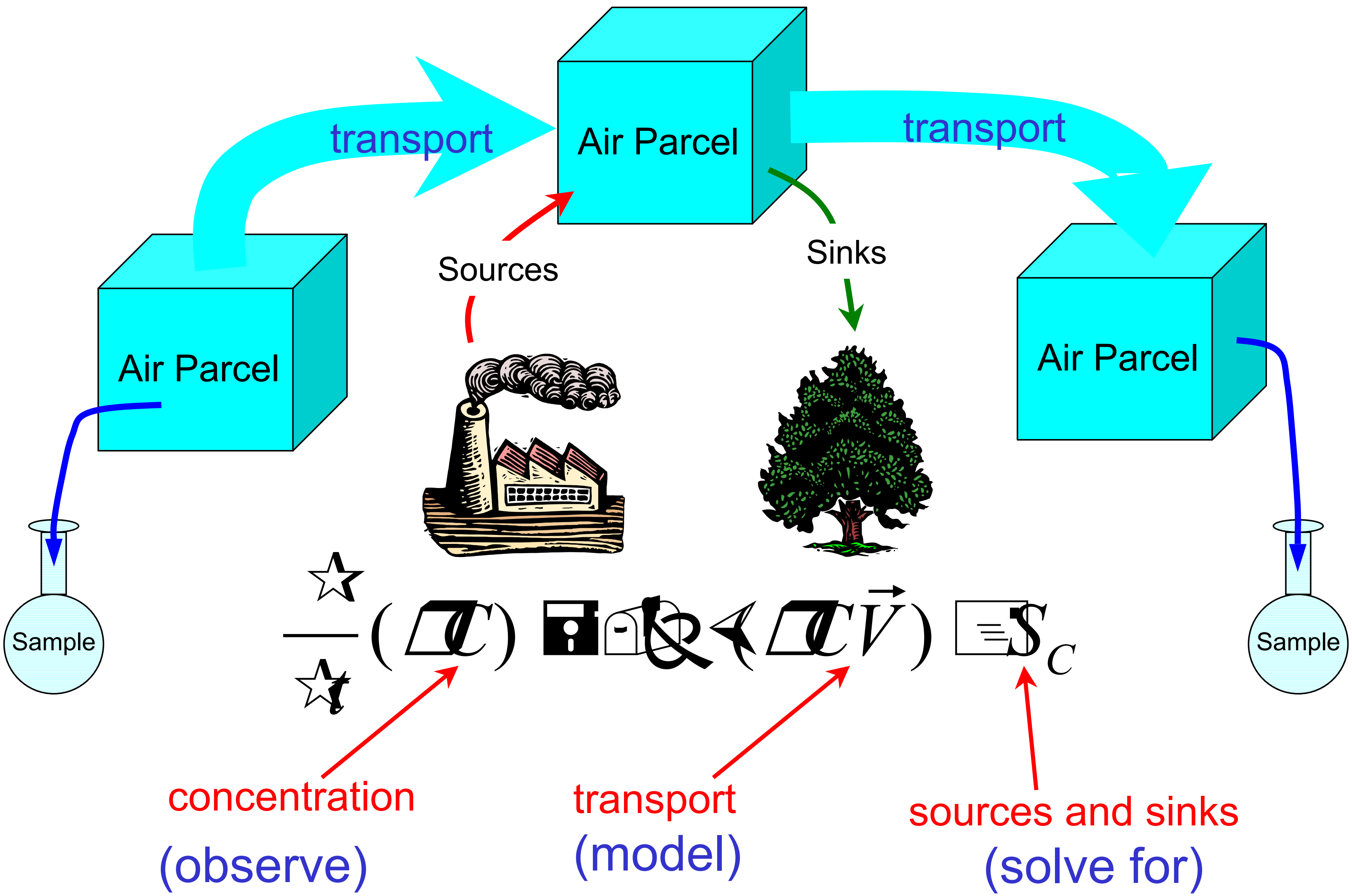
Inverse Modeling of CO_2



Synthesis Inversion

- Decompose total emissions into ***M*** "basis functions"
- Use atmospheric transport model to generate ***G***
- Observe ***d*** and ***N*** locations
- Invert ***G*** to find ***m***

$$\begin{bmatrix} d_1 \\ d_2 \\ \cdot \\ \cdot \\ d_N \end{bmatrix} = \begin{bmatrix} G_{11} & G_{12} & \cdot & \cdot & G_{1M} \\ G_{21} & G_{22} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ G_{N1} & G_{N2} & \cdot & \cdot & G_{NM} \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \cdot \\ \cdot \\ m_M \end{bmatrix}$$

data ***transport*** ***fluxes***

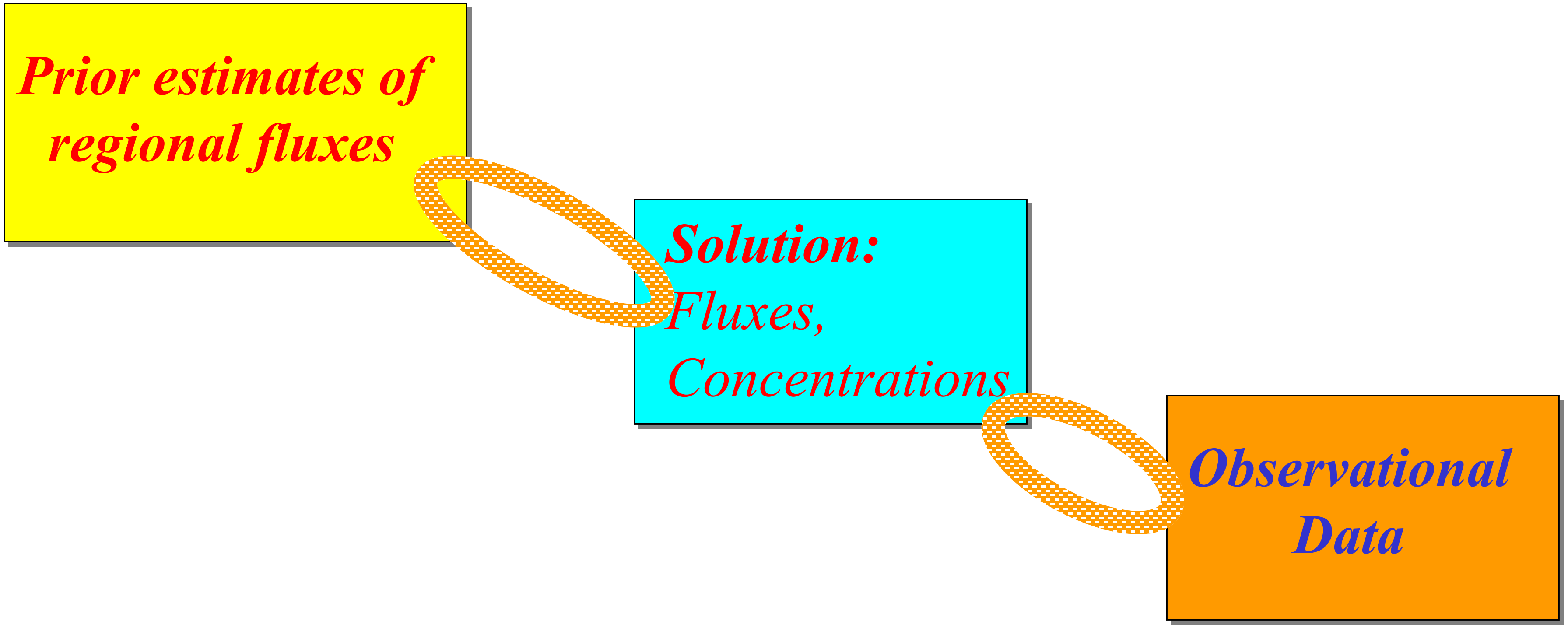
$$d_1 = G_{11}\, m_1 + G_{12}\, m_2 + \ldots + G_{1N}\, m_N$$

CO_2 sampled at **location 1**

partial derivative of CO_2 at **location 1** with respect to emissions of **type 2**

Strength of emissions of **type 2**

Rubber Bands

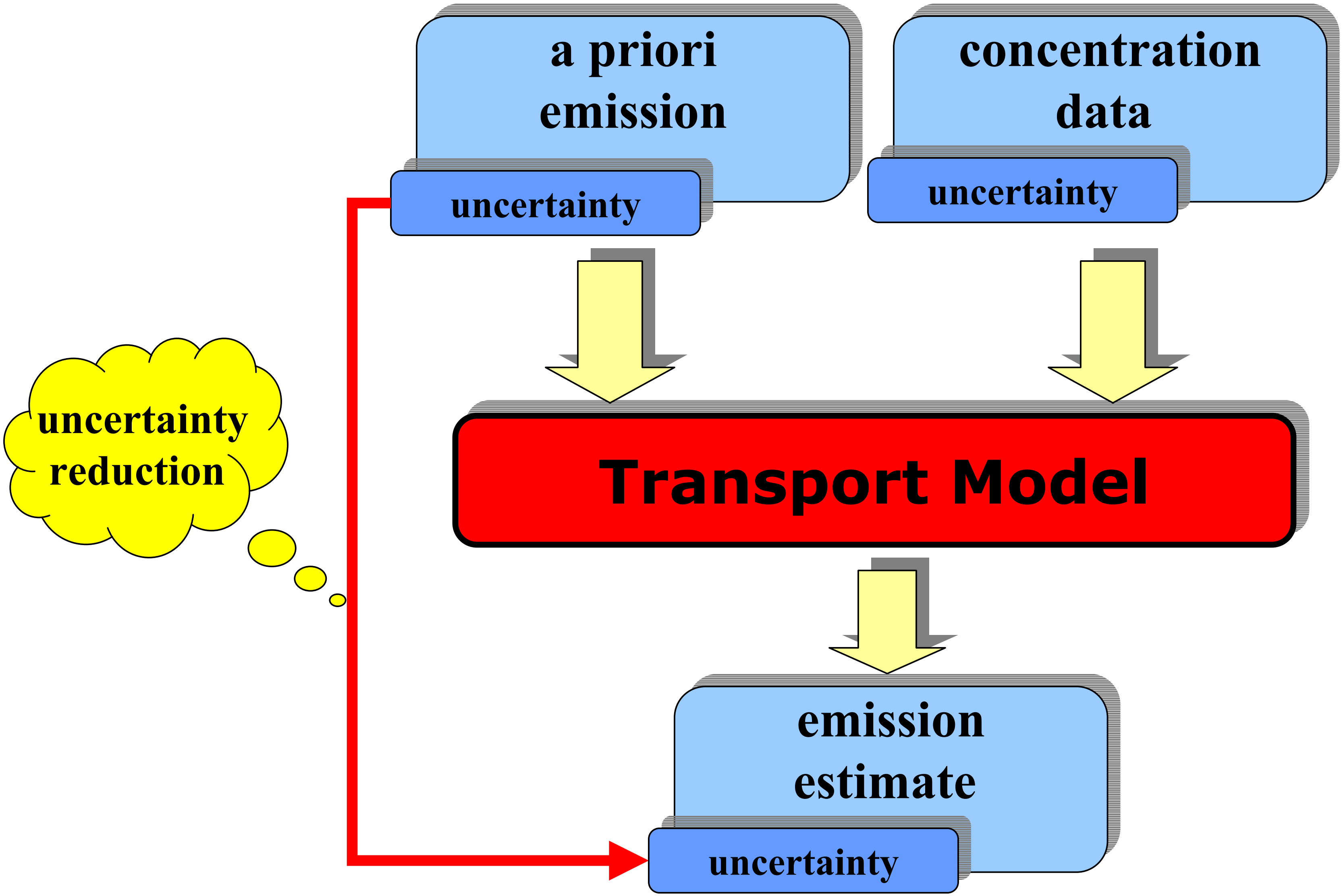


- Inversion seeks a compromise between detailed reproduction of the data and fidelity to what we think we know about fluxes
- The elasticity of these two "rubber bands" is adjustable

Accounting for "Error"

- Sampling, contamination, analytical accuracy (very small)
- Representativeness error (large in some areas, small in others)
- Transport simulation error (large for specific cases, smaller for "climatological" transport)
- All of these require a "looser" fit to the data

Bayesian Inversion Technique



Bayesian Inversion Formalism

Were the problem simple:

$$\vec{d} = \hat{G}\vec{m}; \qquad \vec{m} = \hat{G}^{-1}\vec{d}$$

But problem is ill-conditioned. Use Singular Value Decomposition (SVD) to minimize a cost function:

$$S(m) = \frac{1}{2}\left[\left(\hat{G}\vec{m} - \vec{d}_{obs}\right)^T \hat{C}_d^{-1}\left(\hat{G}\vec{m} - \vec{d}_{obs}\right) + \left(\vec{m} - \vec{m}_p\right)^T \hat{C}_m^{-1}\left(\vec{m} - \vec{m}_p\right)\right]$$

Solution is given by

$$\vec{m}_{est} = \vec{m}_p + \left(\hat{G}^T \hat{C}_d^{-1}\hat{G} + \hat{C}_m^{-1}\right)^{-1} \hat{G}^T \hat{C}_d^{-1}\left(\vec{d}_{obs} - \hat{G}\vec{m}_p\right)$$

Inferred flux ($\vec{m}_{est}$)

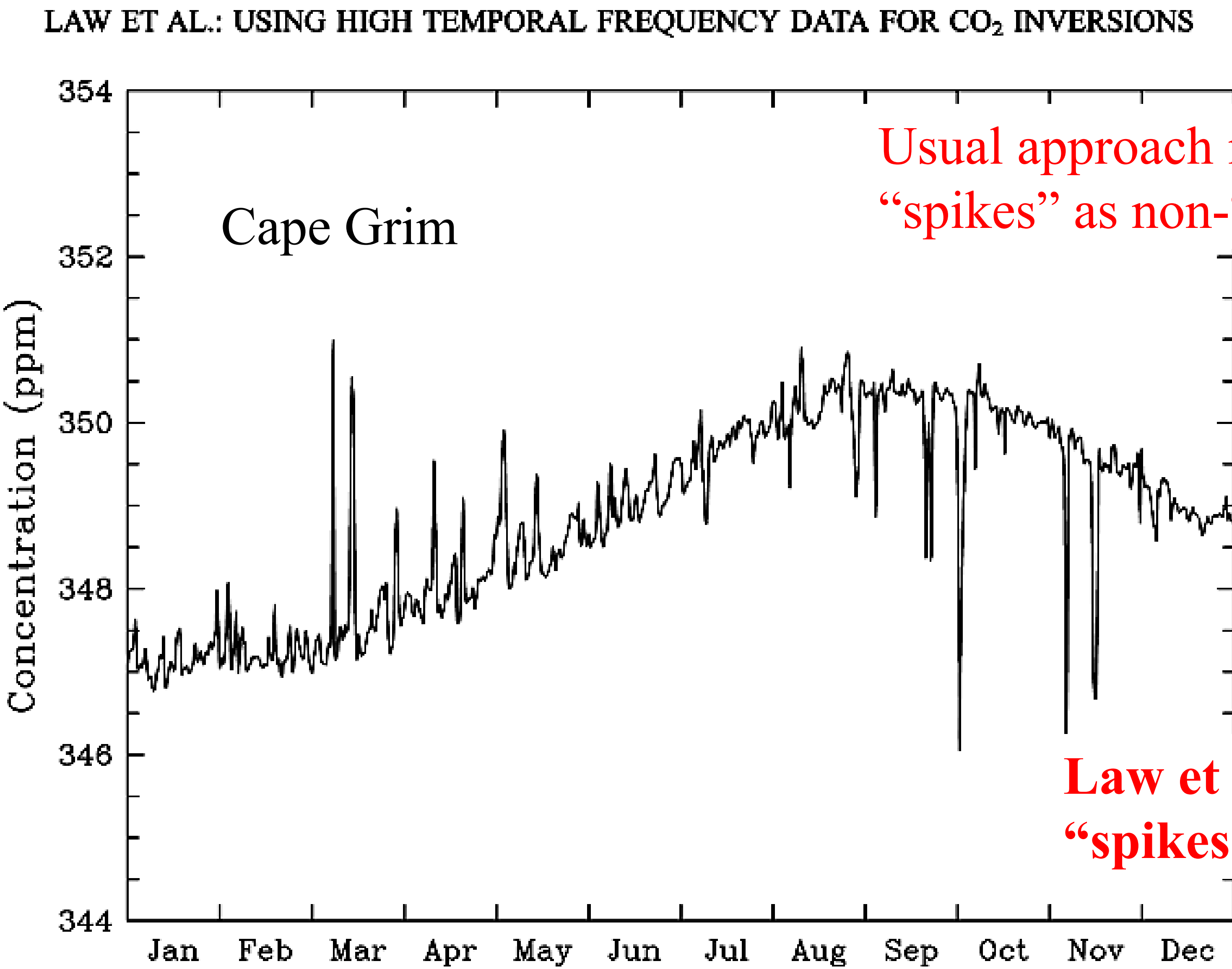
Prior Guess ($\vec{m}_p$)

"Data" Uncertainty ($\hat{C}_d$)

Flux Uncertainty ($\hat{C}_m$)

observations ($\vec{d}_{obs}$)

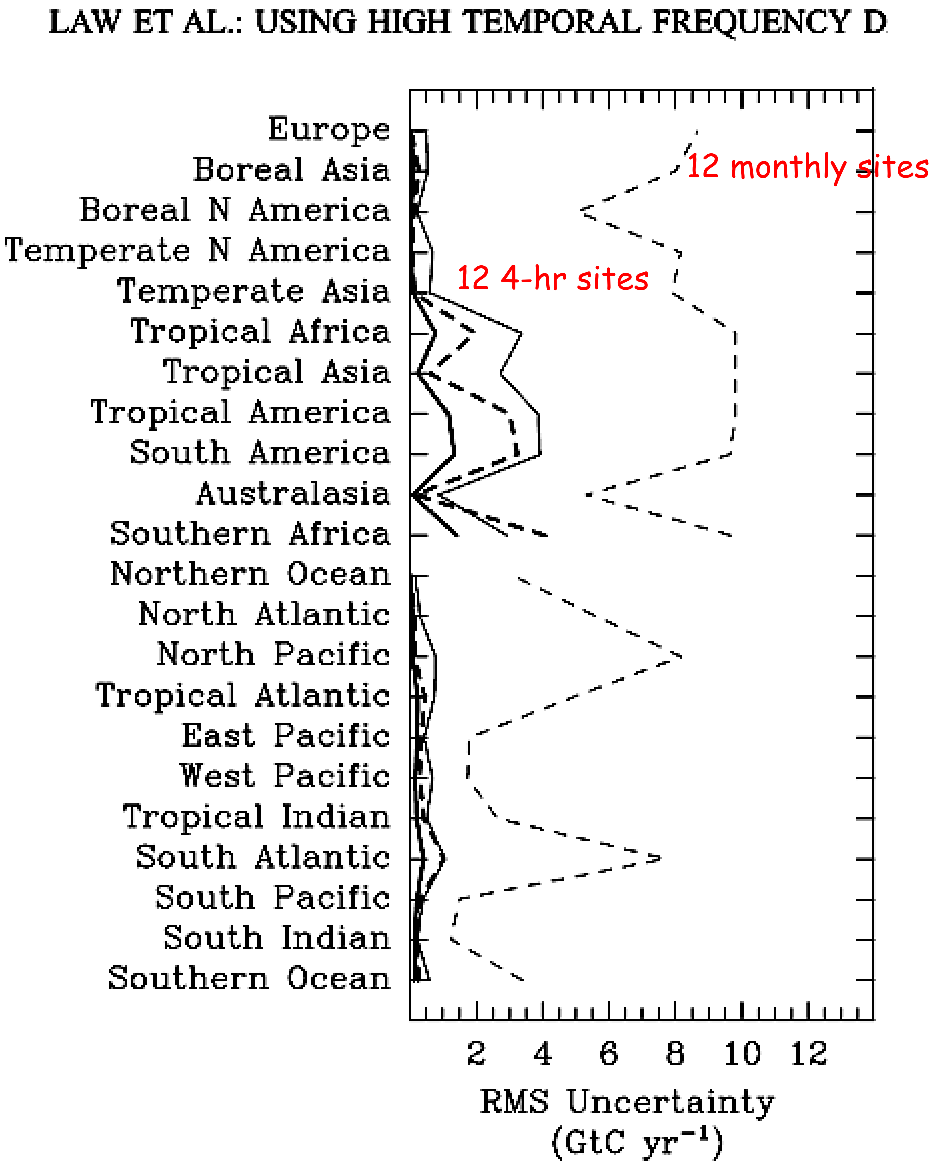
Signal? Noise? Which is which?



Usual approach is to exclude "spikes" as non-"background"

Law et al inverted the "spikes" instead!

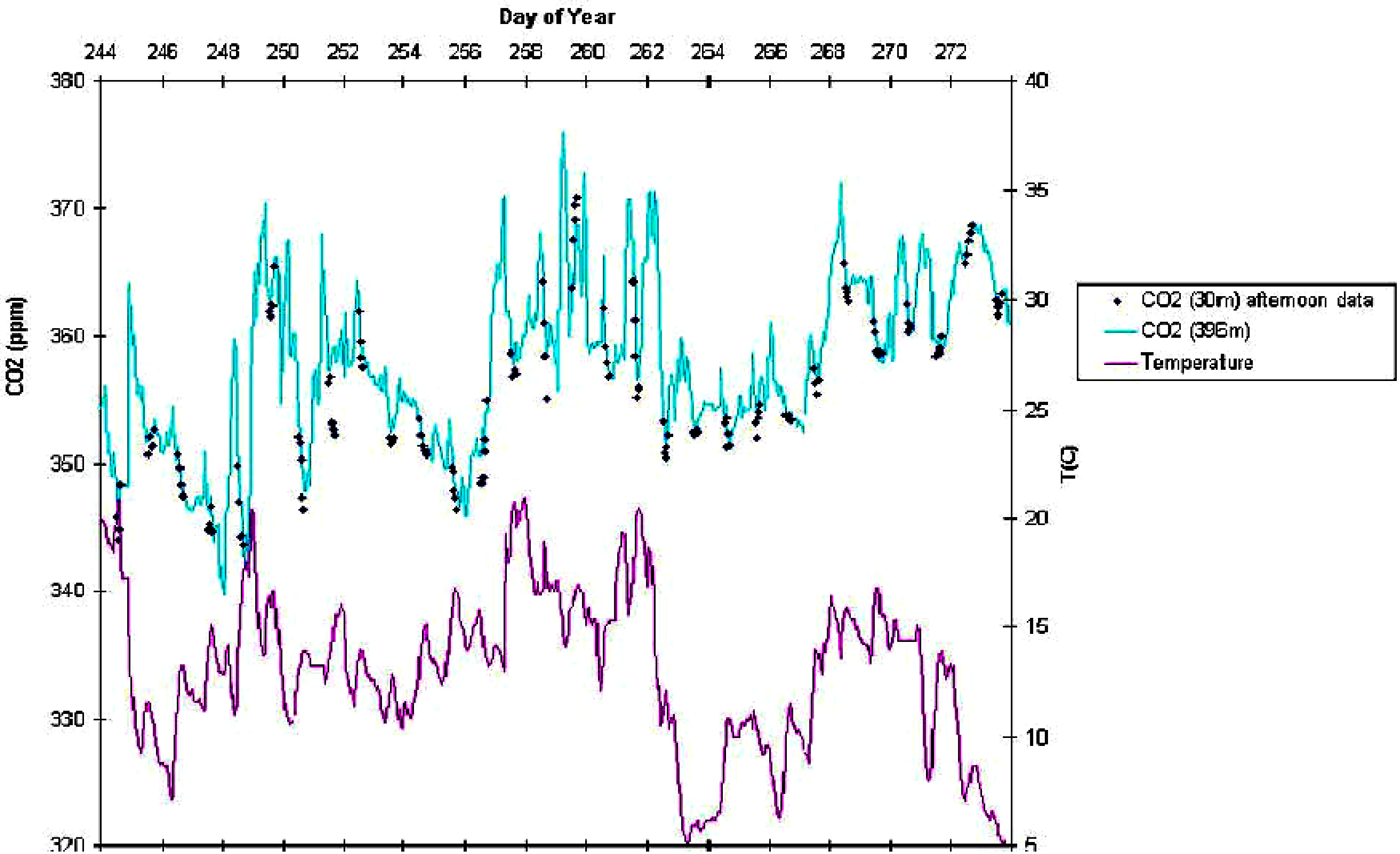
Law et al Inversion Result



Used "pseudodata" approach to estimate flux uncertainty for four cases:

- 12 sites with monthly mean data
- Same 12 sites with data every 4 hours
- 83 sites monthly
- 83 sites @ 4 hrs

WLEF: Aug 1997

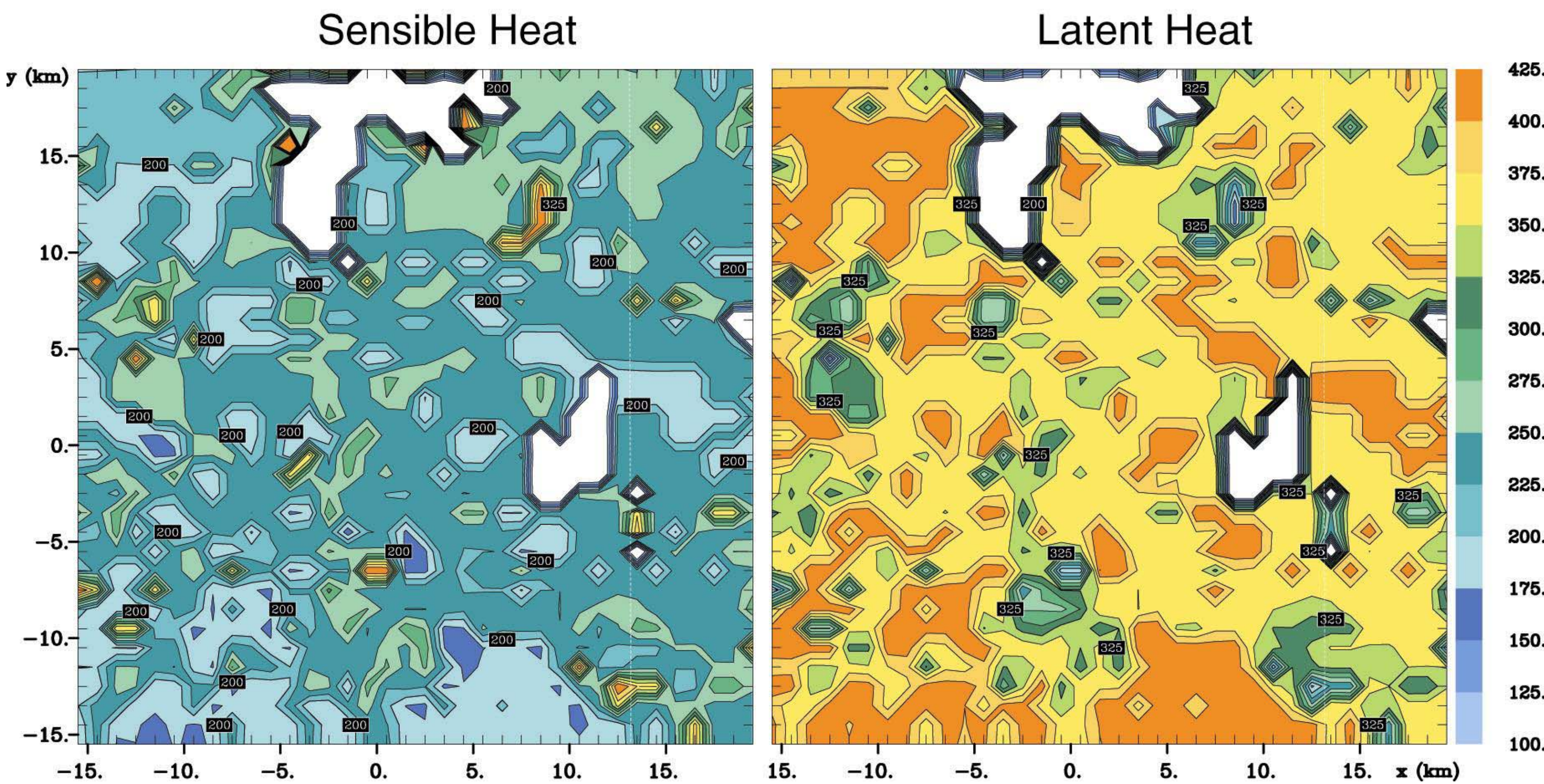


Mesoscale Modeling System

- CSU Regional Atmospheric Modeling System (RAMS)
- Grids may be nested up to six layers deep
- Outer nest as big as North American continent
- Inner nest is a large-eddy simulation (Δx ~ 10 to 50 m)
- Flexible physical parameterizations to handle large range of spatial scales
- Fully coupled to SiB2 with surface parameters defined from remotely-sensed data products

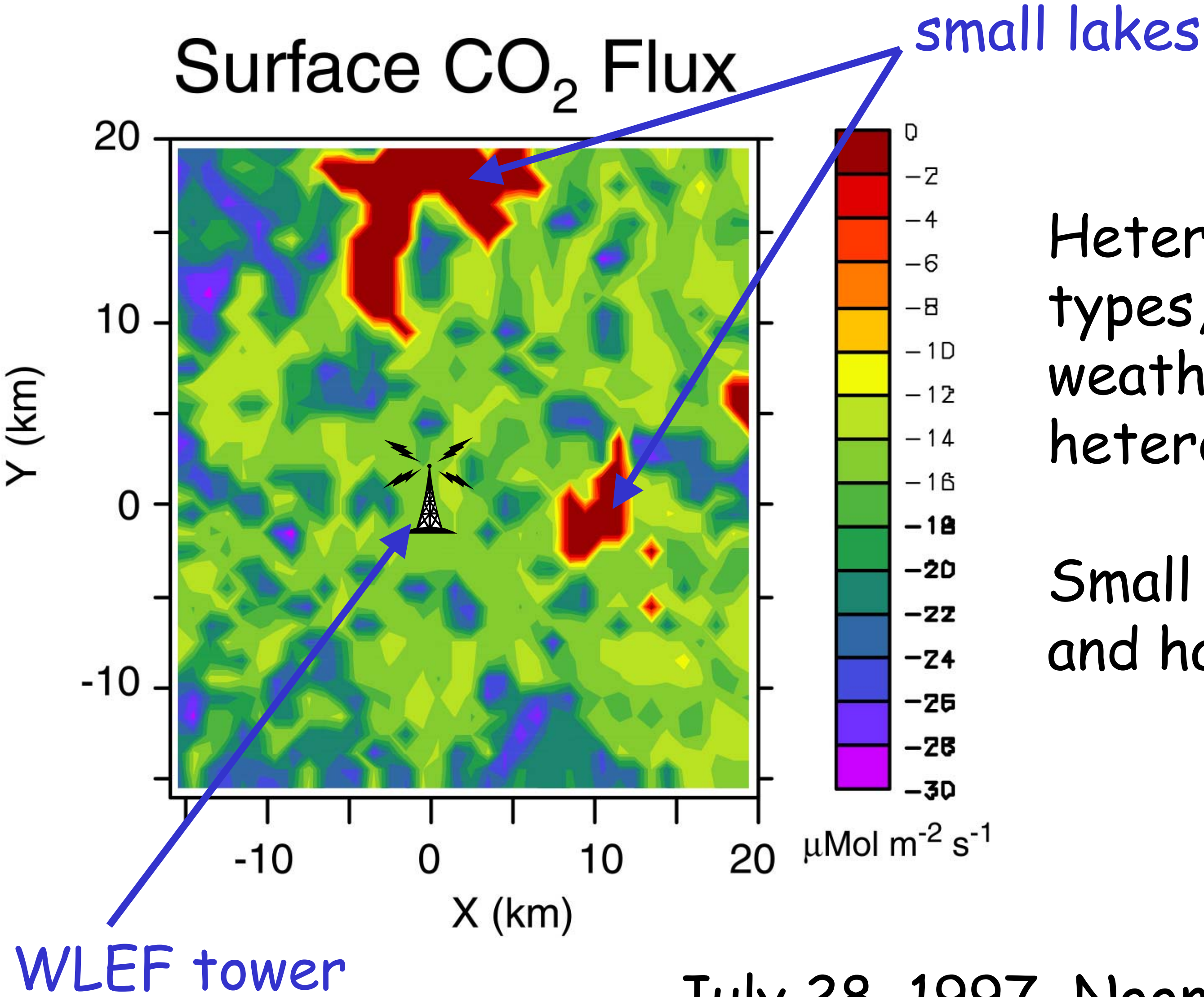
Nicholls et al, 2003

Simulated Energy Fluxes (W m^{-2}) at Noon on Grid 3: Δx = 1 km



- **Variations due to heterogeneous vegetation**
- **White areas are small lakes**

WLEF Vicinity

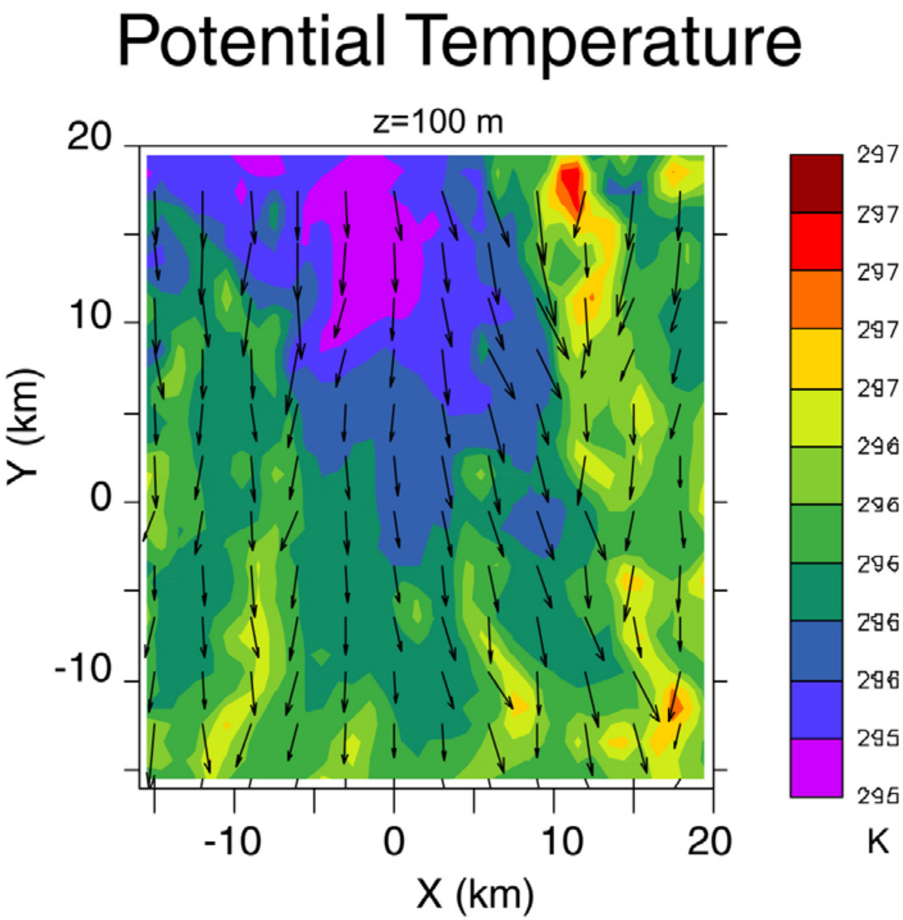


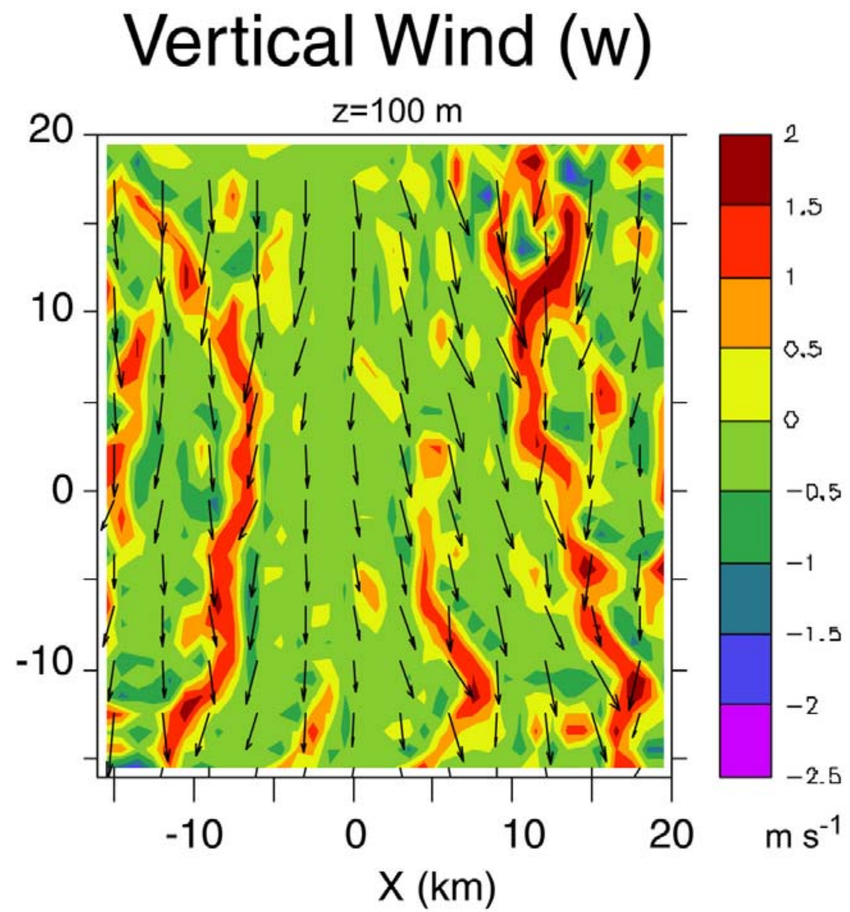
Heterogeneous veg types, LAI, soils and weather produce heterogeneous NEE

Small lakes are cold and have no NEE

July 28, 1997 Noon LT 1 km grid

Local Circulations

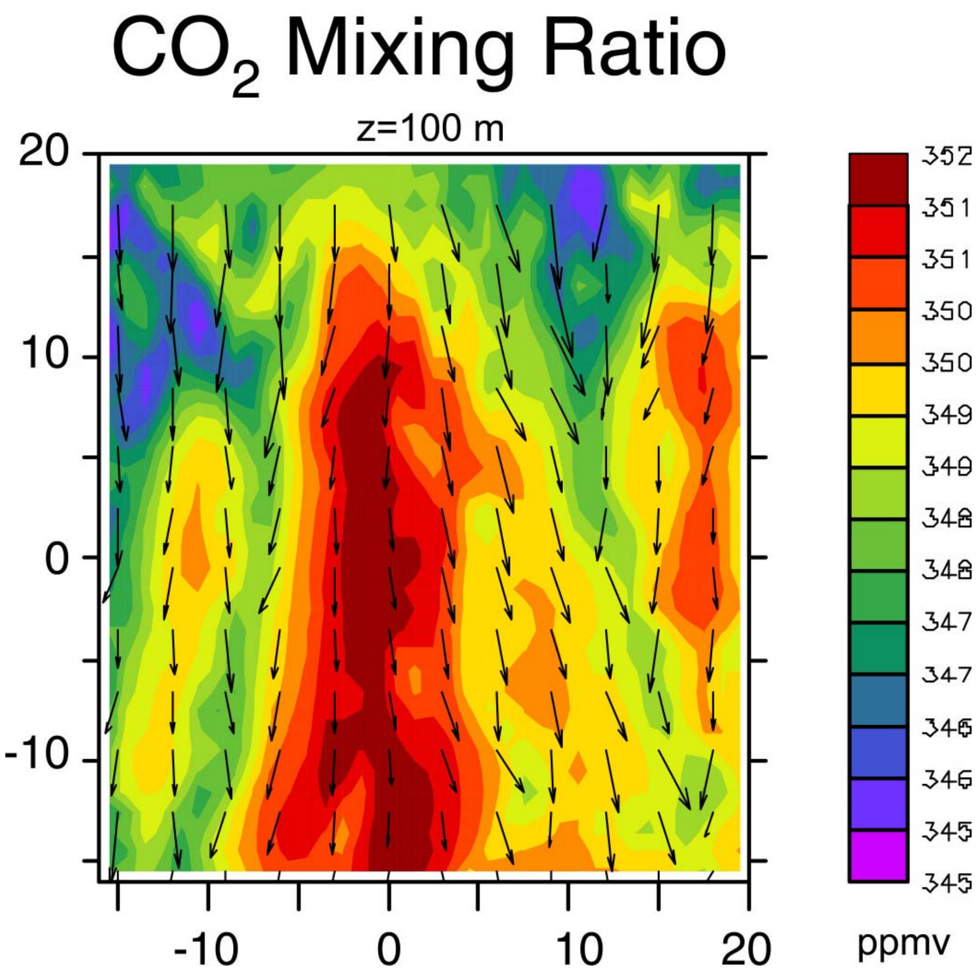




Wind is northerly following cold frontal passage
Lake surfaces are cold, distort PBL turbulence

July 28, 1997 Noon LT 1 km grid z=100 m

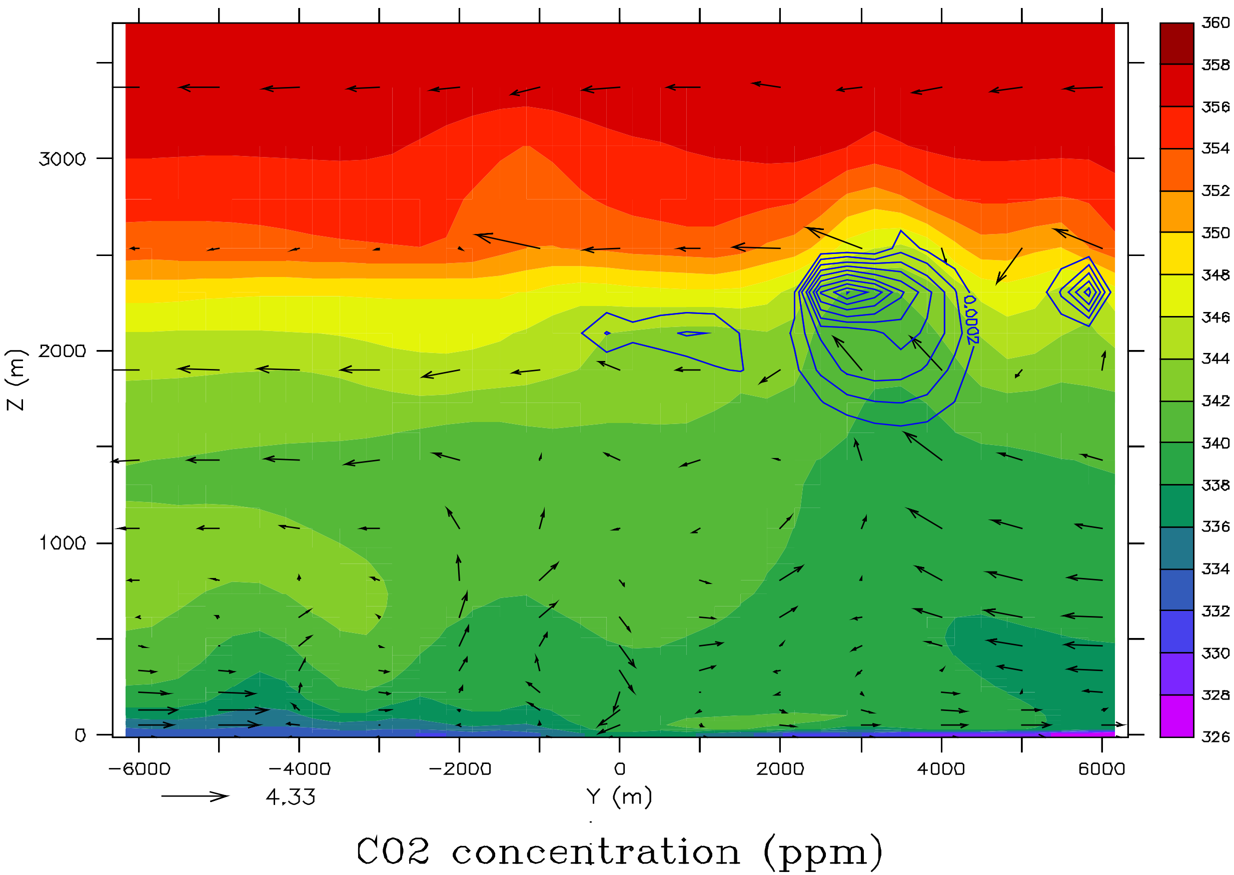
Local "Signals"



- Presence of lakes produces a "plume" of higher CO_2 downwind
- Vertical gradient above forest is perturbed by mesoscale "rolls" in flow
- Mesoscale variations of ~6 ppmv in CBL CO_2 due to these effects
- Is this "signal" or "noise"

July 28, 1997   Noon LT   1 km grid   z=100 m

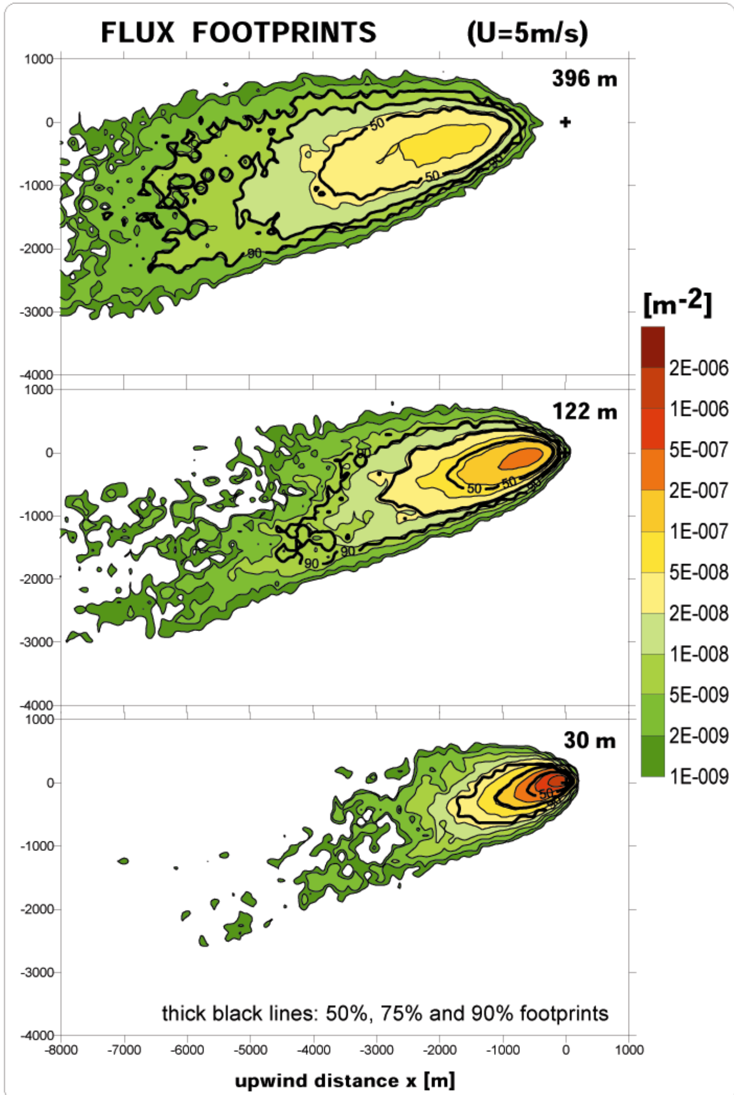
Effects of PBL-top clouds



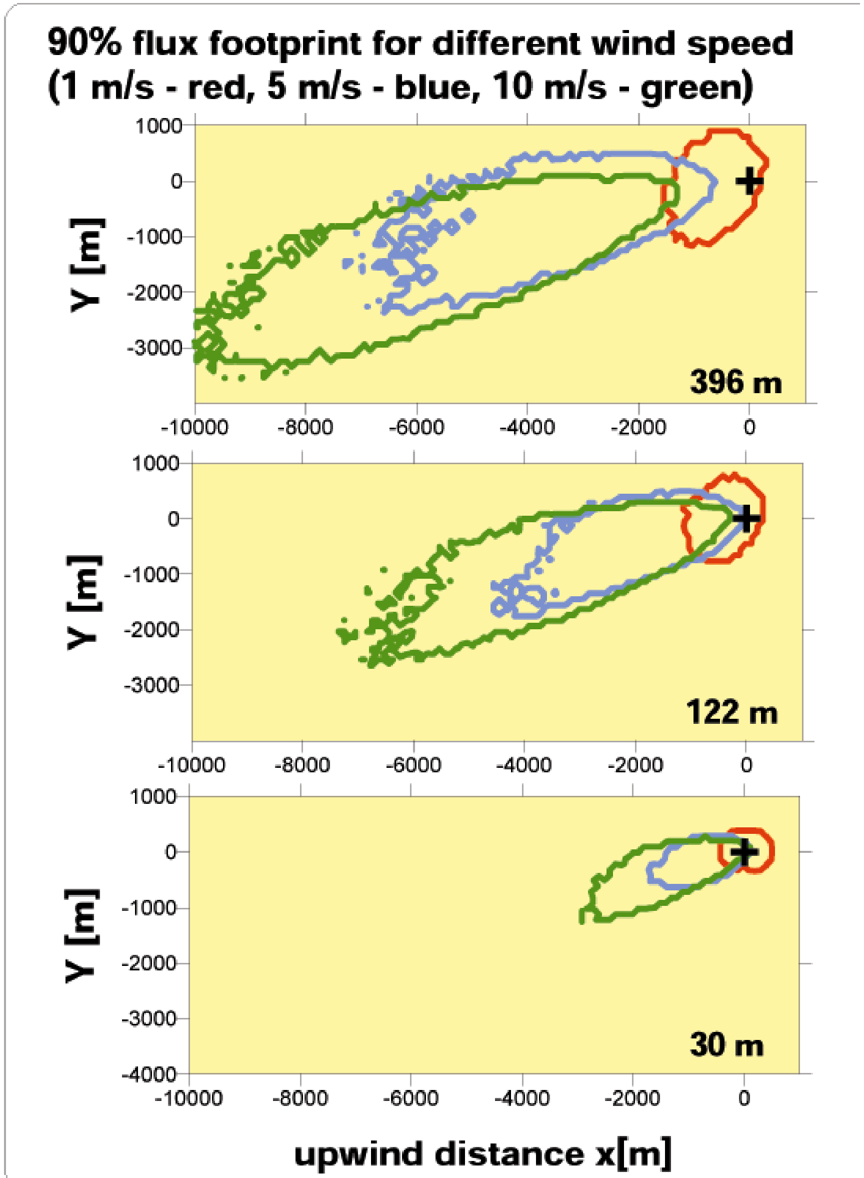
- Thermals carry forest signal to PBL top
- Clouds transports ventilate PBL into free troposphere

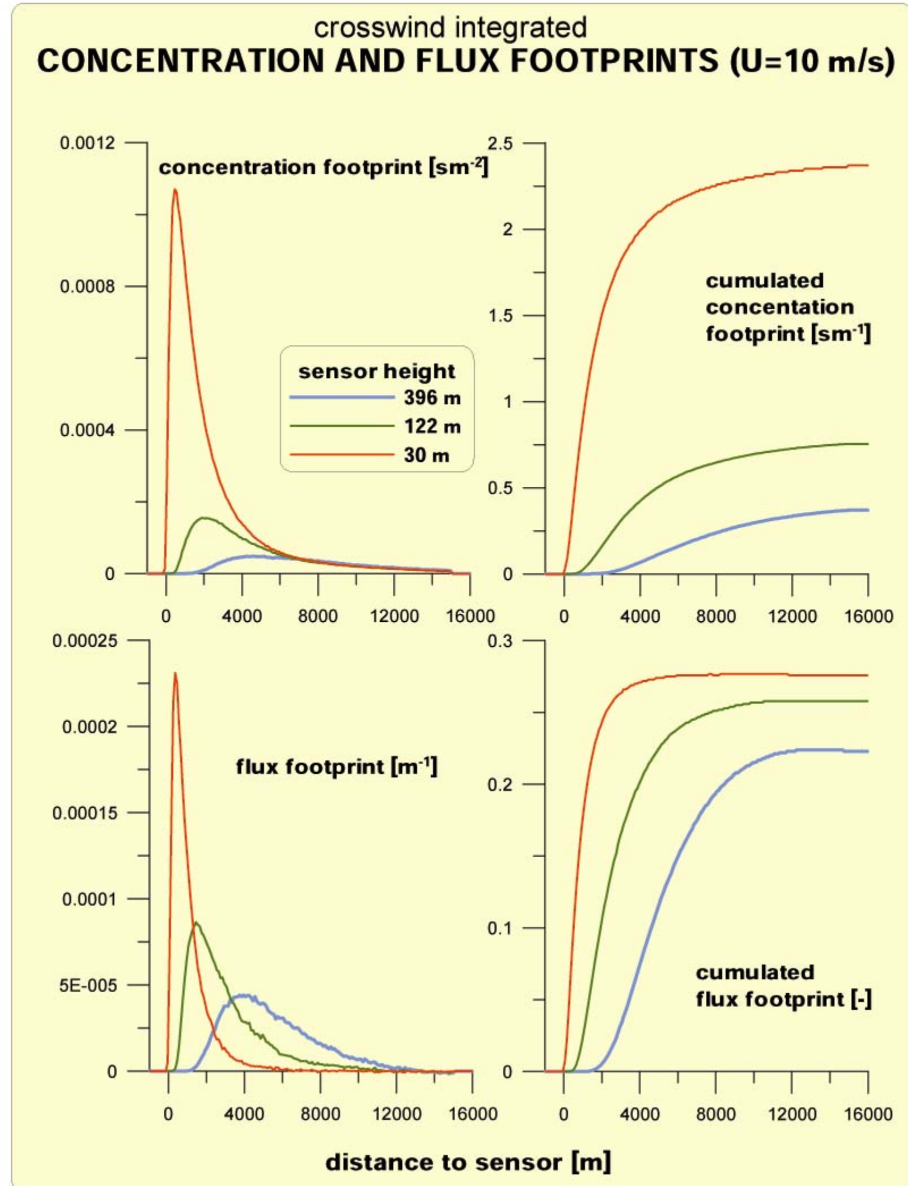
Color: CO_2 contours: cloud liquid water vectors: wind

Lagrangian Particle Tracer Analysis



- Massless "particles" are released into an eddy-resolving RAMS simulation of boundary-layer turbulence
- Population of particles reaching the tower detectors carry information about their points and times of origin in the underlying forest
- Defines "footprints" of tower (or aircraft) data


90% flux footprint for different wind speed
(1 m/s - red, 5 m/s - blue, 10 m/s - green)
Y [m]
396 m
122 m
30 m
upwind distance x[m]


crosswind integrated
CONCENTRATION AND FLUX FOOTPRINTS (U=10 m/s)
concentration footprint [sm-2]
sensor height
396 m
122 m
30 m
cumulated concentration footprint [sm-1]
flux footprint [m-1]
cumulated flux footprint [-]
distance to sensor [m]

Animation

modeling framework

CSU RAMS

↓

LPD model

↓

influence functions

- for concentration
- for vertical flux

↓

Bayesian inversion

influence function for concentration measurements C*

concentration sample

surface fluxes

initial concentration

inflow fluxes

$$\Phi(C) =$$

$$\int_0^T \int_0^{L_x} \int_0^{L_y} C^*\Big|_{z=0} q\,dxdydt +$$

$$\int_0^{L_x} \int_0^{L_y} \int_0^{H} C^*\Big|_{t=0} C_0\,dxdydz +$$

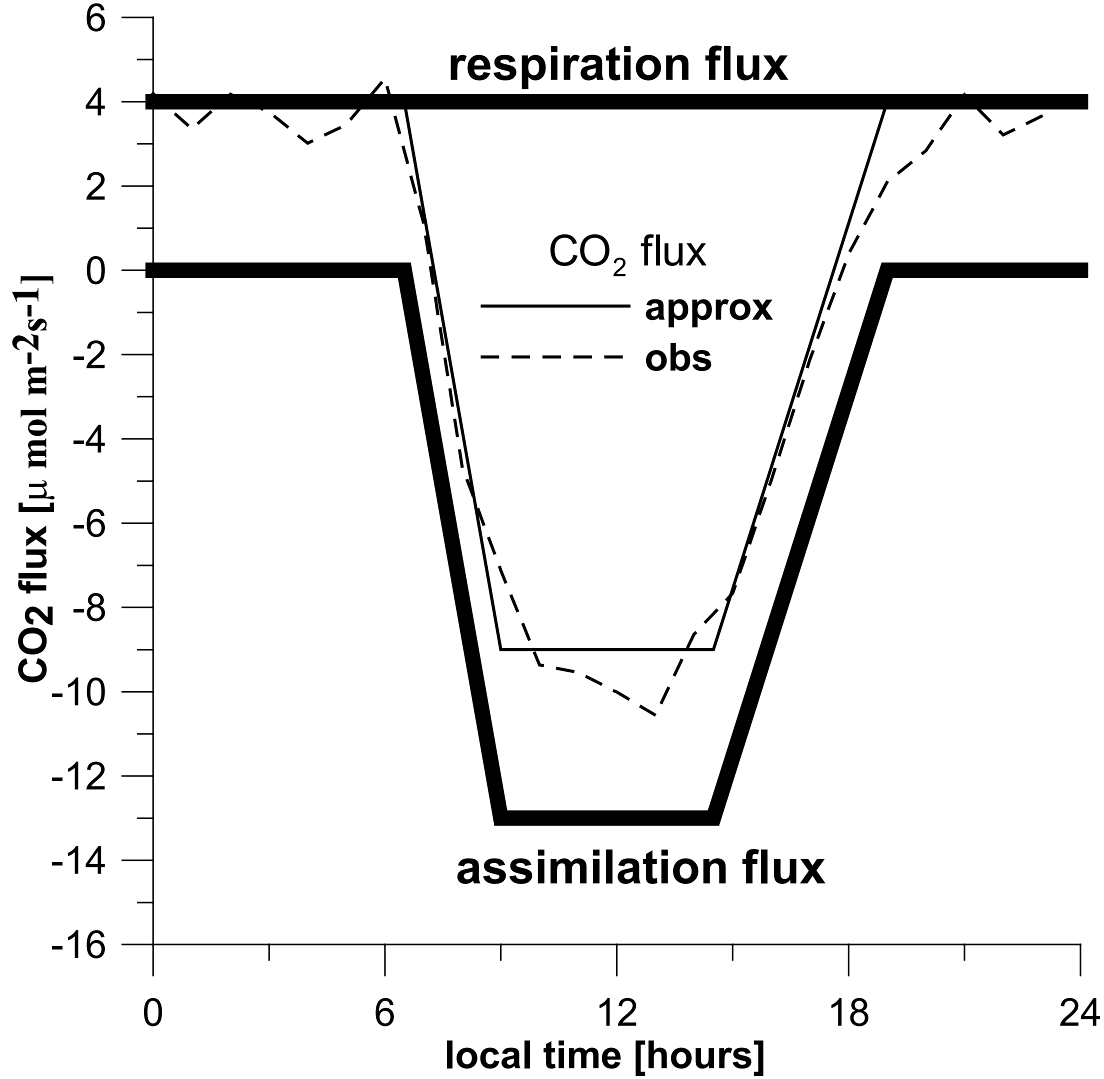
$$\int_0^T \int_0^{L_y} \int_0^{H} (\tilde{u}C^*\Big|_{x=0} C_W + \hat{u}\,C^*\Big|_{x=L_x} C_E)dydzdt + \int_0^T \int_0^{L_x} \int_0^{H} (\tilde{v}C^*\Big|_{y=0} C_S + \hat{v}\,C^*\Big|_{y=L_y} C_N)dxdzdt$$

Tests with a 1D RAMS Simulation

(Uliasz and Denning, JAM, in review)

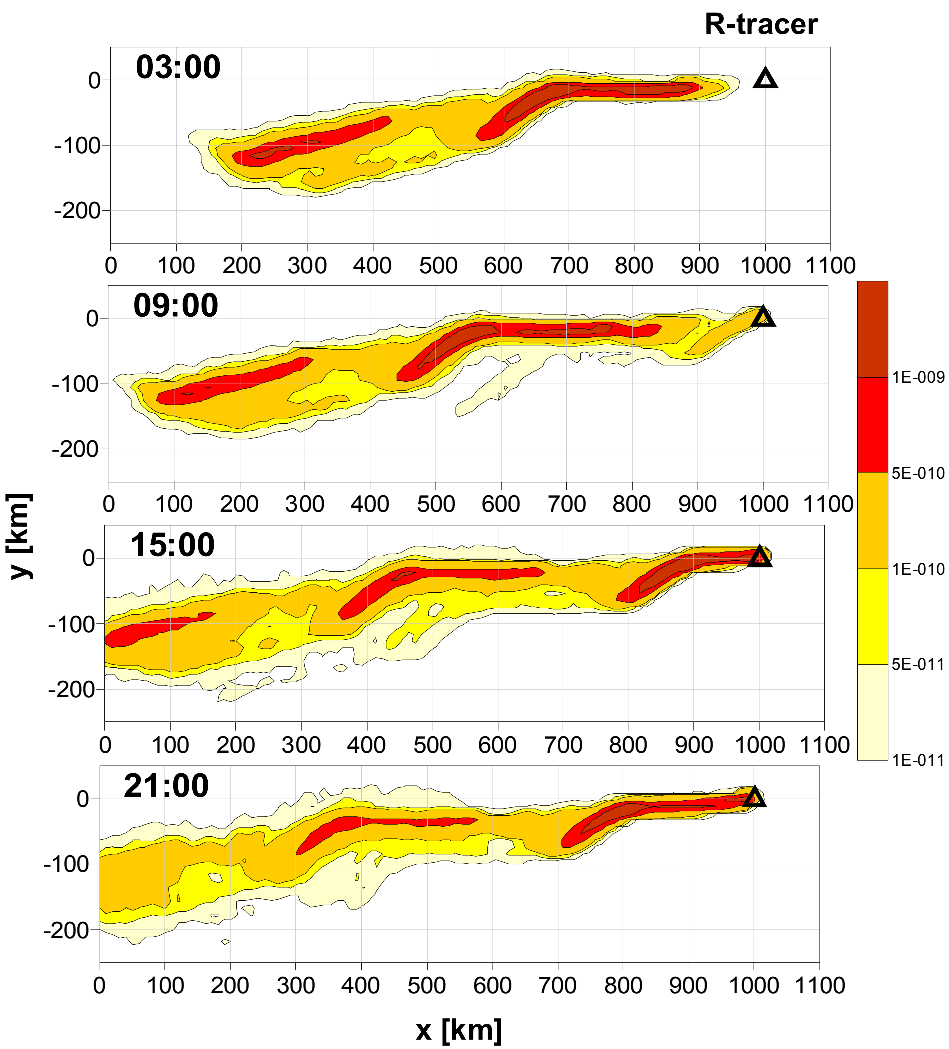
- Diurnal cycle of surface fluxes, PBL and FT exchange
- Clear weather
- Steady geostrophic wind = 5 m s^{-1} aloft
- Use Lagrangian Particle Dispersion Model to calculate concentration footprints for specified sampling strategies
- Separately estimate fluxes due to assimilation (A) and respiration (R)

Figure 2

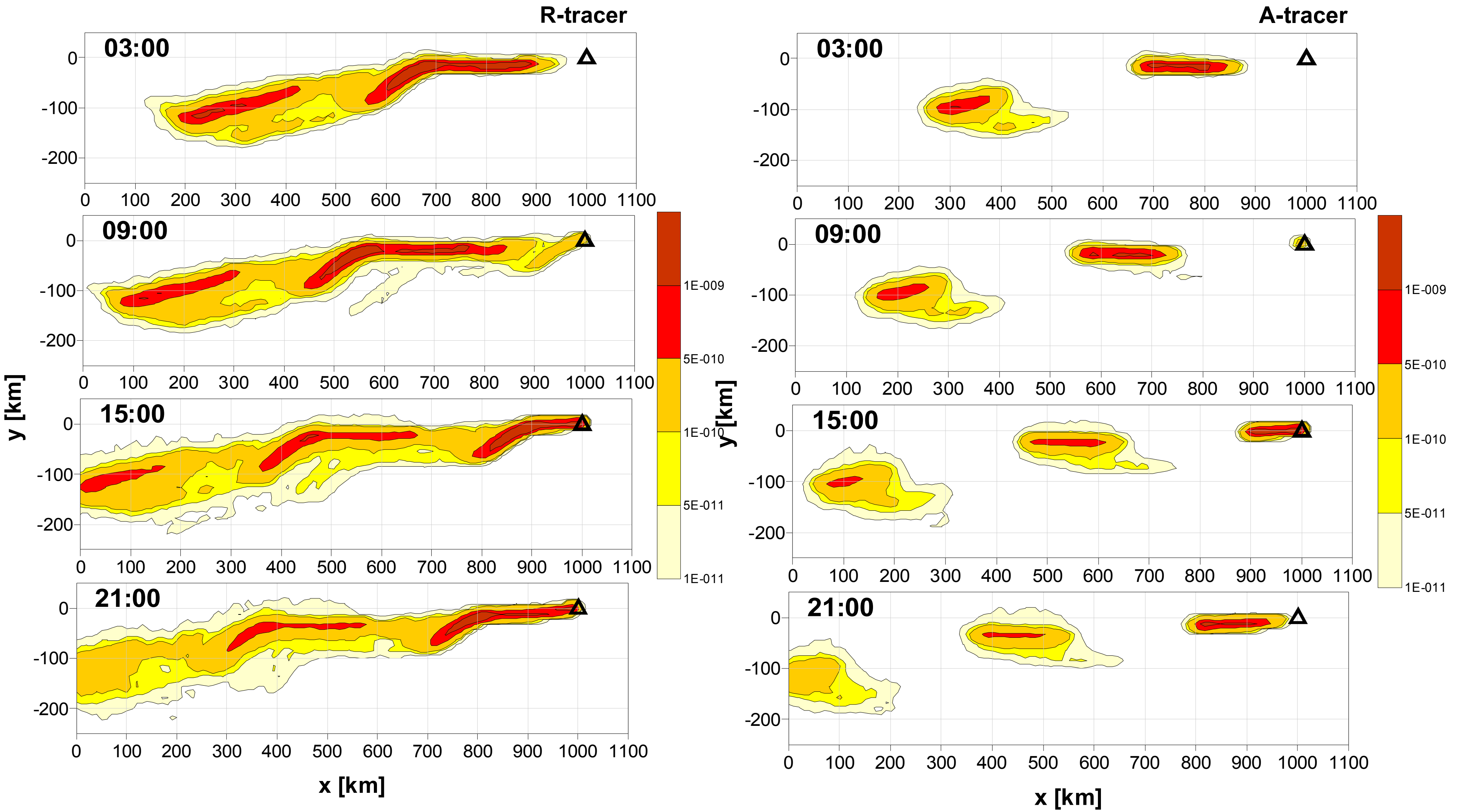


respiration flux
assimilation flux
CO2 flux
approx
obs
CO2 flux [μ mol m-2s-1]
local time [hours]
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
-16
0
6
12
18
24

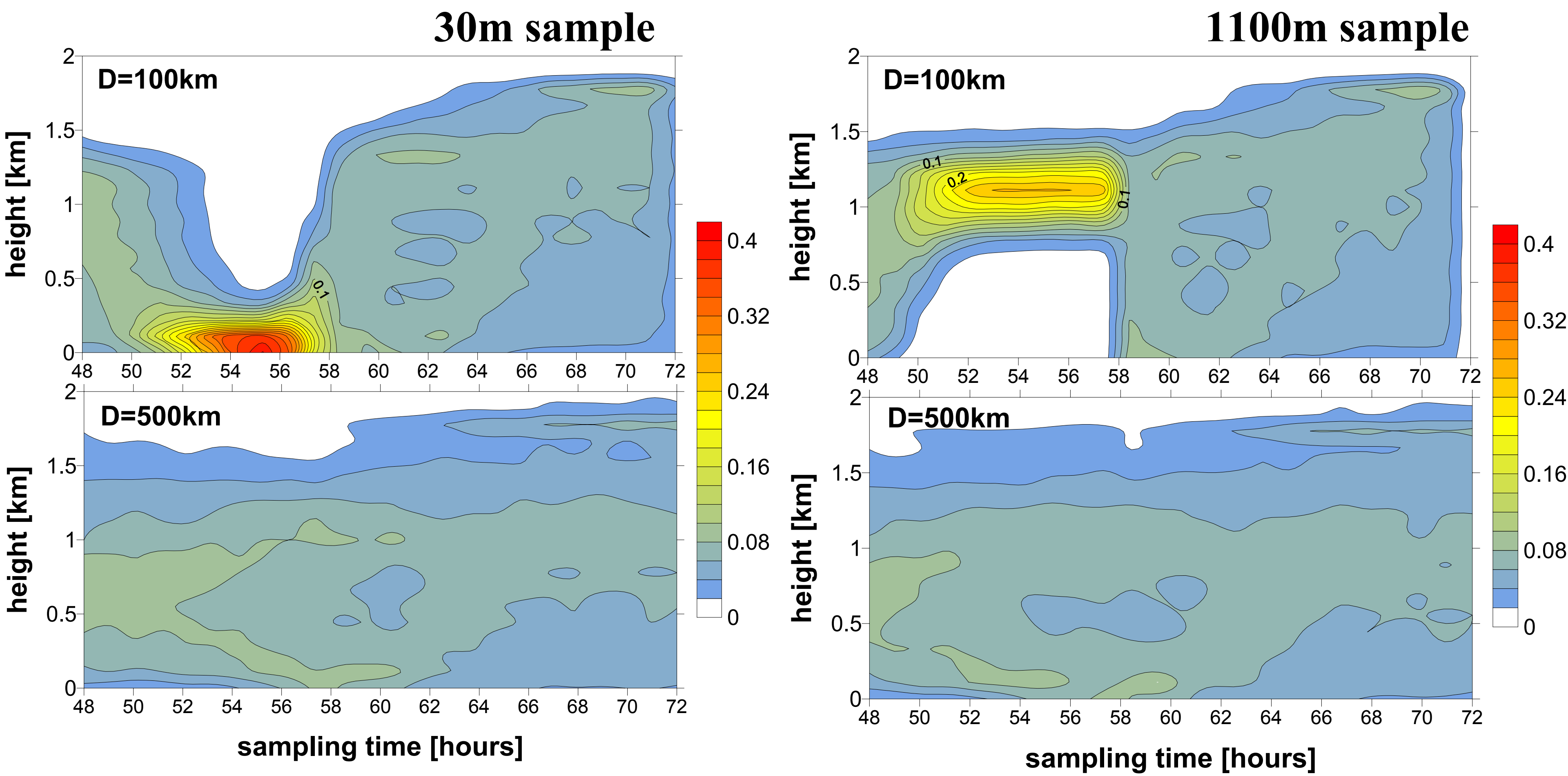
influence functions for surface fluxes: 1D PBL



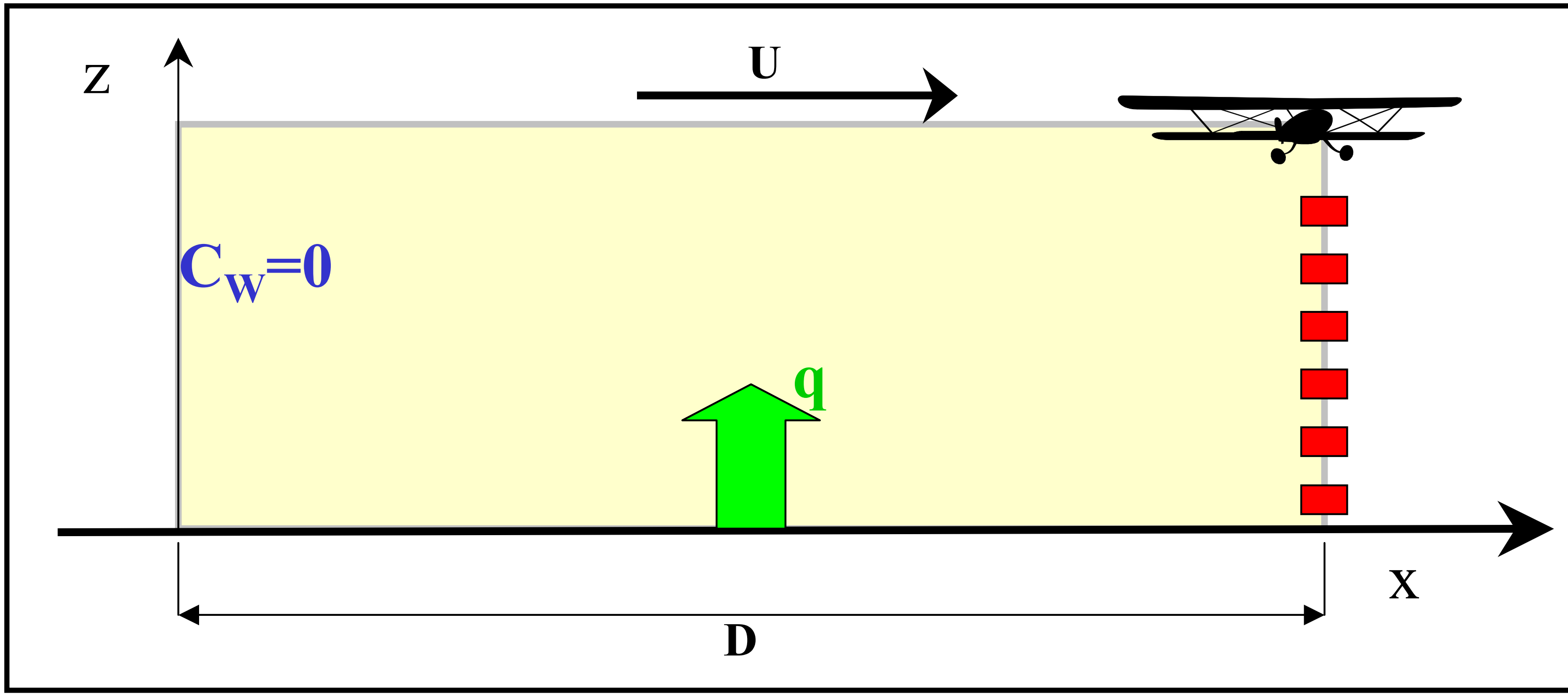
influence functions for surface fluxes: 1D PBL



influence functions for inflow fluxes: 1D PBL

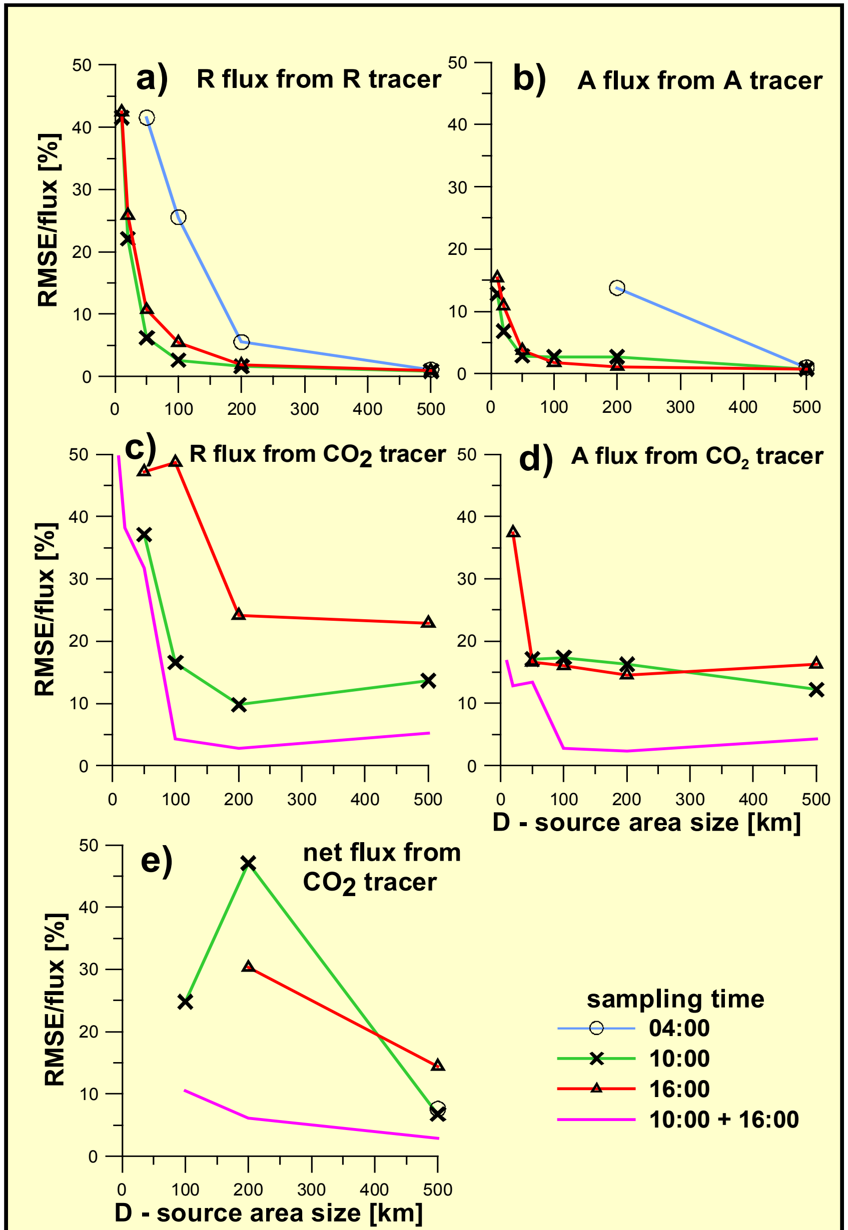


Aircraft Sampling Experiment



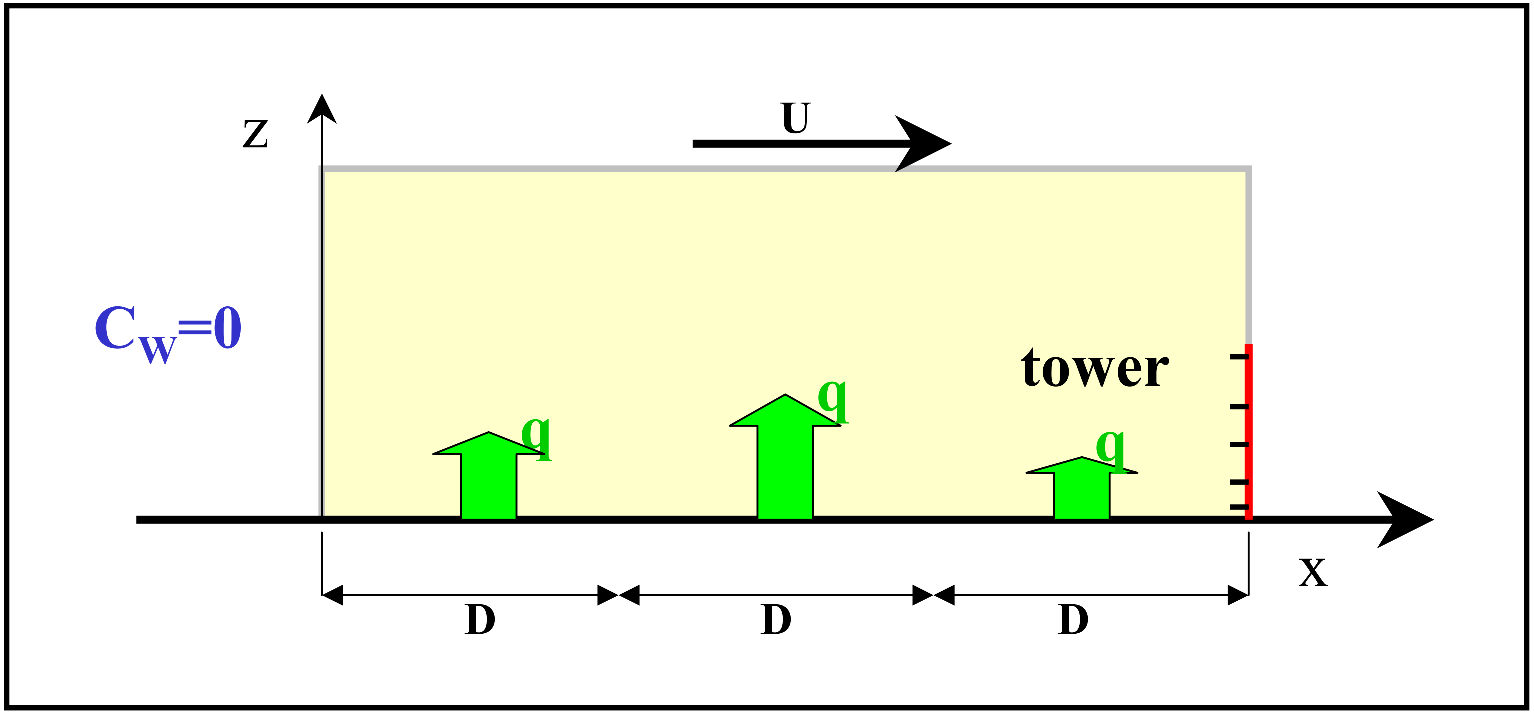
- Vertical profile of airborne samples
- Estimate area average flux upstream over a distance D
- Assume inflow fluxes at lateral boundary known

Aircraft Experiment Results



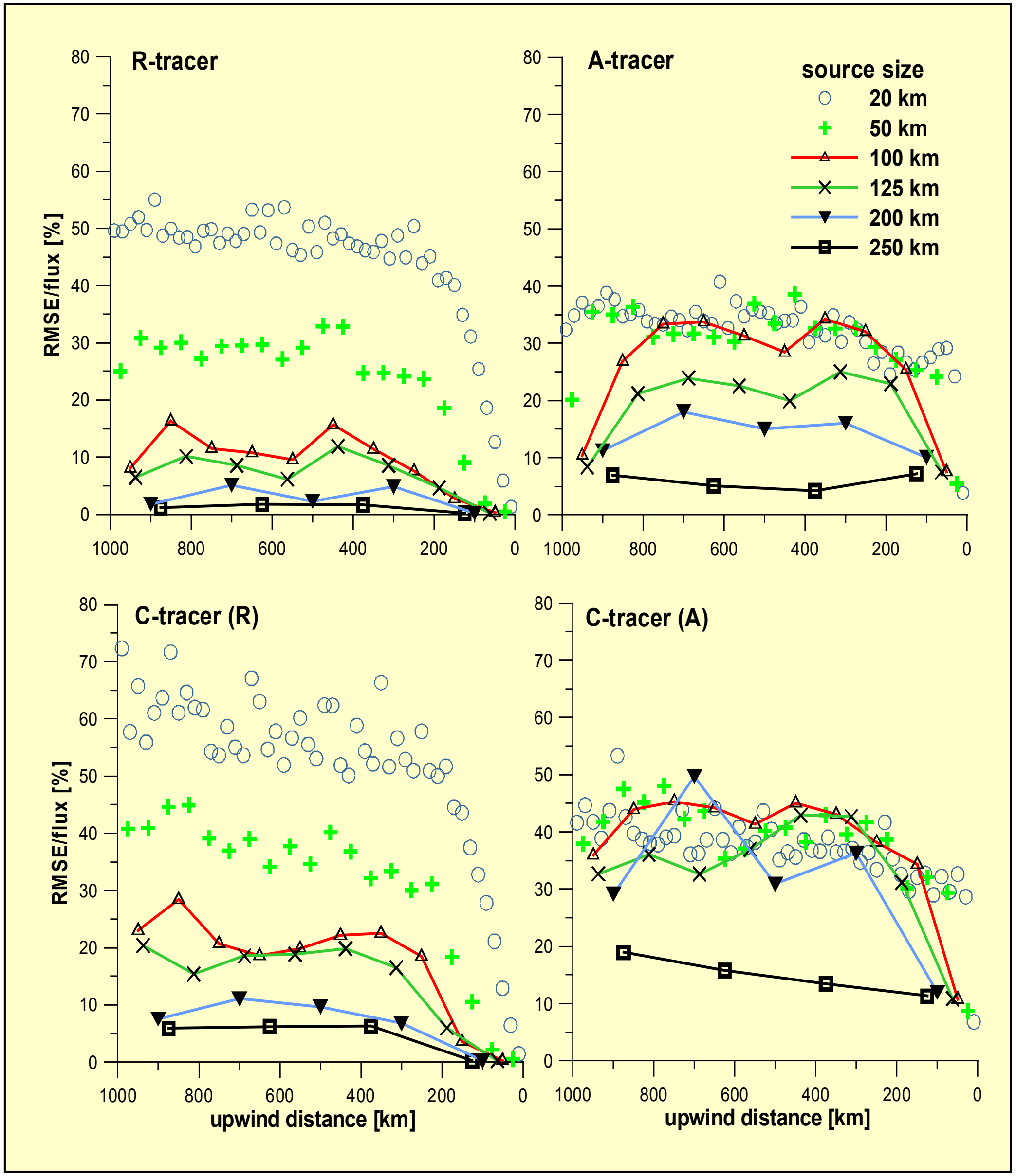
- Estimation better for R than A (diurnal cycle)
- Best result for twice-daily sampling at 10 AM and 4 PM
- Excellent recovery of A and R for large "patch sizes"
- Much worse for net flux from total CO2
- Inversion fails when inflow fluxes unknown!

Tower Timeseries



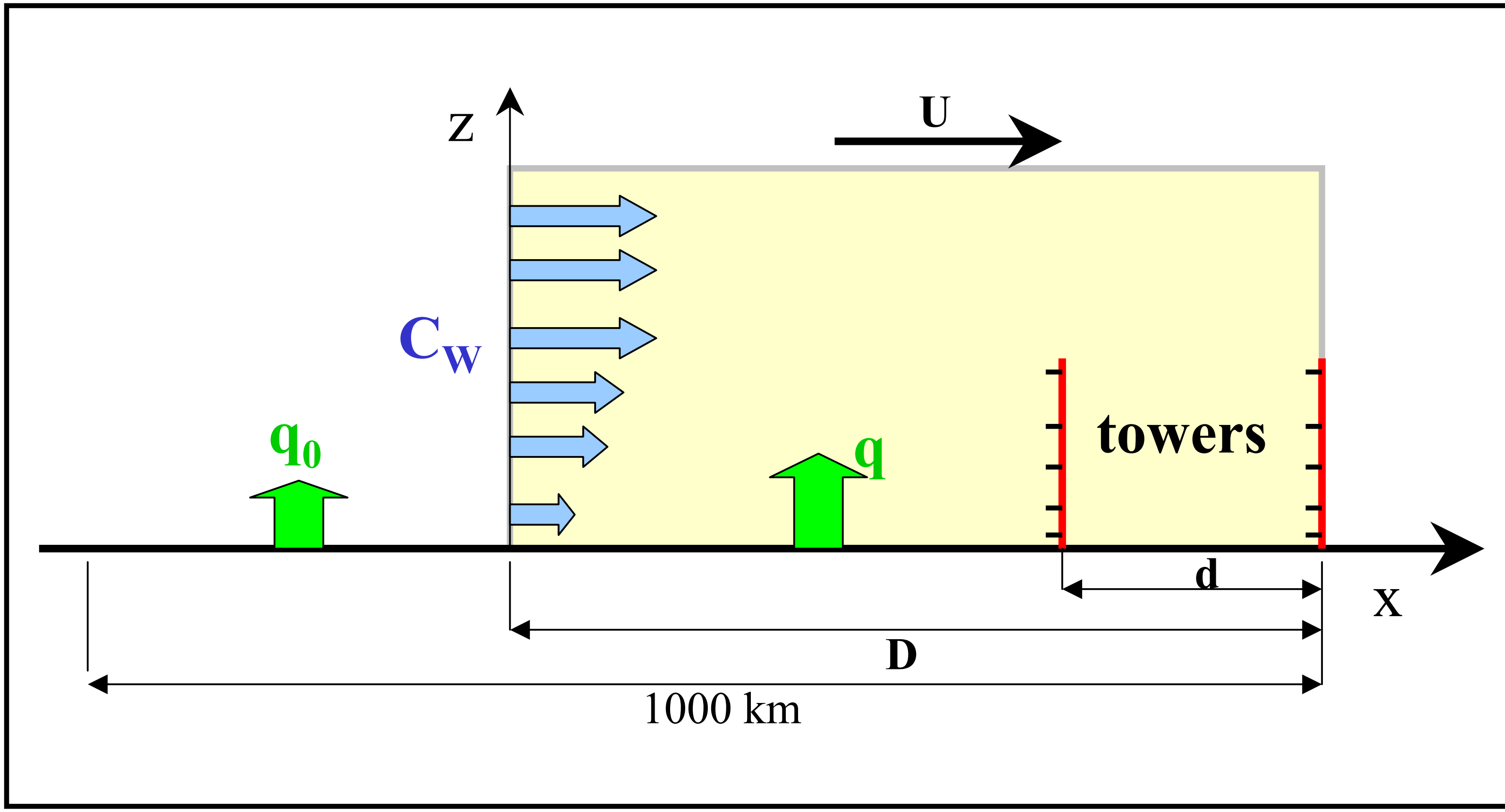
- Hourly vertical profiles of CO2 at WLEF
- Known inflow flux
- Separately estimate A and R over a set of upstream "patches" of length D

Tower Timeseries Results



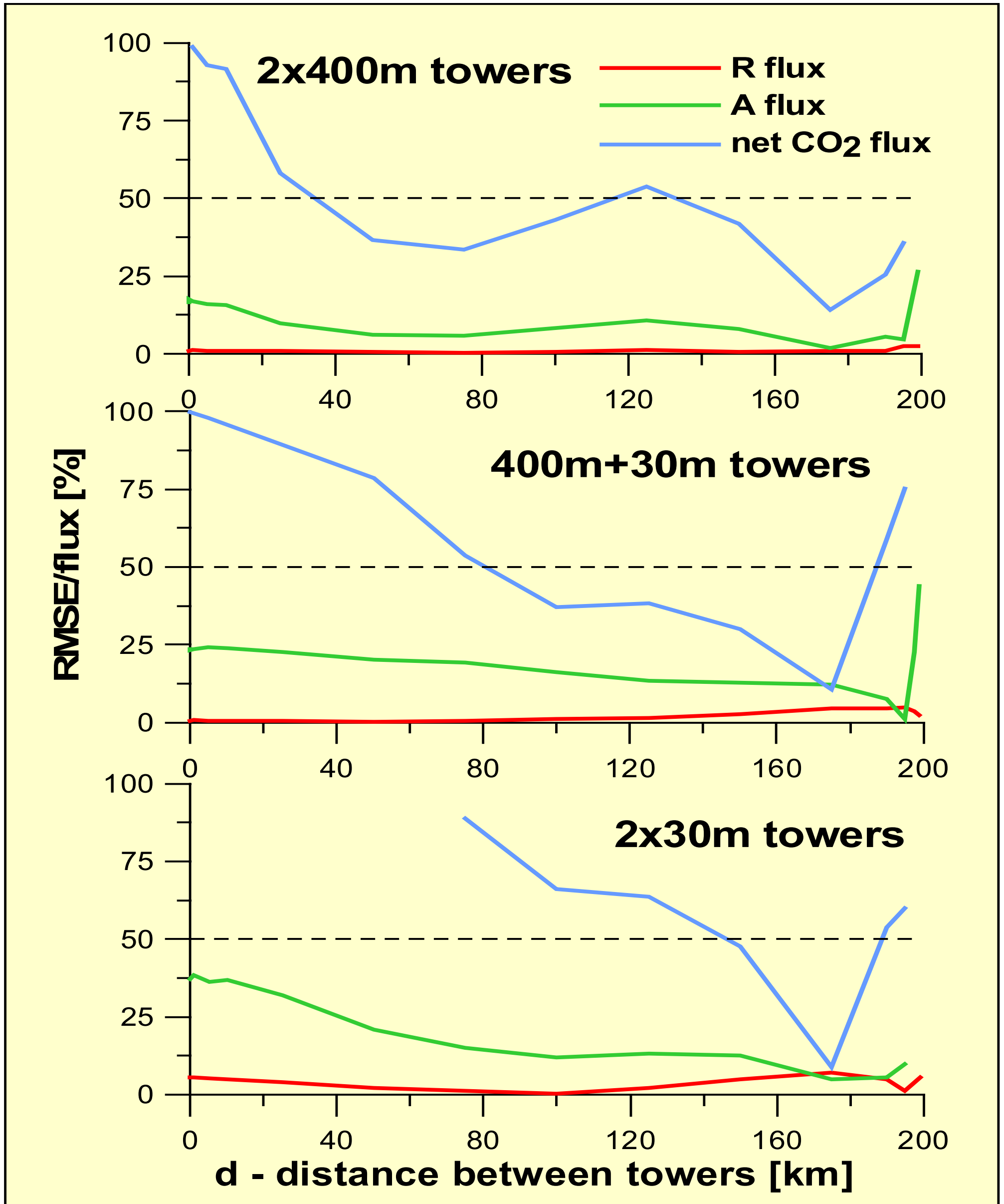
- Better constraint than daily or twice-daily airborne profiles
- Estimation is better for larger patch sizes
- Separate R and A estimates quite good for D > 200 km

Problem with Unknown Inflow Fluxes



- Uniform flux from a patch of size D
- Inflow flux varies in time and height
- Two towers with continuous [CO2] distance d apart

Two-Tower Inversions



- R is very well estimated
- A isn't bad
- NEE very hard to estimate with unknown inflow
- Best estimates when towers are spaced optimally w.r.t. travel time (daytime)