CarbonTracker-Lagrange: A new tool for regional- to continental-scale flux estimation

Arlyn Andrews

For the NASA CMS Atmospheric Validation Working Group

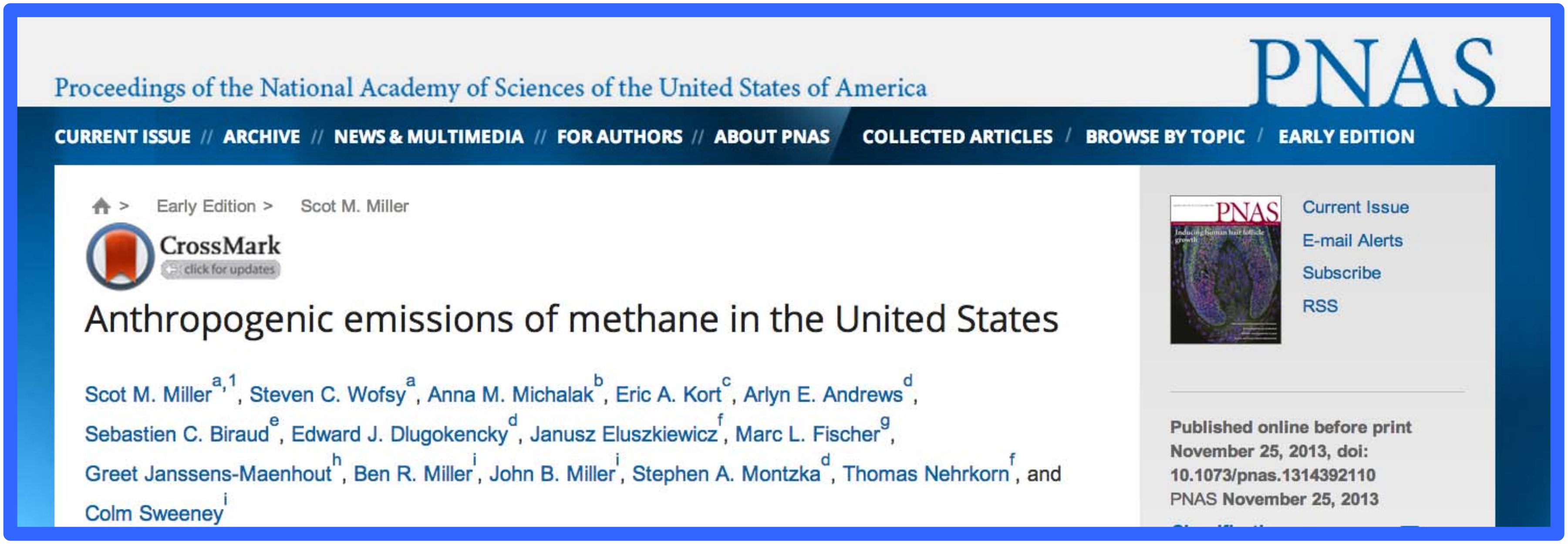
8 October 2010

Outline

- Motivation for CarbonTracker-Lagrange
- Overview
- Mechanics
- Preliminary Results
- Plans for CMS 2014

Motivation

Recent studies have demonstrated the usefulness of regional Lagrangian inverse modeling for greenhouse gas flux estimation:



Proceedings of the National Academy of Sciences of the United States of America

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> Early Edition > Scot M. Miller

CrossMark click for updates

Anthropogenic emissions of methane in the United States

Scot M. Miller[a,1], Steven C. Wofsy[a], Anna M. Michalak[b], Eric A. Kort[c], Arlyn E. Andrews[d], Sebastien C. Biraud[e], Edward J. Dlugokencky[d], Janusz Eluszkiewicz[f], Marc L. Fischer[g], Greet Janssens-Maenhout[h], Ben R. Miller[i], John B. Miller[i], Stephen A. Montzka[d], Thomas Nehrkorn[f], and Colm Sweeney[i]

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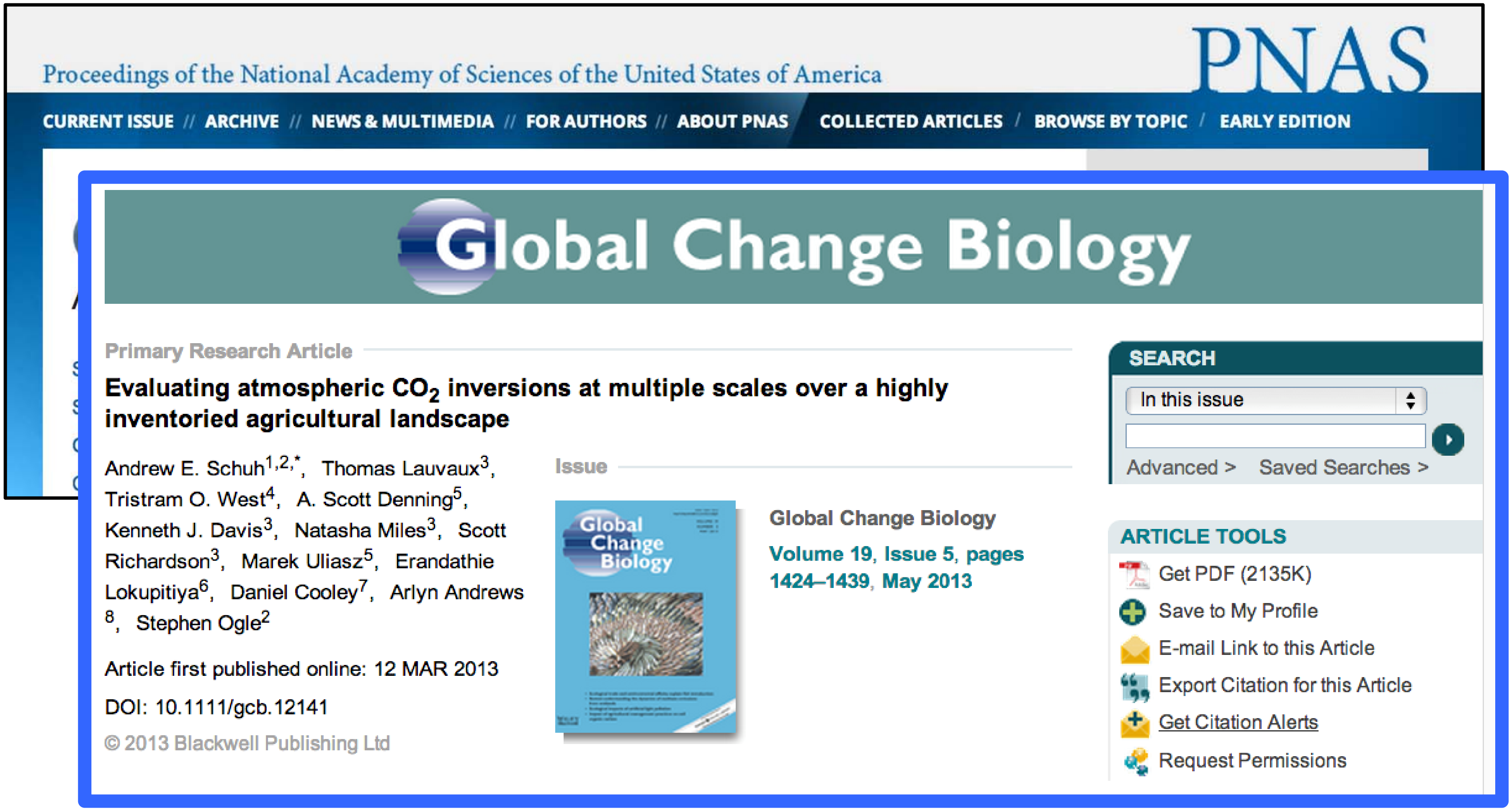
PNAS November 25, 2013

Recent studies have demonstrated the usefulness of regional Lagrangian inverse modeling for greenhouse gas flux estimation:



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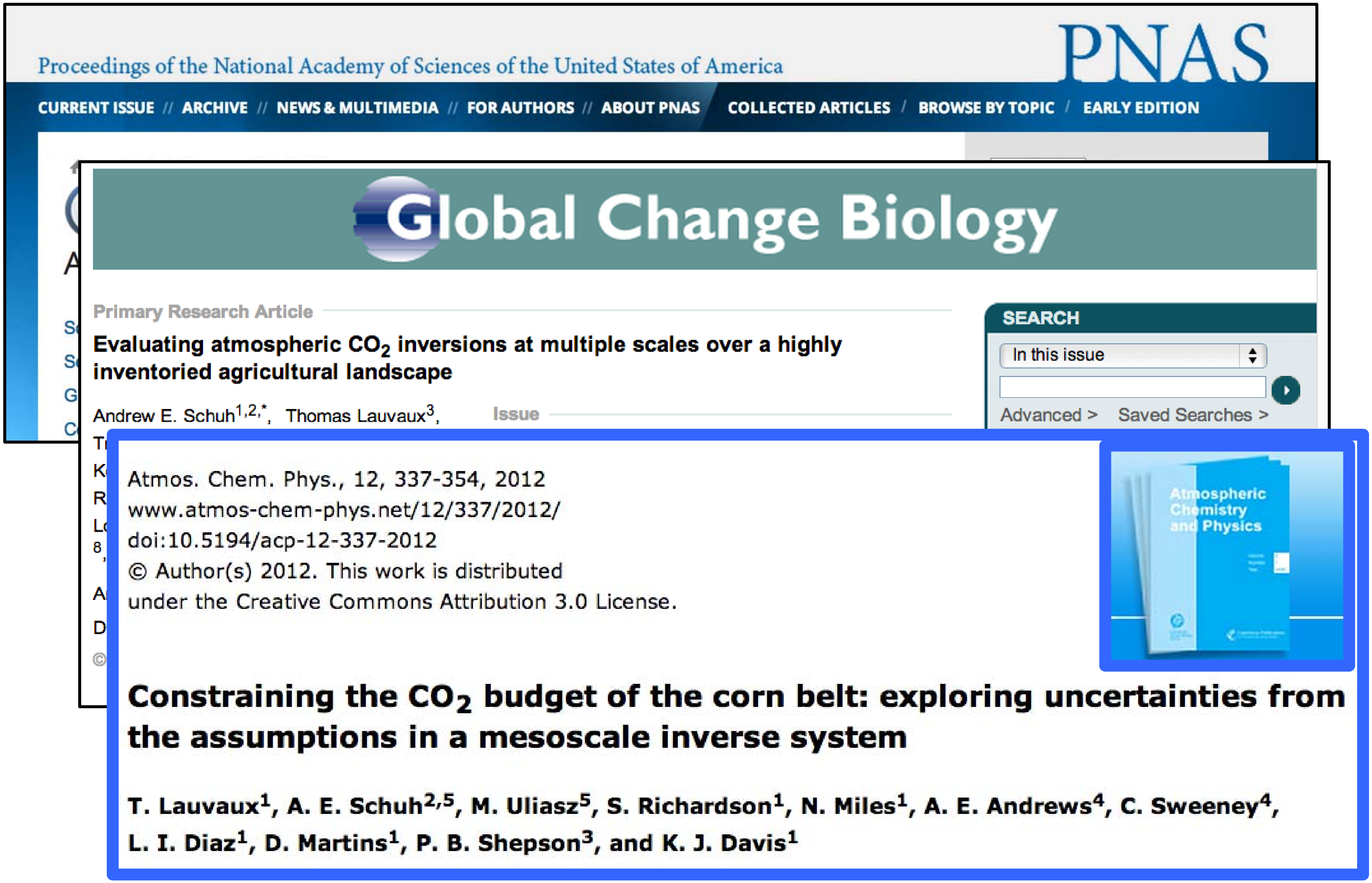

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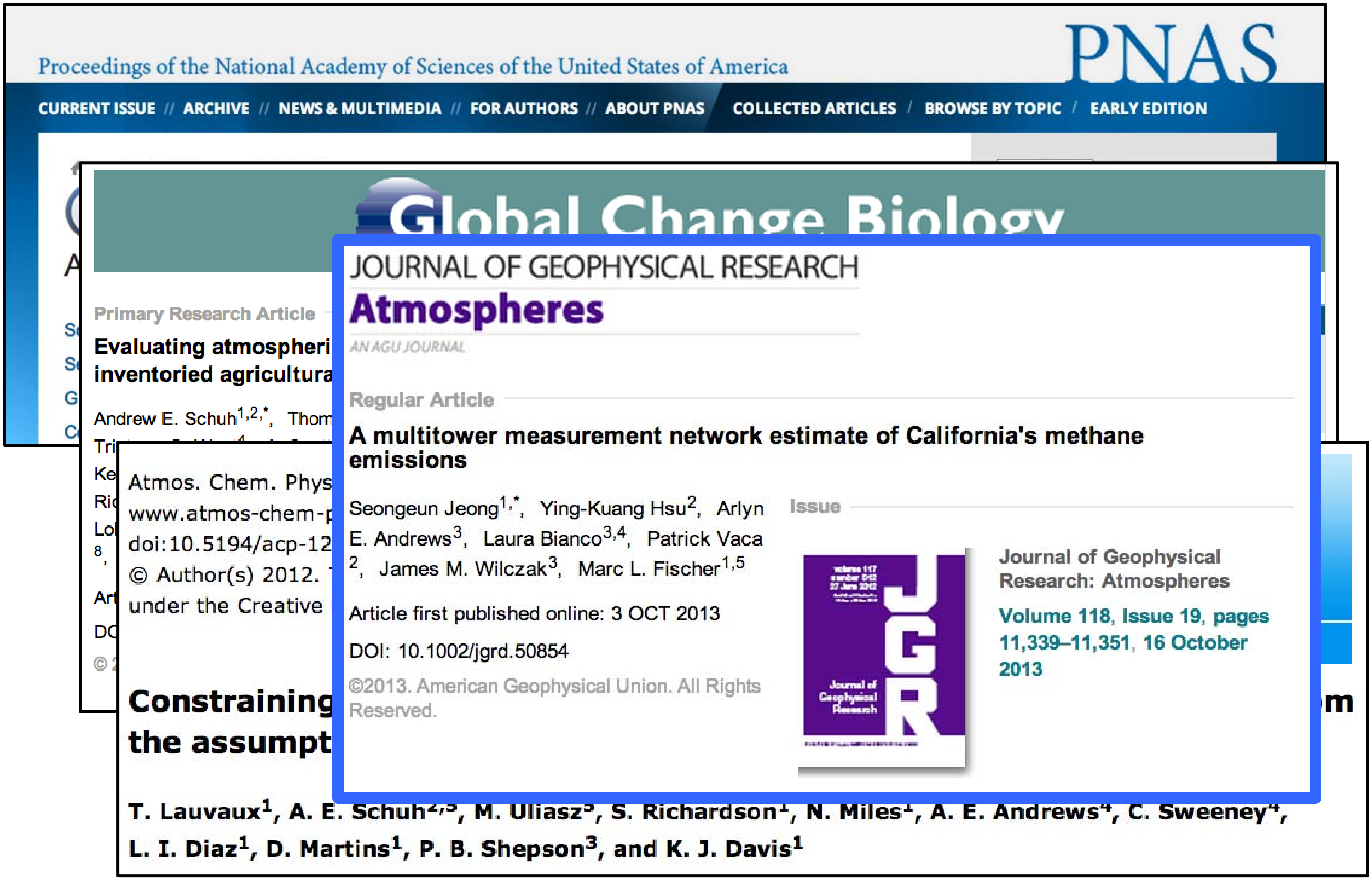

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Global Change Biology

Primary Research Article

Evaluating atmospheri
inventoried agricultura

Andrew E. Schuh[1,2,*], Thom

Atmos. Chem. Phys
www.atmos-chem-p
doi:10.5194/acp-12
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Constraining
the assumpt

T. Lauvaux[1], A. E. Schuh[2,3], M. Uliasz[3], S. Richardson[1], N. Miles[1], A. E. Andrews[4], C. Sweeney[4], L. I. Diaz[1], D. Martins[1], P. B. Shepson[3], and K. J. Davis[1]

JOURNAL OF GEOPHYSICAL RESEARCH

Atmospheres

AN AGU JOURNAL

Regular Article

A multitower measurement network estimate of California's methane emissions

Seongeun Jeong[1,*], Ying-Kuang Hsu[2], Arlyn E. Andrews[3], Laura Bianco[3,4], Patrick Vaca[2], James M. Wilczak[3], Marc L. Fischer[1,5]

Article first published online: 3 OCT 2013

DOI: 10.1002/jgrd.50854

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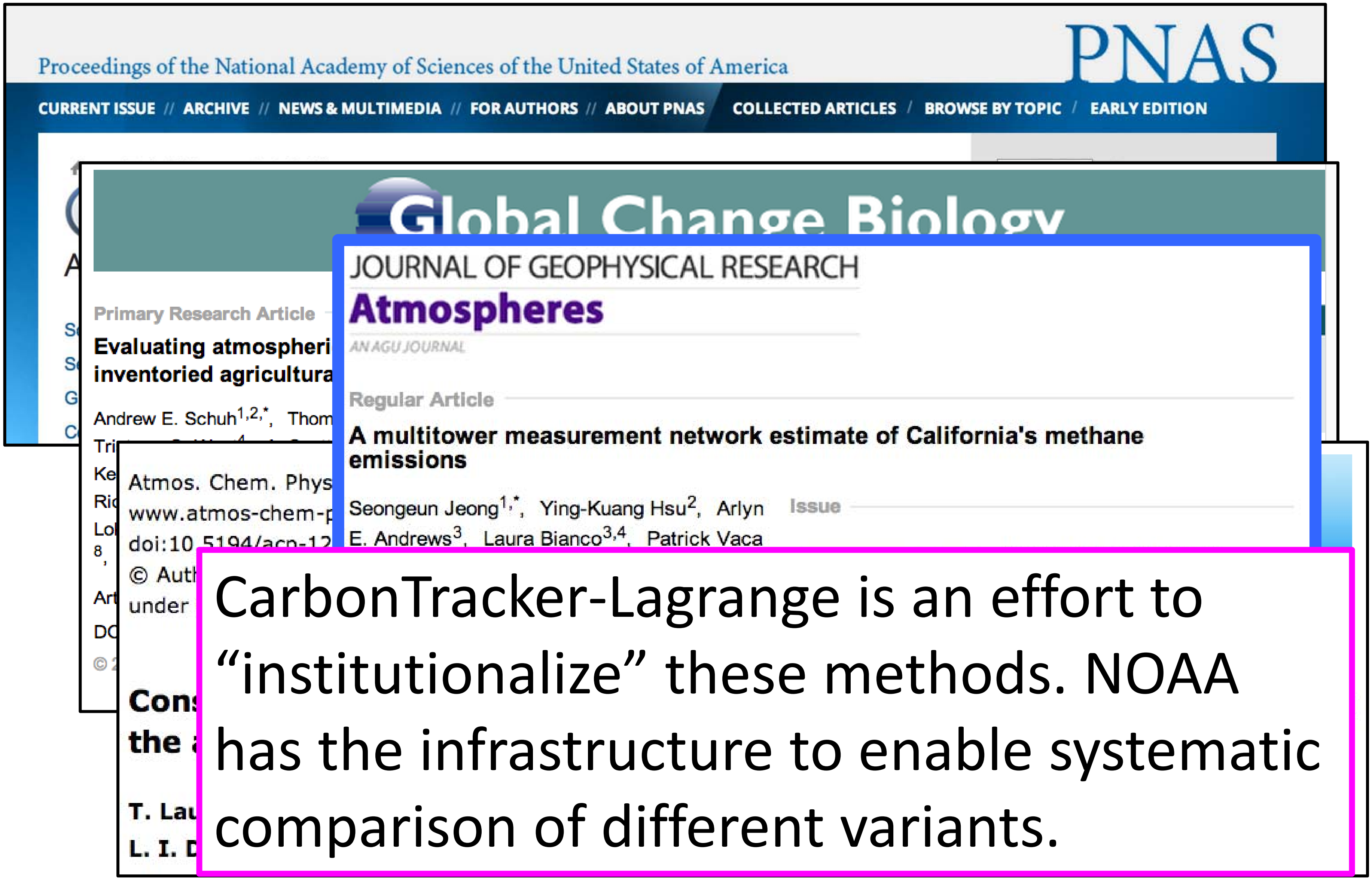
Issue

Journal of Geophysical Research: Atmospheres

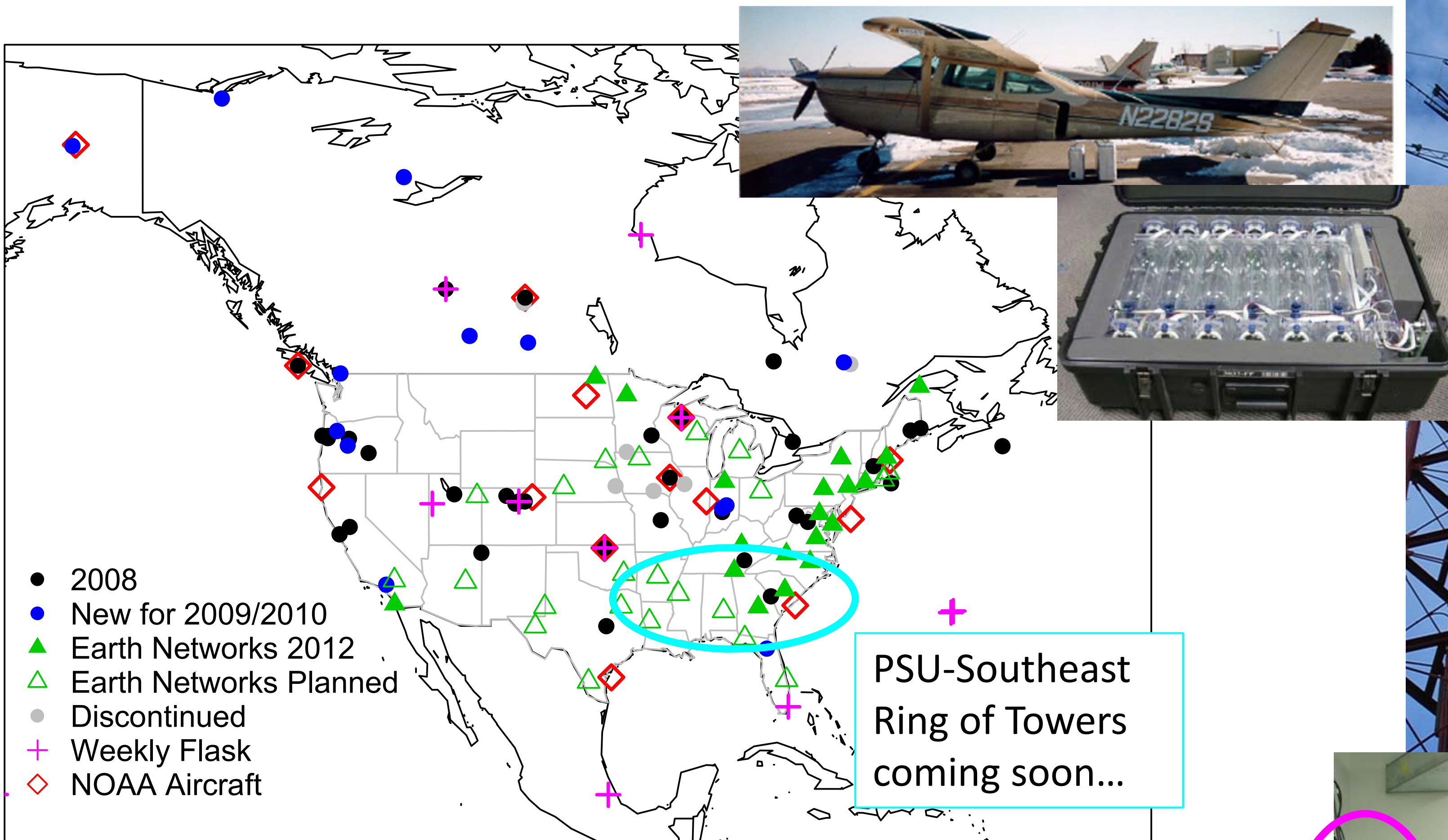
Volume 118, Issue 19, pages 11,339–11,351, 16 October 2013

Recent studies have demonstrated the usefulness of regional Lagrangian inverse modeling for greenhouse gas flux estimation:



CarbonTracker-Lagrange is an effort to "institutionalize" these methods. NOAA has the infrastructure to enable systematic comparison of different variants.

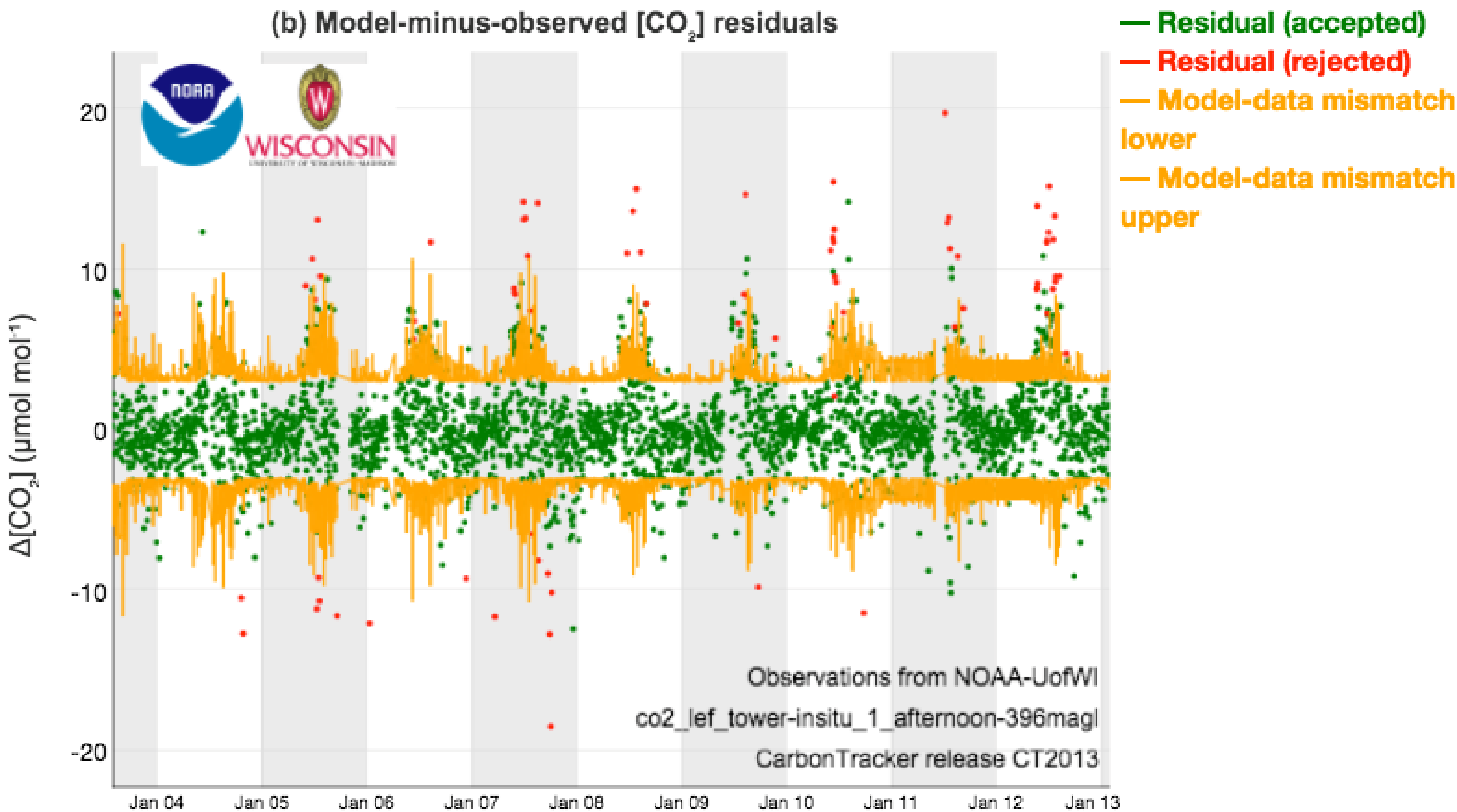
The North American Carbon Program +



PSU-Southeast Ring of Towers coming soon…

- Lots of new data.
- ~50 sites online in Summer 2012 , (~100 by 2014)
- Careful calibration necessary to ensure comparability across networks

CarbonTracker2013 (Eulerian CT) Residuals plot for Park Falls



- Summertime residuals persistently large and positive
- Many values rejected
- Lagrangian methods can potentially enable more effective use of data

Overview

CarbonTracker-Lagrange: A new tool for regional- to continental-scale flux estimation

- New Lagrangian inverse-modeling framework under development at NOAA Earth System Research Laboratory in collaboration with many partners to take advantage from measurements and datasets developed under the North American Carbon Program.

- Initial support from NOAA Climate Program Office's Atmospheric Chemistry, Carbon Cycle, & Climate (AC^4) Program. NASA Carbon Monitoring System funding has enabled inclusion of satellite and TCCON data.

- High-resolution WRF-STILT atmospheric transport model customized for Lagrangian simulations (Nehrkorn et al., *Meteorol. Atmos. Phys.*, *107*, 2010). AER, Inc. is responsible for STILT-WRF runs. Also testing HYSPLIT-NAM, HYSPLIT-HRRR and HYSPLIT-HRRR (High Resolution Rapid Refresh, an experimental real time 3-km simulation from NOAA-ESRL).

- Pre-computed footprints combined with efficient matrix inversion code enables testing of many variants of inversion.

CarbonTracker –Lagrange Contributors

Modeling team:

- NOAA & CIRES: A. Andrews, K. Thoning, M. Trudeau, J. Miller, K. Masarie, R. Draxler, A. Stein, L. Hu
- AER, Inc.: J. Eluszkiewicz, T. Nehrkorn, M. Mountain
- Carnegie Institution for Science/Stanford: A. Michalak, V. Yadav, M. Qui
- Colorado State University: C. O'Dell
- Harvard University: S. Wofsy, S. Miller, J. Benmergui

Data Providers:

- NOAA Earth System Research Laboratory's Global Monitoring Division
- Environment Canada (D. Worthy)
- Penn State University (K. Davis, S. Richardson, N. Miles)
- NCAR (B. Stephens)
- Oregon State University (B. Law, A. Schmidt)
- Lawrence Berkeley National Lab (M. Torn, S. Biraud, M. Fischer)
- Earth Networks (C. Sloop)
- Harvard University (S. Wofsy, J. W. Munger)
- U of Minnesota (T. Griffis)
- TCCON team; CalTech (D. Wunch, P. Wennberg; S. Newman) & JPL (G. Toon)
- GOSAT-ACOS team
- OCO-2 team

CarbonTracker-Lagrange Products

– Multi-laboratory CO_2 in situ data package (ObsPack)
– WRF Meteorological Simulations
  - North America: 2007-2010, plans to extend through 2015
  - Amazonia: dates TBD, will include 2015
– Footprint Library
– Optimized CO_2 Fluxes, optimized 4D Boundary Values, Posterior simulated CO_2 corresponding to observations

ObsPack Framework for Data Distribution

Earth Syst. Sci. Data Discuss., 7, 495–519, 2014
www.earth-syst-sci-data-discuss.net/7/495/2014/
doi:10.5194/essdd-7-495-2014

Open Access Earth System Science Data Discussions

This discussion paper is/has been under review for the journal Earth System Science Data (ESSD). Please refer to the corresponding final paper in ESSD if available.

ObsPack: a framework for the preparation, delivery, and attribution of atmospheric greenhouse gas data

K. A. Masarie[1], W. Peters[2], A. R. Jacobson[1,3], and P. P. Tans[1]

Discussion Paper | Discussion Paper |

ESSDD
7, 495–519, 2014

The ObsPack Framework and Atmospheric Greenhouse Gas Data

K. A. Masarie et al.

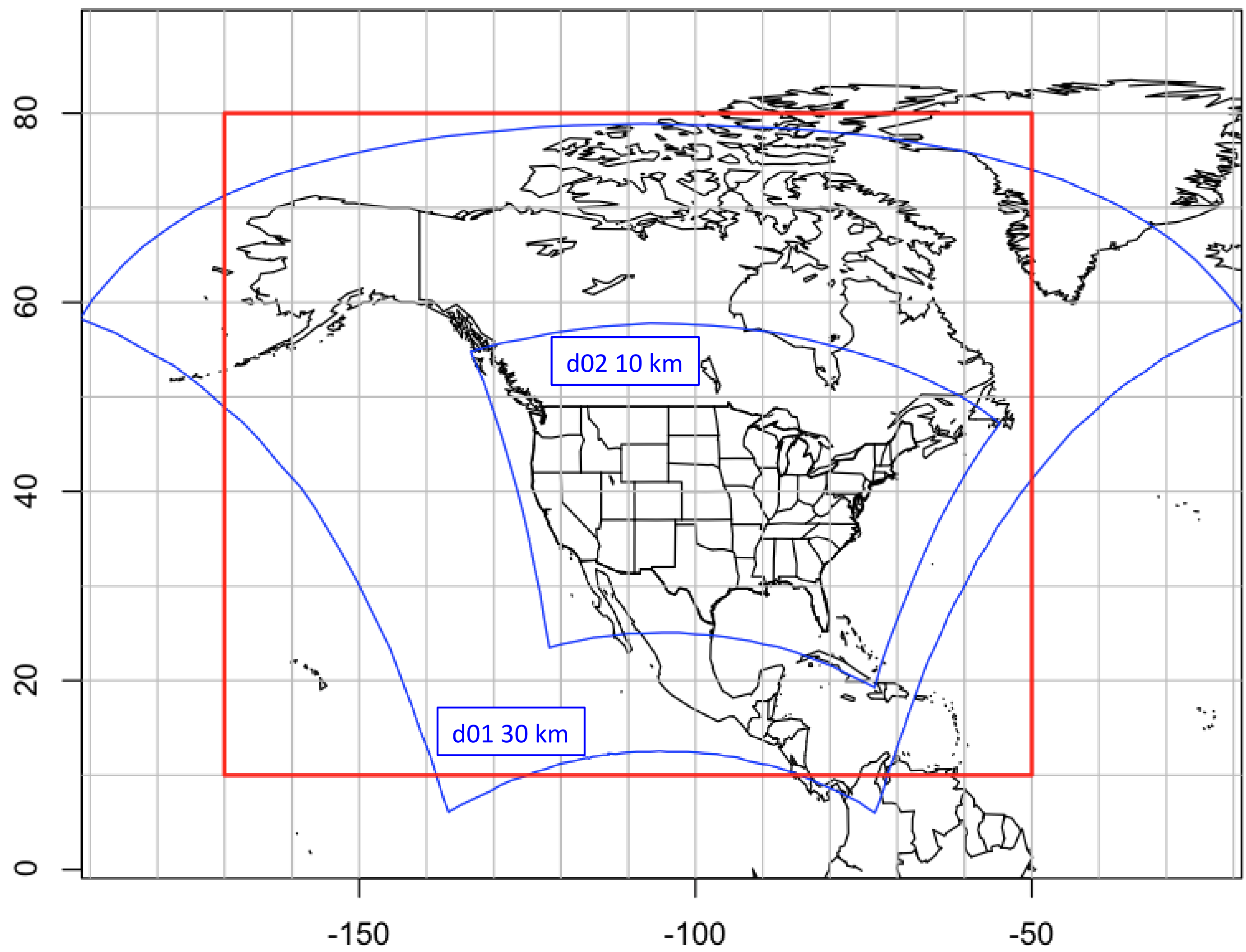
Title Page

Abstract | Instruments

Features

- Comprehensive Metadata
- Flagging and Uncertainty Information
- Data Attribution and Partner Acknowledgement

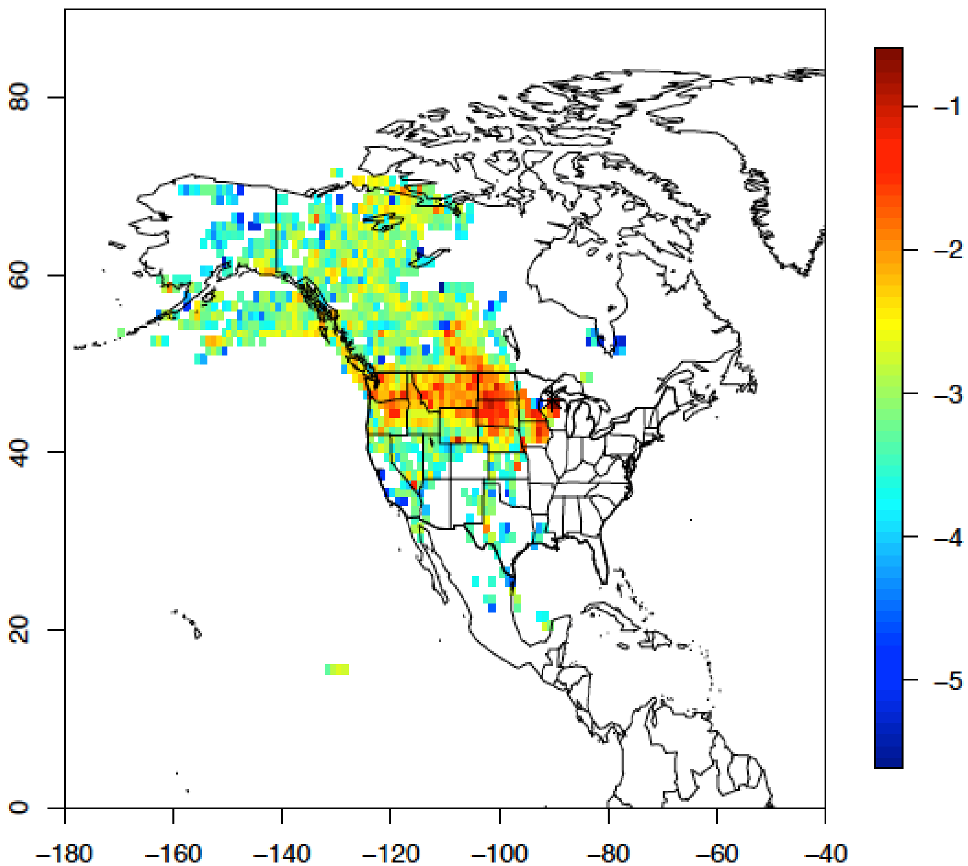
AER WRF Simulations



- CT-Lagrange North America 2008-2010 WRF domains (blue) with 1° footprint domain in red.
- WRF simulations are allowed to evolve (version updates, increased vertical levels, domain changes etc.)

STILT Footprints

LEF Tower 396m: 2010-07-22 18:10

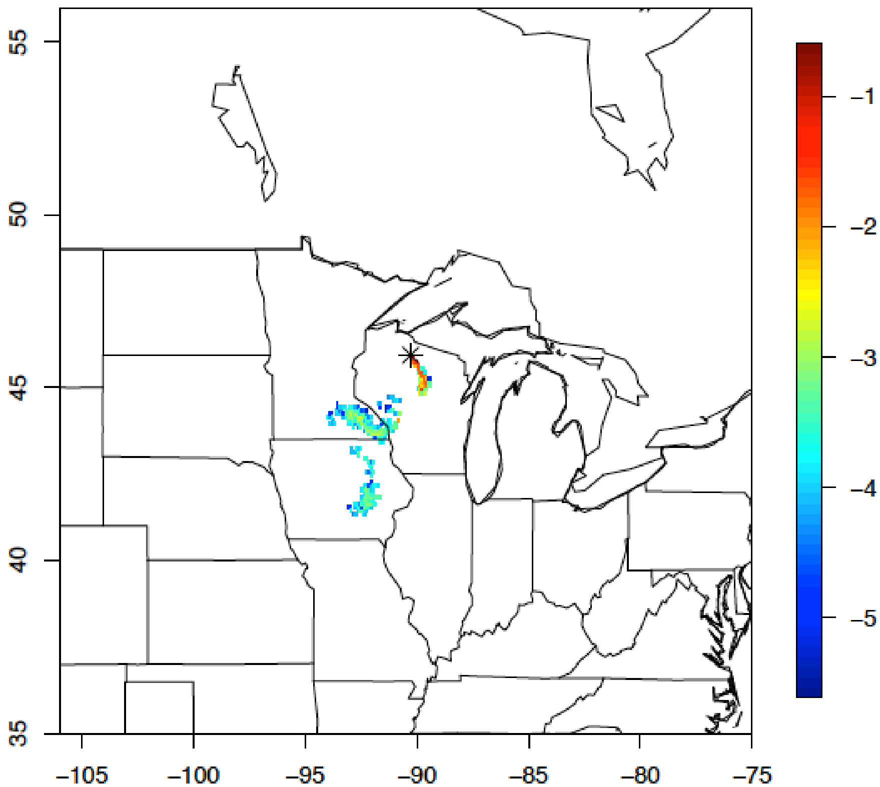


$$\log_{10}\left(\frac{ppm}{\mu mole \cdot m^{-2} s^{-1}}\right)$$

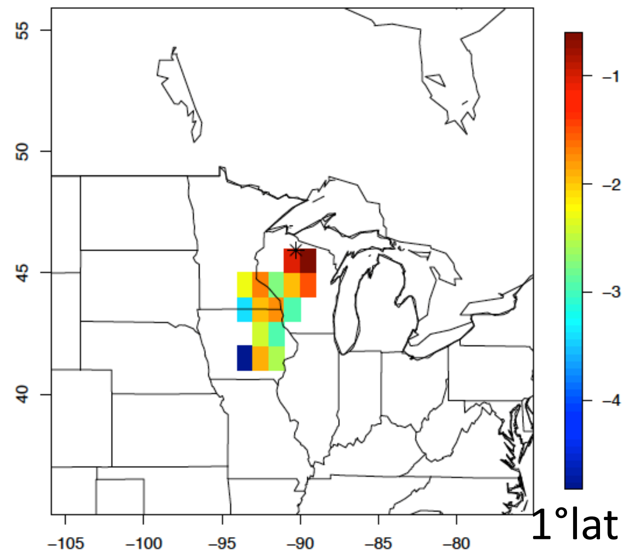
- 10-day footprints computed with 1°lat × 1° lon × hourly resolution
- Second footprint computed with 1°lat × 1.25° lon × hourly for compatibility with NASA CMS and other NASA MERRA products
- Nearfield footprint computed for subdomain with 0.1°lat × 0.1° lon × hourly for 24 hours
- Particle trajectories archived as snapshots with decreasing frequency going backward in time
- Convolutions with CarbonTracker and Goddard CASA-GFED3 (CMS) fluxes
- All products archived in single Climate-Forecast Compliant NetCDF file (v4.0 with compression)

STILT Nearfield Footprint

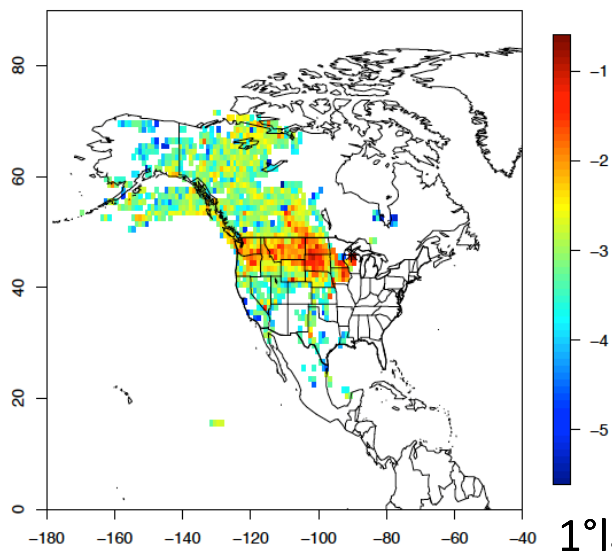
LEF Tower 396m: 2010-07-22 18:10
0.1°lat × 0.1° lon × hourly
24 hours duration



$$\log_{10}\left(\frac{ppm}{\mu mole \cdot m^{-2}s^{-1}}\right)$$



1°lat × 1° lon × hourly
Hours: 0 - 24



1°lat × 1° lon × hourly
10 days duration

CarbonTracker-Lagrange: Footprint Library

Species-independent footprints corresponding to > 1 million well-calibrated CO_2 in situ (continuous and discrete) measurements have been computed. Plans to extend through 2015.

2007-2010

- Surface and tower sites with continuous CO_2 and CH_4 traceable to WMO scales maintained by NOAA/ESRL's Global Monitoring Division. Eight footprints per day to resolve diurnal cycle, synched to solar 2 pm.
- Surface and aircraft flask samples from NOAA's Global Greenhouse Gas Monitoring Network.
- North American TCCON sites. Two column simulations per day: (1) solar noon and (2) time of day corresponding to SZA = 70°
- GOSAT simulations for July 2009 – Dec 2010 were added with support from NASA's Carbon Monitoring System.

Summer 2012 Network Design Case Study

- Augmented surface network (new real and candidate future sites)
- Additional candidate TCCON sites
- OCO-2/ ASCENDS synthetic data
- Augmented aircraft network
- Transport model comparisons

Column-observations are simulated and stored as profiles. Footprints and boundary values from individual altitudes are weighted according to the retrieval averaging kernel and taking into account water vapor.

CarbonTracker-Lagrange: A new tool for regional- to continental-scale flux estimation

- Efficient algorithm uses sparse matrix methods for explicit matrix inversion (Yadav and Michalak, *Geosci. Model Dev.*, *6*, 583-590, 2013). Computational speed enables many permutations of the inversion, such as:
  - Multiple data-weighting scenarios
  - Varied mathematical construct
    - Form of state vector
    - Bayesian or Geostatistical optimization
  - Multiple priors
  - Generalized to enable space/time varying prior error

- Modular python software enables fast incorporation of new techniques and facilitates use of multiple transport models.

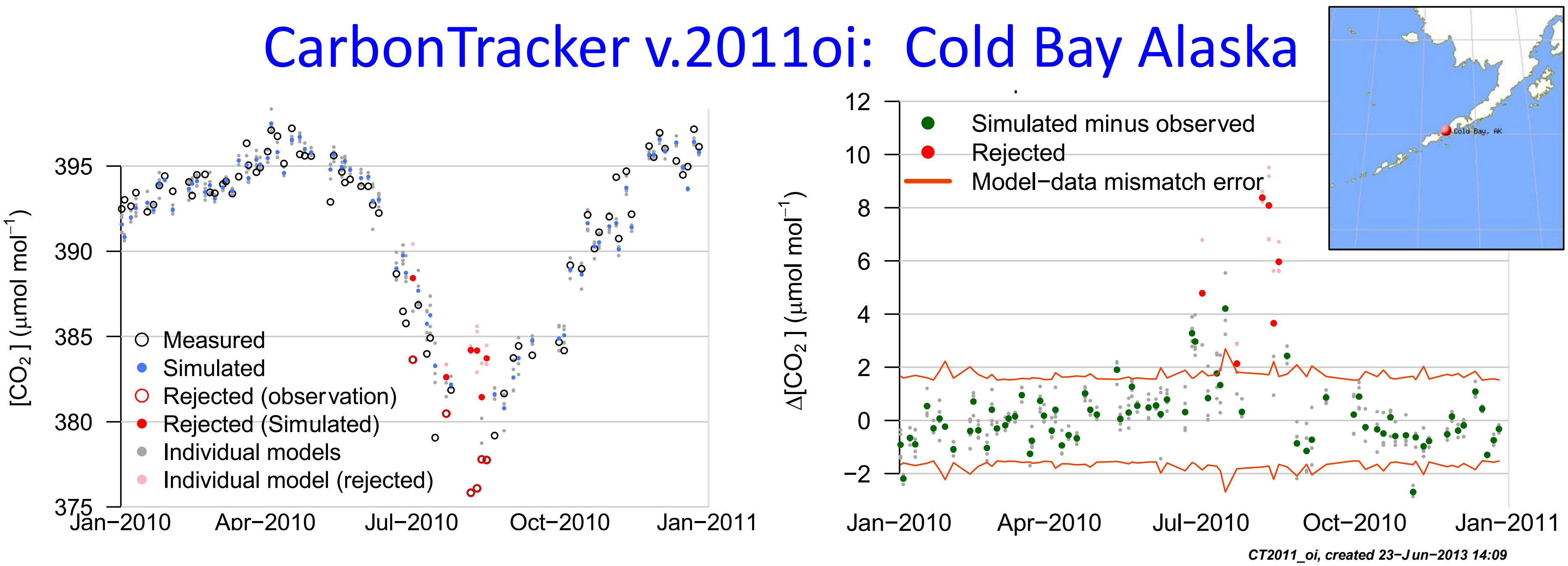
- New boundary value optimization capability has been implemented and is undergoing testing. Success requires vertically resolved measurements that are differently sensitive to surface flux and boundary errors (e.g. aircraft profiles, or surface plus column).

- Initial focus is on continental-scale CO_2 and CH_4 inversions for North America, with plans to move to finer spatial scales and simulate additional species.

Why is simultaneous estimation of boundary inflow and surface influence necessary?

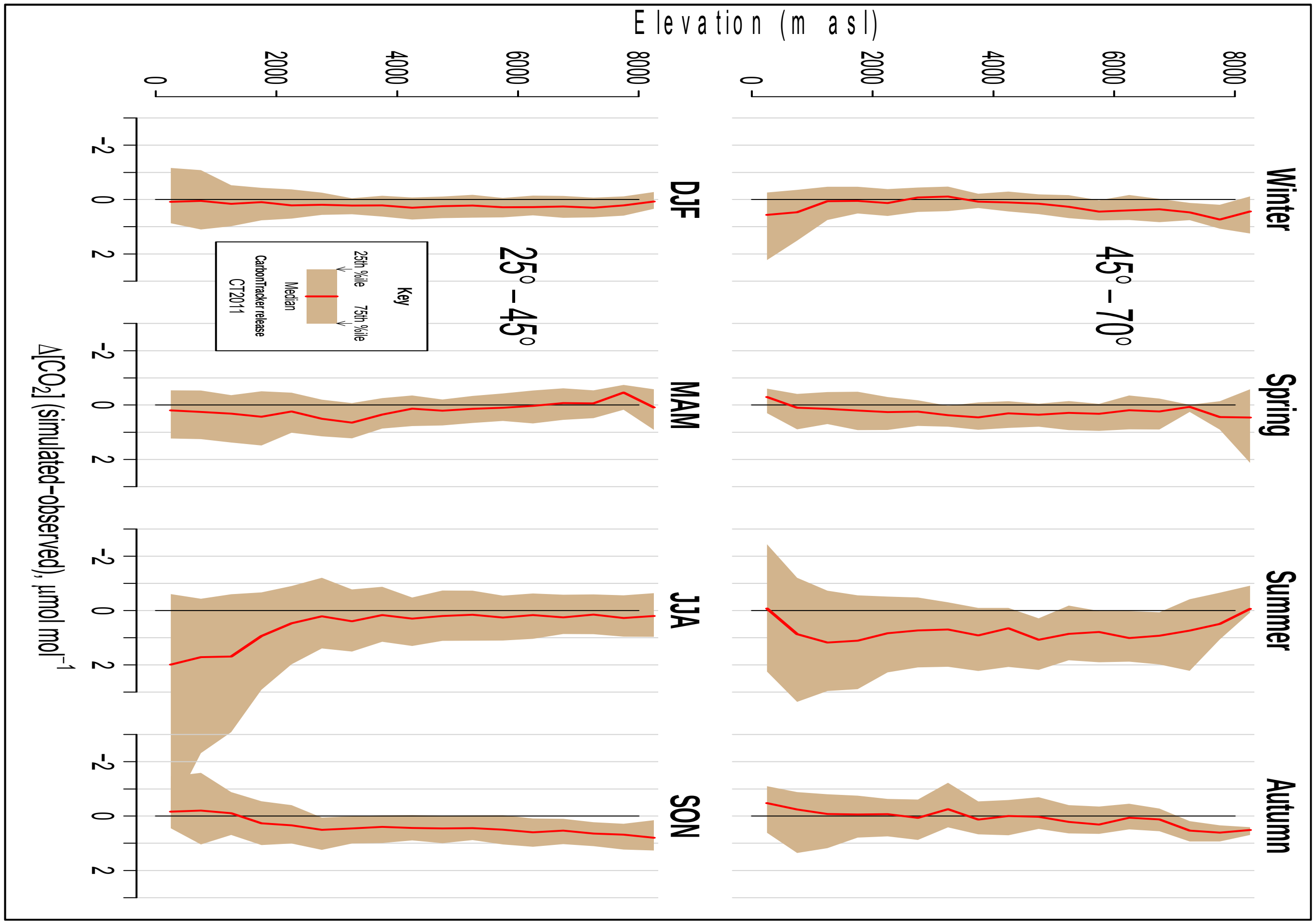
1. Accurate 4-dimensional estimates of the boundary inflow are not readily available.

CarbonTracker v.2011oi: Cold Bay Alaska



- Model is biased high by several ppm during summer.
- Seasonal pattern of residuals for 2010 is typical of all years.

Comparison with NOAA/ESRL aircraft data shows that CT2011oi summertime bias is pervasive in the Northern Hemisphere:



NOAA/ESRL Global Monitoring Division Aircraft Program:

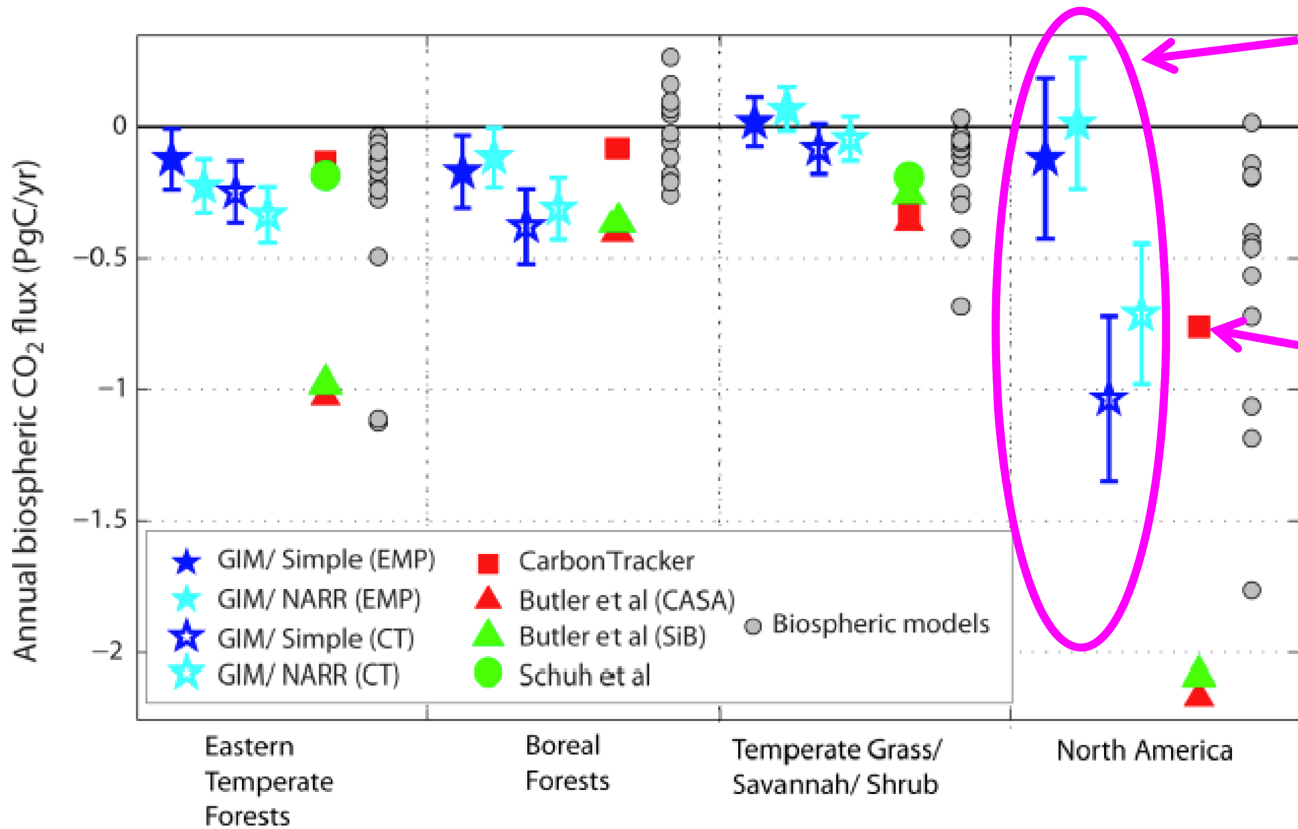
http://www.esrl.noaa.gov/gmd/ccgg/aircraft/data.html

Principal Investigator: Colm Sweeney

A NOAA contribution to the North American Carbon Program

Why is simultaneous estimation of boundary inflow and surface influence necessary?

2. Flux estimates are apparently very sensitive to errors in assumed boundary values.



Changing the boundary condition makes the North American carbon sink disappear!

Using CarbonTracker for the boundary condition produces a flux estimate similar to CarbonTracker's.

S. Gourdji et al., "North American CO_2 Exchange: Inter-Comparison of Modeled Estimates with Results from a Fine-Scale Atmospheric Inversion." *Biogeosciences* (2012)

Mechanics

CarbonTracker-Lagrange Inversion Framework

$$\hat{\mathbf{s}} = \mathbf{s}_p + (\mathbf{HQ})^T (\mathbf{HQH}^T + \mathbf{R})^{-1}(\mathbf{z} - \mathbf{Hs}_p)$$

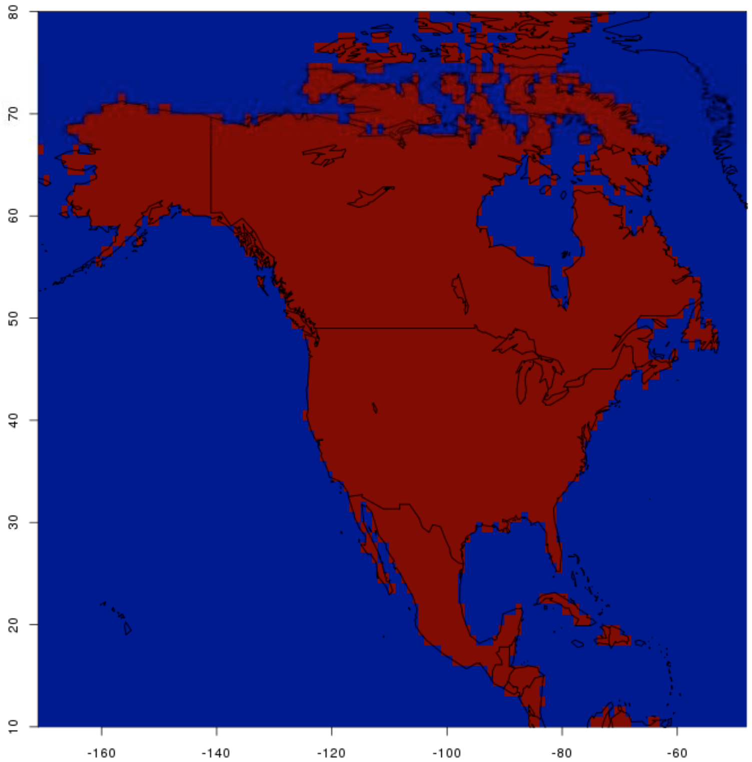
Yadav and Michalak, *Geosci. Model Dev.*, *6*, 583–590, 2013

H is atmospheric transport operator (i.e. the footprints)
Q is the prior error covariance matrix
R is the model-data mismatch matrix
s_p is a vector containing the prior flux estimate
$\hat{s}$ is a vector containing the revised fluxes

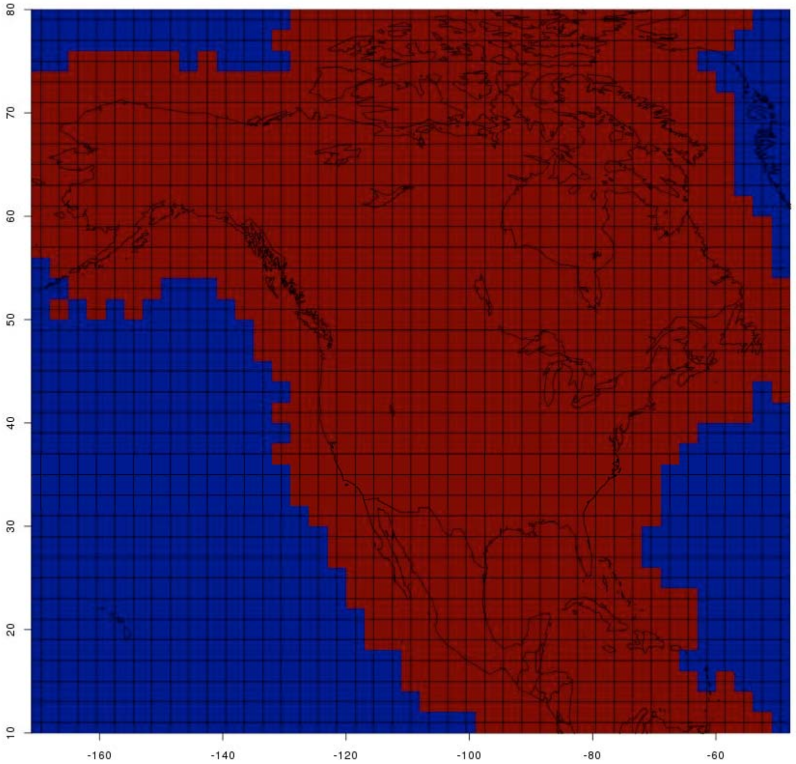
Modified framework for boundary optimization:

- H has additional columns for boundary value grid cells
- s_p and $\hat{s}$ contains additional elements
- Q contains additional rows and columns. No cross-correlation between boundary values and fluxes

CarbonTracker-Lagrange: Boundary Value Optimization



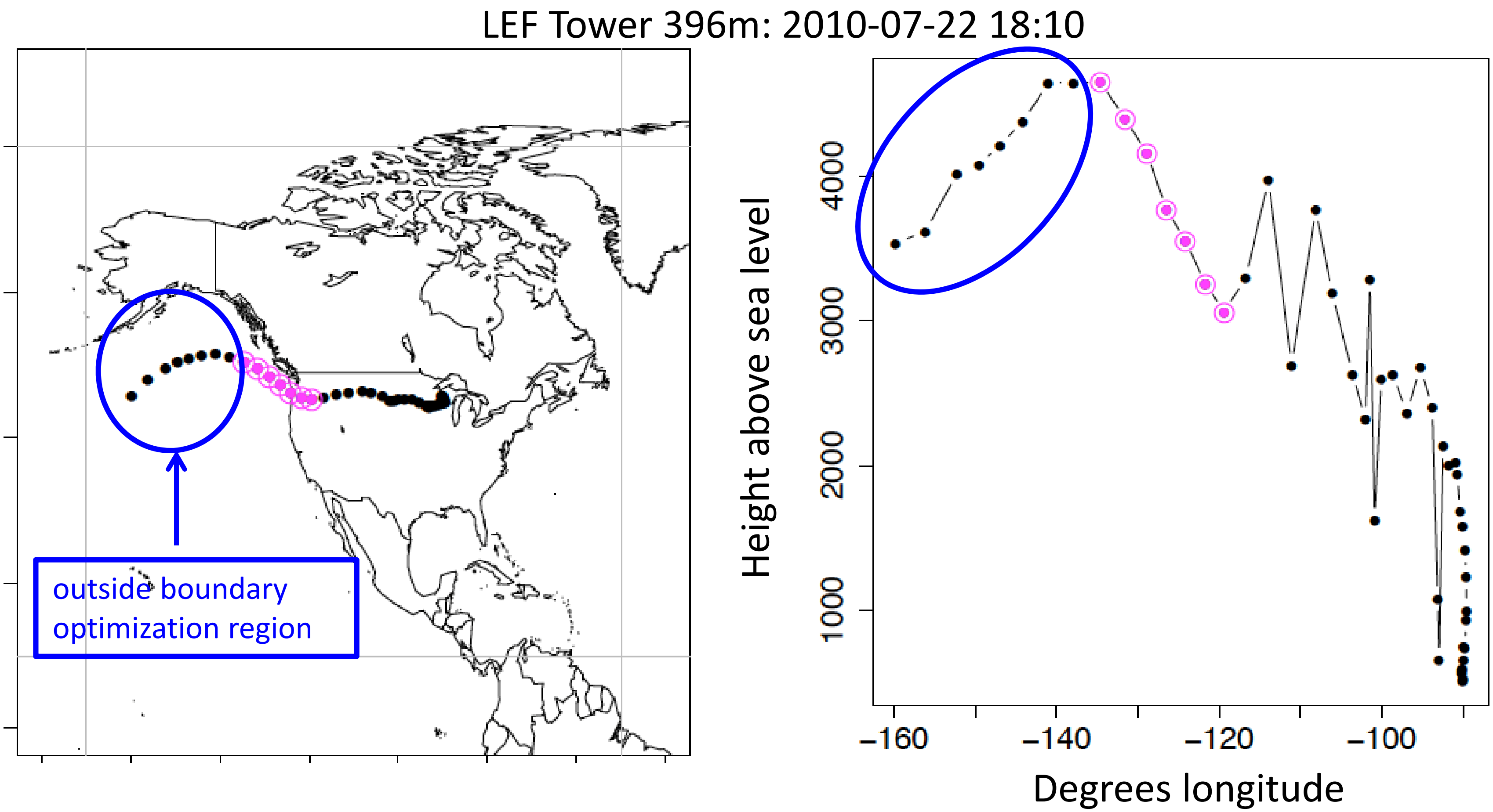
Flux Grid Cells
(1deg lat, 1 deg lon, 3 hourly)



Boundary/ Initial Condition Cells
(2deg lat, 3 deg lon, daily)

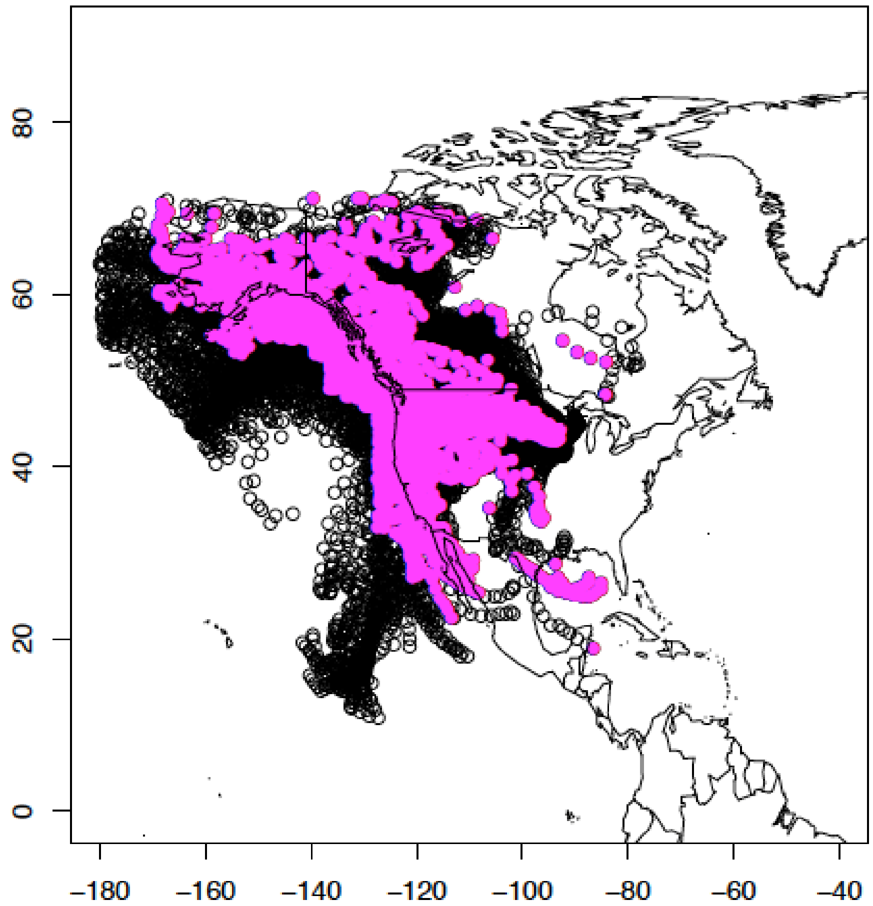
- Flux estimation is for land grid cells only (CT land mask)
- Boundary/initial value optimization region restricts inversion to area where most aircraft data are collected

Example: mid-afternoon trajectory from LEF tall tower 396 magl



- Magenta circled points correspond to trajectory locations outside the flux estimation region and within the initial value estimation region

LEF Tower 396m: 2010-07-22 18:10



Black = all trajectory points

Magenta = points that are within the boundary estimation region and that have permanently exited the continental surface layer.

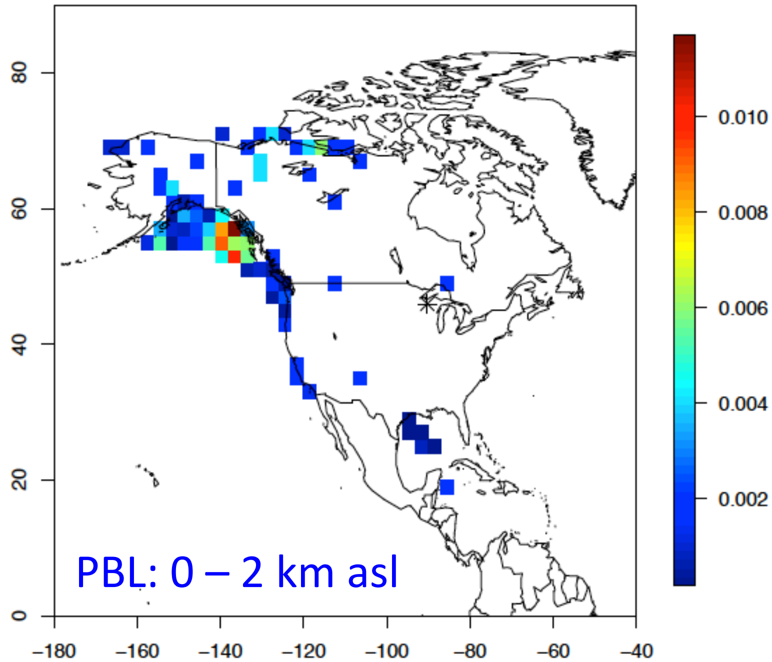
3 conditionals for selecting endpoints:

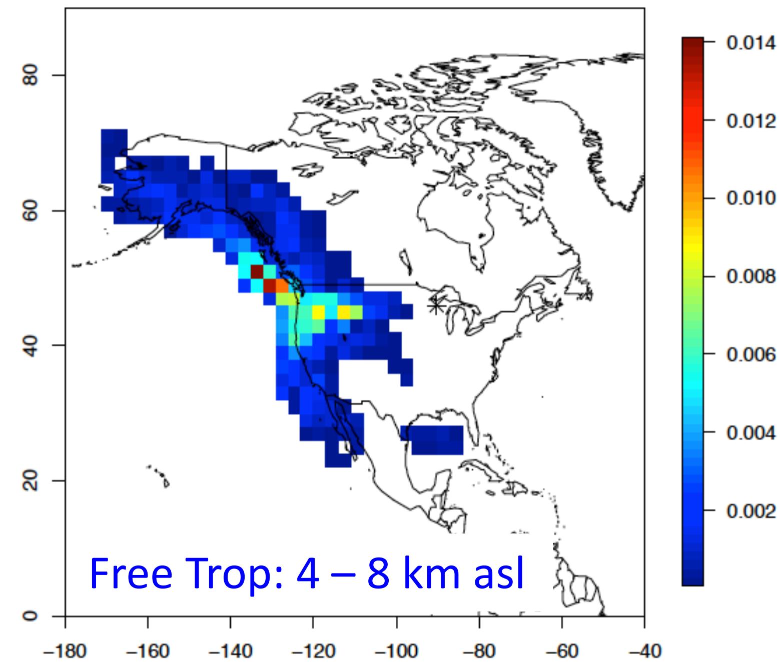
(1) exits laterally via mbl

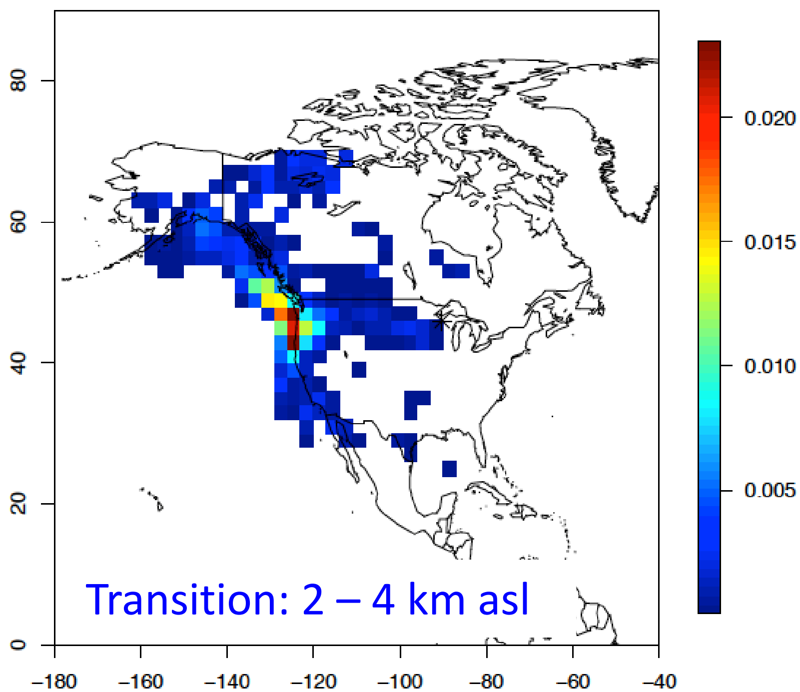
(2) exits vertically via free troposphere

(3) still in cbl at end of 10-day run

LEF Tower 396m: 2010-07-22 18:10







- Gridded boundary footprints: Use all trajectory points within the mole fraction estimation domain.
- Resolution: daily x 3 lon x 2 lat x three vertical bins.
- Each trajectory gets 1/500th of the weight, but trajectories may have different number of points included.
- Units are ppm per ppm.

Prior Error Covariance Q

Yadav and Michalak, GMD, 2013:

$$\mathbf{Q} = \sigma_s^2 \overbrace{\left[exp\left(-\frac{\mathbf{X}_\tau}{l_\tau}\right)\right]}^{\substack{temporal \\ covariance}} \otimes \overbrace{\left[exp\left(-\frac{\mathbf{X}_s}{l_s}\right)\right]}^{\substack{spatial \\ covariance}}$$

- Consider: $\mathbf{D}$ as temporal covariance and $\mathbf{E}$ as spatial covariance:

$$\mathbf{D}_{(p\times q)} \otimes \mathbf{E}_{(r\times t)} = \begin{pmatrix} d(1,1)\mathbf{E} & \cdots & d(1,q)\mathbf{E} \\ \vdots & \ddots & \vdots \\ d(p,1)\mathbf{E} & \cdots & d(p,q)\mathbf{E} \end{pmatrix} \in \mathbf{Q}_{(pr\times qt=m\times m)}$$

We have generalized to allow space- and time-varying sigma:

$$\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_{m-1}, \sigma_m)$$

$$\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}^T = \begin{bmatrix} {\sigma_1}^2 & \cdots & \sigma_1\sigma_m \\ \vdots & \ddots & \vdots \\ \sigma_m\sigma_1 & \cdots & {\sigma_m}^2 \end{bmatrix}$$

$$\mathbf{I}_{\boldsymbol{\sigma}} = \begin{bmatrix} {\sigma_1}^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & {\sigma_m}^2 \end{bmatrix}$$

I_σ is the diagonal matrix of standard deviations: $I_\sigma[ij]=\sigma_i$ for i=j, 0 for i≠j.

$$\mathbf{Q} = (\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}^T) \times (\mathbf{D} \otimes \mathbf{E}) = \mathbf{I}_{\boldsymbol{\sigma}} \cdot (\mathbf{D} \otimes \mathbf{E}) \cdot \mathbf{I}_{\boldsymbol{\sigma}}$$

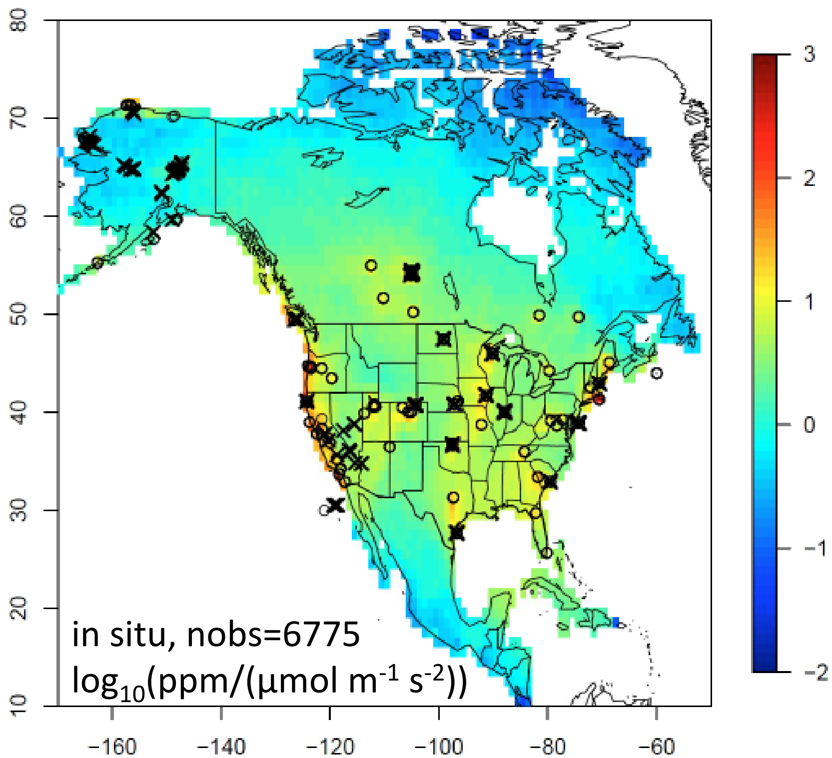
Beta algorithm (in testing) that leverages Yadav and Michalak framework to avoid building full Q and full $\sigma \cdot \sigma^T$.

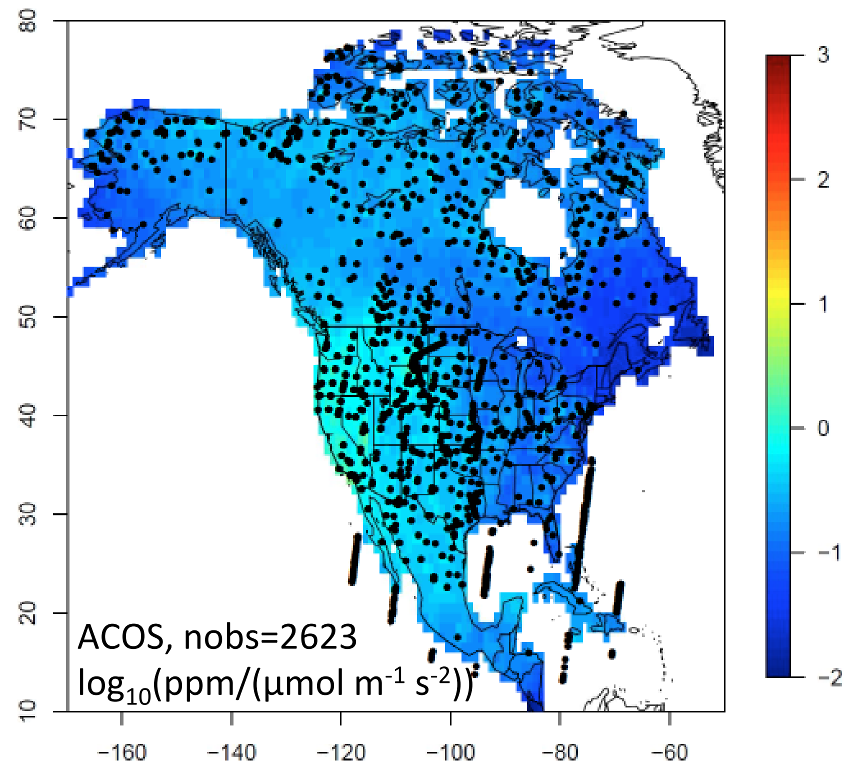
Model-Data Mismatch Matrix R

- Many studies assume R varies slowly, e.g., assigned site by site with a seasonal cycle but no day to day or within day variability
- CT-L bottom up model for R informed by:
  - standard deviation for each observation (e.g. does measurement occur during or proximal to a frontal passage, wind shift, etc.)
  - Modeled and/or measured vertical gradient information
  - Proximity to flux gradients (e.g. coastlines, urban areas)
  - Complex terrain
- So far no off-diagonal elements

Preliminary Results

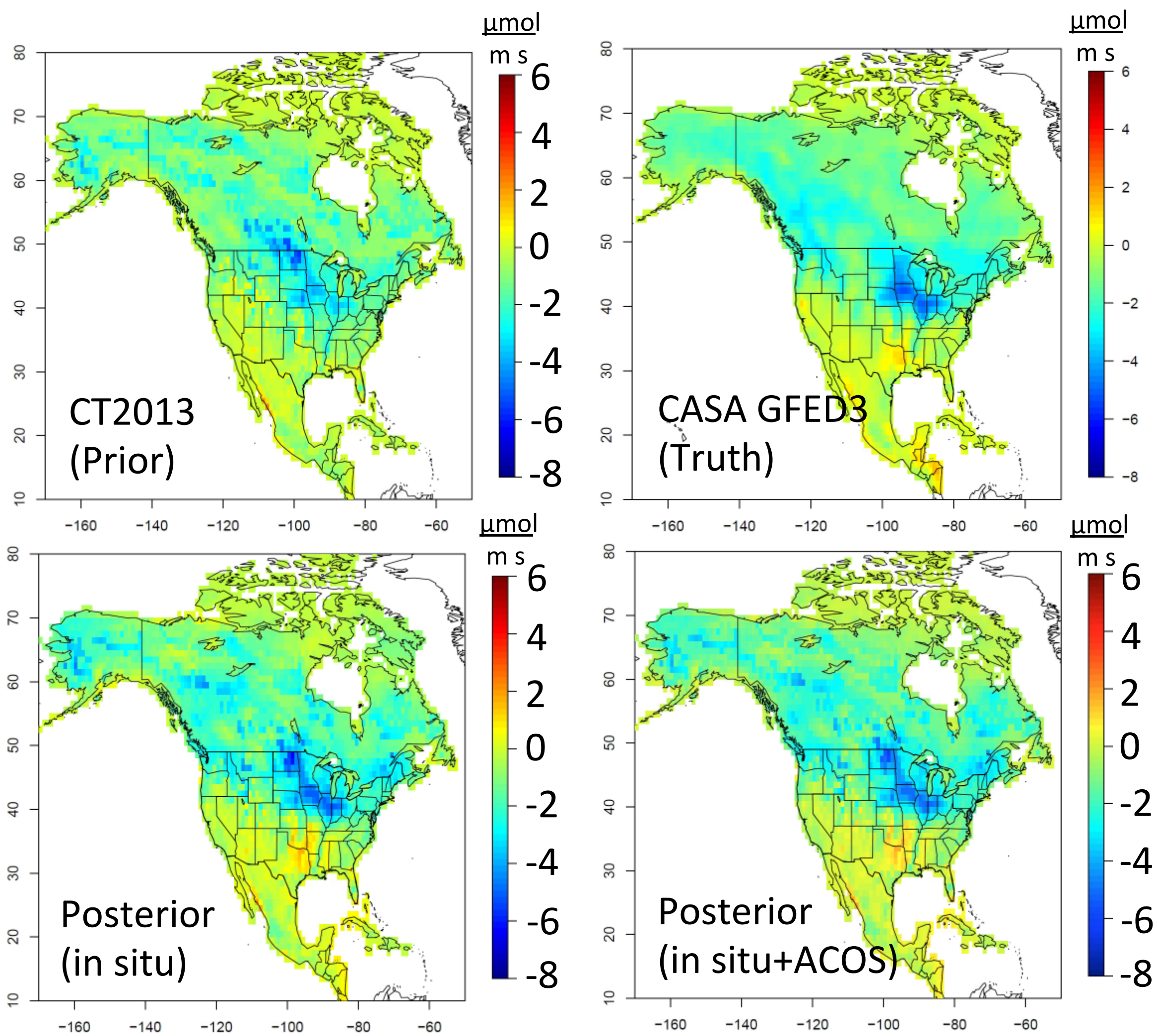
July 2010 Cumulative Sensitivity to Surface Flux for In Situ (Flask and Continuous) and ACOS GOSAT quality controlled data





- Number of GOSAT observations is relatively low and sensitivity to surface fluxes is much lower than for in situ data
- Increased sensitivity for column data may be achieved by extending domain further over the Atlantic

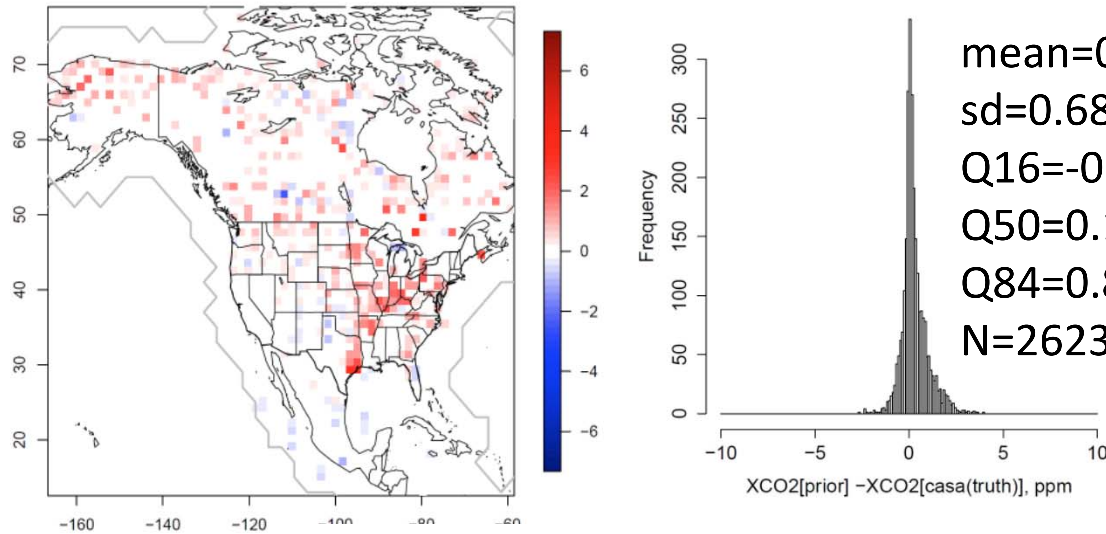
July 2010 Synthetic Data Inversion; Monthly Mean Fluxes



- Idealized case: perfect transport, perfect observations (no noise), no boundary value errors
- Including GOSAT ACOS observations does not significantly change results

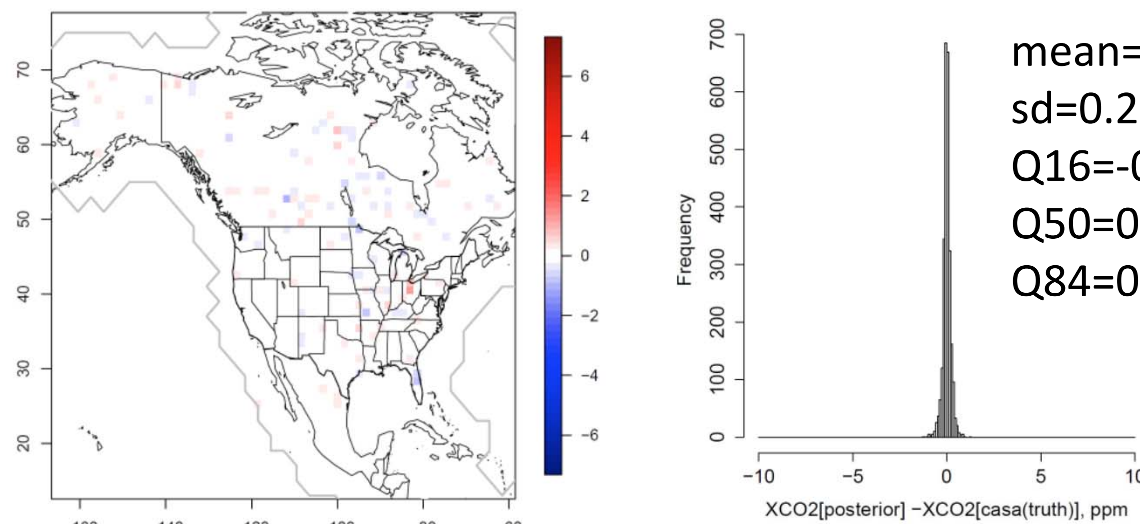
July 2010 Synthetic Data Inversion; ACOS GOSAT Residuals

Prior Simulated OBS – CASA OBS



mean=0.28
sd=0.68
Q16=-0.2
Q50=0.14
Q84=0.83
N=2623

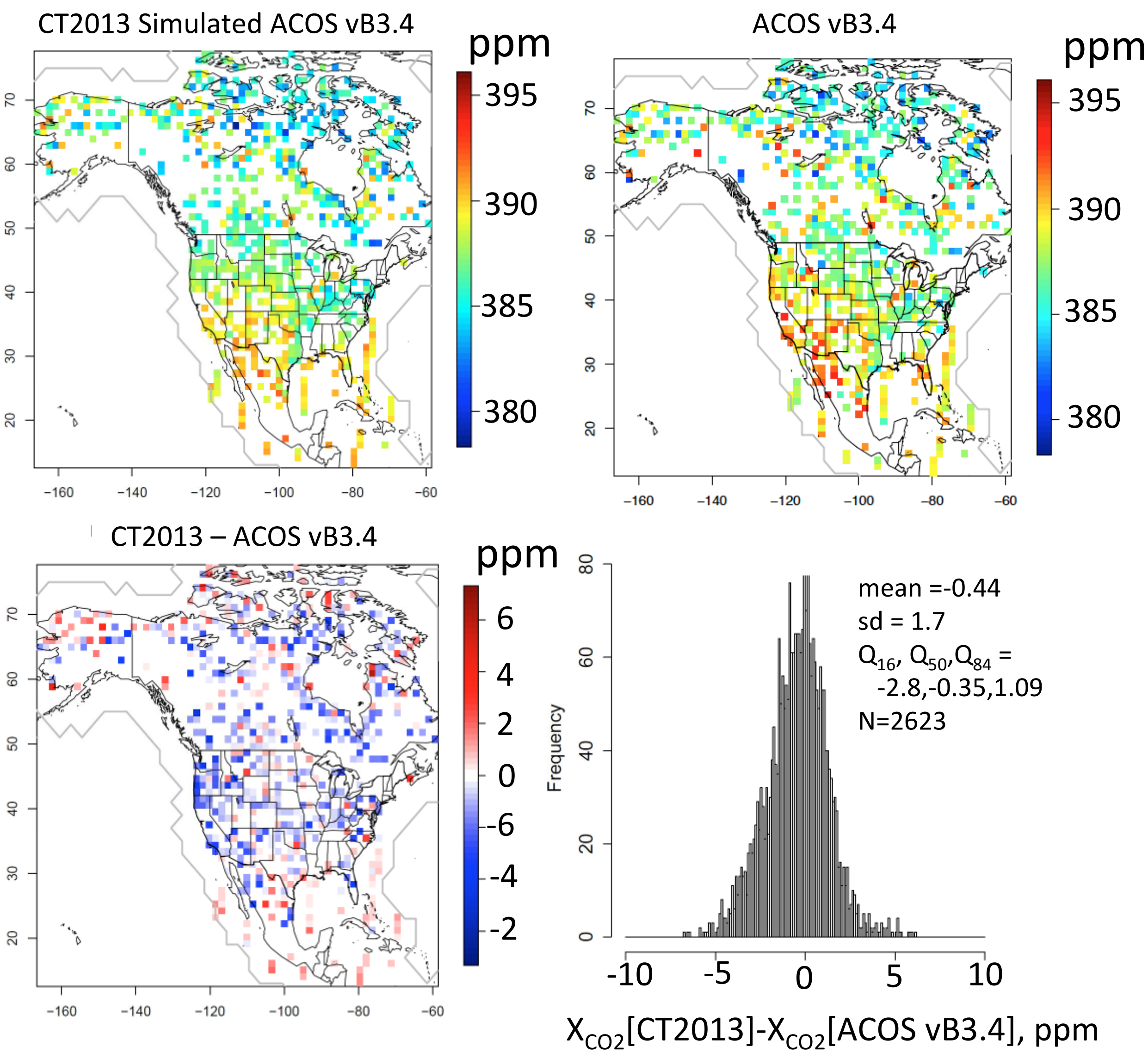
Posterior Simulated OBS – CASA OBS



mean=0
sd=0.2
Q16=-0.14
Q50=0
Q84=0.16

Despite similarity of posterior fluxes with and without GOSAT ACOS observations, improvement in residuals is evident.

July 2010 Forward Simulation: STILT-WRF Footprints Convolved with CT2013 fluxes and with CT2013 Boundary Values

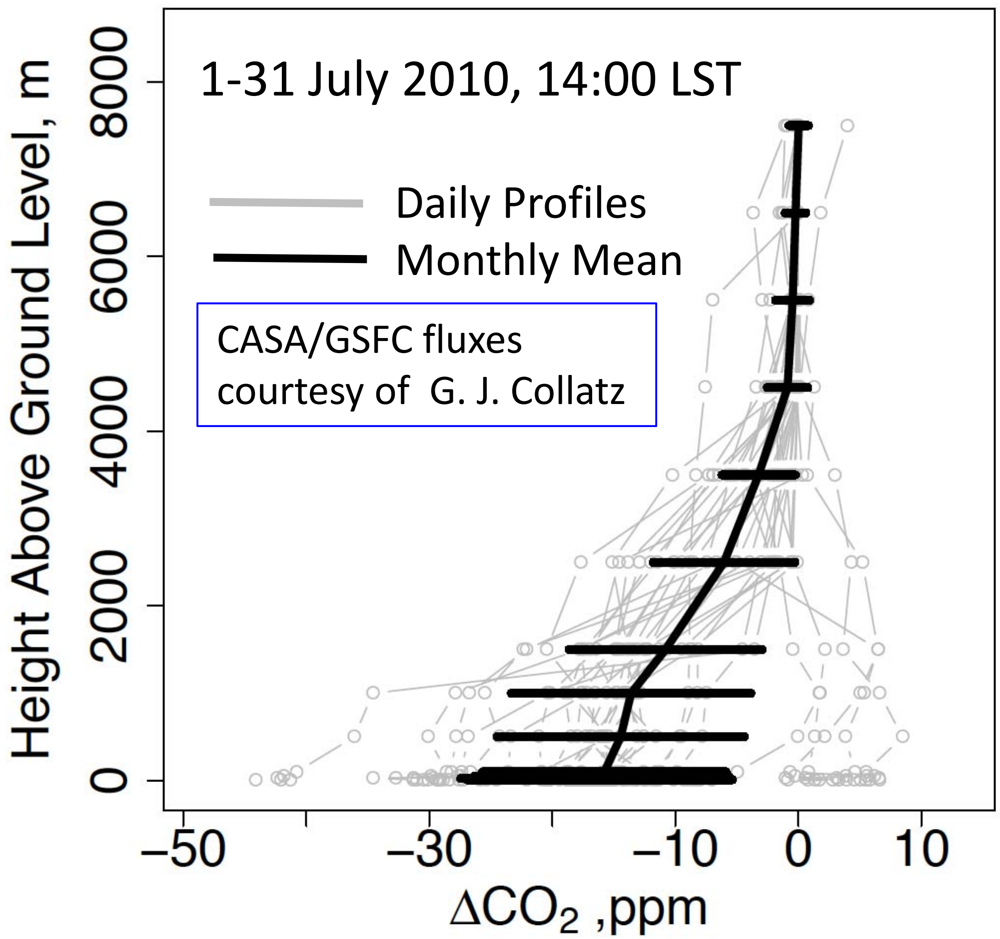


CT2013 has already been optimized against in situ observations, but comparisons show significant* biases and considerable scatter compared to ACOS observations.

*Significant compared to magnitude of flux signatures in X_{CO2}

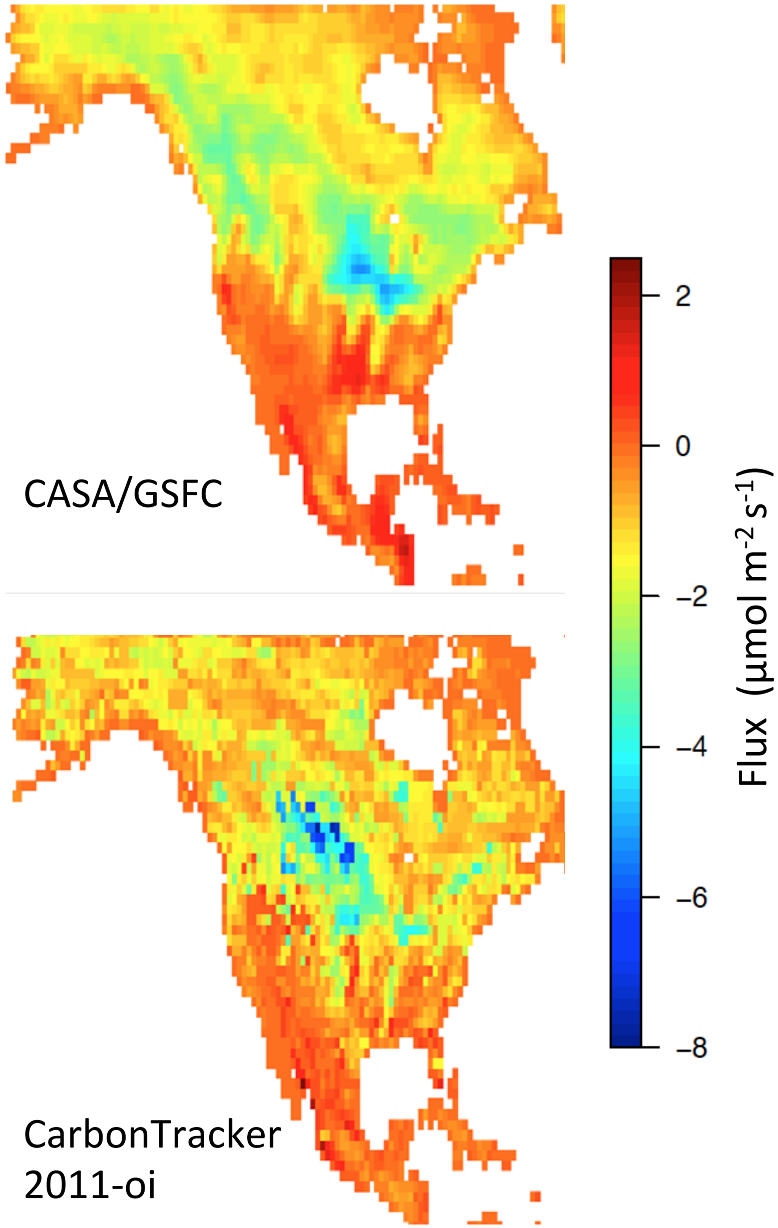
CarbonTracker-Lagrange profiles corresponding to the Park Falls NOAA/UWI WLEF-TV Tall Tower and TCCON site:

CASA/GSFC Net Ecosystem Exchange

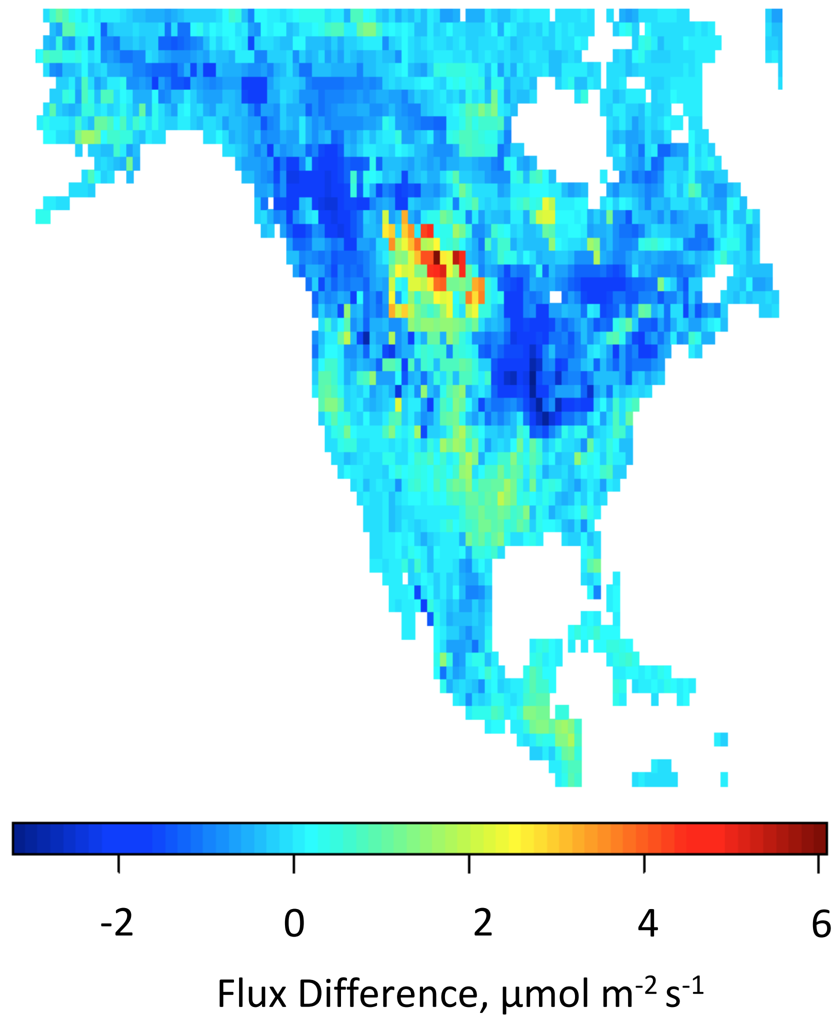


- Contrast between surface and column data provides information about surface versus boundary influences.
- Aircraft versus surface is even better, but aircraft data is very sparse.

Consider differences between two biological flux estimates:

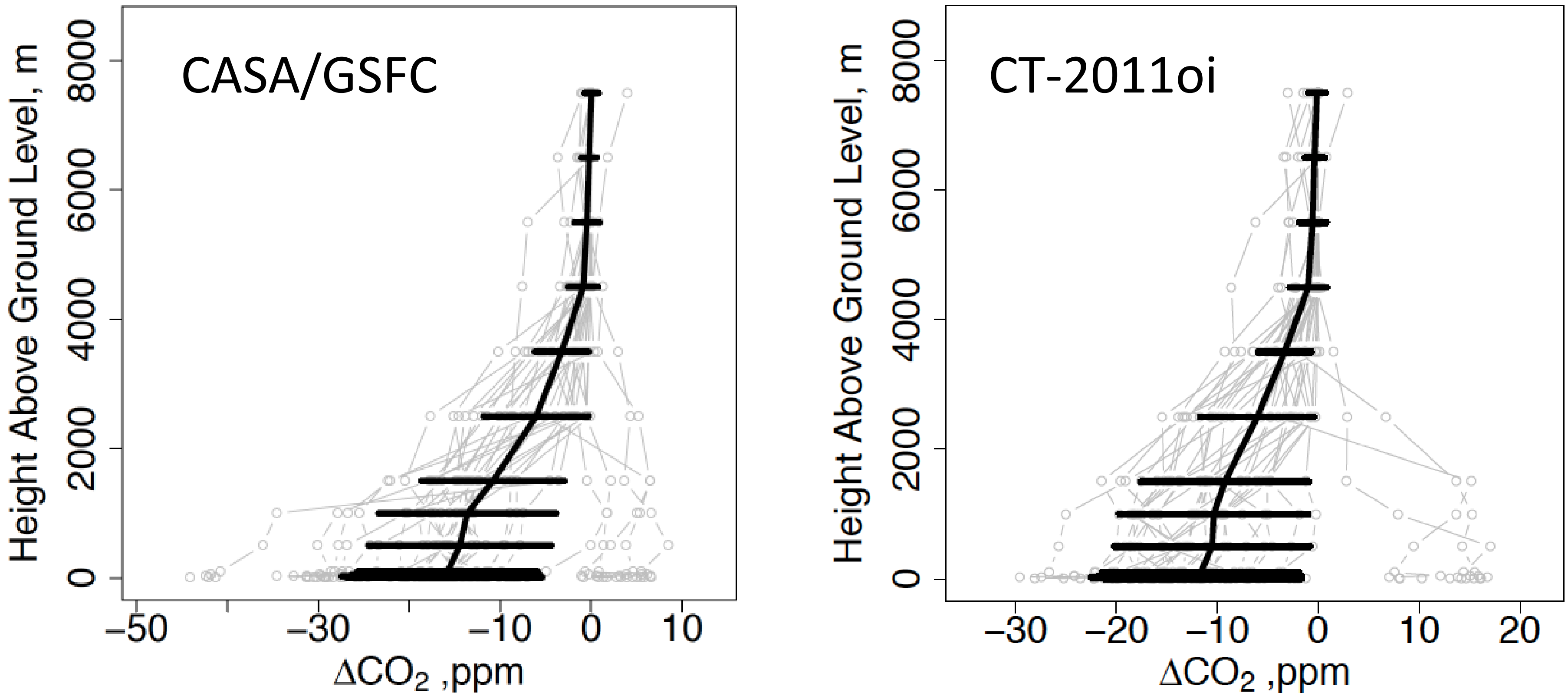


Monthly Mean July 2010
CASA/GSFC minus CarbonTracker



CASA/GSFC fluxes courtesy of G. J. Collatz; CarbonTracker fluxes courtesy of A. Jacobson.

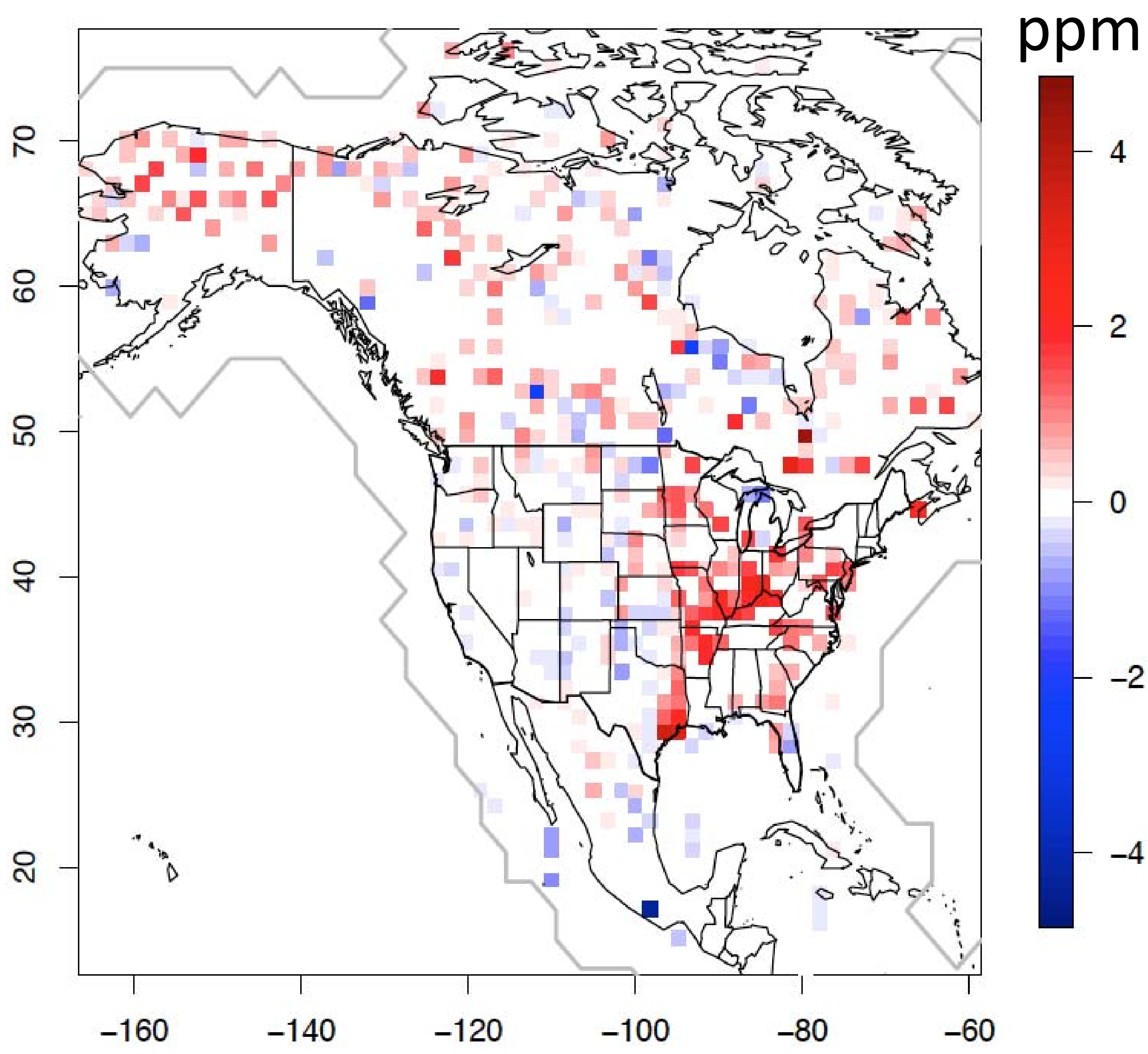
Net Ecosystem Exchange



- Mean profiles look similar, but CASA/GSFC has higher uptake (note x-axis scales are different).

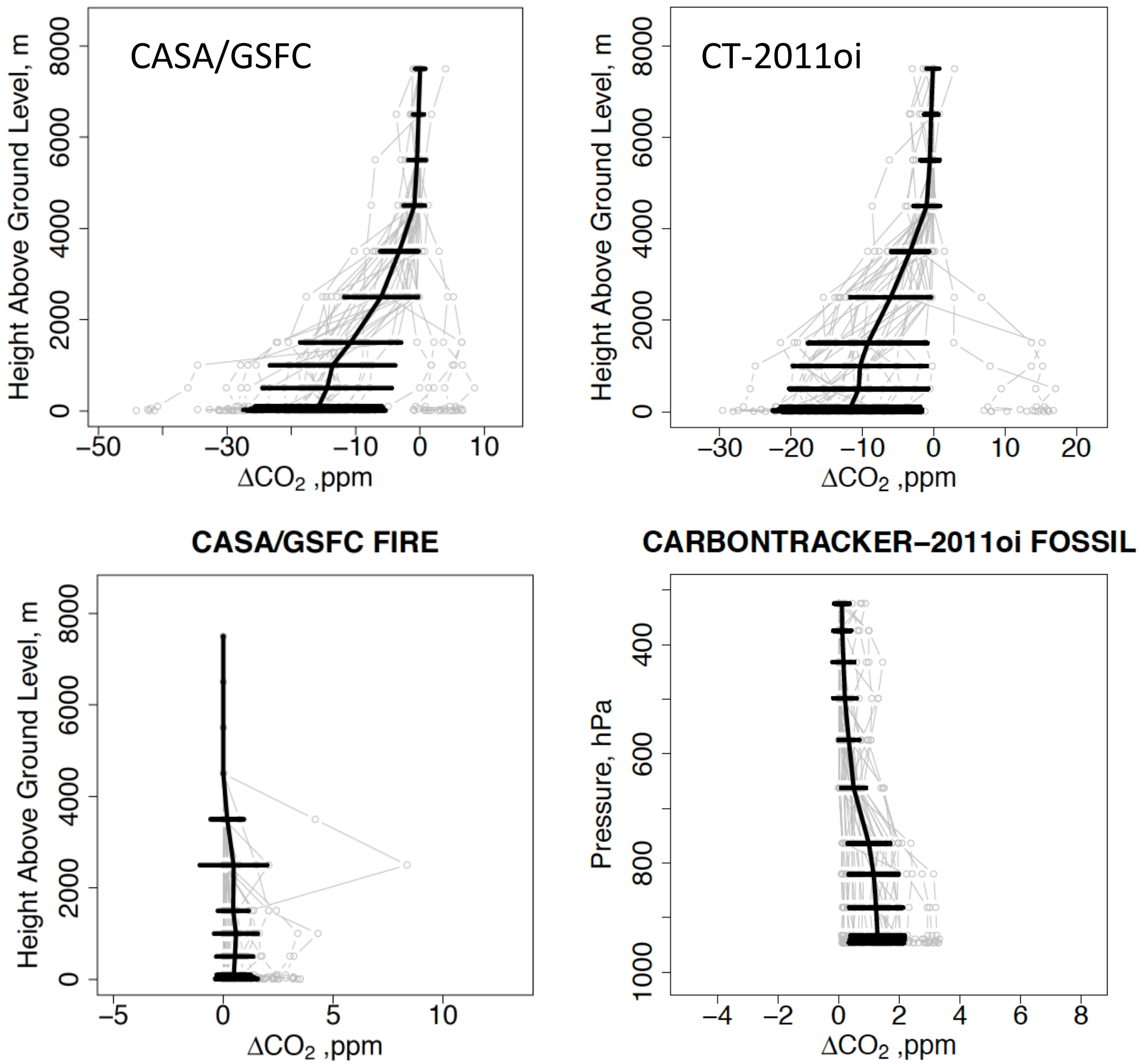
- CASA/GSFC fluxes courtesy of G. J. Collatz
- CarbonTracker fluxes courtesy of A. Jacobson

CarbonTracker –CASA NEE



CarbonTracker-Lagrange profiles corresponding to Park Falls, WI:

Net Ecosystem Exchange



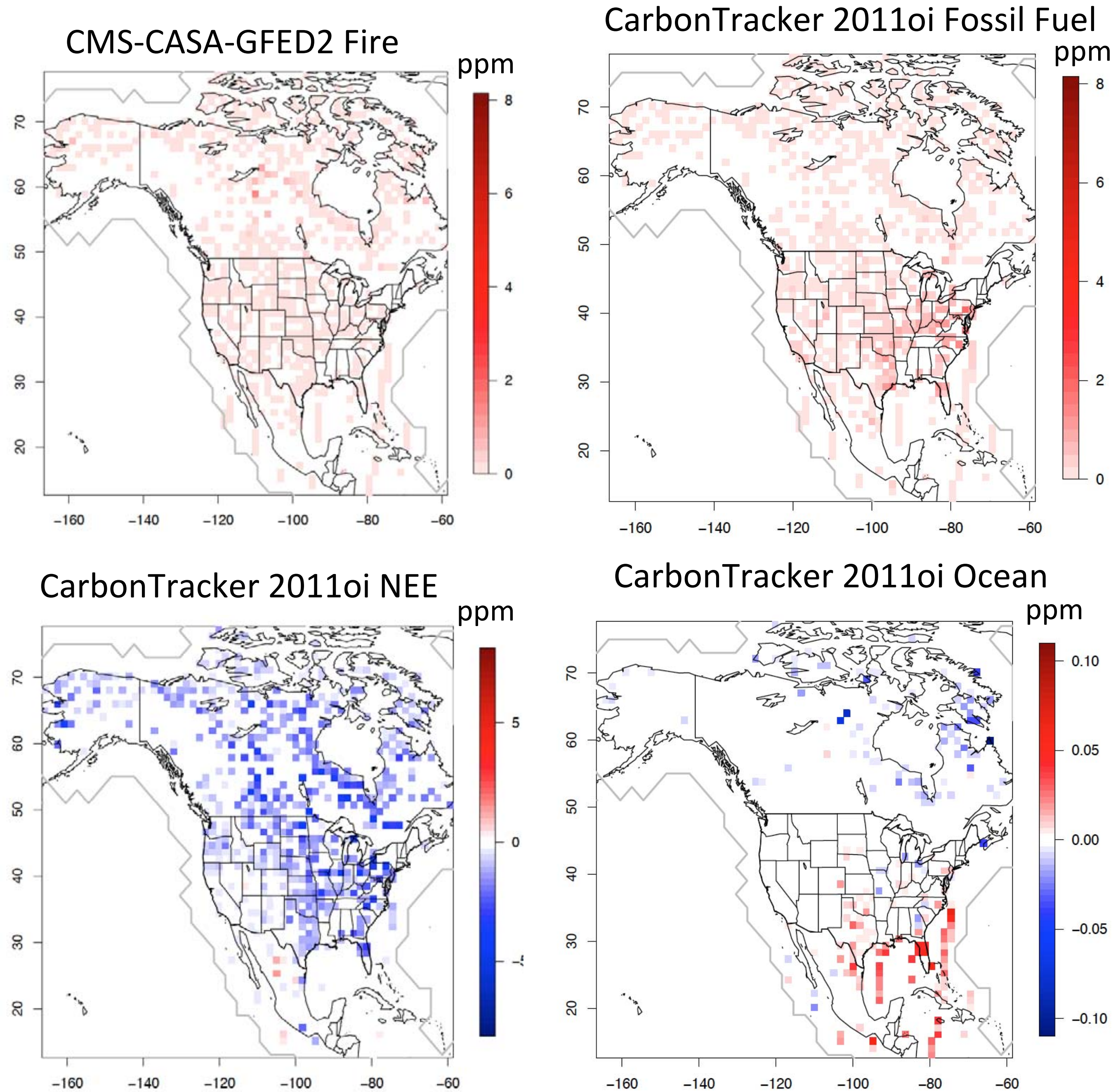
1-31 July 2010, 14:00 LST

Daily Profiles

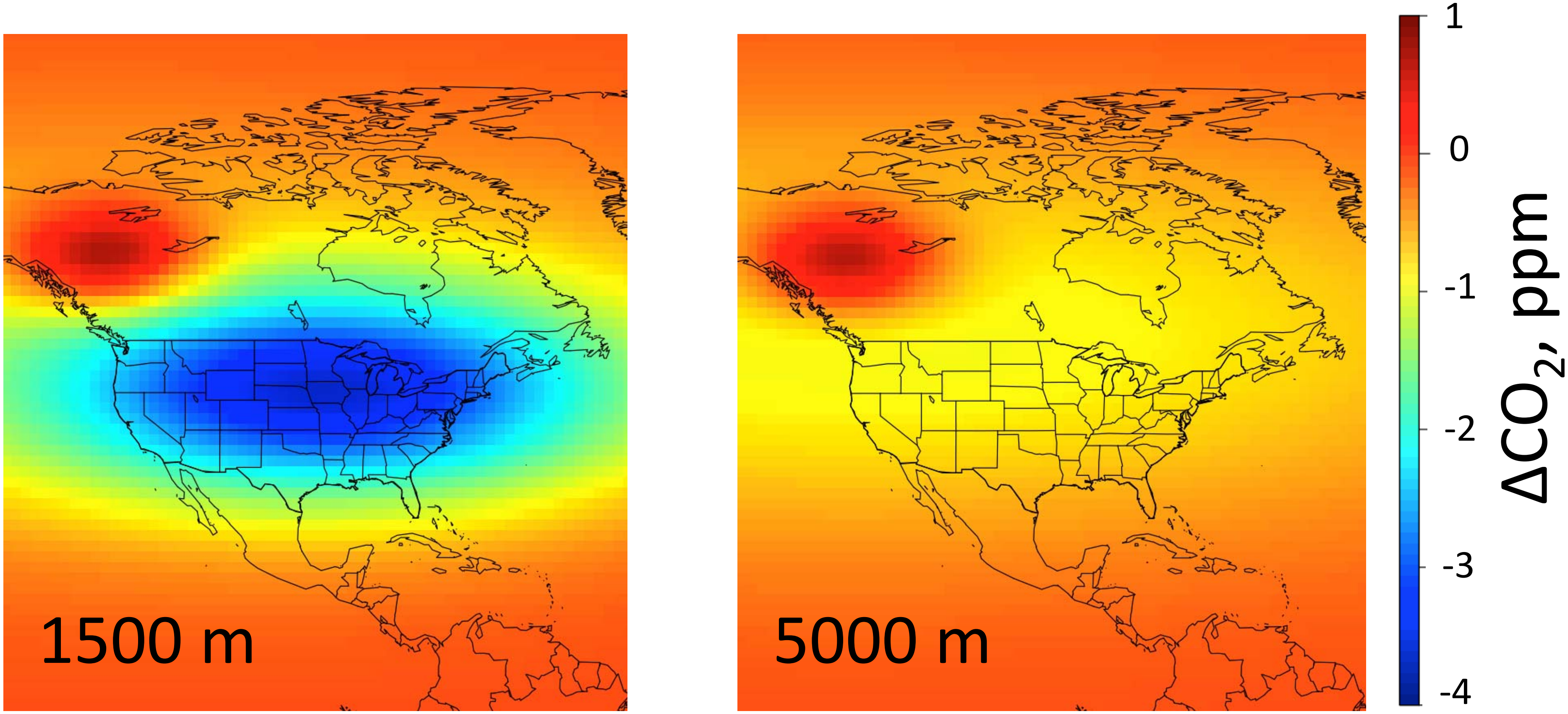
Monthly Mean

- Impact of surface fluxes minimal above 3000m
- CASA/GSFC versus CT-2011oi NEE differences subtle
- Sporadic fire influence aloft.
- Small fossil fuel signal.

- CASA/GSFC fluxes courtesy of G. J. Collatz
- CarbonTracker fluxes courtesy of A. Jacobson

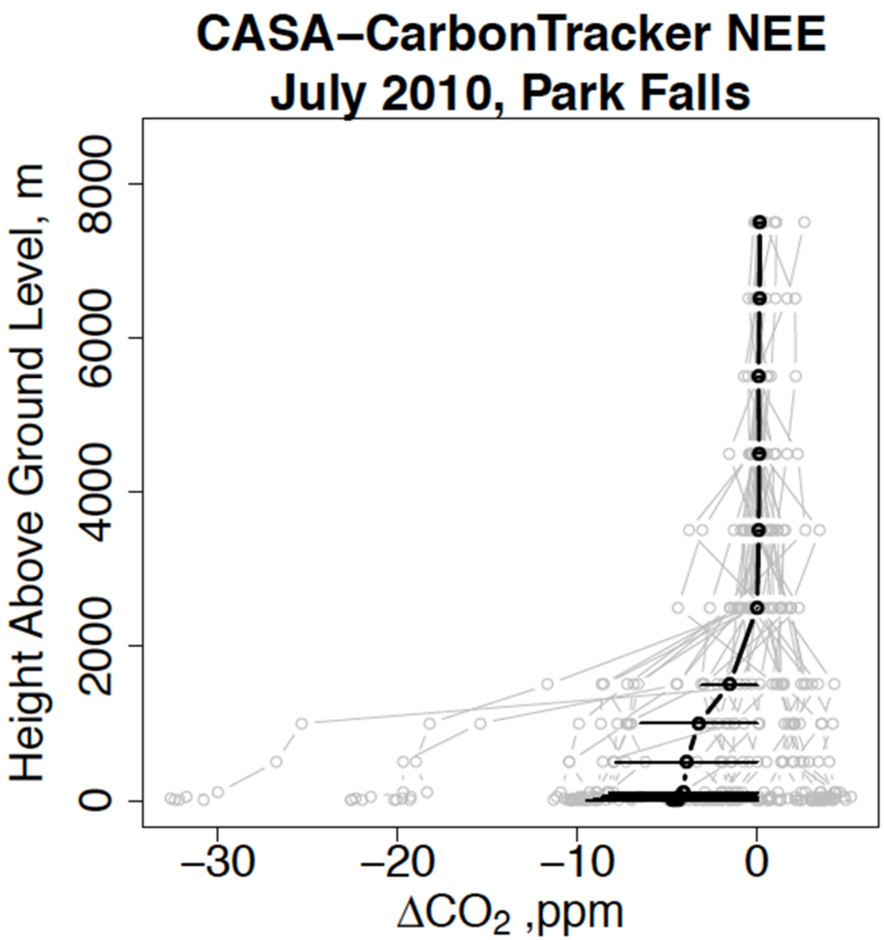

CMS-CASA-GFED2 Fire
ppm
0
2
4
6
8
CarbonTracker 2011oi Fossil Fuel
ppm
0
2
4
6
8
CarbonTracker 2011oi NEE
ppm
0
5
CarbonTracker 2011oi Ocean
ppm
0.10
0.05
0.00
−0.05
−0.10
20
30
40
50
60
70
−160
−140
−120
−100
−80
−60

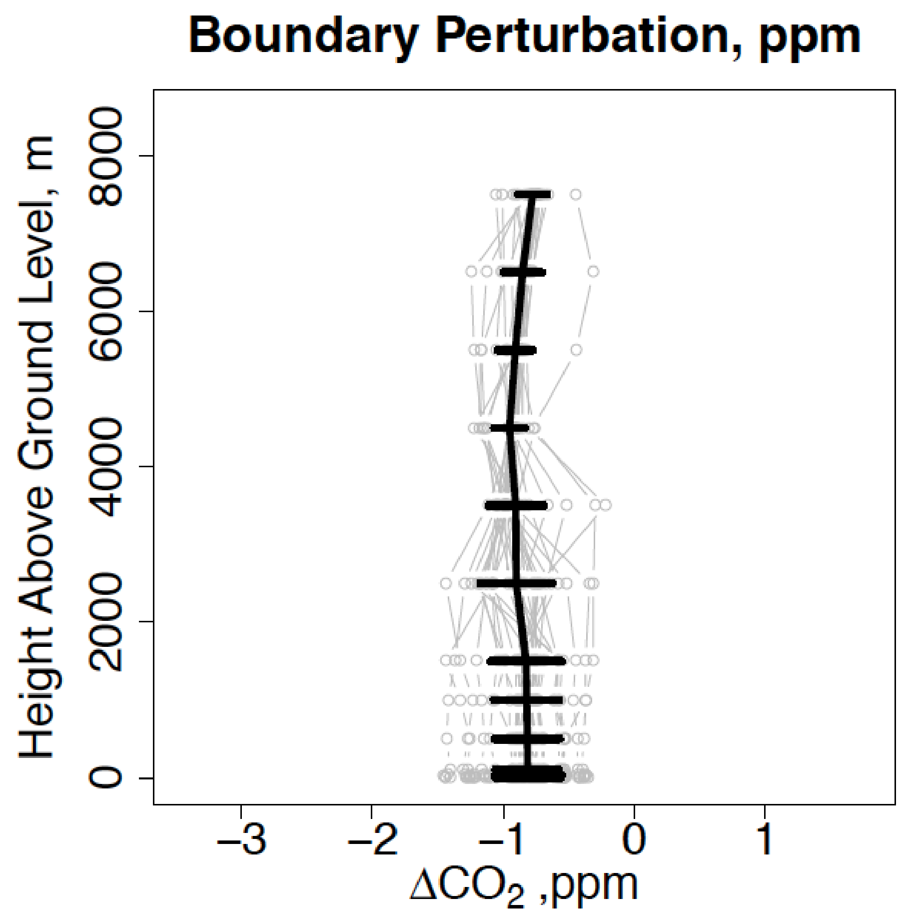
Hypothetical Boundary/Initial Value Perturbation



- Sum of exponential perturbations f(time, lat, lon, alt)
- Roughly consistent with CarbonTracker Simulated minus Observed

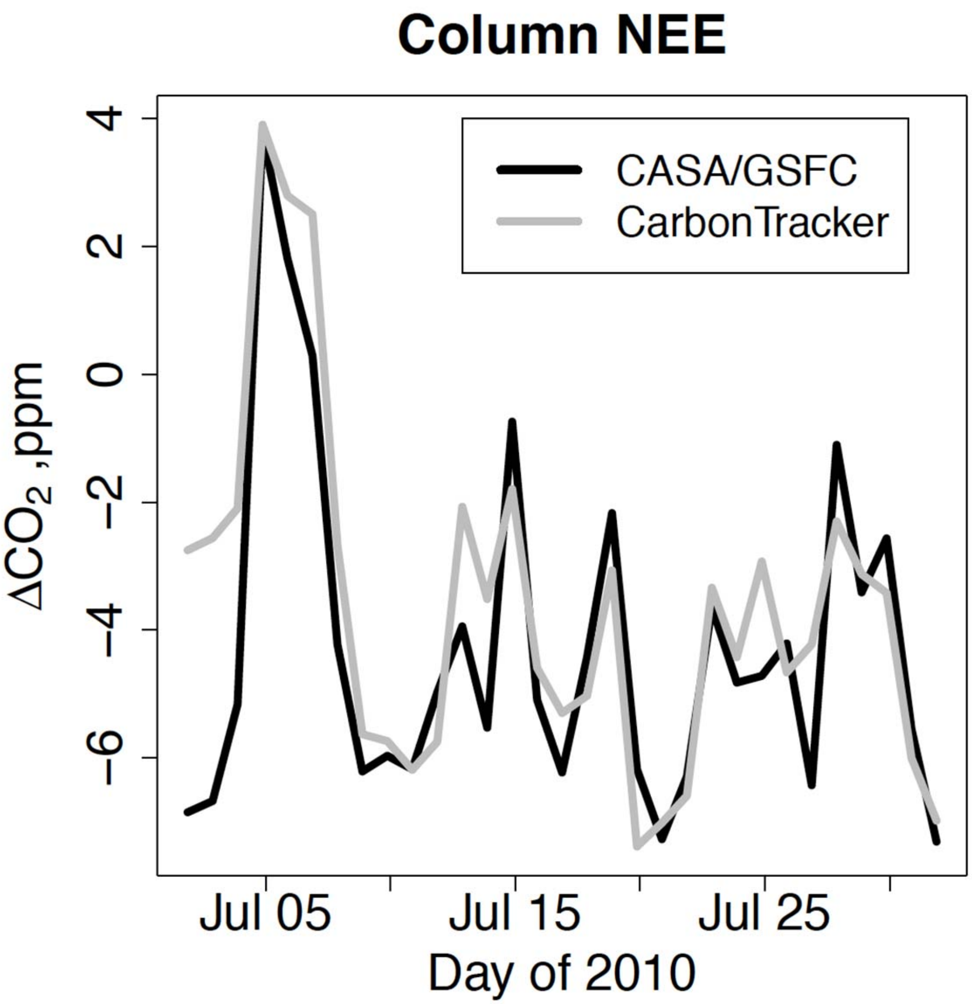
Flux Differences versus Boundary Perturbation: Profile Simulations





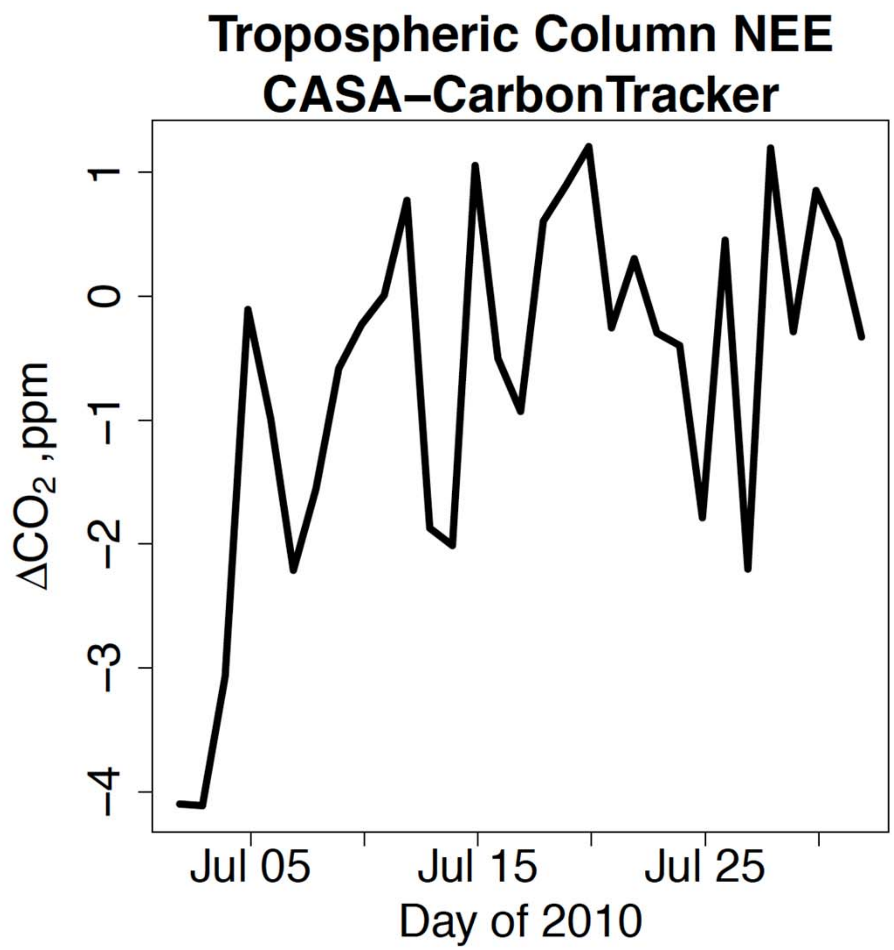
Flux differences confined to lowest 2 km. Boundary perturbation evenly distributed over all altitudes.

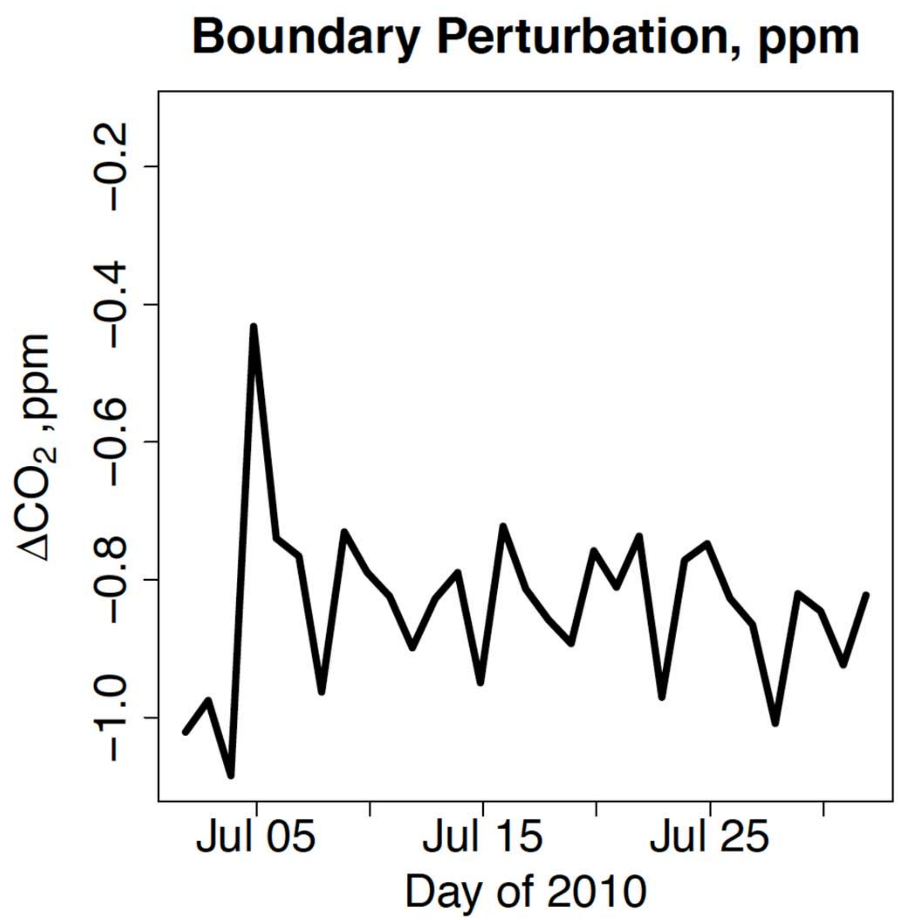
Different Flux Scenarios: Column Simulations



- Signature of flux difference in the column is subtle
- Idealized tropospheric column: uniform weighting function up to 8 km and zero weight at higher altitudes.

Flux Differences versus Boundary Perturbation: Idealized Column Simulations





Similar magnitude. Could be difficult to distinguish between boundary and surface influences if using only column data.

Plans for CMS 2014

- **Team:** A. Andrew s (NOAA), J. Miller (U of CO & NOAA), C. O'Dell (CSU), A. Michalak (Carnegie Inst. for Science & Stanford), M. Mountain (AER), T. Nehrkorn (AER)
- Merger of A. Andrews CMS – 2012 (North America) and J. Miller CMS-2012 (Amazonia) Lagrangian Modeling efforts
- Improve, Extend and Apply CT-L modeling tools using remote sensing and in situ data.
  - Amazonia: 2010-2011, 2015
  - North America: 2007-2015
  - Geostatistical Inversions, e.g., use of OCO-2 fluorescence
- Transport model comparisons
- Develop and implement strategy for simulating OCO-2 observations
  - Too many observations to simulate each scene, along track averaging will be required
  - Increase sensitivity to North America by extending domain over the Atlantic?
- Compare with NASA-CMS flux project optimized fluxes and mole fractions
- Investigate consistency between in situ and remote sensing data

LETTER

doi:10.1038/nature12957

Drought sensitivity of Amazonian carbon balance revealed by atmospheric measurements

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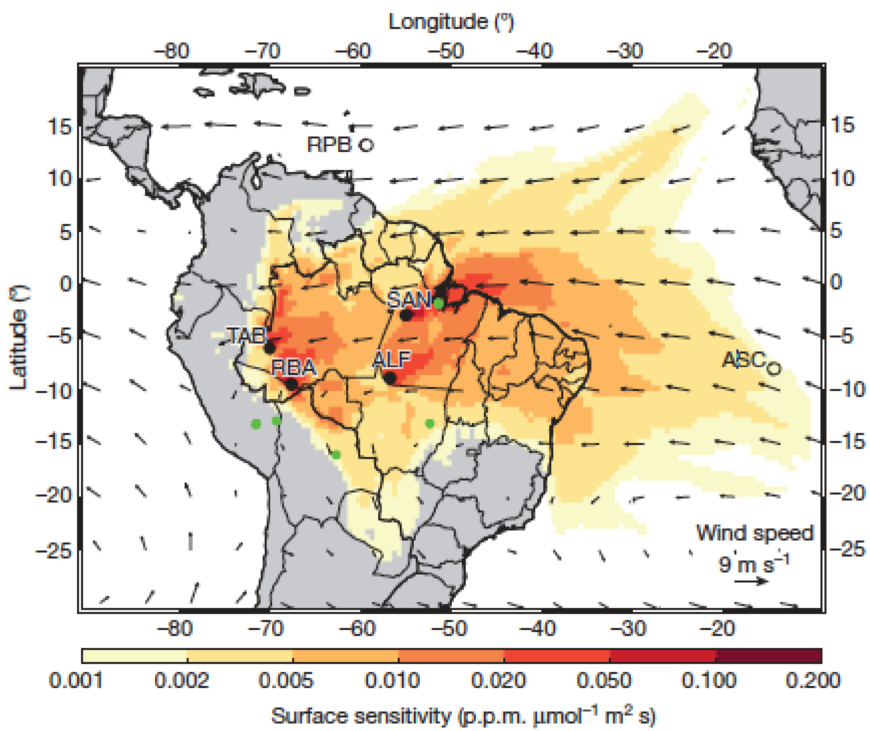

- Mass balance study of Amazon carbon fluxes using newly available aircraft observations
- We will apply Lagrangian modeling tools to the same 2010-2011 dataset and to 2015 with OCO-2 data
- Transport model comparisons are planned (BRAMS-STILT versus WRF-STILT)

Table 1 | Summary of annual carbon flux estimates

Sites	TAB	RBA	SAN	ALF	
	2010 fluxes ($g C m^{-2} d^{-1}$)				Scaled 2010 flux ($Pg C yr^{-1}$)†
Total	0.15 ± 0.10	0.17 ± 0.11	0.33 ± 0.50	0.29 ± 0.15	0.48 ± 0.18
Fire	0.13 ± 0.05	0.17 ± 0.06	0.57 ± 0.45	0.28 ± 0.09	0.51 ± 0.12
NBE	0.02 ± 0.11	0.00 ± 0.13	−0.25 ± 0.70	0.01 ± 0.17	−0.03 ± 0.22
	2011 fluxes ($g C m^{-2} d^{-1}$)				Scaled 2011 flux ($Pg C yr^{-1}$)†
Total	−0.10 ± 0.07	−0.04 ± 0.07	0.46 ± 0.20	0.24 ± 0.06	0.06 ± 0.10
Fire	0.08 ± 0.03	0.09 ± 0.03	0.44 ± 0.51	0.16 ± 0.04	0.30 ± 0.10
NBE	−0.18 ± 0.08	−0.13 ± 0.08	0.02 ± 0.84	0.08 ± 0.07	−0.25 ± 0.14
Area of influence ($\times 10^6 km^2$)*	2.53	3.67	0.59	1.31	

The uncertainties are standard errors calculated by propagating uncertainties in all equations using a Monte Carlo approach, and then taking half the value of the 16th–84th percentile range. A bootstrapping approach to calculate the standard error (2.5th–97.5th percentile range) yields slightly smaller values.

* Back-trajectory ensemble envelope (that is, the total area of influence of a measuring site as estimated from wind back-trajectory ensembles).

† 'Scaled' means the flux estimates have been scaled to the tropical South America forested area, assuming an Amazon forest area of $6.77 \times 10^6 km^2$ (ref. 30).

Big difference between wet and dry years.