Spatial Variability of Trace Gases during DISCOVER-AQ: Planning for Geostationary Observations of Atmospheric Composition

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Motivation

The Tropospheric Emissions: Monitoring of Pollution (TEMPO) instrument will be the first NASA mission to make atmospheric composition observations from geostationary orbit and partially fulfills the goals of the Geostationary Coastal and Air Pollution Events (GEO-CAPE) mission

Follette-Cook et al. (2015, *Atmos. Environ.*) related observed and simulated variability to the precision requirements defined by the science traceability matrices of these space-borne missions

In that work, we quantified the spatial and temporal variability of column integrated and in-situ observations of trace gases over the Baltimore/Washington, DC area using output from WRF/Chem for the entire month of July 2011, coinciding with the first deployment of the NASA Earth Venture program mission DISCOVER-AQ (Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality)

Here, we expand that analysis to include the other three deployments of DISCOVER-AQ

Maryland Analysis Highlights – Follette-Cook et al. (2015)

Follette-Cook et al. (2015) quantified the variability seen in the Maryland/DC DISCOVER-AQ P-3B trace gas data and found it compared well with our WRF/Chem simulation

Questions addressed in that analysis:

- How much does each species vary spatially and temporally throughout the campaign? (i.e. one month)
- How much of that variability would a TEMPO-like instrument see?
- Is the resolvable variability sufficient answer the relevant science questions?

Precision Requirements (PR) for GEO-CAPE/TEMPO

Species	Altitude range	STM Precision		Temporal Revisit
O_3	0-2 km	10 ppbv	1.7 DU*	2 hr
O_3	Tropospheric column	10 ppbv	6.2 DU*	1 hr
CO	0-2 km	20 ppbv	0.91×10^{17} molec/cm²*	1 hr
CO	2 km - tropopause	20 ppbv	2.5×10^{17} molec/cm²*	1 hr
CO	Tropospheric column		3.4×10^{17} molec/cm²*	1 hr
NO_2	Tropospheric column	1×10^{15} molec/cm²	~1 ppbv**	1 hr
HCHO	Tropospheric column	1×10^{16} molec/cm²		3 hr
SO_2	Tropospheric column	1×10^{16} molec/cm²		3 hr

* calculated quantity
** Lok Lamsal, personal communication

TEMPO spatial resolution: 8x4.5 km

Structure Functions

Structure functions are a useful way to quantify variability in both space and time

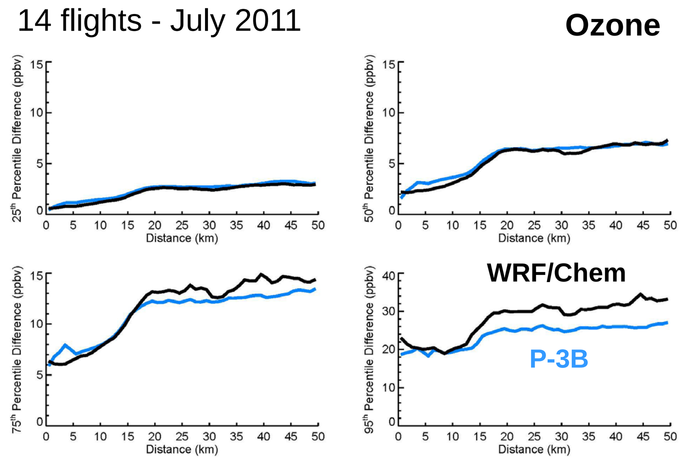
$$f(Z, y) \equiv \langle |Z(x+y) - Z(x)|^q \rangle$$

- < > = the average of data pairs separated by distance *y*
- Z = variable of interest at given location *x*
- q = scaling exponent (here q =1)

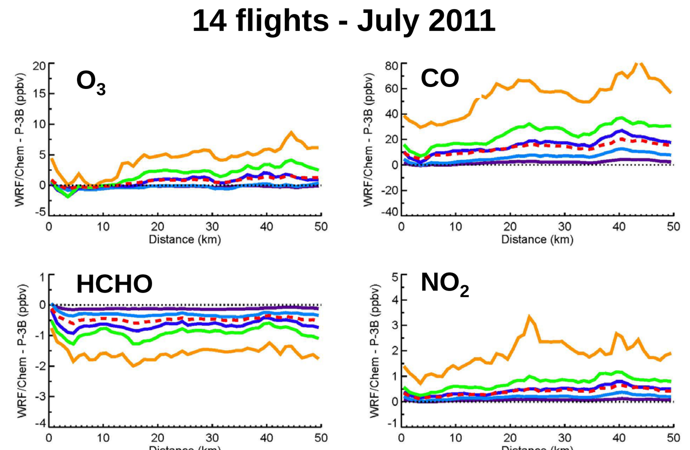
Calculate structure functions using data from DISCOVER-AQ P-3B in-situ aircraft (14 flights for MD)
Criteria:
- Both points must be **below 2 km (AGL)**
- The points must be **< 2 hrs apart (1.75 hrs for MD)**
- The 1-second merge data was used for this analysis
- Model output was sampled along the P-3B flight track

Can WRF/Chem capture the variability seen in the MD DISCOVER-AQ observations?

Percentiles of observed and simulated differences
14 flights - July 2011



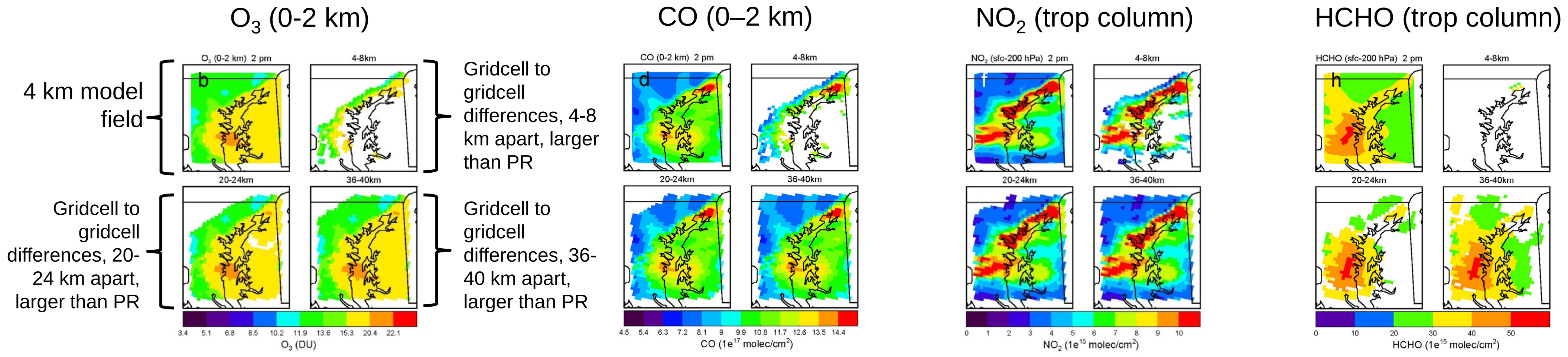
WRF/Chem – P-3B Percentiles
14 flights - July 2011



- WRF/Chem reproduces the variability in O_3 well
- Slightly overestimates the variability of CO and NO_2
- Underestimates the variability in HCHO

What is the geographic coverage of observable differences?

7/29/2011 2 pm EDT – "Code Orange" Day (8-hr max O3 between 76 and 95 ppbv)



These results indicate that the TEMPO instrument would be able to observe O_3 air quality events over the Mid-Atlantic area, even on days when the violations of the air quality standard are not widespread.

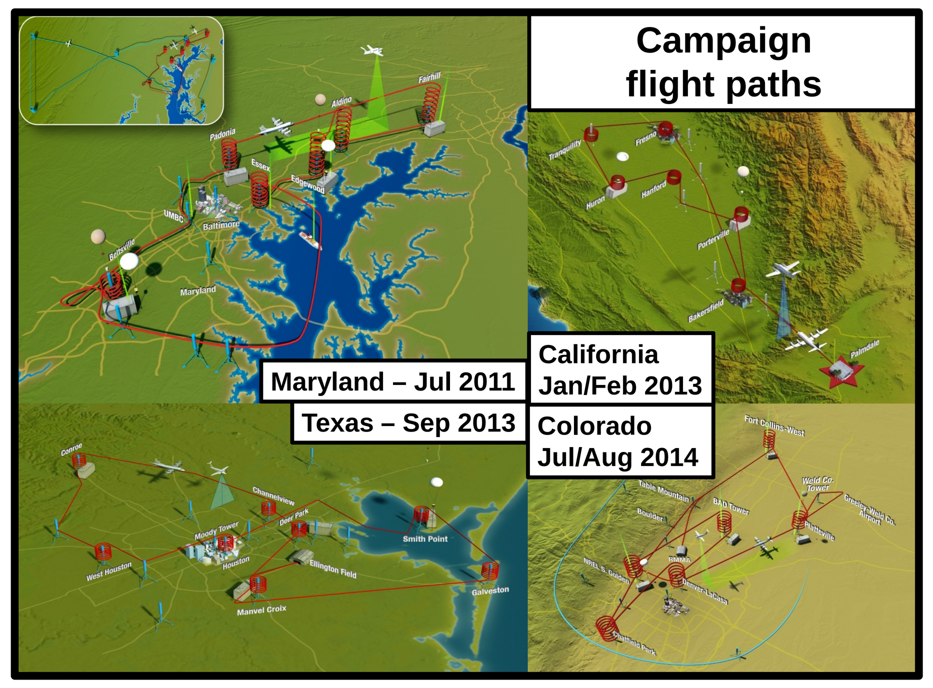
- The maximum differences in NO_2 are in the morning and early evening, so 2 pm represents a minimum in what would be observable
- Despite that, the major features in the tropospheric column field can be seen in the plot of the visible differences at 4 – 8 km distances

In MD, sources of HCHO include oxidation of hydrocarbons with both biogenic and anthropogenic sources. Thus, greater variability in HCHO is seen at longer distances, i.e. greater than 20 km, and would be hypothetically resolvable by TEMPO

DISCOVER-AQ observations and simulations

Objective:
Characterize the relationship between air quality at the surface and in the tropospheric columns that can be measured from a satellite

Observing strategy:
Concurrent in-situ and remote sensing observations from a network of ground sites and two research aircraft

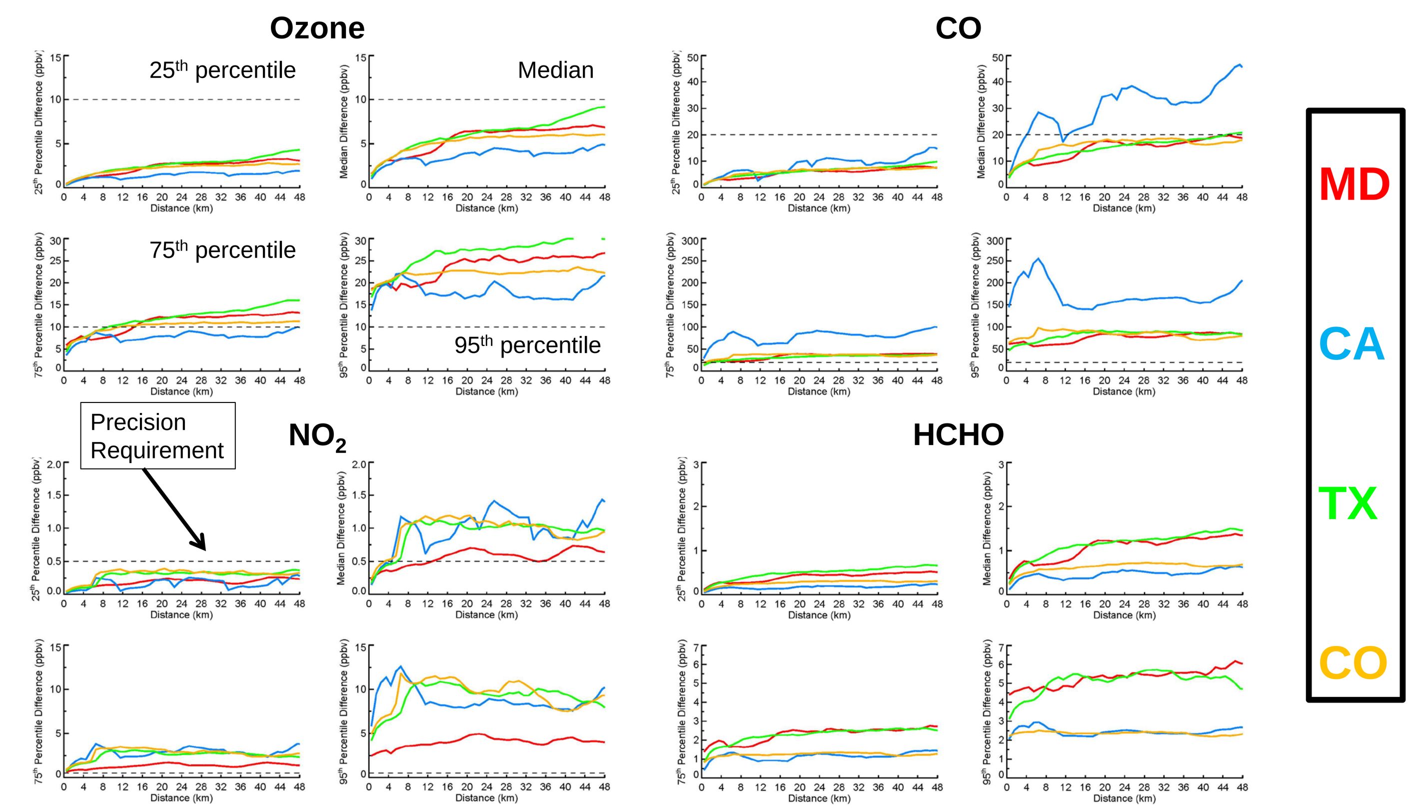


Simulations:
- **Maryland – Follette-Cook et al. (2015)**
  - WRF/Chem v3.3.1 – 4 km
- **California – W. Appel**
  - Coupled WRF/CMAQ v5.0.2 – 4 km
- **Houston – C. Loughner**
  - WRF/CMAQ v5.0.2– 4 km
- **Colorado – G. Pfister**
  - WRF/Chem – 3 km

Inter-Campaign Variability

The results from the MD analysis suggest that the PRs for TEMPO and GEO-CAPE are sufficient for addressing the science questions they are tasked to answer

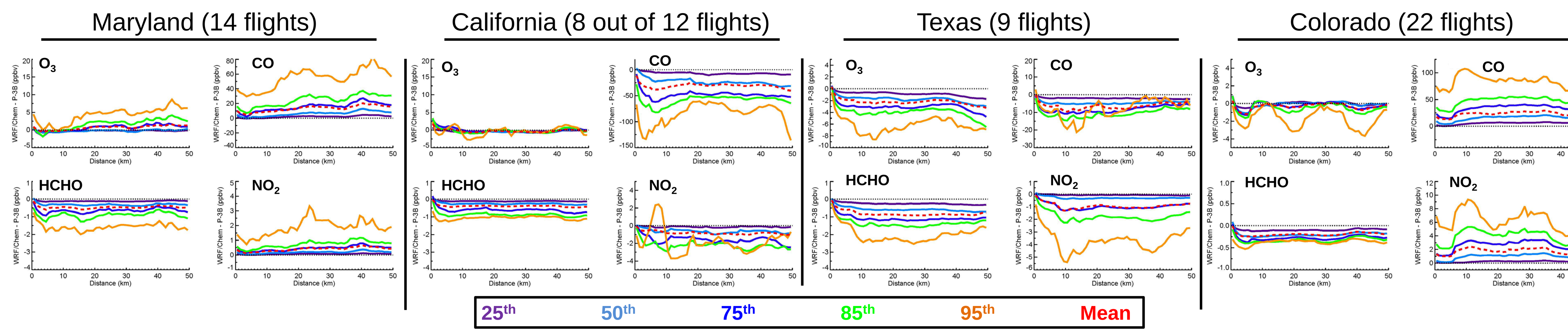
How does the variability seen in the other three deployments compare to that seen in MD?



O_3 – TX, CO, and MD show comparable differences to MD. *Air quality events in these regions will likely be observable by TEMPO*
CO – Variability of all campaigns similar, except for CA, which was much larger
NO2 – MD shows the lowest variability of any campaign, and the variability during the MD campaign was large enough to be well-resolved by TEMPO. *Therefore, with respect to variability, TEMPO's NO_2 PR is more than sufficient for these other regions as well.*
HCHO – MD and TX show largest differences. In MD, larger differences in HCHO are seen at longer distances (> 20 km) and would be hypothetically resolvable by TEMPO. These results indicate that *HCHO variability in the San Joaquin Valley and Denver, CO regions might be too small to be resolvable at ~20 km distances.*

How well do models capture the variability seen in the DISCOVER-AQ observations?

Model – P-3B Percentiles



Conclusions

- Results from an in-depth analysis of trace gas variability in MD indicated that the variability in this region was large enough to be observable by a TEMPO-like instrument
- The variability observed in MD is relatively similar to the other three campaigns with a few exceptions:
  - CO variability in CA was much higher than in the other regions; HCHO variability in CA and CO was much lower; MD showed the lowest variability in NO2
- All model simulations do a reasonable job simulating O_3 variability. For CO, the CA/CO simulations largely under/overestimate the variability in the observations. The variability in HCHO is underestimated for every campaign. NO2 variability is slightly overestimated in MD, more so in CO. The TX simulation underestimates the variability in each trace gas. This is most likely due to missing emissions sources (C. Loughner, manuscript in preparation).
- *Future Work:* Where reasonable, we will use these model outputs to further explore the resolvability from space of these key trace gases using analyses of tropospheric column amounts relative to satellite precision requirements, similar to Follette-Cook et al. (2015).