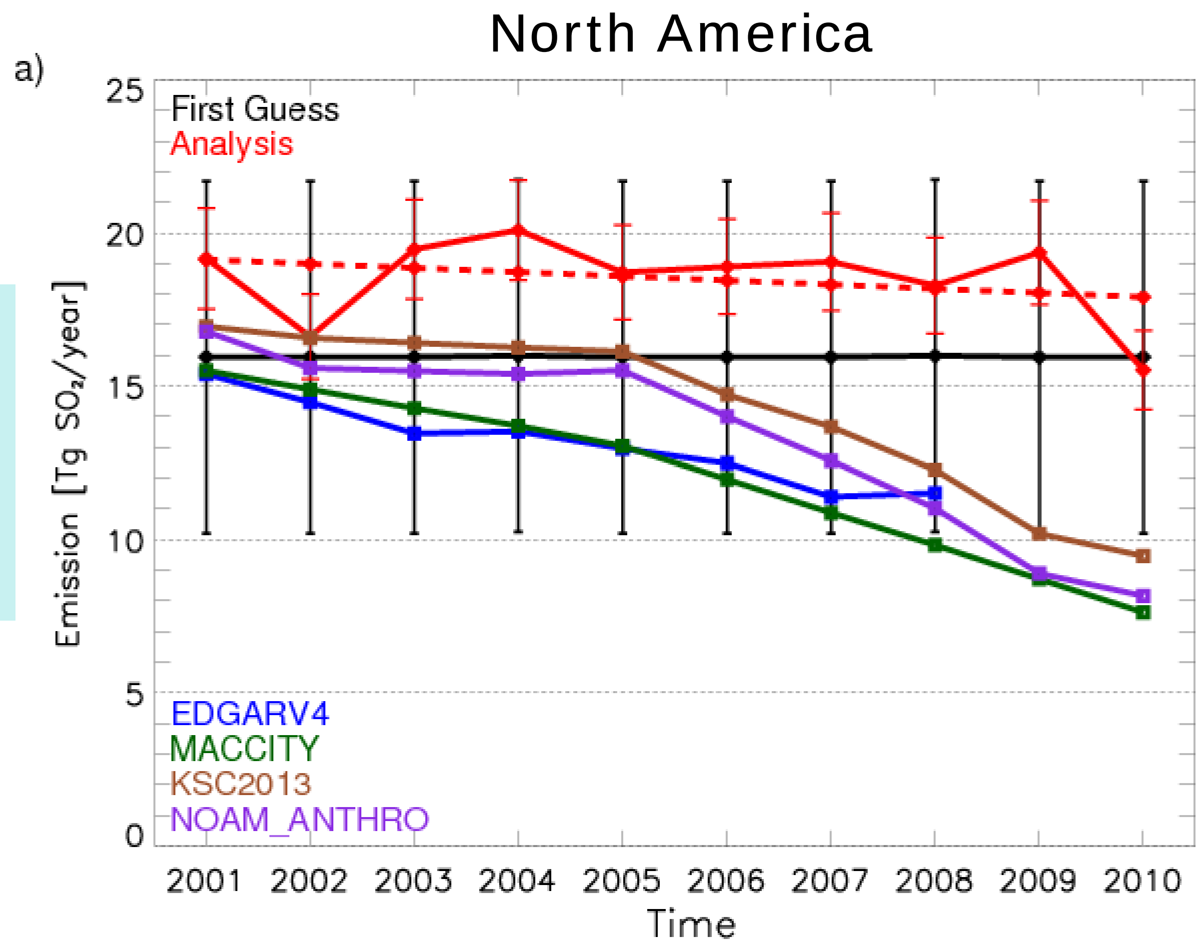
Towards meaningful flux increments

- Some regional emission budgets are very well documented.
- Stringent benchmark.

SO_2 emissions inverted from MODIS AODs vs. emission inventories

Nicolas Huneeus (personal comm., 2013)



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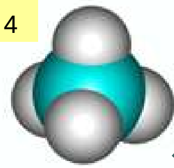
Outline

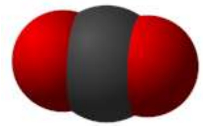
CO

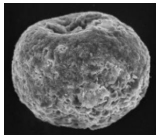
CO$_2$

Aerosols

CH$_4$



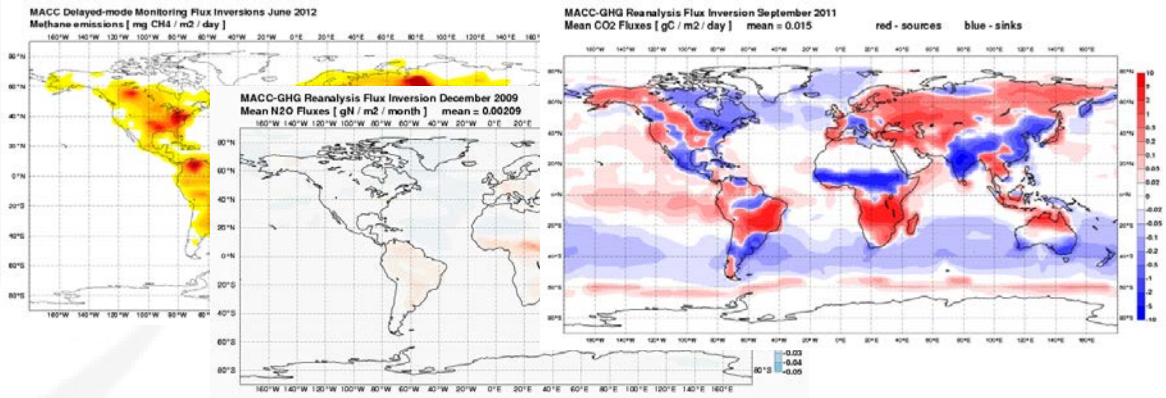




N$_2$O

PYVAR,
TM5-4DVAR,
IFS?

$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}) - \mathbf{y})$$



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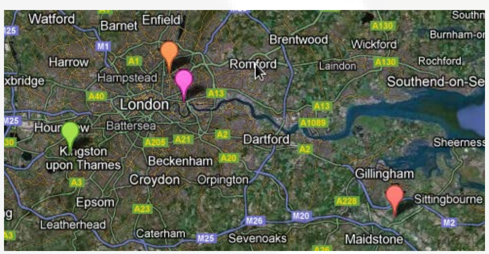
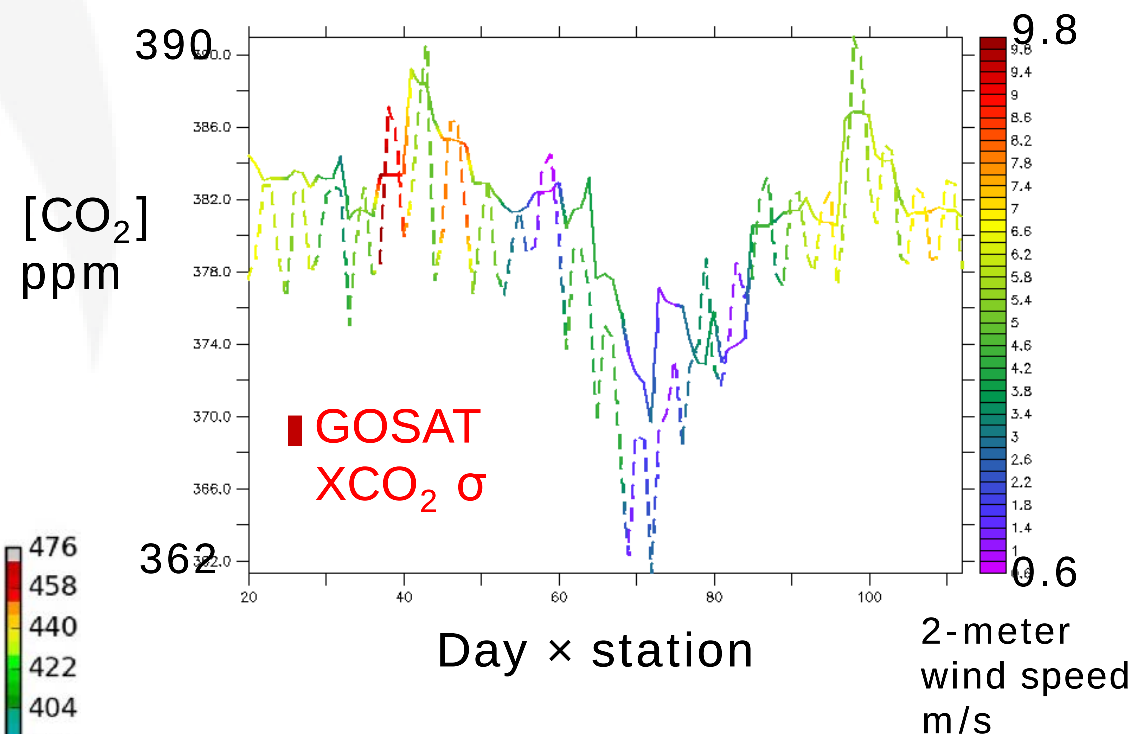
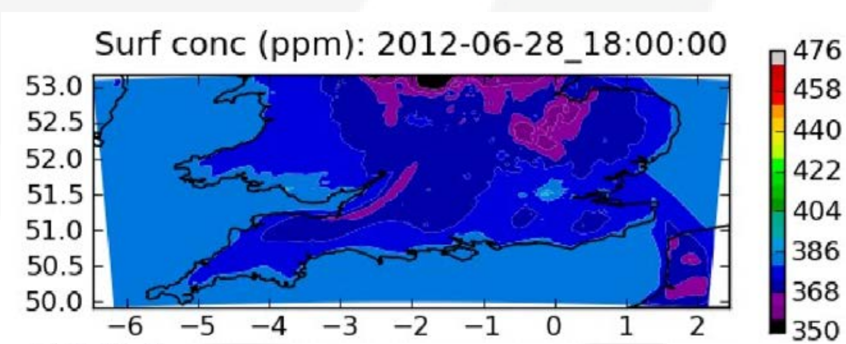
$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}) - \mathbf{y})$$

– **y** – CO_2

- July simulation of CO_2 at 4 sites in London (CHIMERE@2 km).
  - $[CO_2]$ @ 15 UTC = UK fluxes from the past 36 h + Lateral boundaries
  - Sum of the two components (continuous line) and lateral boundaries only (dashed line).



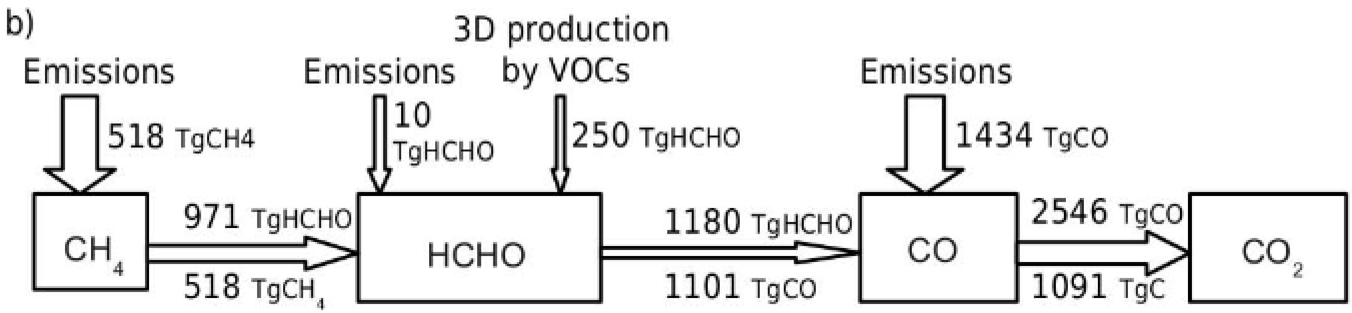




$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x})-\mathbf{y})$$

– y – CO

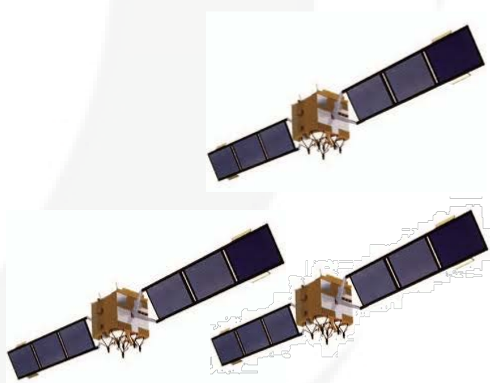
- Atmospheric production and loss: example of CO



Fortems-Cheiney et al. (2011, 2012)

TgCO/year

	USA	China	Canada	Western Europe	Global
EDGAR3.2+ GFED2 (our prior)	105	108	8	44	1066
Posterior MOPITT+mcf	112	213	49	52	1467
Posterior MOPITT+OMI +mcf +ch4	132	151	54	58	1401
EDGAR 4.2+GFED3	60	96	12	22	1284



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$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}) - \mathbf{y})$$

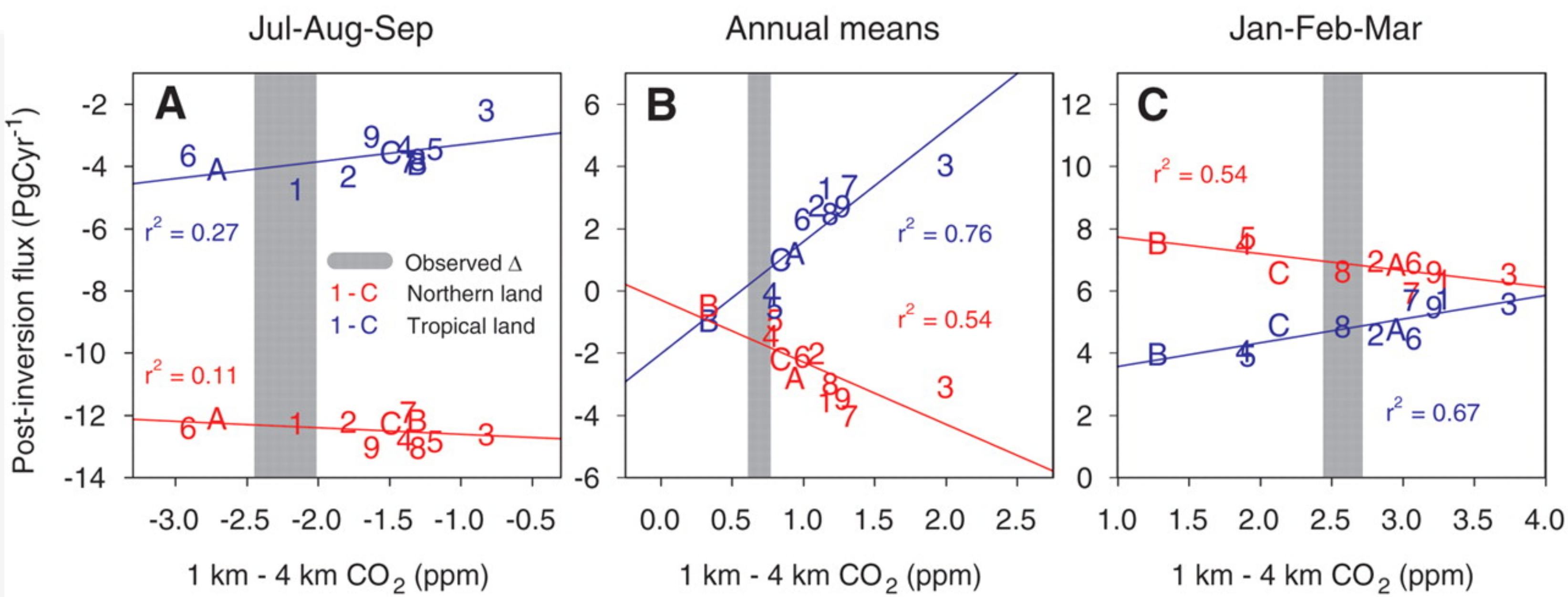
– y –

- Mixture of signals:
  - Surface sources and sinks,
  - Transport,
  - Atmospheric production and loss.
- The signal from the surface fluxes does not necessarily dominate.
- All terms in the atmospheric mass budget ideally should be constrained.

LSCE

– H – long range transport

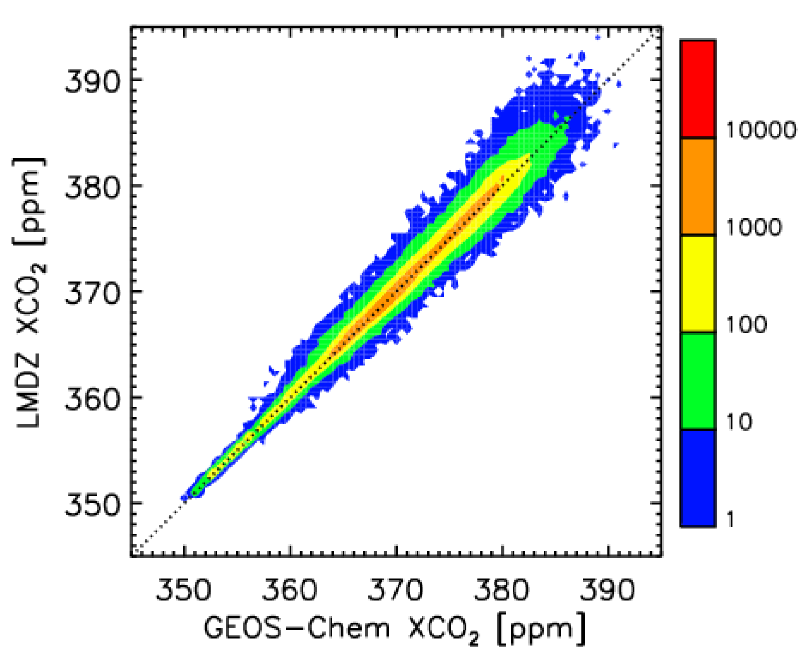
- About 15 global transport models to invert CO_2 fluxes with a standardized method (Stephens et al., Science, 2007).

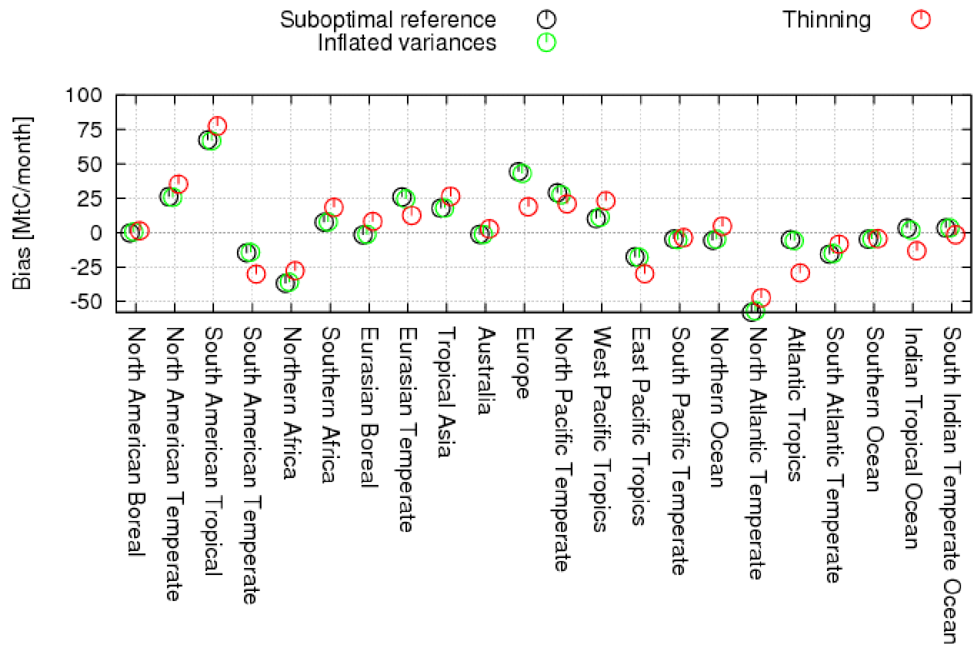


Northern land and tropical land carbon fluxes for the 1992 to 1996 time period estimated by the 12 T3L2 models plotted as a function of the models' post-inversion predicted mean vertical CO_2 gradients for seasonal intervals.

– **H** – long range transport

- Inversion of CO_2 fluxes from simulated GOSAT XCO_2
  - True atmosphere represented by GEOS-Chem.
  - Inversion system uses LMDZ.
- LMDZ vs. GEOS-CHEM : bias = 0.0 ppm, std. dev. = 0.6 ppm
  - XCO_2 variability = 5.6 ppm (std. dev.)
- Inverted fluxes biased by 0.6 GtC/yr over Europe.



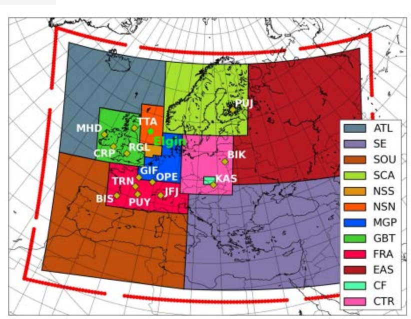


Chevallier, Feng, et al. (2010)

$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}) - \mathbf{y})$$

– **H** – short-range transport

- Most likely (**R**,**B**) tuple given the atmospheric observations.
  - Application to CH_4.
  - Link with boundary layer height (from ECMWF).



Berchet et al. (ACP, 2013)

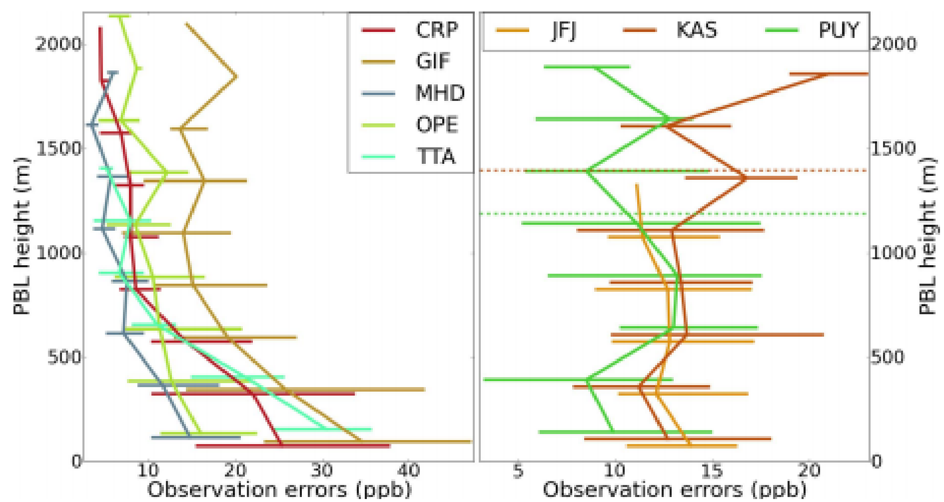


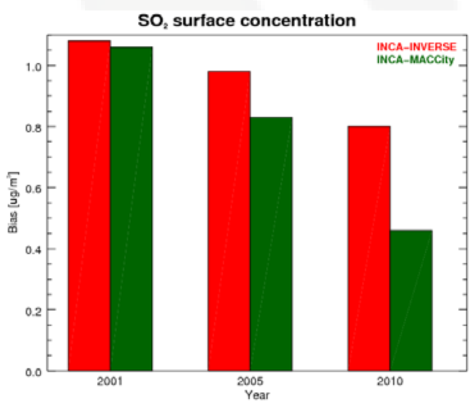
Fig. 3. Statistics of the errors projected along ECMWF-simulated PBL height for ML method: median and inter-quartile gap per 250m-high layer. (Left) sites with strong correlations as calculated in Table 2; not displayed site RGL exhibits the same patterns but with higher errors. (Right) Mountain sites with influence from the PBL less prevailing. Dashed lines refer to the station altitude in the model; JFJ is above the maximum simulated PBL height.

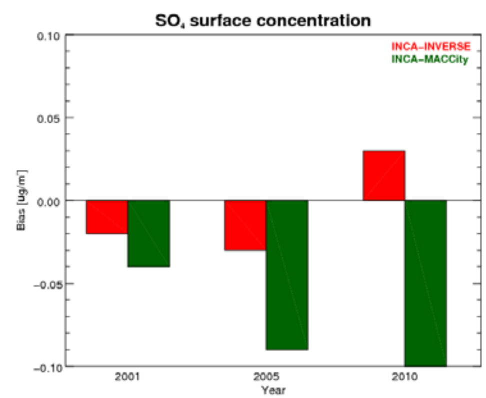
$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}) - \mathbf{y})$$

– H – chemistry

- Compare LMDZ-INCA simulations with SO_2 and SO_4 surface concentrations from the EMEP network:
  - Surface emissions from the MACCity inventory;
  - Surface emissions from the inversion of MODIS AODs (using a simplified chemistry mechanism);
  - Bias shown.

Sulfur dioxide (SO_2)





Sulfate aerosols (SO_4)

Nicolas Huneeus
(personal comm., 2013)

$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}) - \mathbf{y})$$

– H –

- Transport models are flawed at all time scales, despite obvious skills.
  - The flaws are large enough to affect flux inversion.

- Chemistry issues as well.

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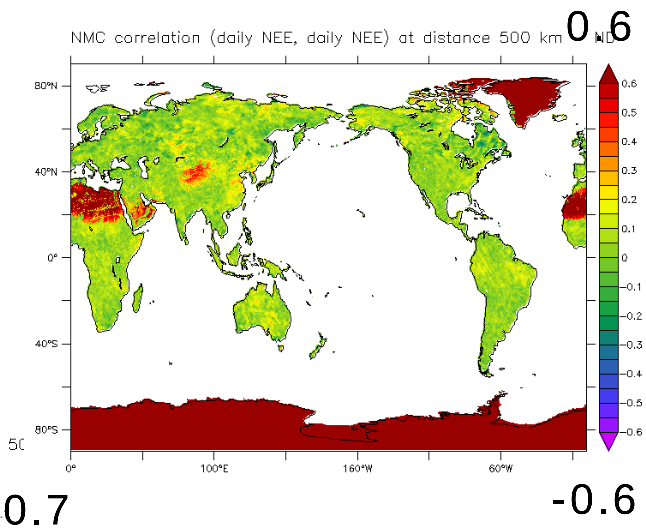
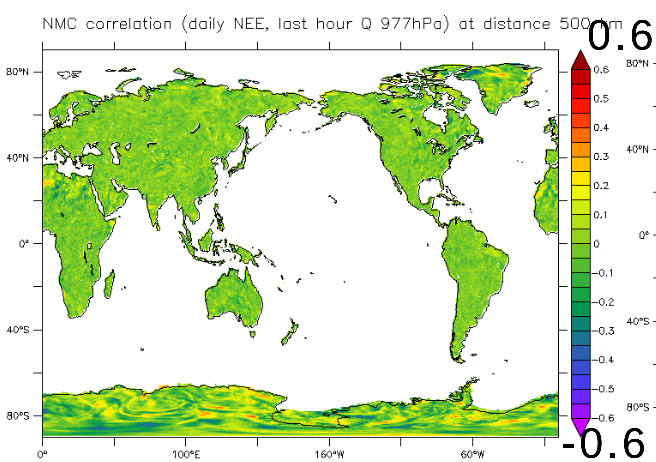
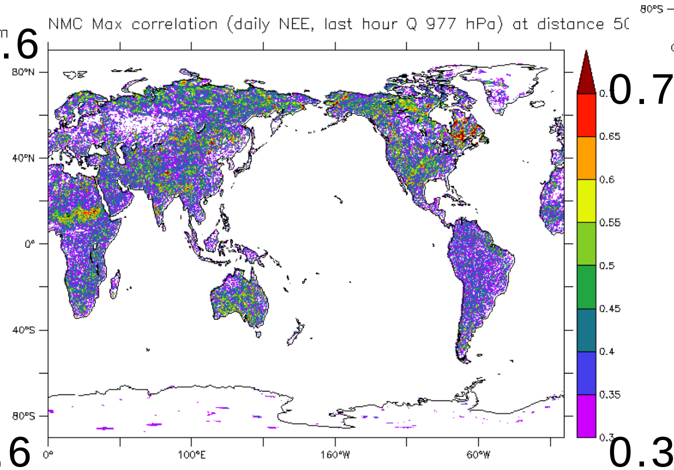
– **B** – short window

- Using the NMC method on the MACC-II NRT forecast to diagnose background error correlations (further to a discussion with W Peters)
  - Mean FCO_2 at ranges 12-36 h and 36-60 h (spin-up, ...)
  - 977 hPa [CO_2] at ranges 36 h and 60 h
  - November-December 2012, 15 km
- No isotropic correlations found.
- Some wind-dependent

  FCO_2 - [CO_2] correlations.





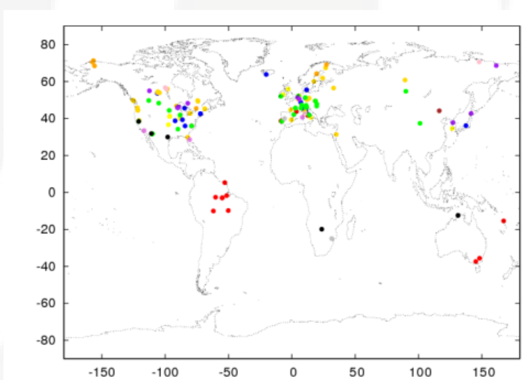


Correlations of the ensemble at lag distance 500 km

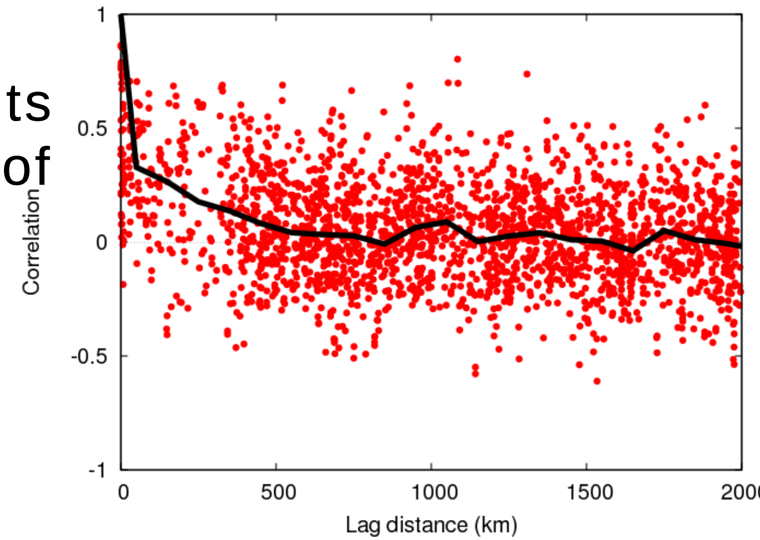
– B – error correlations

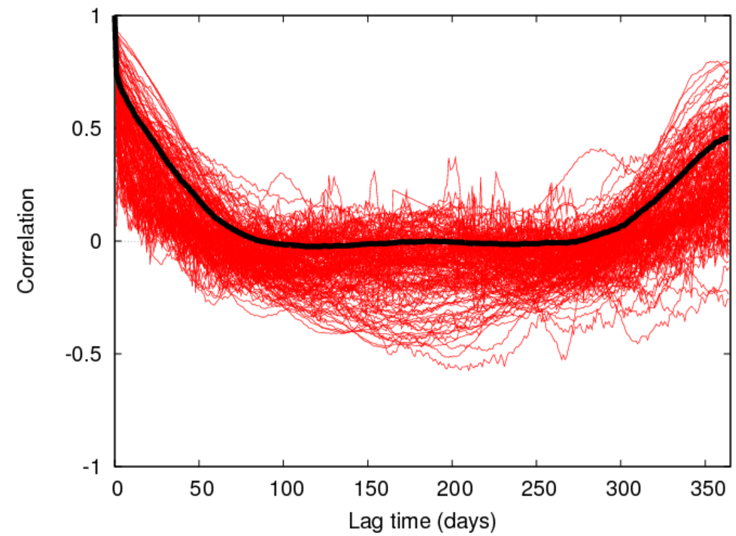
- Use daily-mean eddy-covariance flux measurements to assign the error statistics of the fluxes simulated by the ORCHIDEE model.

- Results:
  - Small spatial correlations,
  - Large temporal correlations.



Chevallier et al. (2012)





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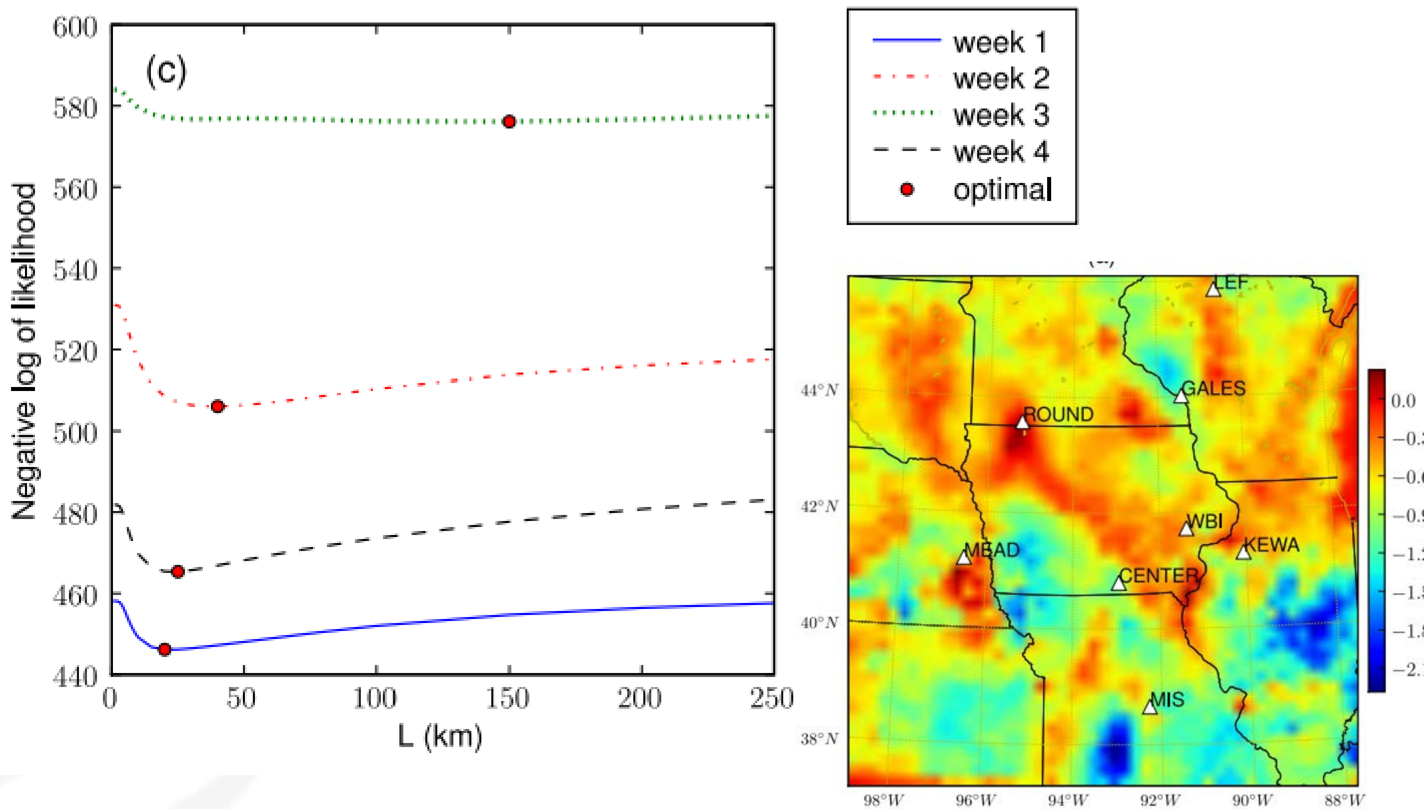
– **B** – error correlations

- Mesoscale regional inversion for NACP's Ring2.
  - Infer the characteristic correlation length of the SiBcrop model from [CO_2] using maximum likelihood.
  - Small error correlations inferred.

Wu et al.
(Tellus B, 2013)



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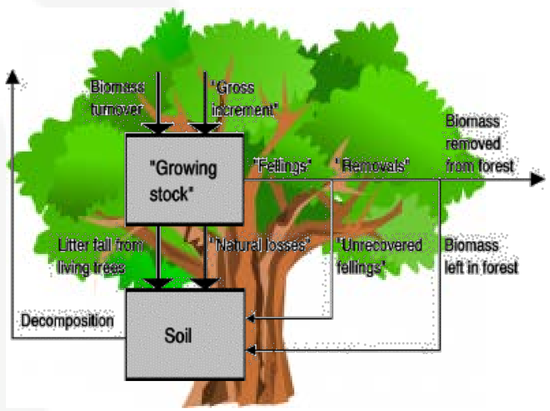
– **B** – parameter inversion

- Invert the parameters of a process model of the fluxes rather than the fluxes directly.
- Prior flux uncertainty $\mathbf{B} = \mathbf{B}_{param} + \mathbf{B}_{struct}$



– B – parameter inversion

- Using Fluxnet data to diagnose $\mathbf{B}_{struct}$ for the ORCHIDEE model.
  - When projected in the space of mole fractions, **the impact of model error ~ transport errors** (L ~ 0, std. = 1.3 ppm for surface CO_2; L = 1200km, std. = 0.5 ppm for XCO_2).

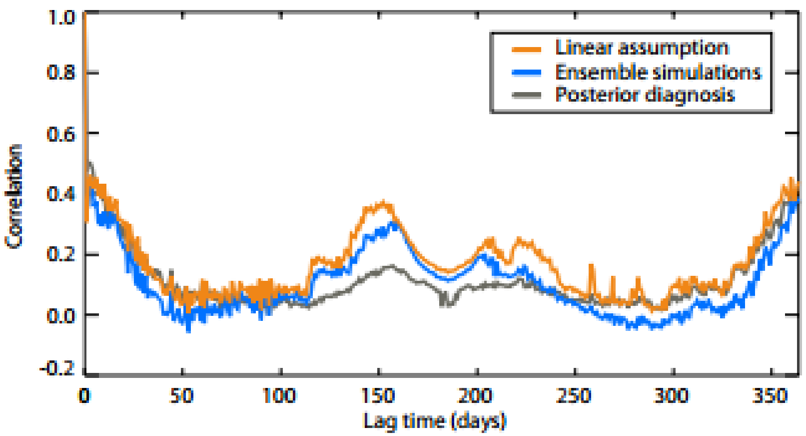


Fig. 2. All-site median of the autocorrelation of the observation error (i.e., model error + measurement error) **R**, estimated at each site with three methods: prior diagnostics with the linear assumption (orange, $\hat{\mathbf{R}}^{prior}$ from Eq. 1), prior diagnostics with ensemble simulations (blue, $\hat{\mathbf{R}}^{prior}$ from Eq. 1), and posterior diagnostics (grey, $\hat{\mathbf{R}}^{post}$ from Eq. 3).

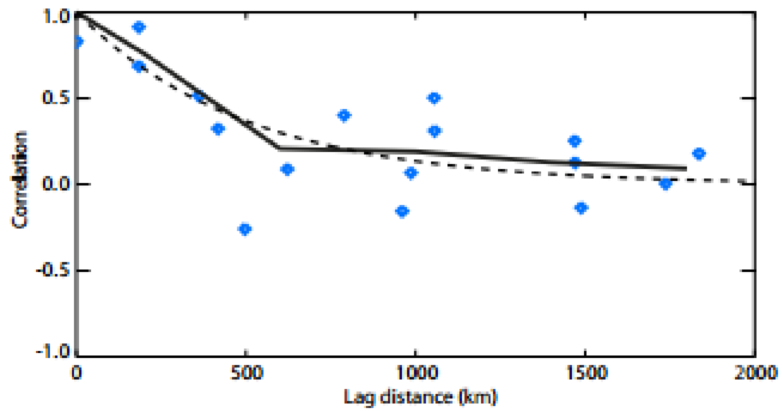


Fig. 3. Distance correlogram of the observation (model+measurement) error $\hat{\mathbf{R}}^{prior}$ estimated from Eq. (1), using pairs of distant sites for a same time. The value represented by each blue diamond includes all the common years of one site pair. The thick black line represents the overall median using 400-km bins, and the dotted line an exponential decay with an e-folding length of 500 km.

Kuppel et al. (Biogeosciences, 2013)

LSCE

– **B** – parameter inversion

- Using Fluxnet data to diagnose $\mathbf{B}_{struct}$ for the ORCHIDEE model.
  - When projected in the space of mole fractions, **the impact of model error ~ transport errors** (L ~ 0, std. = 1.3 ppm for surface CO_2; L = 1200km, std. = 0.5 ppm for XCO_2).

- Mole fraction measurements are not the most effective measurements to constrain process parameters (Koffi et al., ACP, 2013).
  - Atmospheric concentrations are an observation of integrated flux.

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$$\nabla J(\mathbf{x}) = 2\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + 2\mathbf{H}^T\mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}) - \mathbf{y})$$

– B –

- Small spatial correlation lengths of the prior errors (at least for CO_2).
  - Flux increments peak in the vicinity of the measurements.

- Spreading the information via the generic parameters of a process model shifts the problem towards the model errors (within **R**).

- Long temporal correlation lengths.

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Information offered by an air sample

Information offered by an air sample

How atmospheric inverse modelling works

- Accumulating evidence about the fluxes:
  - long atmospheric windows,
  - combination of tracers.

Road map of the talk

"I would therefore appreciate if you could discuss your work and ideas on greenhouse gas inversions within the above framework. Especially, **the potential use of flux increments in the 4D-Var control vector** would be of high relevance."

- Need of specific systems with long assimilation windows (≥weeks) to *properly* extract flux information from atmospheric measurements.
  - Dedicated systems run in // with the IFS.
  - Within shorter data assimilation windows, use other measurement types than atmospheric measurements.
  - Need to get the background errors right

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