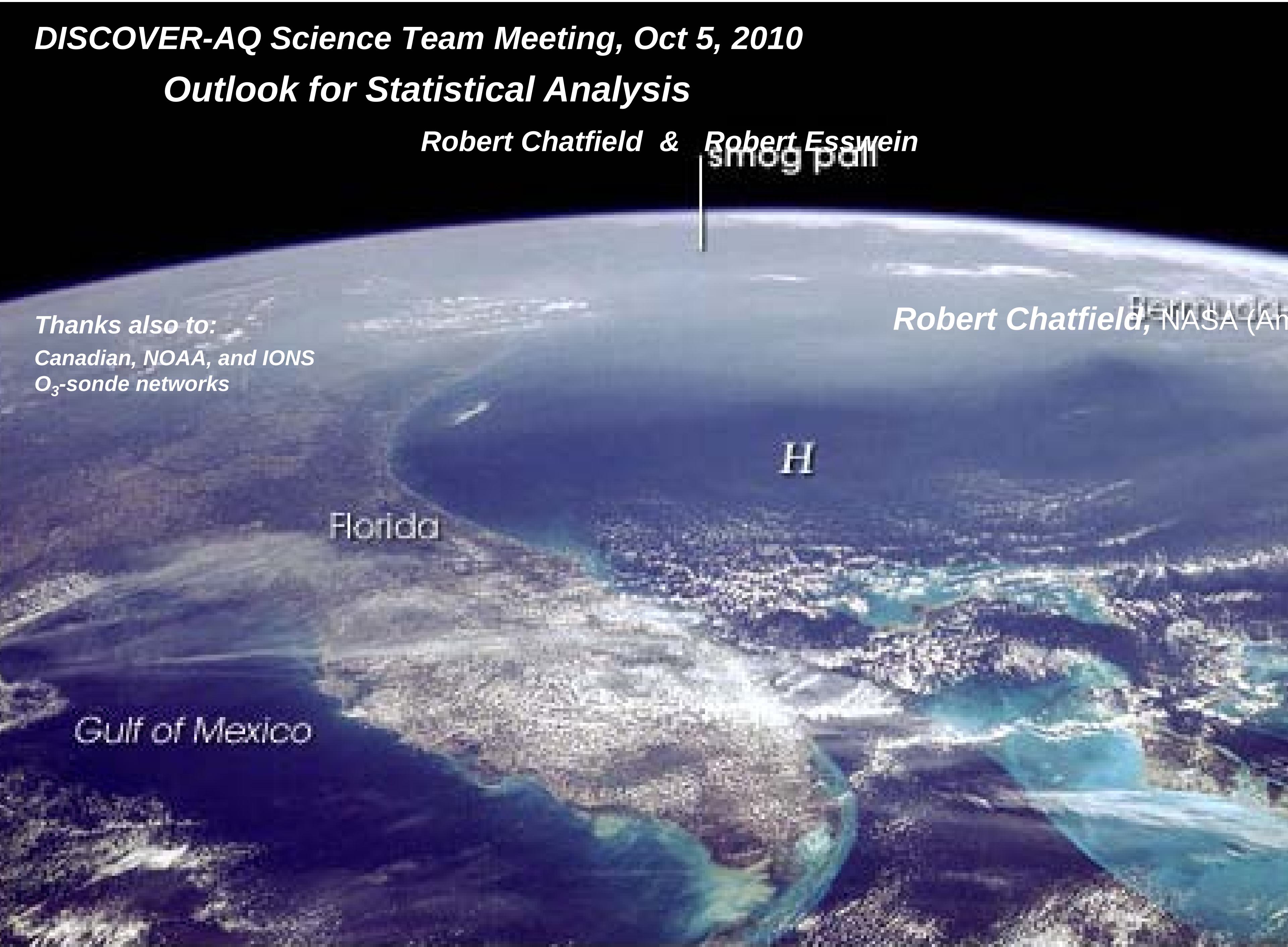
DISCOVER-AQ Science Team Meeting, Oct 5, 2010

Outlook for Statistical Analysis

Robert Chatfield & Robert Esswein

Thanks also to:

Canadian, NOAA, and IONS
O_3-sonde networks



Motivations and Questions for Statistical Analysis
(restated STM questions)

- *How much do we know about pollutant concentrations from current measurement techniques?*
  - O_3, NO_2, HCHO, *absorbing* C *aerosol*, $PM_{2.5}$
  - i.e., how far away can we extrapolate with confidence
    - ***(1)*** Vertically? — *From satellite retrieval*
    - ***(2)*** Horizontally? — From aircraft, satellite retrieval, ground stations
    - ***(3)*** Can we learn to map $PM_{2.5}$ regionally?
    - Can we formulate a "jacknife" methodology to express our knowledge/ignorance?
- *What are spatial patterns of pollutant creation/destruction?*
  - can we model them (enough detail for questions of exposure/compliance?
  - do we understand the details of transformation sufficiently?
  - i.e., (***4b)*** *Chemical production* of O_3 and *Chemical Loss* of NO_2,
  - ***(4a)*** *Chemical production* of absorbing organic aerosol
  - (What are their spatial scales?)

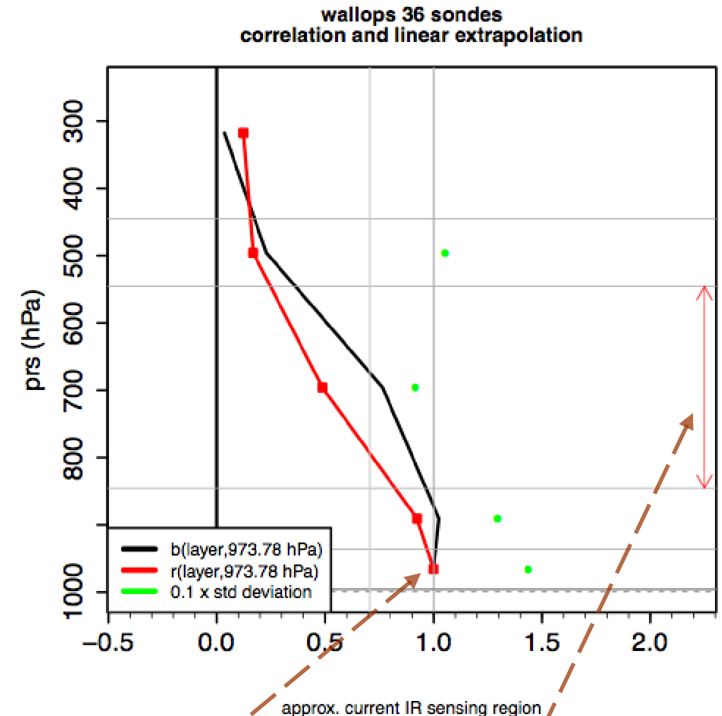
All of these require us to expand our scientific and technical knowledge

ana all have impacts for pollution compliance and (eventually) wiser regulation.

(1) How much do we know about surface pollutant concentrations from current remote measurement techniques?

How much do we know about extrapolating vertically, i.e., from O_3, NO_2 partial columns to surface/lowest-km

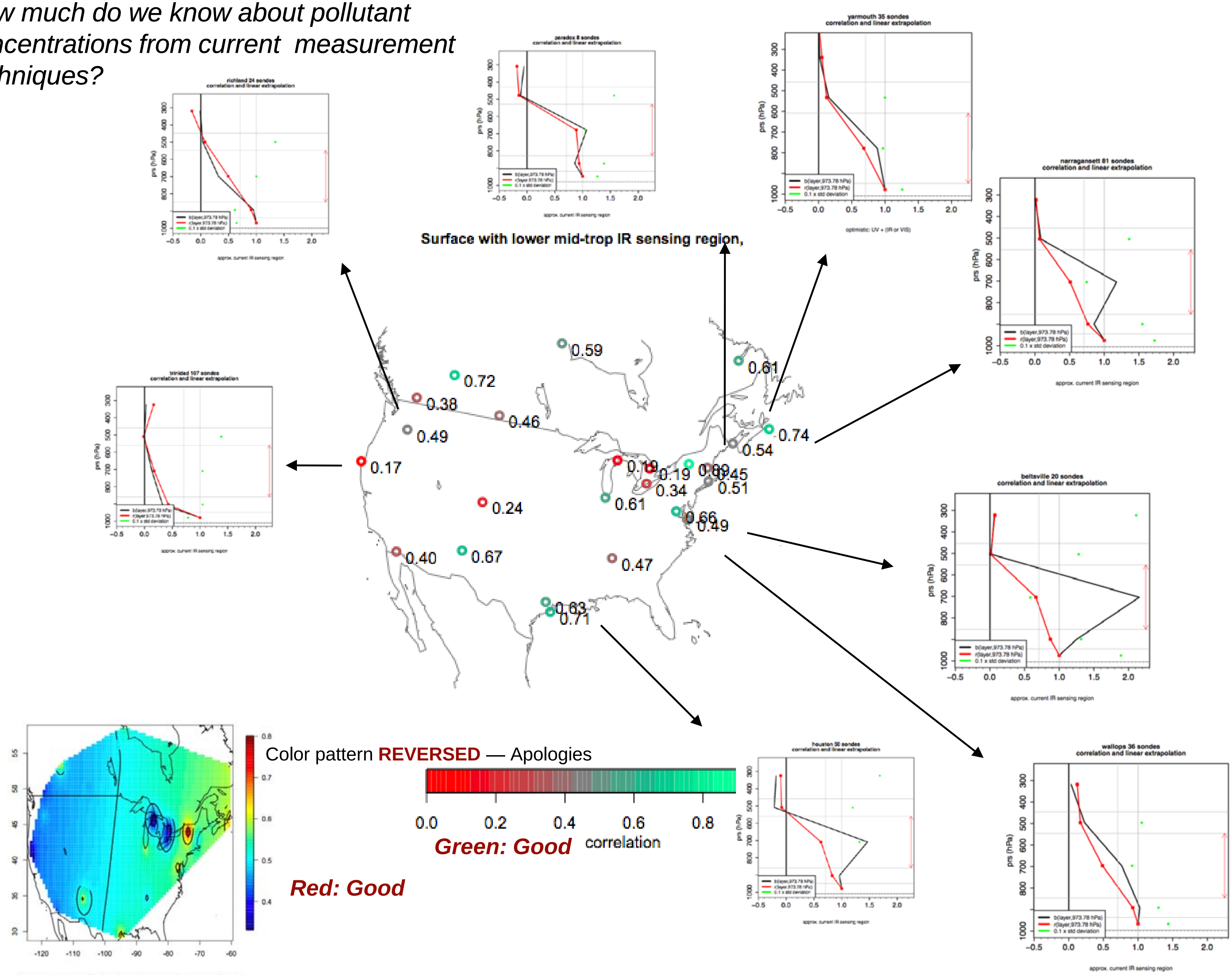
See IGAC-Dalhousie presentation, with a brief discussion in “GEO-CAPE Progress Publication,” (Fishman, ….) *in preparation*



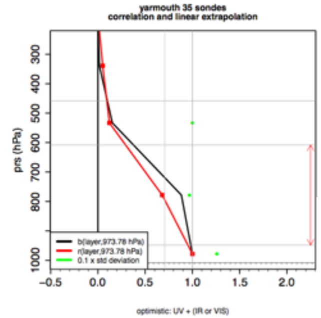
How to estimate O_3 <u>here</u> from <u>this</u> layer average — note r ~ 0.5 when one can retrieve a layer extending from 1.5 to 5 km accurately.

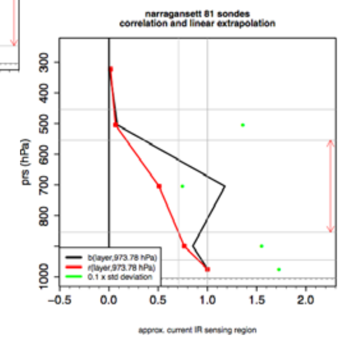
Chatfield et al., 2nd/3rd highest priority for publication

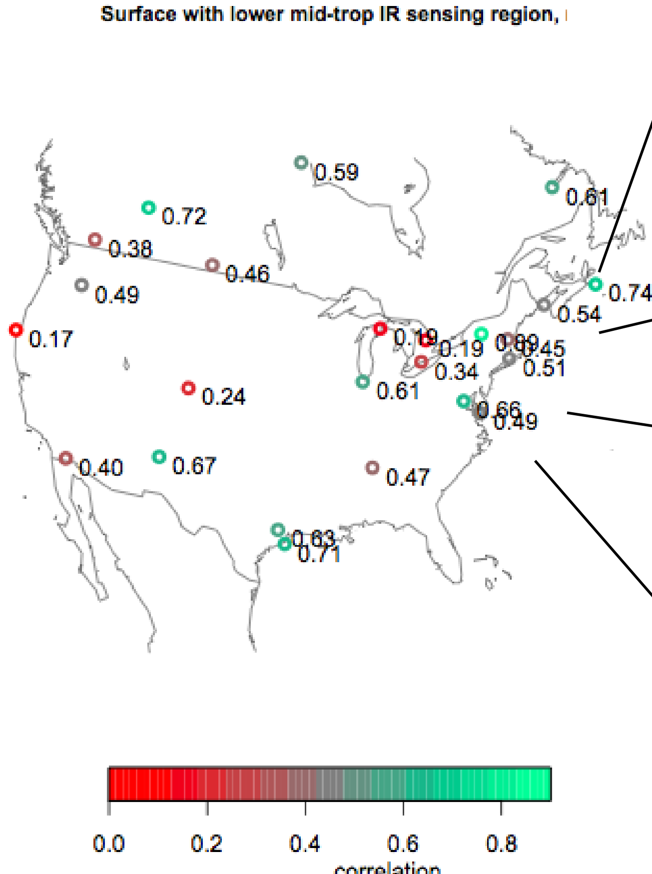
How much do we know about pollutant concentrations from current measurement techniques?



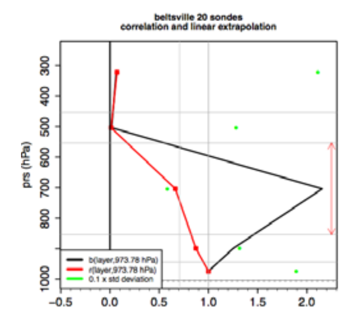
How much do we know about pollutant concentrations from current measurement techniques? East Coast Stations

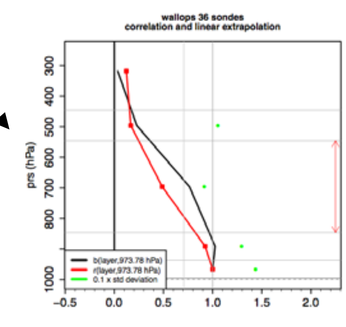






Green: Good





We can apply similar correlation techniques in the DISCOVER-AQ areas

O_3: measurements from aircraft spirals, sondes, ground stations … over the bay

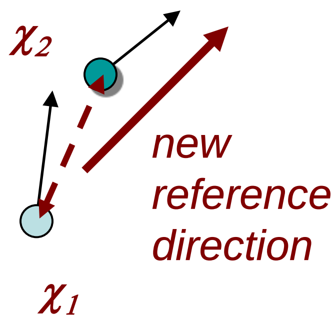
NO_2, HCHO Pandora, ACAM aircraft spirals ground stations

(2) *Describe Horizontal Variability*
Extrapolation of Concentrations Horizontally Needs to Accommodate Directionality … with Windflow

HCHO flow over north east land region, M. Follette-Cook WRF-Chem

- Use wind directions at sampling points (from model analysis … or from weather analysis)

QuickTime™ and a decompressor are needed to see this picture.



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This analysis uses WRF-Chem at 4 km resolution for Northeast Corridor (and to the west)

It needs to be repeated for city simulations, and other regions

It needs to accommodate *slow* wind change.
(Fast wind change => Different airmass?)

….Extrapolation of Long-Lived Species Concentrations Horizontally

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PM2.5, μg m^{-3}

We need a framework, the beginnings of a theory, to describe variability integrating information at apparent Scale-separations: urban, multi-urban region, regional, Continentent-to-ocean.

Each will have a different variogram

- Wind-defined directional variograms for $PM_{2.5}$, CO for the region of the Northeastern US shown. The time is 4 PM EDT on August 8, 2007. Empirical variograms (ppb^2 and for $PM_{2.5}$, (μg m^{-3})^2) are shown.

(3) Aerosol Estimation from Space …extend success from San Joaquin Valley Study

$$PM = \frac{\tau_a}{H_a}\theta\prod_i \frac{m_i}{\sigma_i}$$

6 sites over 400 km
3.5 years
2200 points
reasonable variation

where
τ_a is the AOD,
H_a is the aerosol scale height, H_a
θ is a parameter taking into account seasonal variation (maybe best estimation of
m_i is the aerosol mass concentration for species i and σ_i is the extinction coefficient for species i.

r = 0.74
so far
(previously ~ 0)

Several measures of AOD …

? Measures of Albedo
? 2 wavelengths of MODIS retrieval
? RH only above ~65%

$\log_{10} (PM_{2.5}) = 0.54 + 0.21 \log_{10} (AOD_{47}0) + 0.011 \log_{10} (AOT_{OMI}) + 0.11 \log_{10} (NO2_{OMI})$
$+ \textit{spline} (\log_{10}(AOD_{deep\text{-}blue,470}) + \textit{spline} (Day\_of\_Year),$

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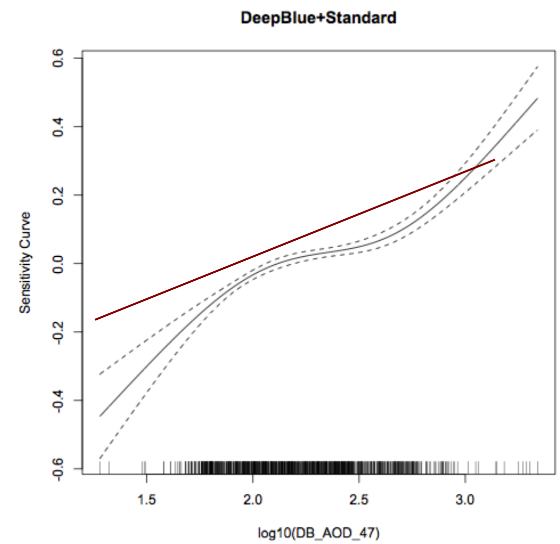
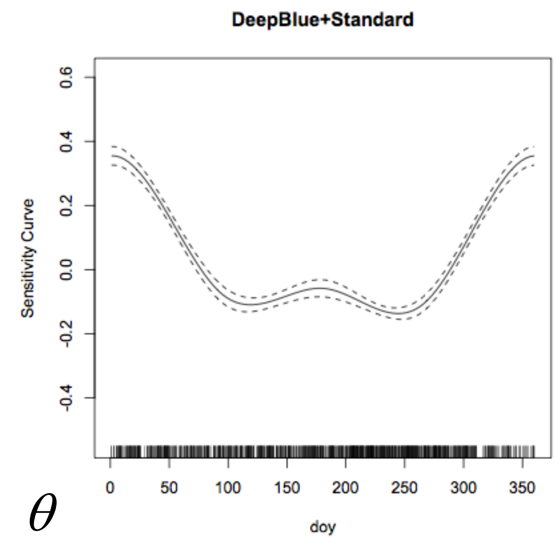
Several measures of AOD
(eg., MODIS standard algorithm, MODIS Deep Blue, OMI), because each may have a best range of greatest applicability and worst of "noise".
The OMI aerosol index (AI) tends to be more sensitive to aerosols at altitude

Chatfield, Strawa, et al, A-Train Symposium …
first results need better understanding



Deep Blue Aerosol

Standard Aerosol

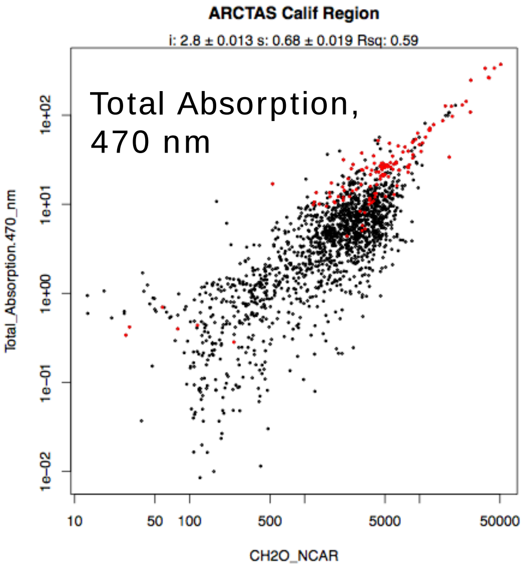


θ

(4a) Understand Chemical Processes

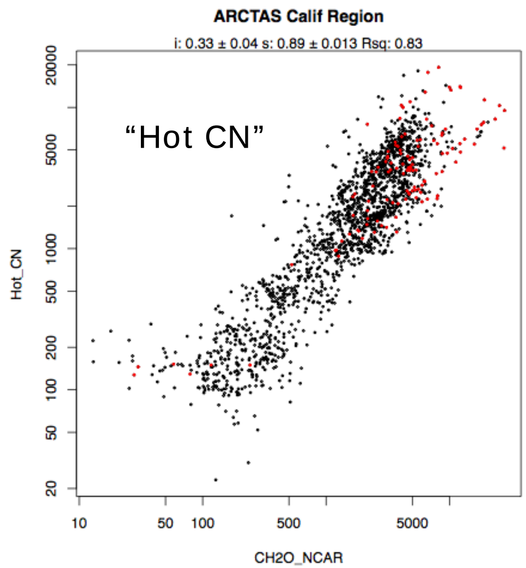
Explain close relationship of organics and fine submicron aerosol

Indicates absorbing aerosol

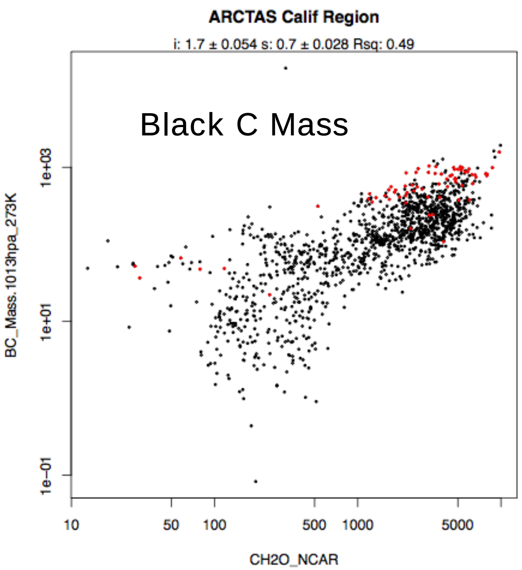


Red points: Smoke using HCN

Indicates *certain* absorbing aerosol



Primary C => absorption *must be "unwound"*



Interesting correlation of small particles to HCHO (and VOC's) in Cal-ARCTAS:

Similar to many previous missions

*(4b) Understand Chemical Processes … Ozone Formation*s

O_3 production and its VOC or NO_x sensitivity

- ***at one location and over a few hours, using networks of relatively simple instruments. This allows us to extend DISCOVER-AQ airborne measurements in both space and time.***
- ***The technique promises to use satellite retrievals if descriptions of PBL HCHO, UV, O_3, and NO_2 become available.***
- ***The technique begins to disentangle O_3 transport, VOC transport, and NOx transport …***

$$P_o(O_3) = C\,(j_{HCHO\text{->}rads}[HCHO])^a\,[NO]^b$$

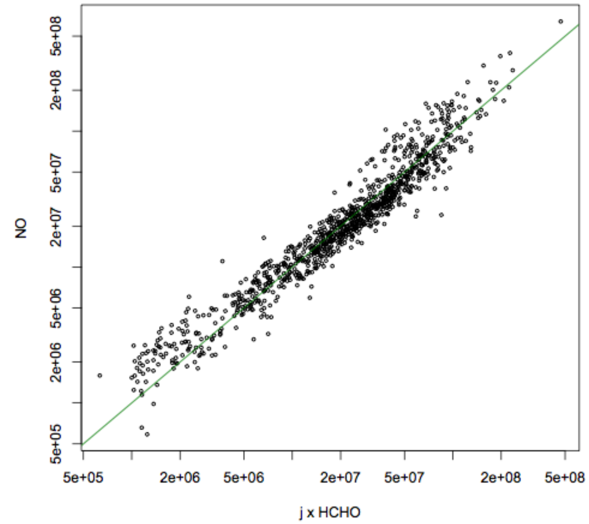
and may help pin down peroxy radical concentrations in models.

- ***The technique works also to estimate the important loss process L_{NO_2} for NO_2 and ozone, OH+NO_2***

- ***References:***

- **Chatfield, R.B. Ren, Xinrong, Brune, Wi. and Staub, J., Controls on Urban Ozone Production Rate as Indicated by Formaldehyde Oxidation Rate and Nitric Oxide, *Atmospheric Environment, in press,* Oct 2010.**
- **Chatfield, R.B., Ren, Xinrong, Brune, William, and Fried, Alan, 2010. Controls on regional ozone production: contrasts between Calfornia and the Eastern States, *submitted for publication (October, 2010), Journal of Atmospheric Chemistry and Physics.***

Regression and Correlation of Model

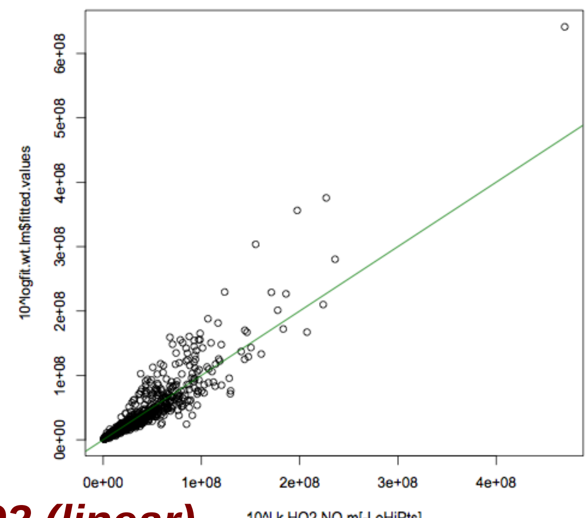


$$Po(O_3) = 10^{-2.46}(j\ [HCHO])^{0.70}[NO]^{0.57}$$

LA Urban Data
From Cal-ARCTAS

California measurements show high exponents compared to NYC and INTEX-NA exponents, $\geq$0.4
Why?

r = 0.93 (log)

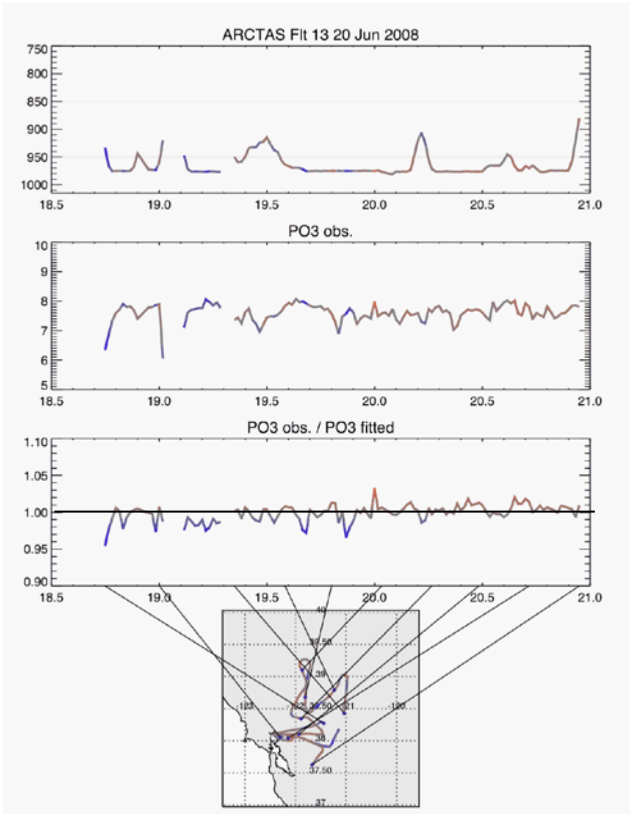


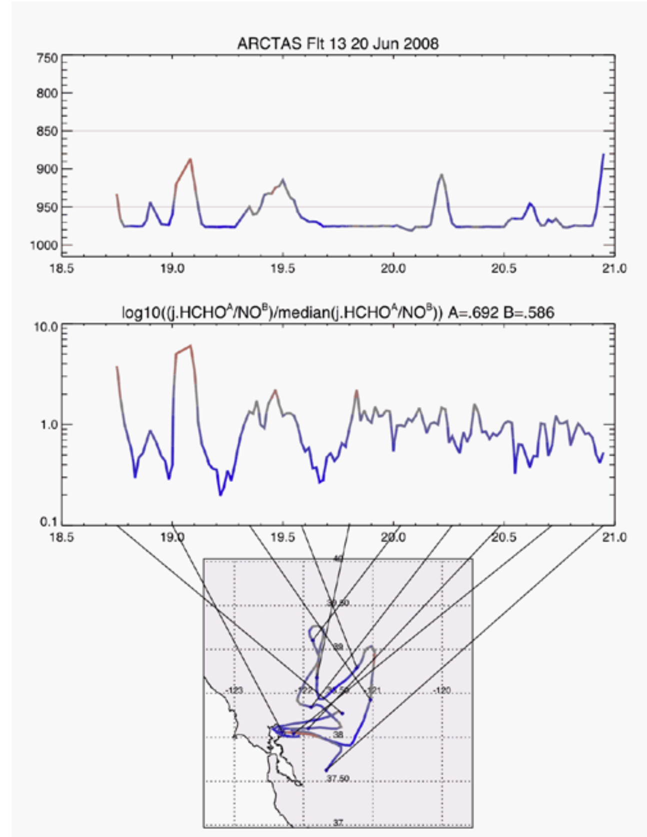
California Regional Data, non-Urban …

Chatfield, R.B., Ren, Xinrong, Brune, William, and Fried, Alan, 2010. Controls on regional ozone production: contrasts between Calfornia and the Eastern States, *submitted for publication (October, 2010), Journal of Atmospheric Chemistry and Physics.*

r = 0.92 (linear)

Reliability of POGO & Variability of NO_x Control





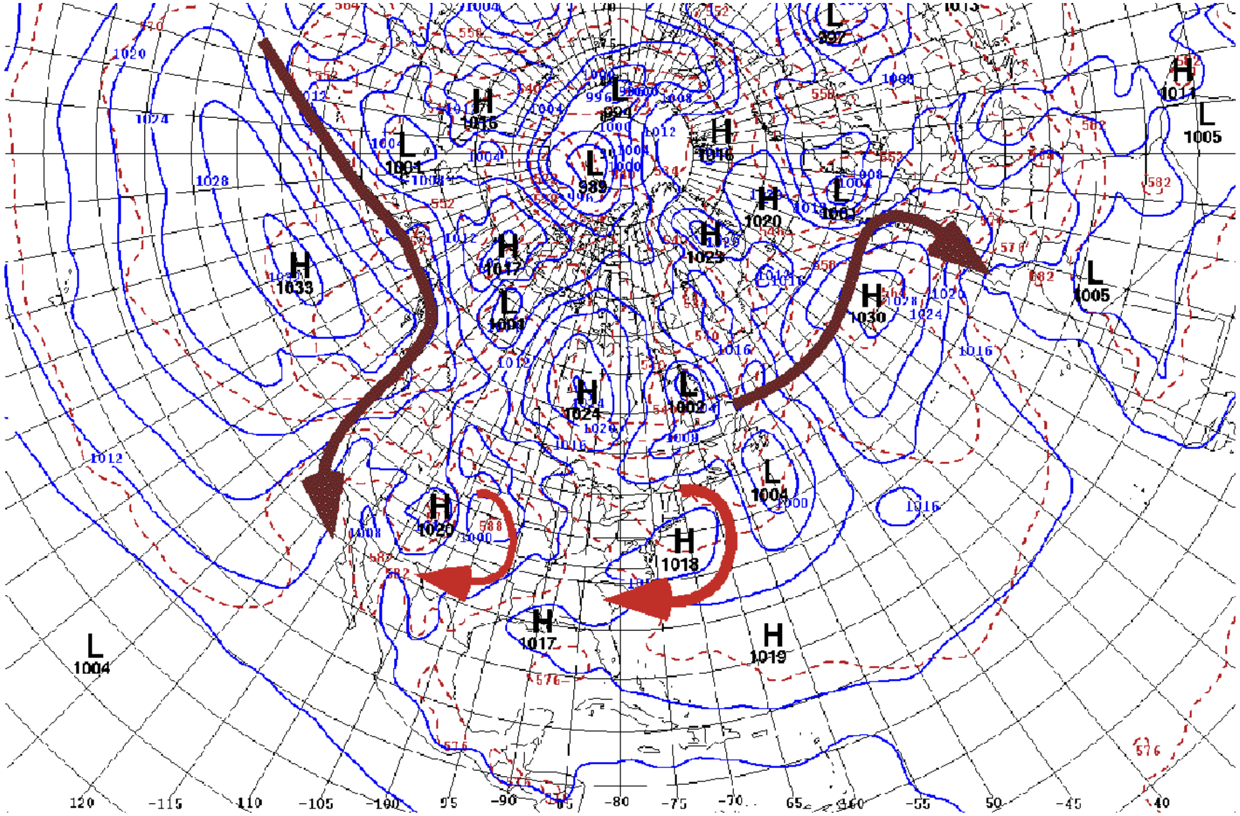
- This San-Francisco-Bay—Sacramento POGO had excellent agreement with (DC-8)-based, Brune/Weinheimer) "observations" of $k_{HO_2\,NO}$ [HO_2] [NO] = $P_o(O_3)$

- Production of ozone alternates rapidly between NOx control and VOC (radical) control. Is this modeled

Background

Why did Vukovich, Fishman, … see smog ozone in total ozone ? … Eastern transient anticyclones include mixing to 2-3 km by clouds: this ozone layer is thicker and much more visible in the UV

- Ozone from the Great Pacific Anticyclone vs East-Coast transitory Anticyclones



08/10/2006 00UTC 000HR FCST VALID THU 08/10/2006 00UTC NCEP/NWS/NOAA

- West Coast: subsidence, PBL affected by subsidence and horizontal inflow ozone, but no symmetrical venting with region above

- East Coast: PBL reaches 1-2 km, exchanges symmetrically with 1-3 km region by means of low clouds and some subsidence

Extrapolation of Concentrations Horizontally Needs to Acomodate Directionality … with Windflow

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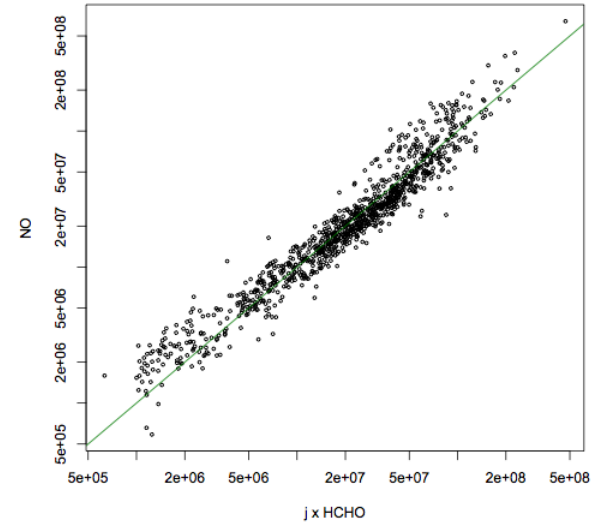
Regression and Correlation of Model

```
Call:
lm(formula = l.k.HO2.NO.m ~ l.j.HCHO.m + l.NO.m,
subset = -LoHiPts,
    weights = (l.k.HO2.NO.m), x = TRUE)

Residuals:
     Min       1Q   Median       3Q      Max
-1.22452 -0.20482  0.05008  0.22725  1.53562

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -2.46722    0.08744  -28.21   <2e-16 ***
l.j.HCHO.m   0.69706    0.01499   46.49   <2e-16 ***
l.NO.m       0.56941    0.00809   70.38   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.3491 on 998 degrees of freedom
Multiple R-squared: 0.9311,   Adjusted R-squared: 0.9309
F-statistic:  6738 on 2 and 998 DF,  p-value: < 2.2e-16
```



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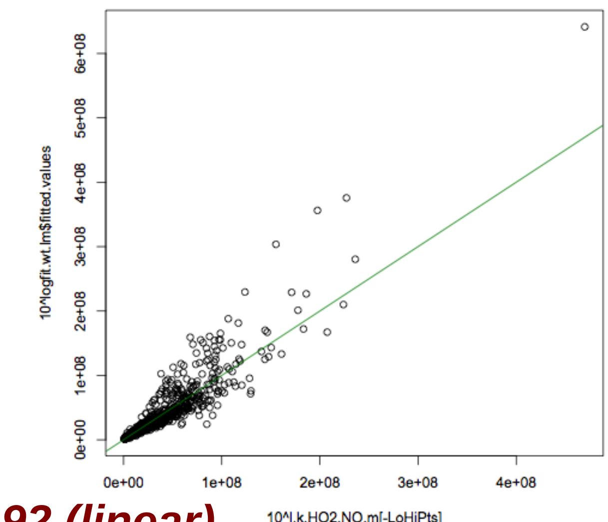

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