Estimation of natural and anthropogenic CO2 fluxes: towards regional atmospheric inversions

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- Explain the basic concepts of CO2 (regional) atmospheric inversions
- Characterize the need for regional inversions
- Give an overview of the initial applications and challenges of regional inversions



#### Outline

- The principles of CO2 atmospheric inversions
- Global inversions of natural fluxes
   the need for regional inversions
- The issues raised or amplified by regional inversions
- Regional inversion of natural fluxes
- Inversion of anthropogenic fluxes at urban scale
- Conclusion: challenges for the regional inversion



# I- The principles of CO2 atmospheric inversions



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#### The basic concept: fluxes and atmospheric gradients

- Gradients in atmospheric concentrations bear the signature of CO2 fluxes
  - Top-down approach: going back to the fluxes using proxies of the atmospheric transport Mauna Loa Monthly Mean Carbon Dioxide



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#### Can the atmospheric transport be inverted ?



• The CO2 concentration integrates the fluxes along the atmospheric trajectory

The atmospheric transport cannot be inverted to separate local flux contributions to a gradient in concentrations



#### Can the atmospheric transport be inverted ?



• The relationship between the flux / obs could be inverted if nb<sub>obs</sub>=nb<sub>unknowns</sub>



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## Can the atmospheric transport be inverted ?



• However: unkown errors in the atmospheric modeling and in the finite representation of the fluxes so  $nb_{unknowns} > nb_{obs}$ 

Atmospheric inversions are "generalized (statistical) inversions"



#### The need for "bottom-up" estimates of the fluxes

- The top-down retrieval of the fluxes can bear large uncertainties
  - need to be combined with independent & valuable information
- Large gaps in the atmospheric observation coverage
  - → need to constrain the estimates using other data for many regions
- > In general, the atmospheric inversion is not a purely top-down estimation







A typical in situ observation

## The correction of the bottom-up "prior" estimate



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observation space: CO2 at the time/location of the measurements = y
control parameters (e.g. fluxes at a specific space and time resolution) = f

**Observation operator H:** conversion of the control parameters into transport model input parameters, **atmospheric transport model** and extraction of the transport model output concentrations at observation time/location

**offset y**<sup>fixed</sup>: component of CO2 not controlled by the control vector (e.g. background concentration when the control vector = flux parameters only)

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projection of s into y: y=Hf + y<sup>fixed</sup>
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```
measurements = y^{\circ}
prior estimate of the control variables = f^{\circ}
prior misfits = y^{\circ} - Hf^{\circ} - y^{fixed}
```



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## The mathematical framework of data assimilation (2)

#### Statistical representation of the errors/uncertainties

Definition of the "true" control parameters and concentrations:  $f^{true}$  and  $y^{true}$ Information from the prior and from the data:  $p(f^{true} | f^{b})$  and  $p(f^{true} | y^{o})$ **Uncertainties in the prior information:**  $p(f^{b} - f^{true} | f^{b})$ **Observation error:**  $p(y^{o} - Hf^{true} - y^{fixed} | y^{o})$  $\Rightarrow$  includes model error:  $Hf^{true} + y^{fixed} - y^{true} + measurement error: <math>y^{o} - y^{true}$ 

Unbiased / Gaussian assumptions: p(f<sup>b</sup> - f<sup>true</sup> | f<sup>b</sup>)=N(0,B)

A typical spatial structure of the covariance matrix B for uncertainties in the gridded estimates of European fluxes





and  $p(\mathbf{y}^{\circ} - \mathbf{Hf}^{true} - \mathbf{y}^{fixed} | \mathbf{y}^{\circ}) = N(\mathbf{0}, \mathbf{R})$ 

isotropic correlations in space between a German location and other points



## The mathematical framework of data assimilation (3)

**Bayesian update: the equations for the inversion problem** 

**Bayesian equation:**  $p(\mathbf{f}^{true} | \mathbf{f}^{b}, \mathbf{y}^{o}) = p(\mathbf{y}^{o} | \mathbf{f}^{b}, \mathbf{f}^{true}) p(\mathbf{f}^{true} | \mathbf{f}^{b}) / p(\mathbf{y}^{o} | \mathbf{f}^{b})$ 

=  $\alpha_1 p(\mathbf{y}^\circ | \mathbf{f}^{true}) p(\mathbf{f}^{true} | \mathbf{f}^{b})$ 

#### Unbiased / Gaussian assumption:

$$p(\mathbf{y}^{o} | \mathbf{f}^{true}) = \alpha_{2} \exp(-1/2 [\mathbf{y}^{o} - \mathbf{H}\mathbf{f}^{true} - \mathbf{y}^{fixed}]^{T} \mathbf{R}^{-1} [\mathbf{y}^{o} - \mathbf{H}\mathbf{f}^{true} - \mathbf{y}^{fixed}])$$
$$p(\mathbf{f}^{true} | \mathbf{f}^{b}) = \alpha_{3} \exp(-1/2 [\mathbf{f}^{b} - \mathbf{f}^{true}]^{T} \mathbf{B}^{-1} [\mathbf{f}^{b} - \mathbf{f}^{true}])$$

→ p(f<sup>true</sup> | f<sup>b</sup>, y<sup>o</sup>) = 
$$\alpha_4 \exp(-1/2 J(f^{true}))$$

where  $J(\mathbf{f})=[\mathbf{f}^{b}-\mathbf{f}]^{T}\mathbf{B}^{-1}[\mathbf{f}^{b}-\mathbf{f}] + [\mathbf{y}^{o}-\mathbf{H}\mathbf{f}-\mathbf{y}^{fixed}]^{T}\mathbf{R}^{-1}[\mathbf{y}^{o}-\mathbf{H}\mathbf{f}-\mathbf{y}^{fixed}]$   $\Rightarrow p(\mathbf{f}^{true} | \mathbf{f}^{b}, \mathbf{y}^{o}) = N(\mathbf{f}^{a}, \mathbf{A})$  where  $\mathbf{f}^{a} = \mathbf{f}^{b} + \mathbf{A}\mathbf{H}^{T}\mathbf{R}^{-1}(\mathbf{y}^{o} - \mathbf{H}\mathbf{f}^{b} - \mathbf{y}^{fixed})$   $\mathbf{f}^{a} \text{ minimizes } J \text{ (least square min)}$  $\mathbf{A}=(\mathbf{B}^{-1} + \mathbf{H}^{T}\mathbf{R}^{-1}\mathbf{H})^{-1}$ 

Optimal estimate: f<sup>a</sup>

Uncertainty in the optimal estimate: A



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## **Practical implementation and interpretation (1)**

**Optimal estimate:**  $\mathbf{f}^{a} = \mathbf{f}^{b} + \mathbf{B}\mathbf{H}^{T}(\mathbf{H}\mathbf{B}\mathbf{H}^{T}+\mathbf{R})^{-1}(\mathbf{y}^{o} - \mathbf{H}\mathbf{f}^{b} - \mathbf{y}^{fixed})$ 

Meaning of adjoint  $\mathbf{H}^{\mathsf{T}}$ : if  $g(\mathbf{f})=G(\mathbf{H}\mathbf{f})=G(\mathbf{y})$  then  $\nabla_{\mathbf{f}}g = \mathbf{H}^{\mathsf{T}}\nabla_{\mathbf{y}}G$ 

 $H^{T} \rightarrow$  sensitivity of functions of the conc. to the control param (e.g. "obs footprints")

→ HBH<sup>T</sup>+R and in particular R weight the information from the data

B rescales (STD) / smoothes & extrapolates (correlations) the patterns of the misfit footprints to get the corrections to the fluxes

B and R need to be defined a priori: critical configuration of the inversion

# Typical footprints of atmospheric stations in South America



Typical patterns of optimal correction when using B with isotropic correlations





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## **Practical implementation and interpretation (2)**

<b>Problem:</b> $\mathbf{f}^{a} = \mathbf{f}^{b} + \mathbf{A}\mathbf{H}^{T}\mathbf{R}^{-1} (\mathbf{y}^{o} - \mathbf{H}\mathbf{f}^{b} - \mathbf{y}^{fixed})$ and $\mathbf{A} = (\mathbf{B}^{-1} + \mathbf{H}^{T}\mathbf{R}^{-1}\mathbf{H})^{-1}$	[1]
or $\mathbf{f}^a = \mathbf{f}^b + \mathbf{K} (\mathbf{y}^o - \mathbf{H}\mathbf{f}^b - \mathbf{y}^{fixed})$ and $\mathbf{A} = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{B}$ where $\mathbf{K} = \mathbf{B}\mathbf{H}^T (\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}$	[2]
or $\mathbf{f}^{a} = \operatorname{argmin} J: \mathbf{f} \rightarrow [\mathbf{f}^{b}-\mathbf{f}]^{T}\mathbf{B}^{-1}[\mathbf{f}^{b}-\mathbf{f}] + [\mathbf{y}^{o}-\mathbf{H}\mathbf{f}-\mathbf{y}^{fixed}]^{T}\mathbf{R}^{-1}[\mathbf{y}^{o}-\mathbf{H}\mathbf{f}-\mathbf{y}^{fixed}]$	[3]

- *H* can be non-linear
  - Linearization (derivation or finite-differences)
- H and sometimes  $H^T$  available as operators  $f \rightarrow Hf=y$  and  $\nabla_v G \rightarrow H^T \nabla_v G = \nabla_f g$ 
  - not as matrices
- **Different implementations: analytical, ensemble and variational methods,** solving for different sets of equations [1,2 or 3]
  - → Different constraints on the size of **f** or **y**, or on the structure of **B** and **R**
  - Most of the methods need f or y to be small (except for variational inversion) and R to be easily invertible



#### Some insights on the set-up of inversions

• B and R need to be defined a priori: critical configuration of the inversion

In particular, when R is too small compared to actual model/measurement errors, the inversion will mistakenly correct the fluxes to compensate for these errors

The configuration of the control vector should be driven by the ability to define the uncertainty on its prior estimate (i.e. B)

• Actual errors are hardly unbiased and Gaussian

and

- Lack of knowledge for the characterization of **B** and **R**
- Ifficulties to find "the right" configuration for B and R

Often better to select the data to be assimilated when R likely small only rather than attempt to account for large errors in R

Jusually, definition of relatively long/time correl length in B to smooth/ extrapolate the information from coarse atmospheric networks

# II- Global inversions of natural fluxes and the need for regional inversions



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#### The need for identifying the main Carbon sinks and sources

Global estimates: anthropogenic emissions and natural sinks/sources for 2000-2009



- Global anthropogenic emissions and atmospheric growth relatively well known
- The split between ocean and land natural sinks more uncertain
- Need for anticipating the evolution of the natural sinks/sources with climate change

Requires a knowledge of the spatial/temporal distribution of the sinks/sources and ultimately of the underlying processes



## Traditional configuration of the global inversions



- Attempt to separate the global natural sink between (1) the ocean and land
  (2) Latitudinal bands, mainly: Tropics, Northern/Southern Hemispheres
  (3) the different continents & oceans
- Use of in situ weekly and continuous (hourly) measurements
   inversions based on satellite data exist but are still marginal
- Use of atmospheric transport models at 2-3° horizontal resolution
- Despite its increase, the in situ network still too sparse (e.g. South America)
- → Regions of interest too large/heterogeneous to characterize underlying processes





## The uncertainties in the results

#### Actual uncertainties

- = spread + potential bias of the ensemble of inversions
- > spread of the ensemble of inversions
- > theoretical uncertainties estimated by inversions (due to errors in these estimates)
- Annual to multi-annual budgets from the inversions bear large uncertainties



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#### **Comparison to other types of estimates**

		C-sink
Estimates of the European natural carbon sink (Tg C y <sup>-1</sup> ) between 2001-2005	Inversion-based Inventory-based	-356 ± 330 -201 ± 80
Luyssaert et al., 2012, BGD	Fluxes-based	$-251 \pm 220$

• Other methods (**upscaling of eddy-covariance flux data, biomass & harvest inventories** etc.) seem to provide more robust estimates of (multi-)annual budgets

• Critical role of ecosystem model underlying inversion results



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## Sources of uncertainties in results from global inversions (1)

#### Uncertainties in the anthropogenic emissions

Differences between the estimates of annual flux in Europe from two different inventories (EDGAR and IER) as a function of the spatial resolution

Ciais et al., 2010, GCB

- Global inversions generally assume that their prior estimates of anthropogenic emissions are perfect
- however, significant uncertainties in the anthropogenic inventories at global/annual scale (5-10%) to 2-3° / hourly resolution
- Inversions mistakenly report the errors from anthropogenic fluxes into natural fluxes







### Sources of uncertainties in results from global inversions (2)

#### **Atmospheric transport errors**

- Global inversion generally ignore the error correlations in time
- Comparisons of the meteo data used to force the model and atmospheric measurements reveal sources of biases

Large potential impact of the poor configuration of model error (inversions apply spurious corrections to the fluxes to compensate for the model errors)

Spread of CO2 simulations at the Hungarian tall tower between different atmospheric transport model





12UTC MHs, stations centered on dateline



TRANSCOM PBL inter-comparison



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## Sources of uncertainties in results from global inversions (3)

#### **Representativeness errors (from transport model)**

• The topography, coastline, local atmospheric and flux conditions nearby ground based measurement stations are poorly represented in low resolution models

> data not representative of the mean conc in the corresponding model grid cell

→ by essence, this error can easily be biased or highly auto-correlated in time, and is poorly accounted for by inversions

• Similar issue with the representation of fluxes in heterogeneous / coastal regions

LMDZ grid 3.25° x 2.75° grid cells, the dominant ecosystem within these grid cells and atmospheric measurement stations in Amazonia



## Sources of uncertainties in results from global inversions (4)



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### Sources of uncertainties in results from global inversions (4)

#### Aggregation / flux representativeness error

→ Caused by a too coarse resolution of the fluxes (a too low dimensional control vector) for the inversion or by the use of too long time/space correlations in B

Some patterns of aggregation errors ? (natural 4-year mean fluxes based on the inversion of the fluxes for large regions)



Source: carboscope inter-comparison



### How to decrease these source of uncertainties ?

• The increase in control/atmospheric space resolution naturally decreases the representation/aggregation errors and help solve for anthropogenic emissions

• The set-up of **atmospheric/inversion regional parameters** adapted to regional atmospheric transport / flux or the use of true **mesoscale / high resolution transport model** should help decrease the model error

#### Mean diurnal cycle of CO2 at Ochsenkopf based on data and simulations using low and high spatial resolution transport or fluxes



The drivers of monthly variability in CO2 at sites in USA and in Amazonia



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## Need for resolving high resolution patterns in the fluxes

- to identify underlying processes by separating inhomogeneous sinks/sources
- to exploit the knowledge about the distribution of urban areas and ecosystems
- to solve anthropogenic emissions at scales relevant for policy makers (verification of the emissions at national/city/site scales; identification of local drivers)
  - → Major interest for cities (~70% of the total CO2 emissions)

The strong heterogeneity in the European FAPAR map of Europe from MERIS data ecosystem (photosynthetic activity map) (photosynthetic activity of vegetation) Last 10-days period of September 2011

High resolution estimate of the emissions of CO2 in Europe



Source: ODIAC





#### **Development of regional observation networks**

#### ICOS European network



- GHG atmospheric in situ networks at continental to urban scales
- Several ICOS stations would be binned together in global inversion configurations

# CO2-MEGAPARIS & ICOS network in the Paris area

- CO2 & CO (rouge: CO2-MEGAPARIS, orange: RAMCES-ICOS)
- Hauteur de couche limite





## Use of small domains for high resolution configurations

- Computational resources prevent from operating global models at high resolution
- Need for local configuration of the atmospheric transport and inversion
- regional configurations with regional/local domains, regional mesoscale / high resolution atmospheric transport models and open boundary conditions (nesting in larger configurations)







# III- Issues raised or amplified by regional inversions



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## **Difficulties in modeling the regional transport**

- Better fit to the observed variability but **biases in PBLH** still high
  - Assimilation of hourly data (vs daily/monthly at global scale) but selection of data e.g. at low altitude stations during the afternoon only (as for global inv)



#### **CO2 at Marmande tower**

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#### More unkowns for the inversion problem ?

- The ratio nb obs / nb model grid cell generally lower than for global applications
- Need to solve for different flux components (per ecosystem, emission sectors...)
- Complex **B** (higher resolution → shorter correl length & anisotropy, inhomogeneity)





Definition of a control vector based on dominant ecosystems in Europe

Peters et al. 2009, GCB



Lauvaux et al. 2008, ACP

Land cover and measurement stations in les Landes

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#### **Errors from the boundary conditions**

• Boundary conditions are critical driver of the concentrations in the regional configurations but are **based on CO2 from global inversions** with flux/transport/representation errors  $\rightarrow$  errors in the regional flux inversion

 Global config with zooms to avoid boundaries (problem with the definition of local meteo or inversion parameters)

> Attempts at adjusting the boundary conditions during the inversions (problematic definition of  $\mathbf{f}_{OBC}$ and  $\mathbf{B}_{OBC}$ ) or using "background" measurements



Corrections from European inversions with different control vectors:

#### natural fluxes



#### natural fluxes+boundary conditions



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# **IV- Regional inversion of natural fluxes**



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#### Various scales: continental / national / regional



Broquet et al. 2011 JGR / 2013 ACPD: European Net **Ecosystem Exchange** (NEE) at 0.5°/6-hour res 200



Meesters et al. 2012, JGR: **Resp and Growth Primary Production (GPP) in the** Netherlands at 10km/seasonal res

Gockede et al. 2010, JGR: temporal mean GPP, RH and RA in Oregon for 120 different surface types





Lauvaux et al. 2012a ACP, 2012b Tellus B: daytime and nighttime NEE in the **Cornbelt (lowa &** neighbour states) at 20km/weekly res + boundary conditions



Grossland

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## **Evaluation of results using eddy covariance data**

- Scale of representativeness for flux eddy covariance measurements ~ 1ha / 1km
- Increase in flux resolution by inversions allow for comparisons



Comparison of daytime NEE from inversion at ~8km resolution and eddy covariance data in Les Landes for 3 different 5-day observing periods



Lauvaux et al. 2009, GRL



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#### **Evaluation of results/uncertainties at European scale**

Inversion of NEE at European scale for 2002-2007: 30-day avg NEE (gCm<sup>-2</sup>day<sup>-1</sup>) at eddy cov measurement sites. Shadded areas=+/- std of model uncert.



Theoretical uncertainty reduction = 53% vs 38% reduction in STD for misfits to eddy cov

Broquet et al. 2013, ACPD



#### Robustness of the estimate of the variability in Europe NEE

#### Comparison between the amplitude of the natural variability and the uncertainties from the inversion

#### Mean seasonal cycle of over Europe: 30-day avg NEE (in gCm-2day-1) Shadded areas=+/- std of model uncertainty. Dotted lines=+/- std of the inter-annual variability



- High confidence in the estimate of uncertainties in **NEE at European/monthly** scale
  - The seasonal cycle from inversion is reliable
  - Difficulties to monitor the inter-annual variability (< posterior uncertainties)

Broquet et al. 2013, ACPD



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#### Influence of the prior estimate in the corn belt

CO2 fluxes accumulated from June to



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## Sensitivity to the control vector in the Netherlands

#### The different control vectors and parameters for the associated B

Inversion name	Variables in state vector	Correlation	Optimization units	D.o.f.	$\chi^2$ of innovations
βNEE	βNEE	NA	ecoregions	6	0.4
βRG0.0	$\beta_{\text{RESP}}, \beta_{\text{GPP}}$	0.0	ecoregions	11	0.7
βRG0.5	$\beta_{\text{RESP}}, \beta_{\text{GPP}}$	0.5	ecoregions	9	0.6
βRG1.0	$\beta_{\text{RESP}}, \beta_{\text{GPP}}$	1.0	ecoregions	6	0.3
βRGpixel	$\beta_{\text{RESP}}, \beta_{\text{GPP}}$	0.0	pixels	62	0.3
Parameter	$\beta_{E_0}, \beta_{R_{net}}, \beta_{V_m}, \beta_{aj}$	0.0	ecoregions	22	0.6

**RMS between flux inversion (βRG0.0** and **BRGpixel**) using real data and direct flux measurements from aircraft



#### Two week fluxes based on synthetic data inversion experiments



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# **V-Conclusion**



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### **Challenges for the regional inversion**

• Need for demonstrating the capacity of the method even though observation networks seem to be still inadequate and difficult to sustain

- The "proof of concept" approach (e.g. get the flux right for x% of the time / space)
- Natural/industrial site scale inversions

• Ability to merge different sources of information and to characterize the processes (adjustment of parameters for process models at regional scale)

- Need for breakthrough improvement in the atmospheric transport modeling
- Exploitation of satellite data



## **Supplementary material**



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#### Satellite data: potential and challenges

- Satellite measurement of CO2 vertically integrated column (XCO2): **nearly** daily/weekly global global coverage at 10<sup>2</sup>km to (future) 2km resolution
  - → decrease the role for prior information
  - → decrease the weight of representation error due to spatial resolution
- However:
  - → small signal in XCO2 from the fluxes; problem of vertical extrapolation
  - Iarge measurement errors with large biases

#### Map of Aug 2012 mean XCO2 from GOSAT in 2.5°x2.5° mesh









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## Inversion of anthropogenic fluxes at urban scale



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#### Bottom-up inventories at urban scale

- **Sectoral/spatial/temporal** disaggregation of national total combustion (oil, gas, coal, cement production...)
- Locally & per sector: CO2 emission = activity data x emission factors
- Large uncertainties at high resolution, good estimates of total (annual) fluxes



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## **Objectives for the atmospheric inversions ?**

- Verification vs improvement of inventories
  - different objectives & tasks
- Need for highly accurate total (annual) flux for cities
- Need for good **sectoral estimates** (improve emission factors for climate policies)
- Need for solving high temporal / spatial resolution ? (emission factors function of space ? Identification of sites through urban scale inversions ?) feasibility ?
- How to separate natural vs anthrop fluxes ? Between sectors ?

How to constrain large scales when the correl in time / space are low, flux bear very high heterogeneity / high temporal & spatial variability ?



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## Adequacy of exploratory observation networks ? (1)

SW

#### **CO2-Megacity (Los Angeles)**

DRAFT: (fixed) CO2 monitoring Network\*



Typical CO<sub>2</sub>Data Set ppm 410 37: Aircraft 4000 measurements for 3000 405 381 (m) 2000 2000 1000 Indianapolis 400.381 40.2 395.39! Latitude . 39.1 -85.8 -88 -86.2 390.40; -86.4 Harding St. Power Plant Longitude (deg)

#### **CO2-MEGAPARIS & ICOS** network in the Paris area

- CO2 & CO (rouge: CO2-MEGAPARIS, orange: RAMCES-ICOS)
- Hauteur de couche limite



Continuous stations (5 in Salt Lake city, 3-12 in indianapolis, 5-6 in Paris, 4 in London...), mobile & aircraft campaigns



## Adequacy of exploratory observation networks ? (2)

Some conclusions from Mc Kain et al. 2012, PNAS:

- Models cannot explicitly represent small-scale processes
  - In situ stations should be used to detect regional trends only
- Increase nb of stations: useless for detecting changes in the emissions at monthly scale
- Remote sensing: "the best route for accurate verification of emission inventories"

Hourly observed and modeled CO2 concentrations for two weeks in October 2006 at a site downtown Salt Lake City (Mc Kain et al 2012, PNAS)







## Study of the representativeness in a urban environment

Measured vs modeled concentrations during the afternoon at Teddington (London)



- Local vs remote signal ?
- Contribution of boundaries, natural and anthrop fluxes ?

Use of high resolution modeling to configure the urban meteorology and assess the representativeness of measurements station in the Carbocount-city project (for the Paris area; image from ARIA)







#### **Use of co-emitted species**

• Strong correlations between the emissions of CO2 and CO/NOx/SO2... for a given sector

29.5

→ Use of the co-emitted species to help separate natural & sectoral emissions

Use of CO &NOx inventories, CO/CO2 and NOx/CO2 atmospheric slopes to derive estimates of CO2 fluxes from Houston (Brioude et al 2012, JGR)





CO, flux based on 1 tracer (CO)

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#### Use of carbon isotopes

• The depletion in <sup>14</sup>CO<sub>2</sub> gives insights about CO<sub>2</sub> from anthropogenic emissions





## Potential of satellite data

• The signature of plumes from large cities can be seen using high horizontal resolution space-borne data

Problem of representativeness in time (few hours) and of the requirements of accuracy/precision

384.5

385.0

385.5

386.0

Enhancement of GOSAT concentrations over Los Angeles (Kort et al 2012, GRL)





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Wind Speed [m.s<sup>-1</sup>]