

Boundary layer observations, ensembles, and their use in improving greenhouse gas flux inversions: Result from the ACT-America mission

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Background

- The atmospheric boundary layer (ABL) is a big deal for greenhouse gas and air quality studies.
 - Wind speed and mixing depth (ventilation factor) determines mole fraction enhancements:
 - $\Delta C = \frac{F_C L}{z_i M}$, where ΔC is the mole fraction enhancement, F_C is the flux of C, L is the advection distance, z_i is the mixing depth, and M is the wind speed.
 - ABL wind direction drives plume location.
 - ABL clouds / venting into the free troposphere / large-scale subsidence determines ABL residence time.
- Atmospheric simulations of the ABL have errors – bias and random.

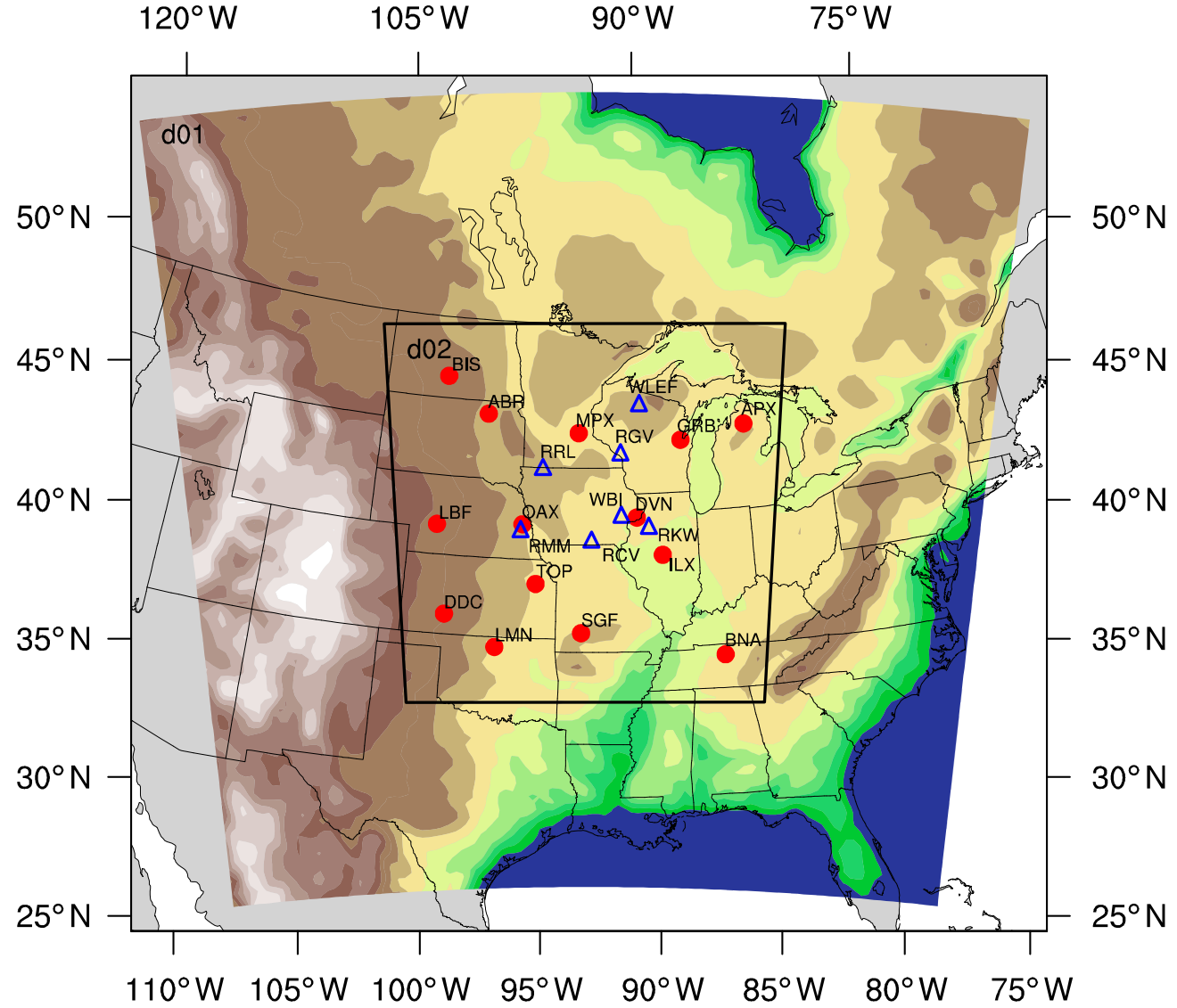
An example...

- How do WRF ABL winds and ABL depth compare to rawinsonde measurements of the same properties in the US midcontinent?

An example...

- How do WRF ABL winds and ABL depth compare to rawinsonde measurements of the same properties in the US midcontinent?
- OK, WRF isn't one model...let's ask this of a WRF ensemble.

Evaluation of WRF-Chem CO₂ simulations in the upper Midwest, summer



Evaluation of *mid-afternoon* CO₂, ABL depth, and ABL winds.

Blue are tower-based CO₂ observation points (PSU, NOAA).

Red are rawinsonde stations (NOAA).

Boxes show the model domains (interior at 10 km).

45-member WRF transport ensemble

Diaz-Isaac et al, ACP, 2018

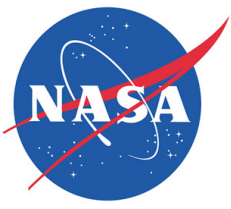
Table 1. Different model configurations used in this study.

Model number	Reanalysis	LSM scheme	PBL scheme	Cumulus scheme	Microphysics schemes
1	NARR	Noah	YSU	Kain-Fritsch	WSM 5-class
2	NARR	Noah	MYJ	Kain-Fritsch	WSM 5-class
3	NARR	Noah	MYNN	Kain-Fritsch	WSM 5-class
4	FNL	RUC	YSU	Kain-Fritsch	WSM 5-class
5	FNL	RUC	MYJ	Kain-Fritsch	WSM 5-class
6	FNL	RUC	MYNN	Kain-Fritsch	WSM 5-class
7	NARR	Thermal dif.	YSU	Kain-Fritsch	WSM 5-class
8	NARR	Thermal dif.	MYJ	Kain-Fritsch	WSM 5-class
9	NARR	Thermal dif.	MYNN	Kain-Fritsch	WSM 5-class
10	NARR	Noah	YSU	Grell-3D	WSM 5-class
11	NARR	Noah	MYJ	Grell-3D	WSM 5-class
12	NARR	Noah	MYNN	Grell-3D	WSM 5-class
13	FNL	RUC	YSU	Grell-3D	WSM 5-class
14	FNL	RUC	MYJ	Grell-3D	WSM 5-class
15	FNL	RUC	MYNN	Grell-3D	WSM 5-class
16	NARR	Thermal dif.	YSU	Grell-3D	WSM 5-class
17	NARR	Thermal dif.	MYJ	Grell-3D	WSM 5-class
18	NARR	Thermal dif.	MYNN	Grell-3D	WSM 5-class
19	NARR	Noah	YSU	Kain-Fritsch	Thompson
20	NARR	Noah	MYJ	Kain-Fritsch	Thompson
21	NARR	Noah	MYNN	Kain-Fritsch	Thompson
22	FNL	RUC	YSU	Kain-Fritsch	Thompson
23	FNL	RUC	MYJ	Kain-Fritsch	Thompson
24	FNL	RUC	MYNN	Kain-Fritsch	Thompson
25	NARR	Thermal dif.	YSU	Kain-Fritsch	Thompson
26	NARR	Thermal dif.	MYJ	Kain-Fritsch	Thompson
27	NARR	Thermal dif.	MYNN	Kain-Fritsch	Thompson
28	NARR	Noah	YSU	Grell-3D	Thompson
29	NARR	Noah	MYJ	Grell-3D	Thompson
30	NARR	Noah	MYNN	Grell-3D	Thompson
31	NARR	Noah	YSU	No CP	WSM 5-class
32	NARR	Noah	MYJ	No CP	WSM 5-class
33	NARR	Noah	MYNN	No CP	WSM 5-class
34	FNL	RUC	YSU	No CP	WSM 5-class
35	FNL	RUC	MYJ	No CP	WSM 5-class
36	FNL	RUC	MYNN	No CP	WSM 5-class
37	NARR	Thermal dif.	YSU	No CP	WSM 5-class
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40	FNL	Noah	YSU	Kain-Fritsch	WSM 5-class
41	FNL	Noah	MYJ	Kain-Fritsch	WSM 5-class
42	FNL	Noah	MYNN	Kain-Fritsch	WSM 5-class
43	FNL	Thermal dif.	YSU	Kain-Fritsch	WSM 5-class
44	FNL	Thermal dif.	MYJ	Kain-Fritsch	WSM 5-class
45	FNL	Thermal dif.	MYNN	Kain-Fritsch	WSM 5-class

Ensemble varies the:

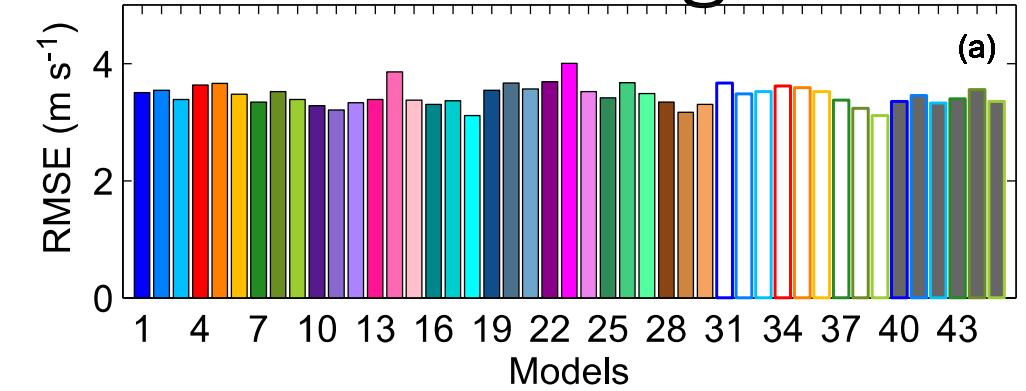
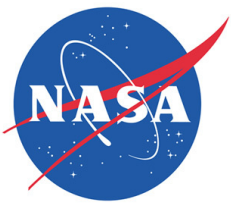
- boundary and initial conditions (2),
- land surface model (3),
- boundary layer parameterization (3),
- cumulus convection parameterization (3) and
- cloud microphysics parameterization (2).

No within-domain meteorological data assimilation.



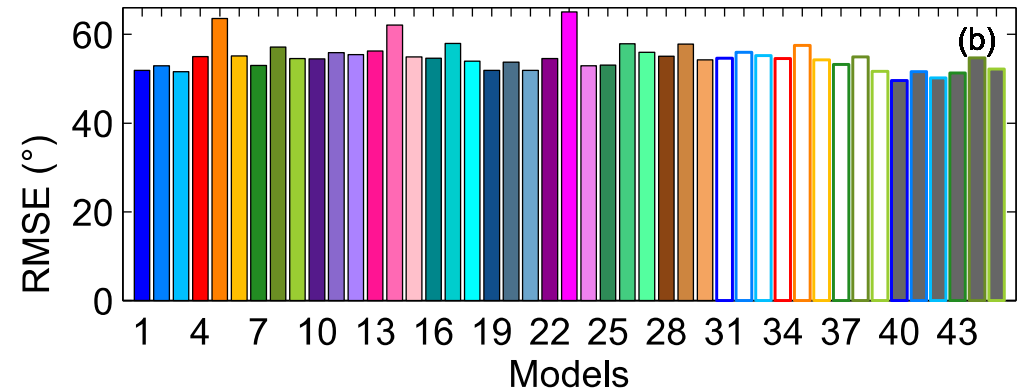


Random errors are significant for *all* model configurations

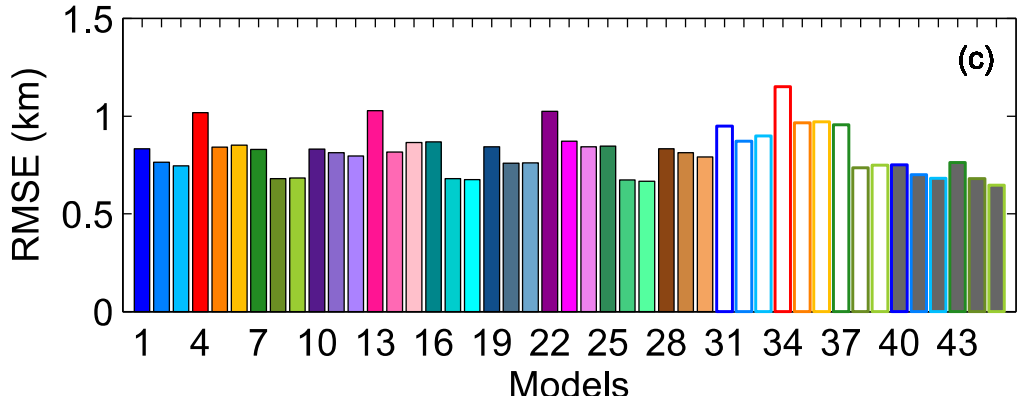


Afternoon conditions, daily comparison.

ABL wind (a) RMSE ~ 3 m/s.



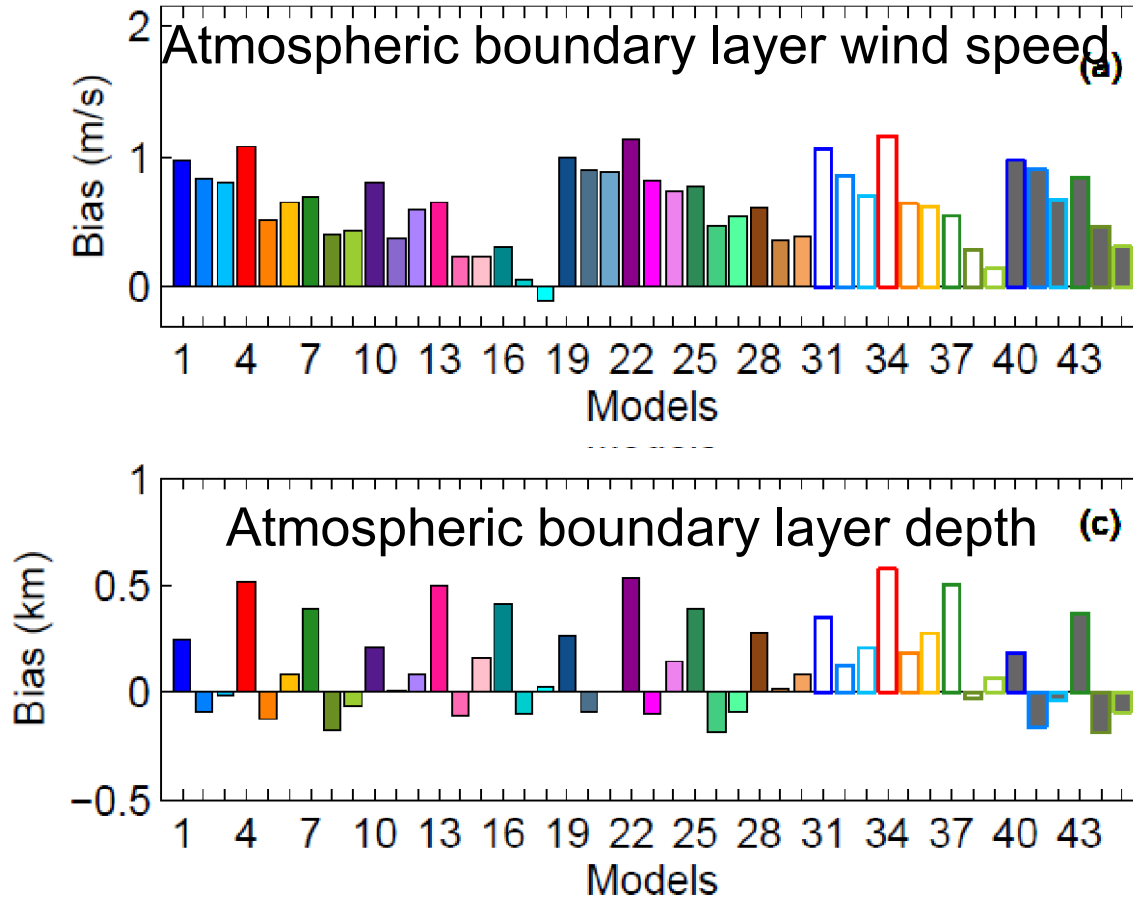
ABL wind direction (b) RMSE ~ 50 degrees.



ABL depth (c) RMSE ~ 700 m. (YSU-RUC consistently high).



Many model configurations show mean biases averaged over the study domain



Nearly all ensemble members overestimate boundary layer wind speeds.

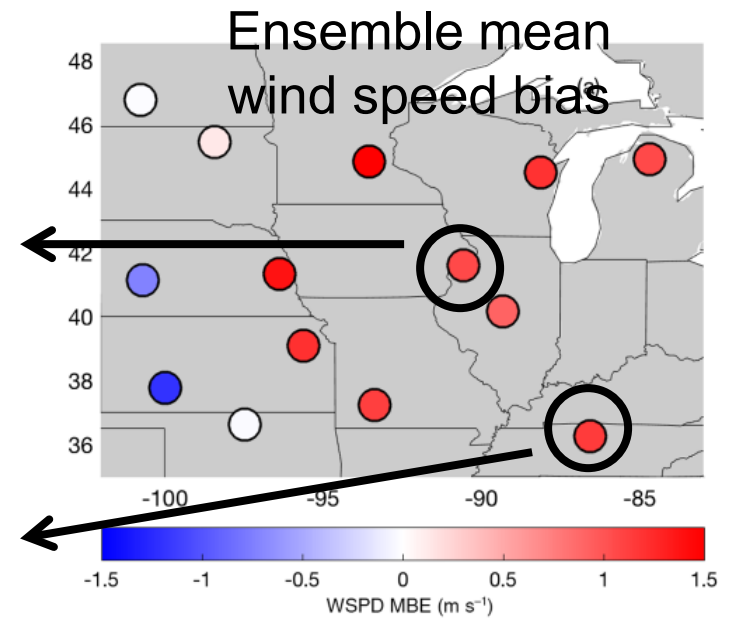
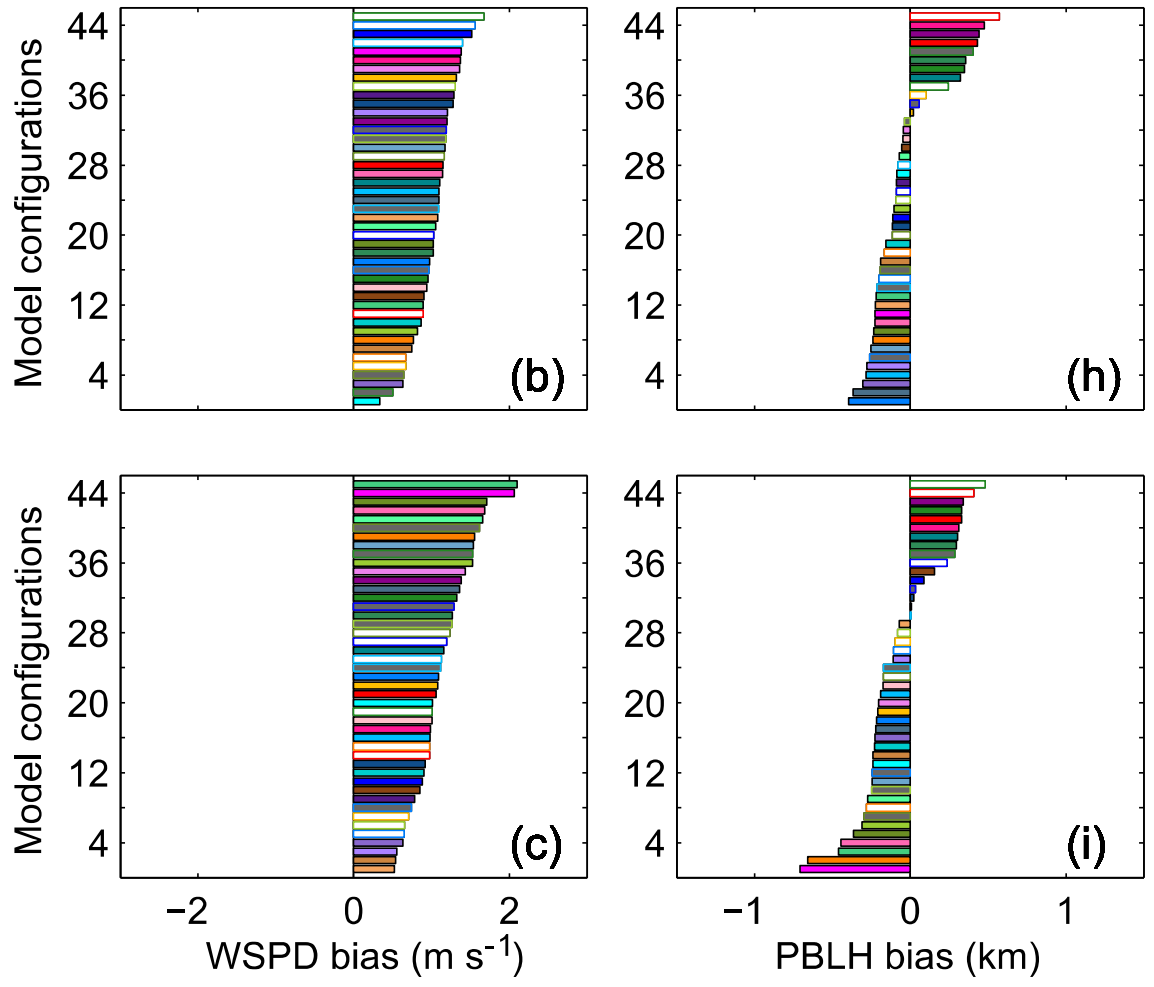
Most ensemble members overestimate boundary layer height.

MYNN with thermal diffusion LSM appears to minimize both biases.

YSU-RUC appears to maximize biases.

No cumulus parameterization increases biases.

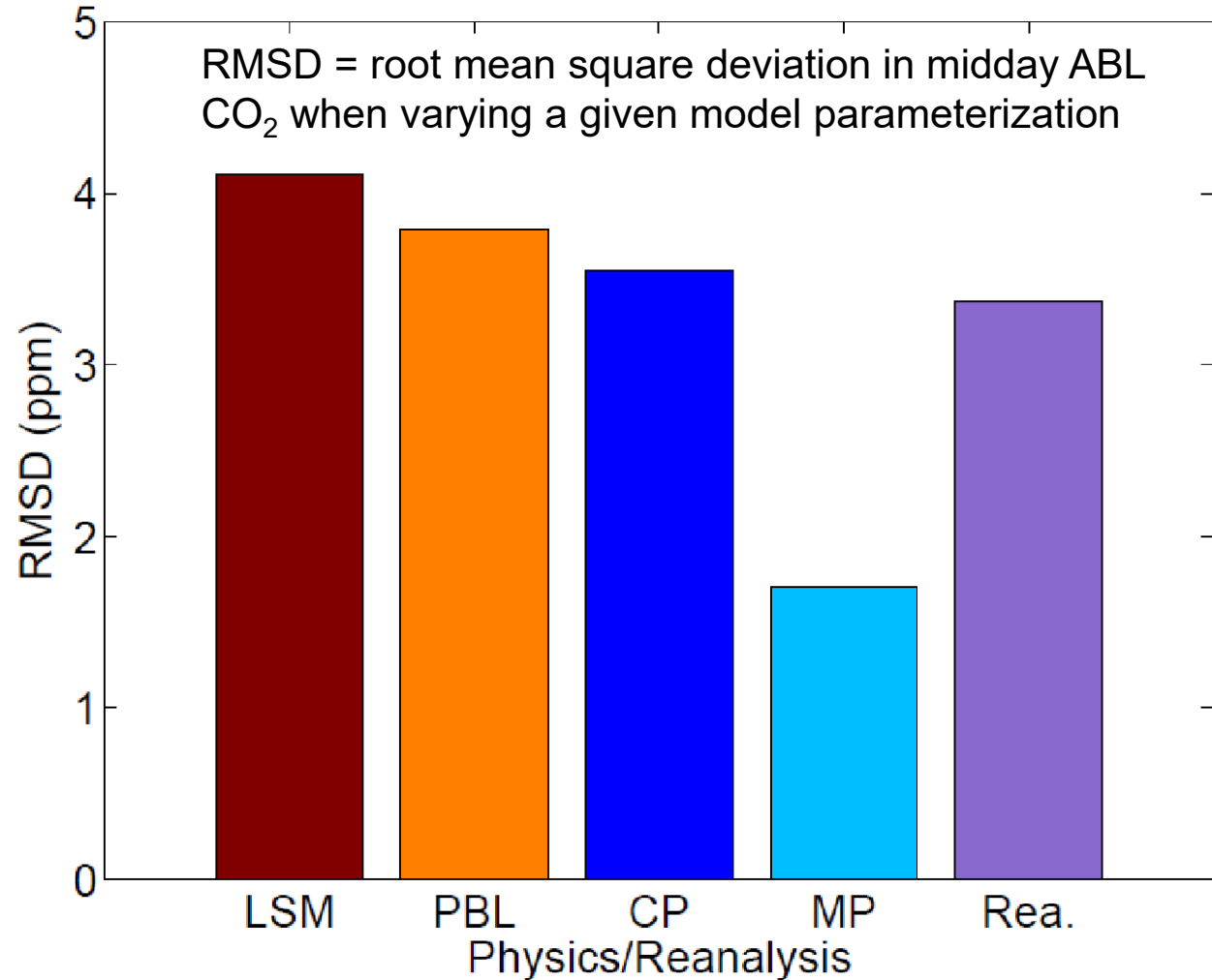
Biases have spatial structure and some locations are always biased



You can find model members with small mean ABL depth bias in these locations. But mean ABL wind speed is always too high.

Ensemble-mean, mean ABL wind speed bias changes sign with longitude.

ABL CO₂ simulations are sensitive to nearly all physical processes in WRF, and the variability is substantial



Land Surface Model (LSM)

Planetary Boundary Layer (PBL)

Cumulus Parameterization (CP)

global meteorological Reanalysis (Rea)

Cloud Microphysics (MP)

Background

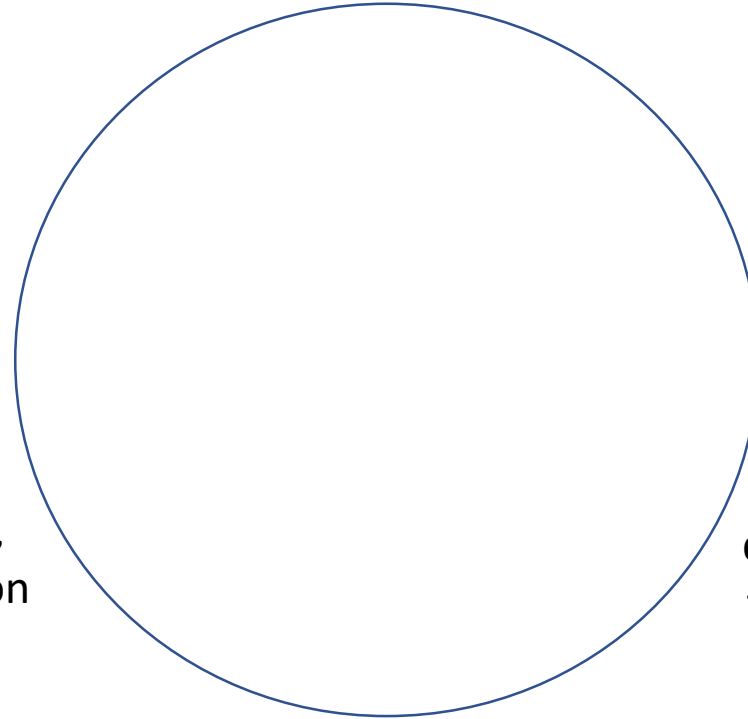
- The source of error are complex.
 - All ensemble elements matter (Diaz-Isaac et al, 2018).
 - Incoming solar radiation at surface is biased, improved land cover data doesn't fix urban ABL problems, urban surface fluxes (energy and momentum) have large errors (Sarmiento et al, 2017).
 - Model ensembles are often biased (sometimes *all members*) (Diaz-Isaac et al, 2018; Sarmiento et al, 2017).

What to do?

- Jim Wilczak. “Wheel of pain”
 - Coupled system
 - Hard to isolate one component

Radiation,
precipitation

Land surface
state and
fluxes



ABL state,
development,
fluxes, clouds

- Pop culture reference.
 - <https://www.dailymotion.com/video/x4blt6l>

What can we do to improve our modeling systems?

- *Fix.*
 - Improve the model physics.
- *Kick.*
 - Use data assimilation to push the model around.
- *Quantify with calibrated ensembles.*
 - Make model ensembles that have minimal bias, and whose spread is a fair measure of model uncertainty.

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- *What do all of these approaches have in common?*

What can we do to improve our modeling systems?

- *Fix.*
 - Improve the ABL model physics.
- *Kick.*
 - Use data assimilation to push the ABL model around.
- *Develop calibrated ensembles.*
 - Make model ensembles that have minimal bias, and whose spread is a fair measure of ABL model uncertainty.
- *What do all of these approaches have in common?*
- *They all require ABL observations.*

ABL observational efforts being presenting today...

- Ankur Desai – Long-term, ecosystem, point or small region, surface flux – ABL observations.
- Sunil Baidar – Long-term, urban system, surface flux - ABL observations.
- Me – Large-area, multi-season, airborne campaign, (surface flux) - ABL observations.

ACT-America ABL-relevant observations, models, and ongoing research

Overarching Goal

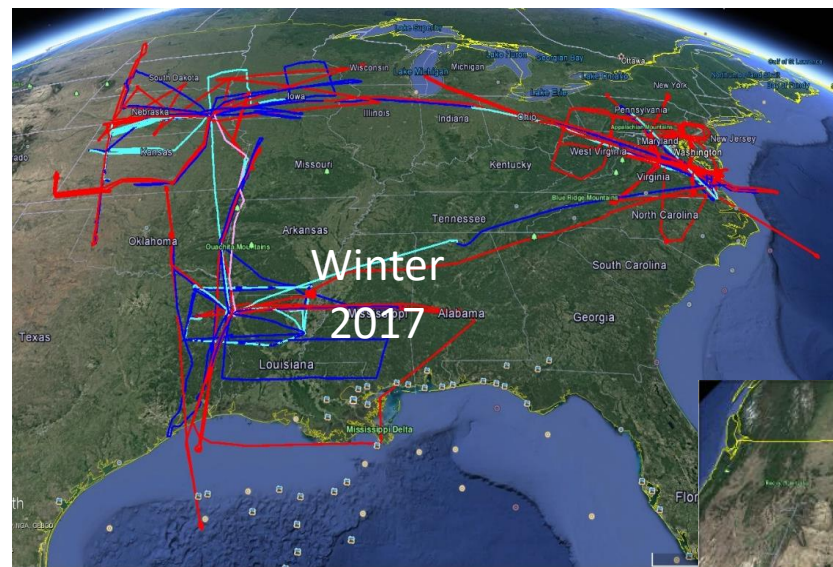
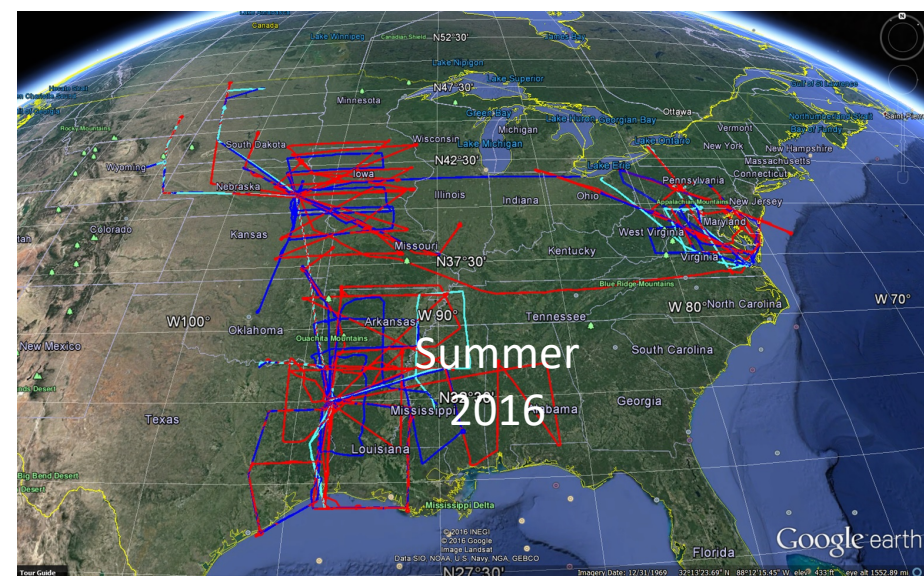
- The Atmospheric Carbon and Transport-America (ACT-America) mission will enable and demonstrate a new generation of atmospheric inversions for quantifying CO₂ and CH₄ sources and sinks at regional scales.
- These inverse flux estimates will be able to:
 - Evaluate and improve terrestrial carbon cycle models, and
 - Monitor carbon fluxes to support climate-change mitigation efforts.

Mission Goals

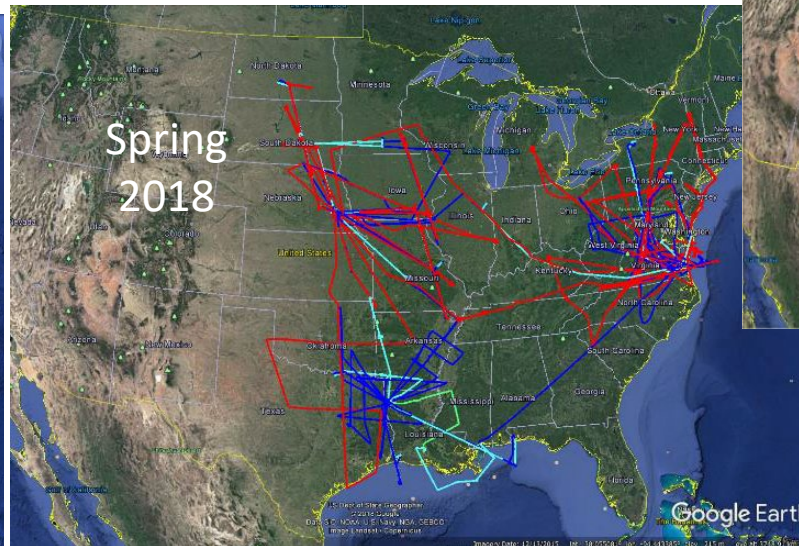
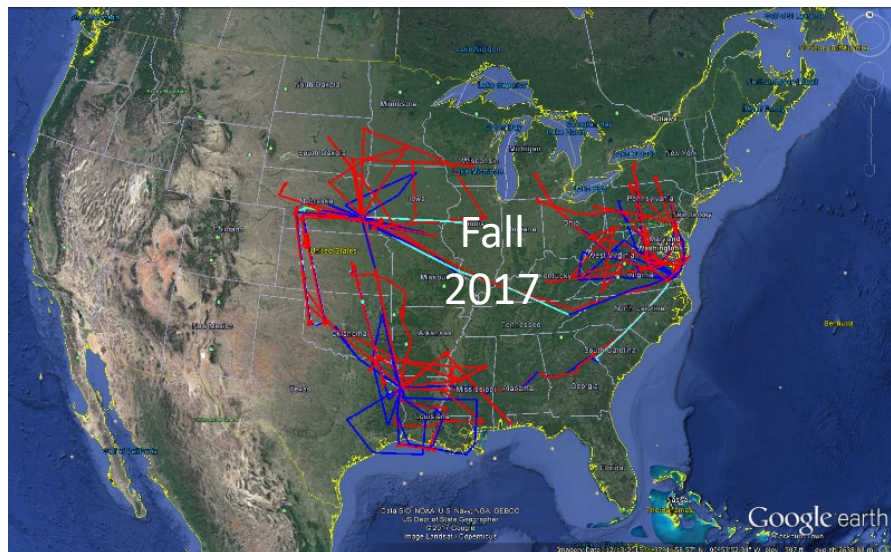
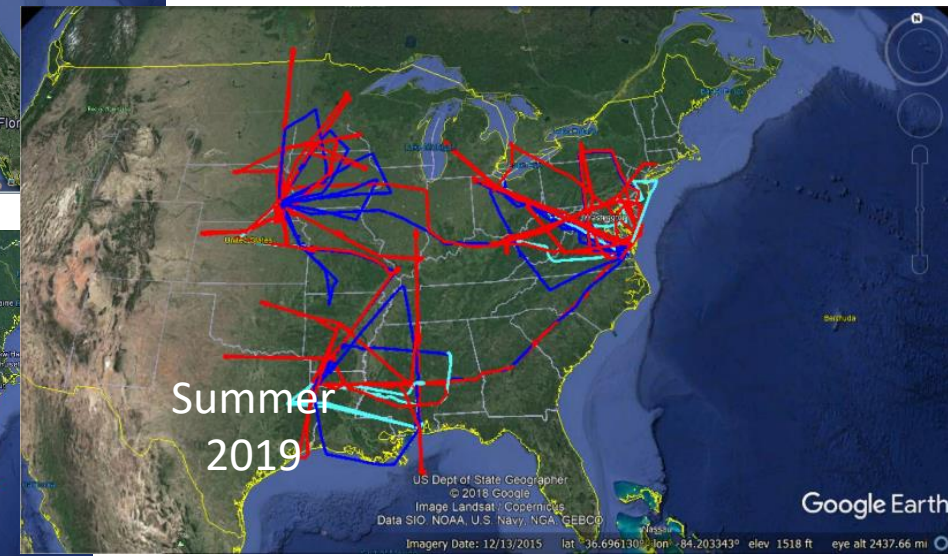
1. Quantify and reduce atmospheric transport uncertainties
 2. Quantify and reduce uncertainties in prior CO₂ and CH₄ flux estimates
 3. Evaluate the sensitivity of Orbiting Carbon Observatory-2 (OCO-2) column CO₂ measurements to regional variability in tropospheric CO₂
- All aimed to be applied to atmospheric inversions that use our long-term atmospheric observing systems.
- Concerned with bias, random error, and spatial structure of errors in all cases.

What's unique about ACT for ABL studies?

- Five-campaign, four-season, east-of-the-Rockies record of:
 - ABL depth (lidar – continuous, about 50,000 km; in situ profiles, ~1,200)
 - Cloud top retrievals (lidar – continuous, probably ~100,000 km)
 - ABL winds (level legs – nearly 200,000 km)
 - Spanning 30-40 weather systems, with pre-frontal, frontal, and post-frontal flights
 - With coincident GHG and other trace gas and meteorological data
- A multi-element ABL-GHG-calibrated ensemble modeling system
 - Transport and GHG ensemble elements
 - Transport calibrated on ABL winds and depth
 - GHG calibrated on flux and mole fraction tower data



ACT-America flight campaigns



- Five, six-week campaigns over 3 years, covering each season and summer twice. ~25 flights / campaign.
- Each campaign: 2 weeks in each of 3 regions across US (MidAtlantic, MidWest, SouthCentral).
- About 50% of the data in the atmospheric boundary layer (ABL).
- 1140 total flight hours. About 1,500 flasks and 1,000 vertical profiles. ~400,000 km of flight data

Ongoing, anticipated and desired analyses

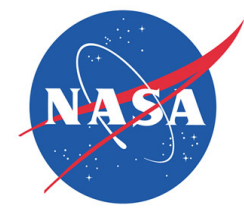
- Create a well-documented, quality-checked data base of ABL observations.
- Evaluate the ABL depth and winds in the models used for atmospheric GHG inversions.
 - Identify biases.
 - Identify less-biased transport models.
 - Improve inverse flux estimates by relying on the less-biased models.
- Use the ACT ABL depth and wind data to create better transport model ensembles. Apply these to atmospheric inversions.
- Develop improved ABL simulations to implement in atmospheric inversion systems.



A little about the observations

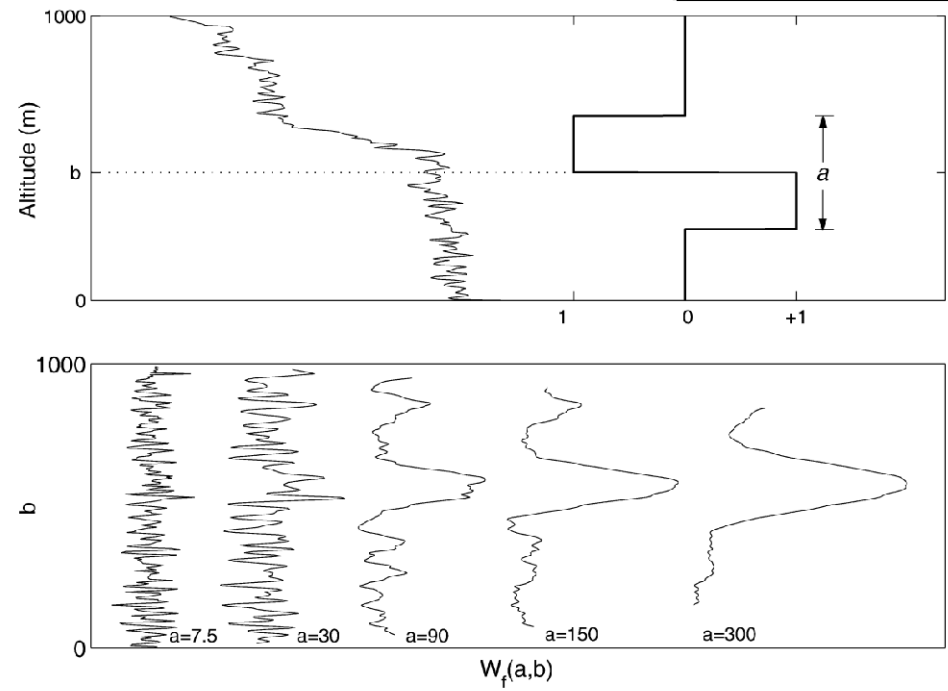
- Winds – multi-level, orthogonal-heading calibration legs flown on each aircraft during each campaign to remove biases.
- Performance suggests biases less than 1 m s^{-1} .
 - Data manuscript in prep with details on wind calibrations
- Lidar ABL depth and cloud top data.
 - Goddard's Cloud Physics Lidar (CPL), first four flight campaigns.
 - Langley's High Altitude Laser Observatory (HALO), for the last flight campaign.
 - Both retrieve cloud top and boundary layer top with high resolution and accuracy using lidar backscatter.





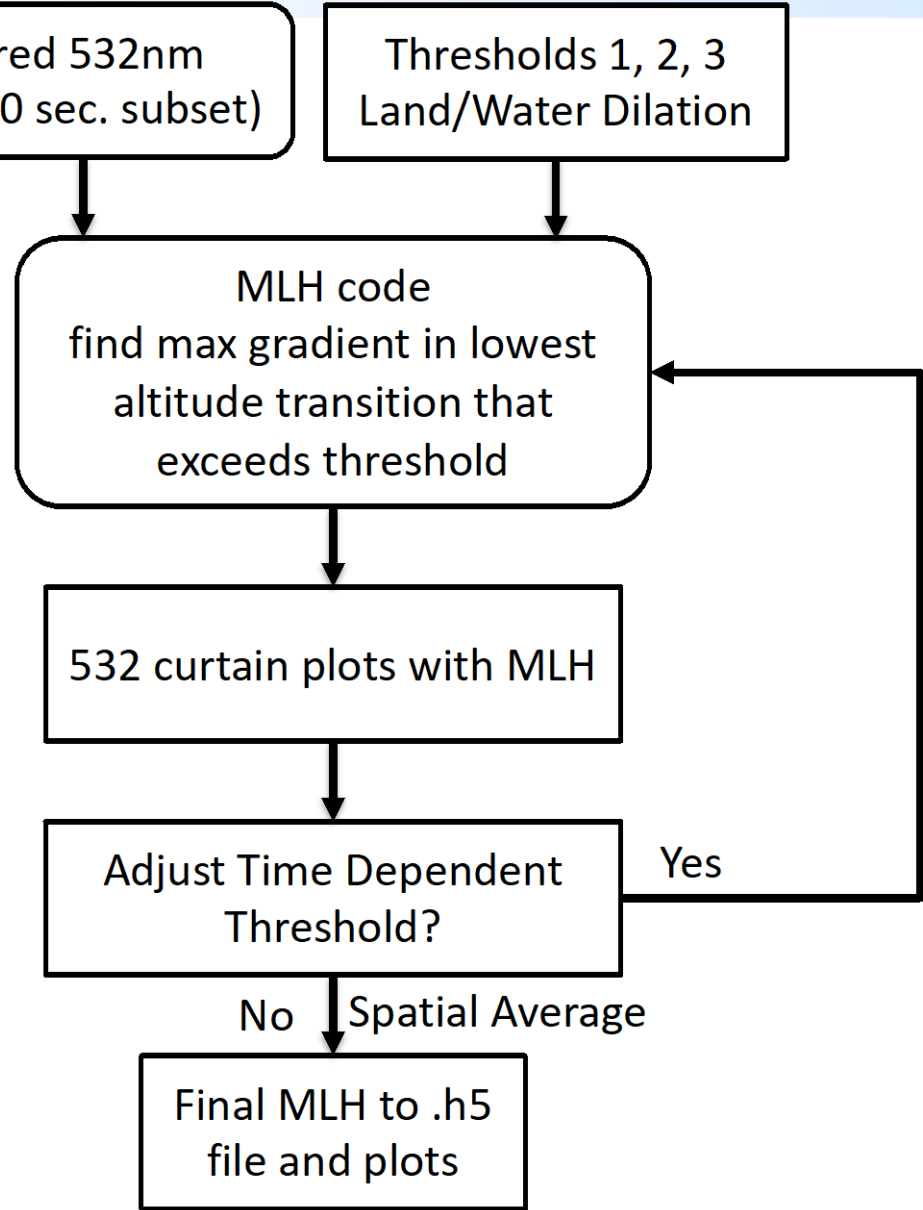
Mixed Layer Height Processing Flow Diagram

Cloud Cleared 532nm Backscatter (10 sec. subset) Thresholds 1, 2, 3 Land/Water Dilation



$$W_f(a, b) = \frac{1}{a} \int_{z_b}^{z_t} f(z) h\left(\frac{z-b}{a}\right) dz$$

Davis et al., 2000
 Brook 2003
 Scarino et al. 2004



HALO wavelet-based ABL depth detection algorithm.

Similar for both CPL and HALO observations.

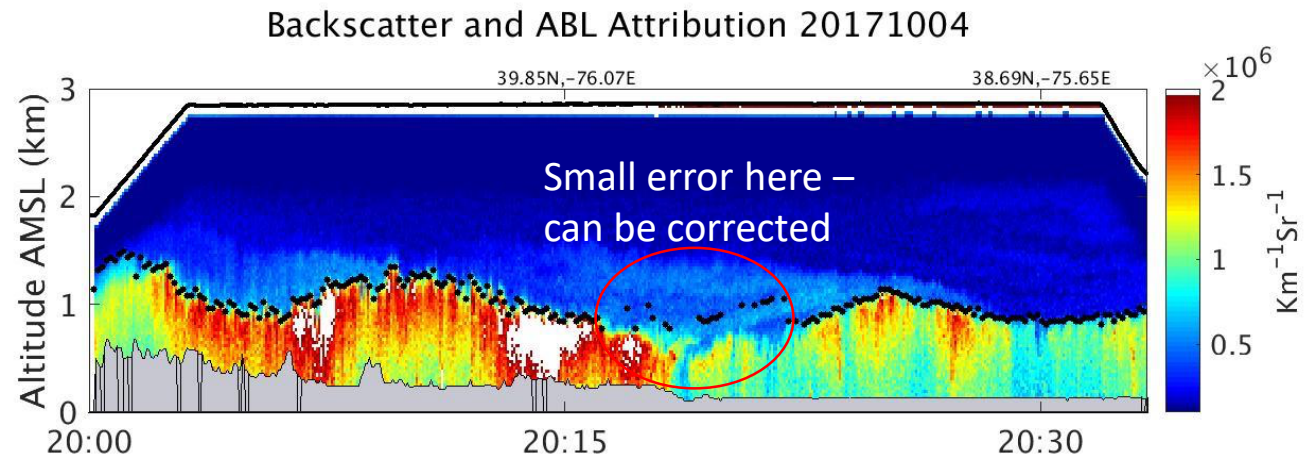
Collins, Nehrir, Kooi, Barton-Grimley, NASA LaRC



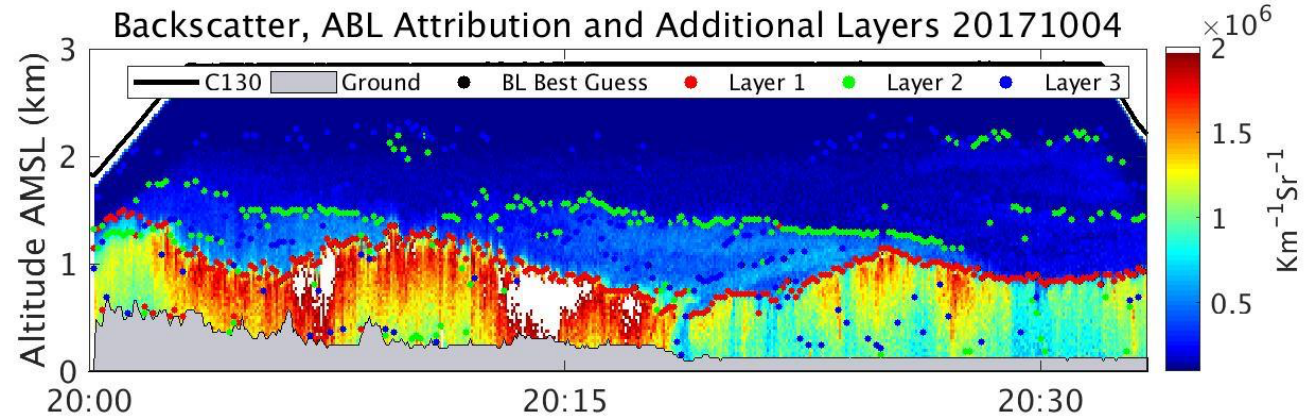
Cloud Physics Lidar ABL depth example. 30 minutes of C130 data.

Pal et al, data set in prep

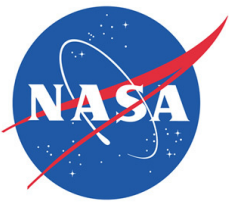
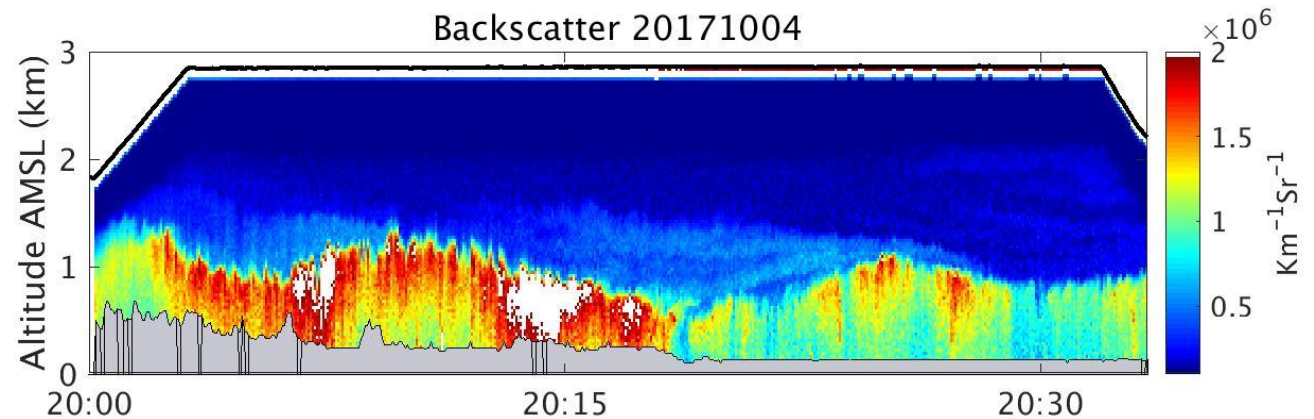
Backscatter with ABL identified



Backscatter with layers

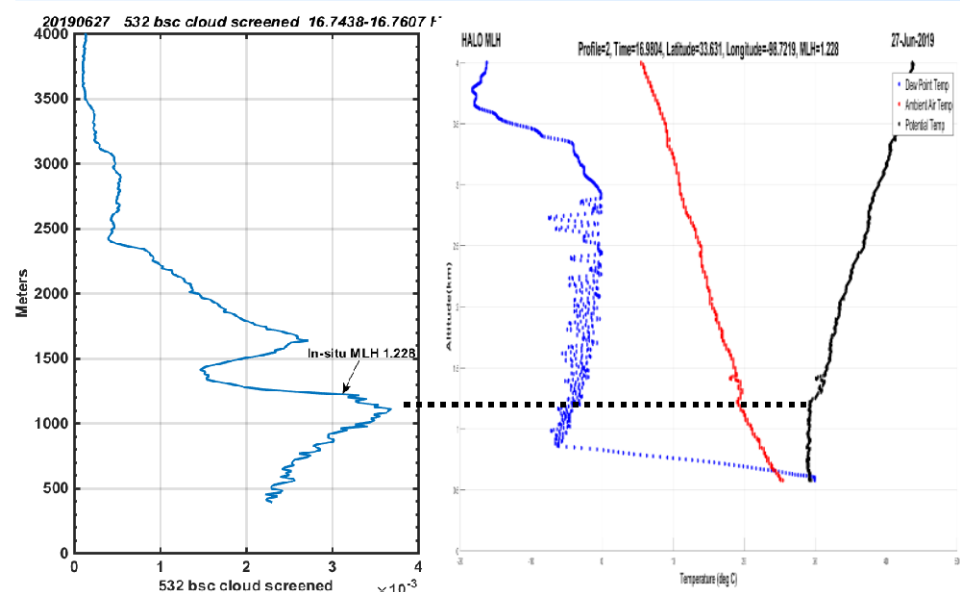
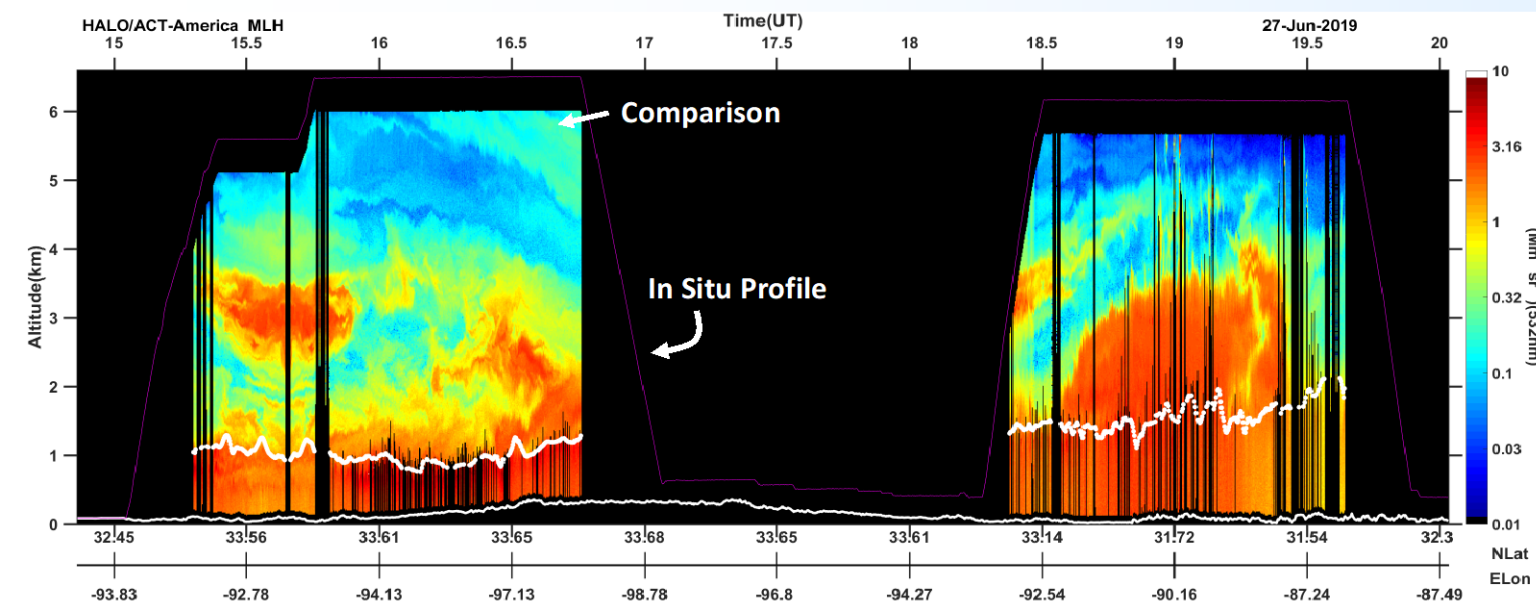


Backscatter

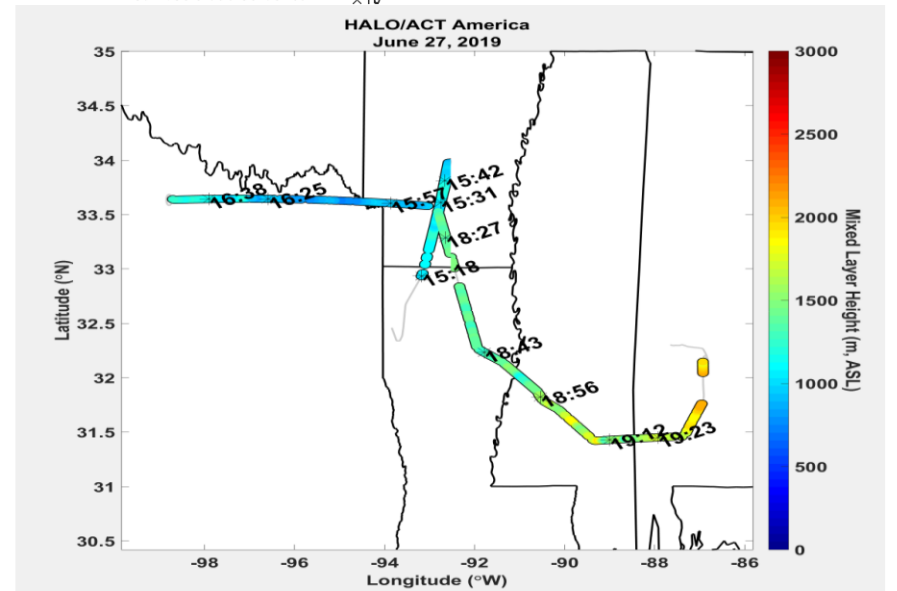




Comparison with Potential Temperature in optimal conditions

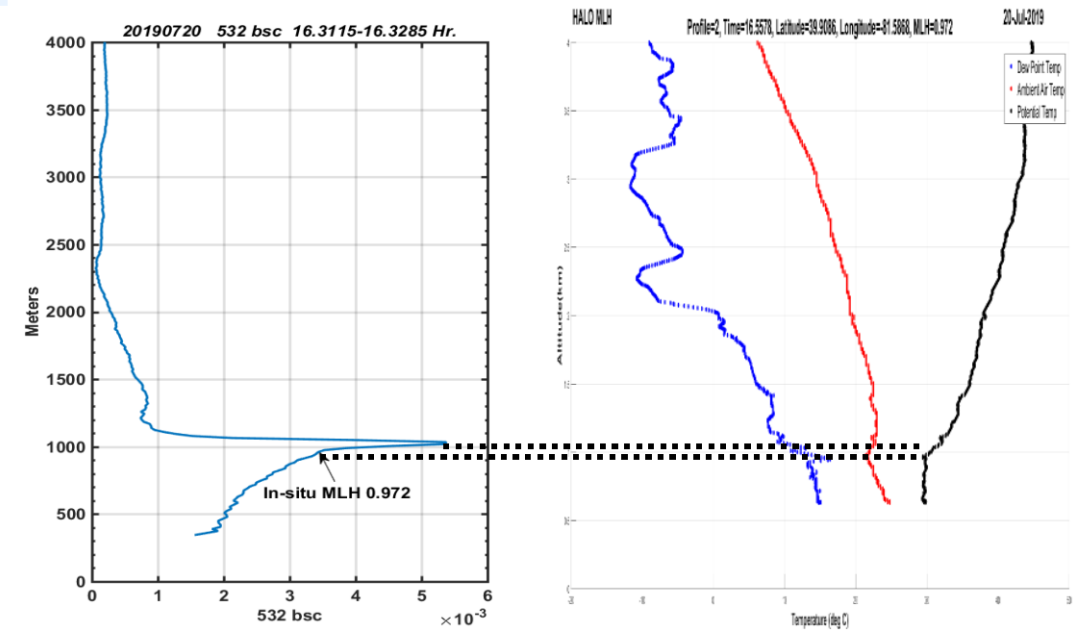
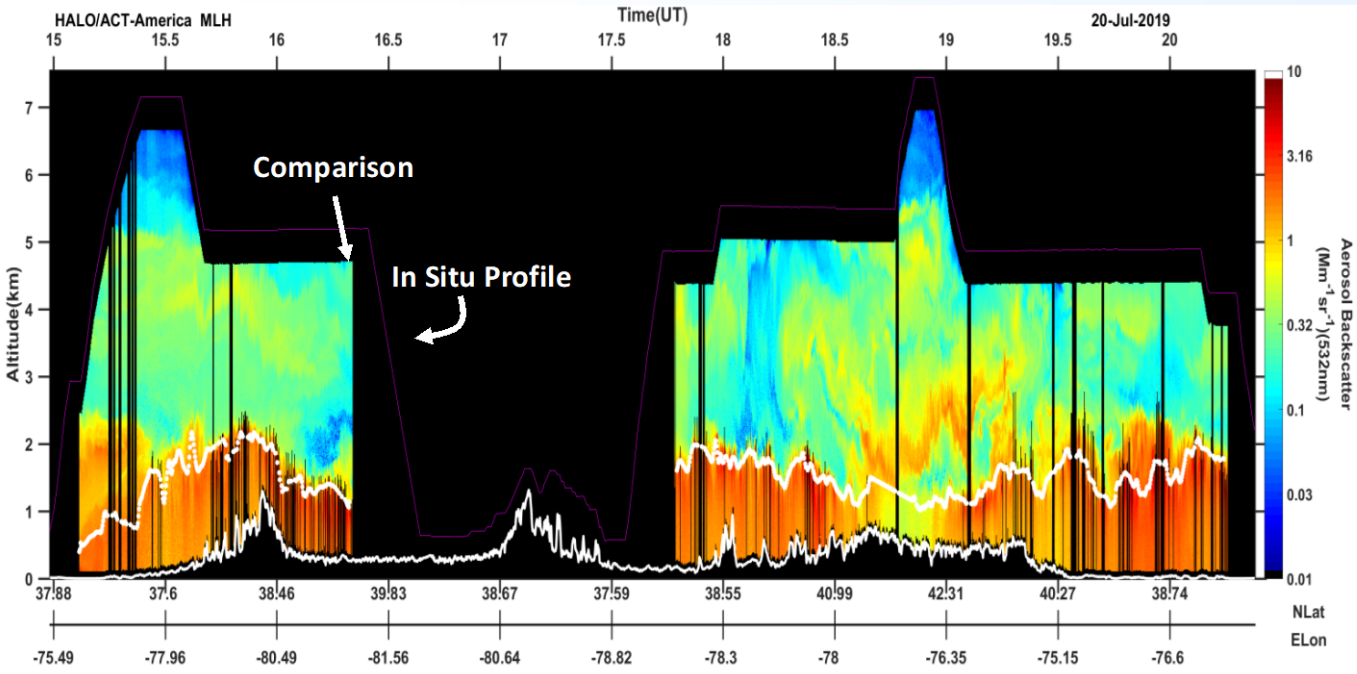


- Potential temperature derived MLH = 1.228 km
- HALO derived MLH = 1.236 km
- Fair weather cu and well defined mixed layer...easy for lidar



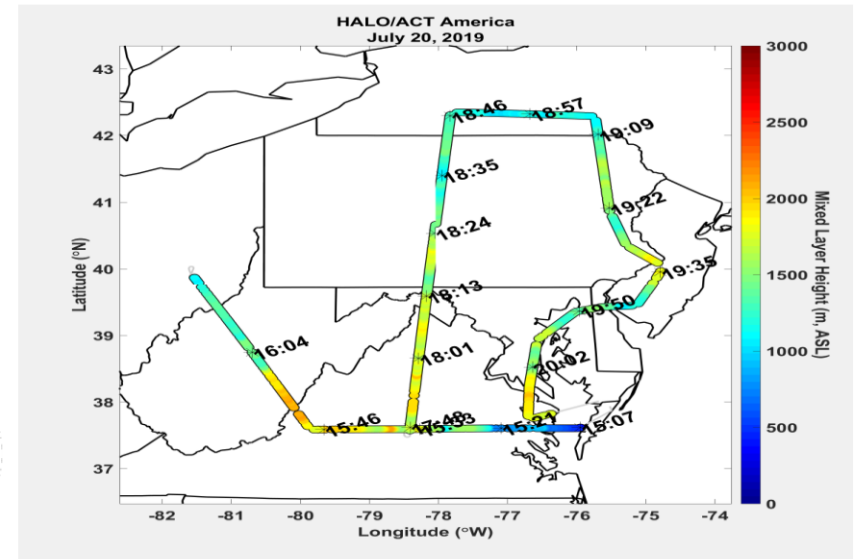
Collins, Nehrir, Kooi, Barton-Grimley, NASA LaRC

Example – PBL top humidification

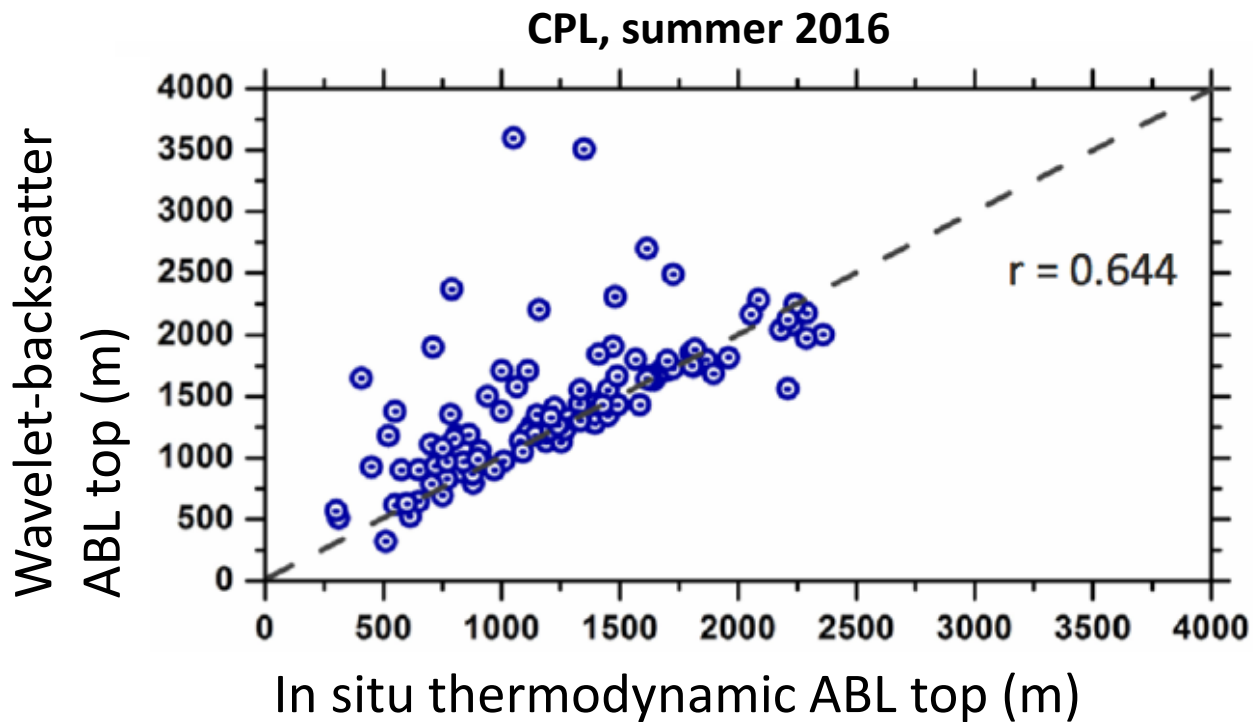


- Potential temperature derived MLH = 0.972 km
- HALO derived MLH = 1.098 km
- Humidification at PBL top could confound lidar retrieval

Collins, Nehrir, Kooi, Barton-Grimley, NASA LaRC

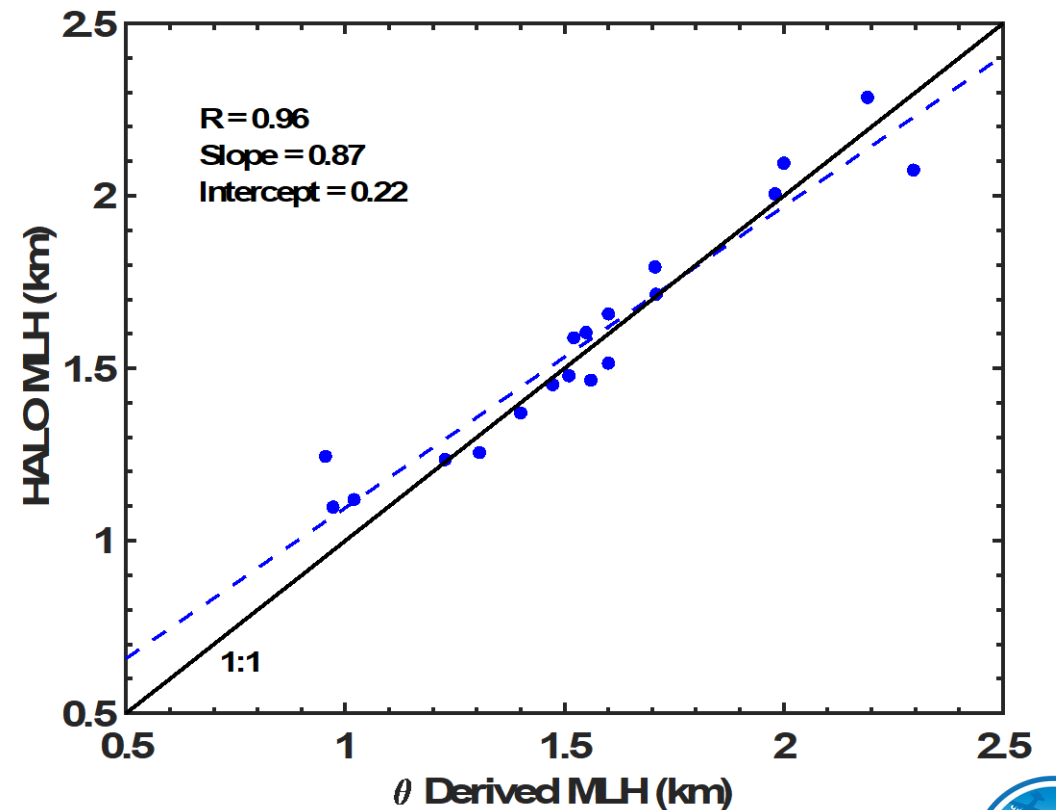


Comparison of in-situ and lidar ABL depth retrievals



Elevated aerosol layers likely cause the outliers. These cases have probably already been screened out.

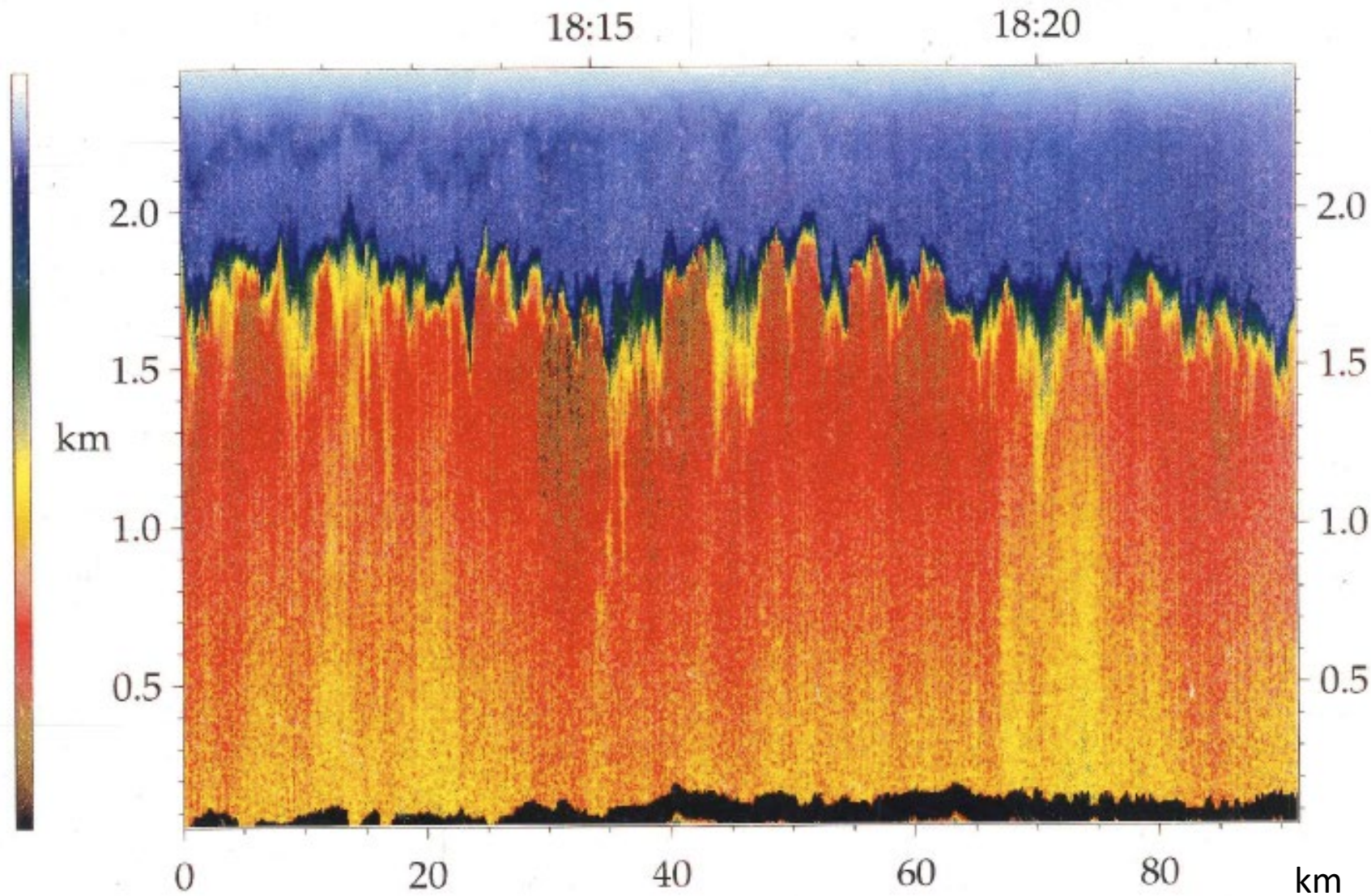
HALO ABL top compares very well with in situ soundings.



This isn't brand new technology

- BOREAS (1994), SGP (1997), IHOP (2002) all had substantial airborne lidar campaigns.

BOREAS – 1994 – central Canada



Kiemle et al, 1997
Davis et al., 1997

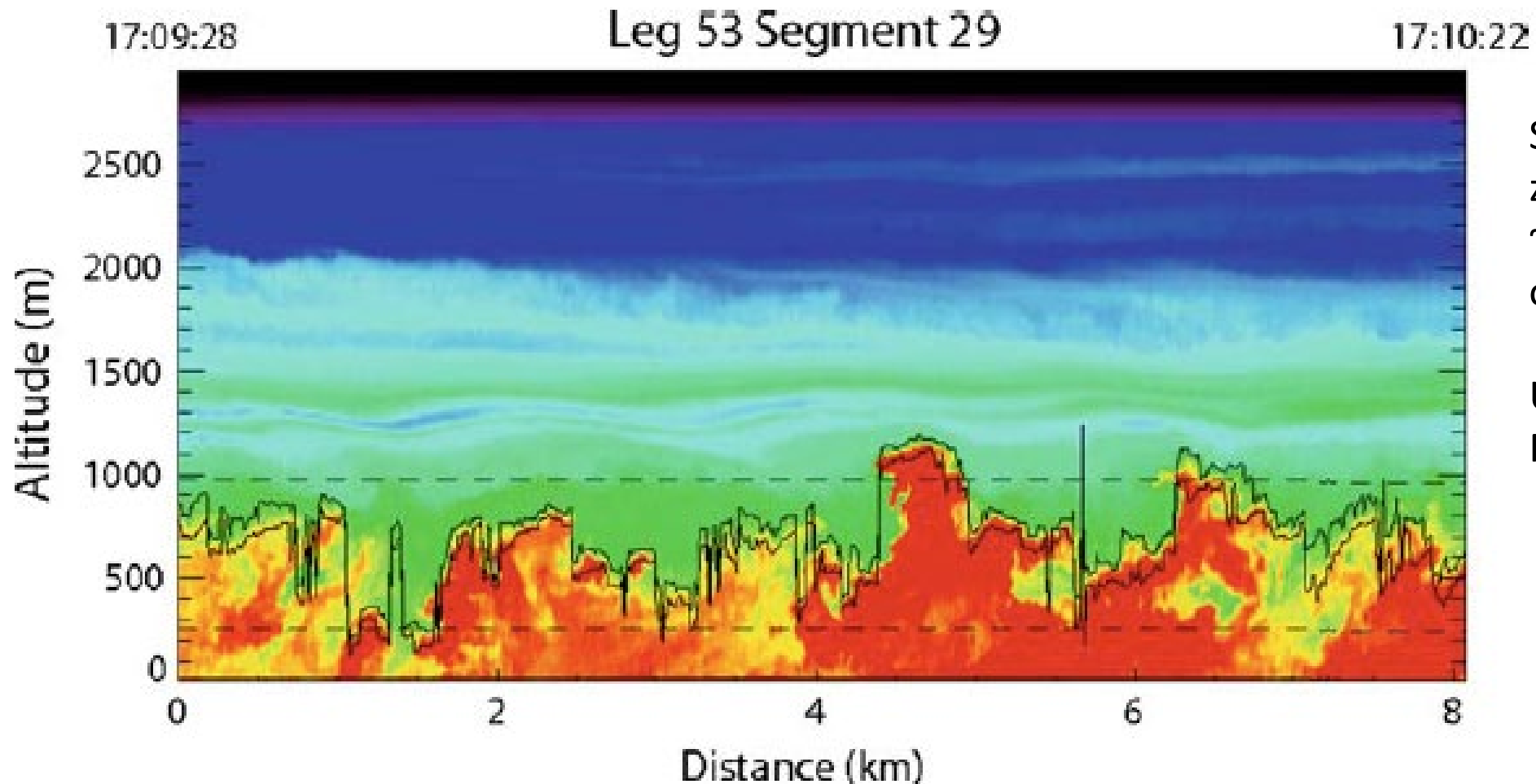
Studies of ABL top structure, statistics, entrainment, relation to surface thermodynamic fluxes, link to water.

Multiple summer flights over central Canada

Classic daytime clear air convective boundary layer case.

BOREAS airborne lidar backscatter. Local standard time at top. Warm colors = more backscatter. Note horizontal scale is highly compressed.

IHOP: 7 June, 2002: Weak inversion, rapid morning ABL growth



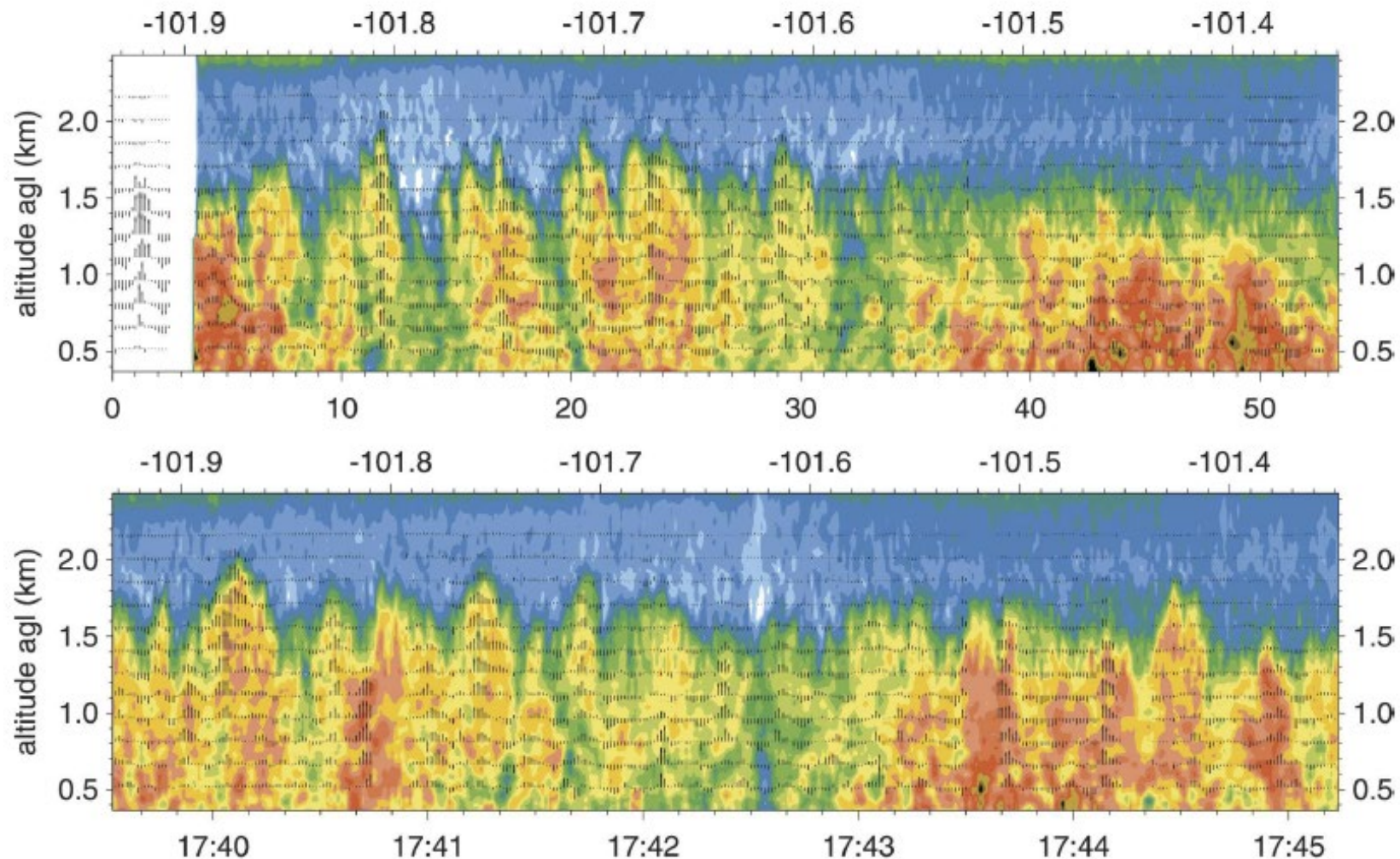
Study of entrainment zone structure using ~6,000 km of lidar ABL observations.

US southern Great Plains, spring 2002.

Fig. 5 A lidar backscatter image from an 8- km segment from with Leg 53 on June 7. Altitude, ground colour coding, and time are indicated as explained in Fig. 3

“Extreme entrainment” situation...ML scaling violated.

Grabon et al., 2010, BLM



DLR DIAL Water Vapour Mixing Ratio and NOAA HRDL Wind Velocity on 7.6.02., Legs 3 and 4

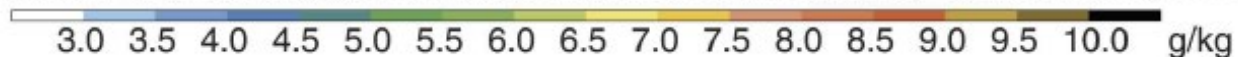


FIG. 2. Vertical cross sections of water vapor (colors) and vertical velocity (arrows) for the Falcon flight legs 3 and 4 oriented west–east at 37.4°N over southwestern Kansas. The aircraft flew (top) leg 3 from right (east) to left (west) and turned back at 102°W to (bottom) fly leg 4 on the same track. Top axis is longitude, bottom axis distance (km), and UTC time, 7 h ahead of LT. Maximum vertical wind velocities are -4.2 m s^{-1} in downward and 6.6 m s^{-1} in upward directions. An arrow length corresponding to 150-m altitude difference is 7 m s^{-1} in vertical velocity. The aspect ratio is about 1:7; that is, the cross sections are compressed horizontally by a factor of 7. It is evident that strong contributions to the flux emanate from the largest thermals.

IHOP 2002

Airborne lidar observations of vertical velocity (NOAA) and water vapor (DLR).

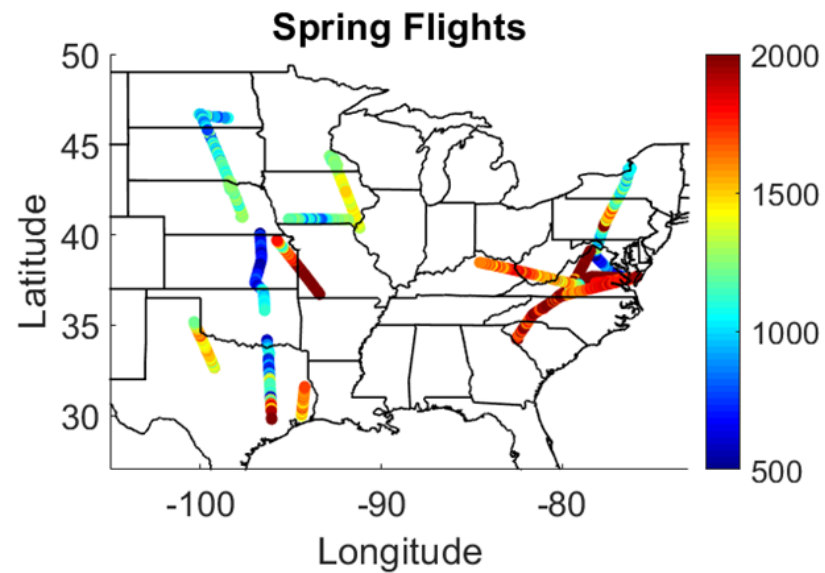
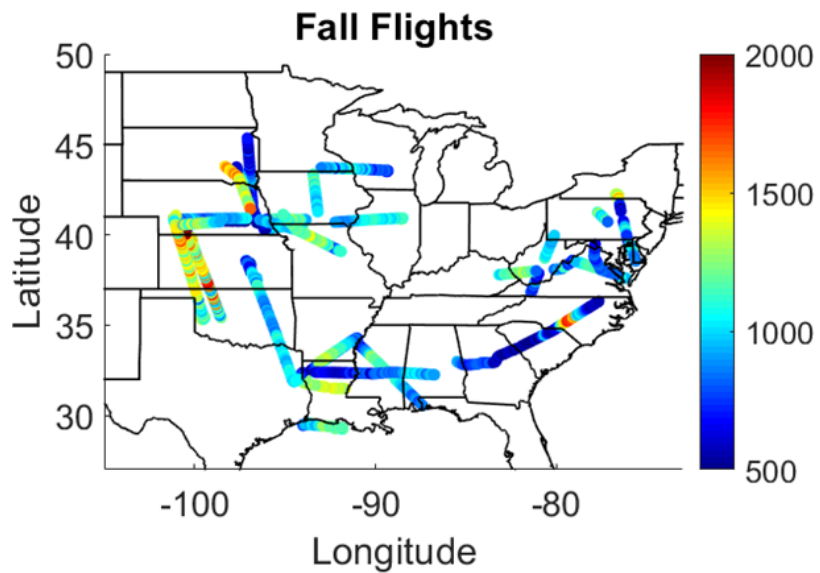
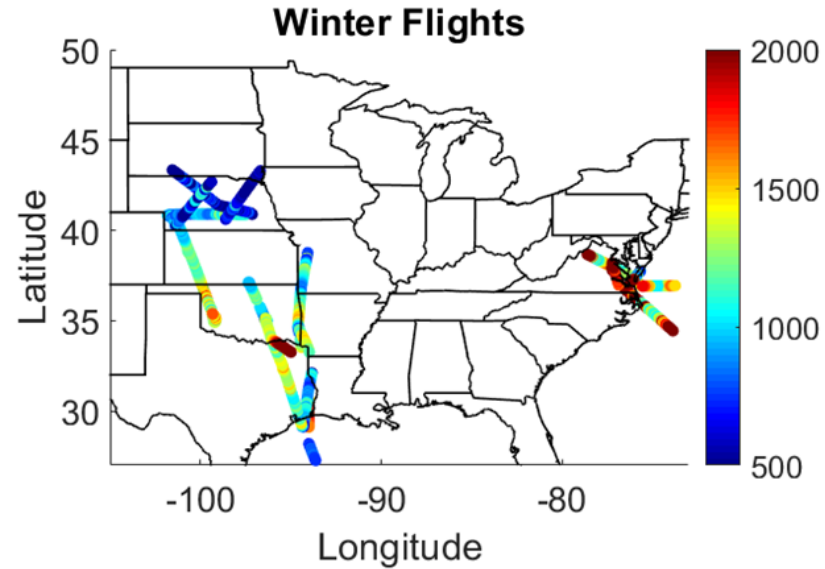
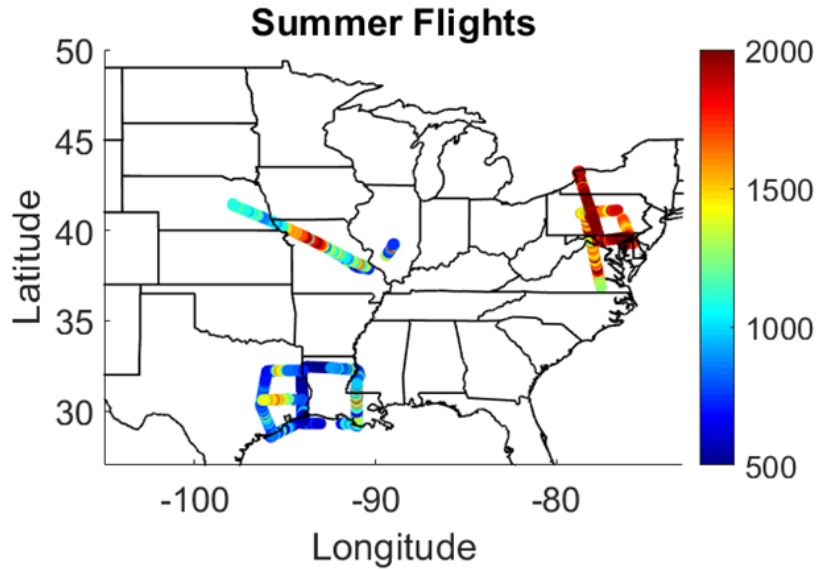
Airborne eddy covariance flux profile measurement demonstration.

This isn't brand new technology

- BOREAS (1994), SGP (1997), IHOP (2002) all had substantial airborne lidar campaigns.
- But none of these past campaigns are as extensive in space and time as ACT, and none have the coincident density of in situ winds and GHG measurements.
- And it has been slow work getting the atmospheric modeling community to work with these data.

Beginnings of comprehensive model-data comparisons

CPL ABL depth maps

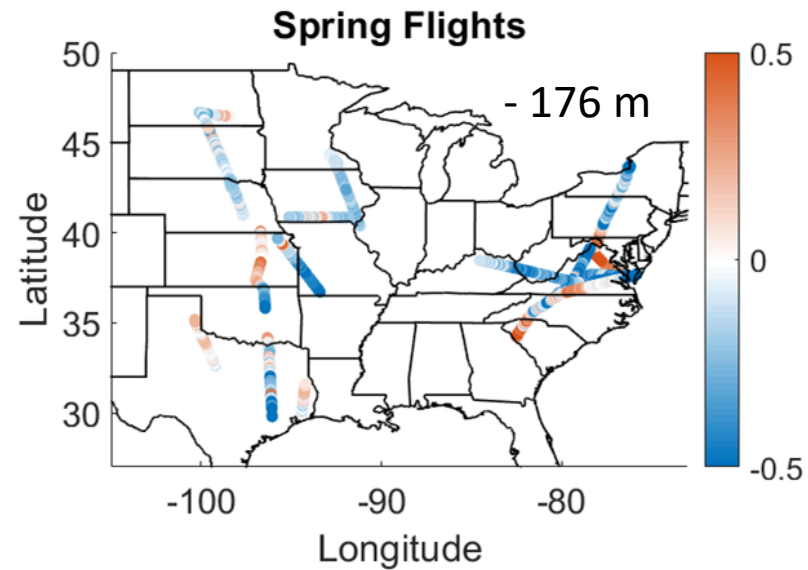
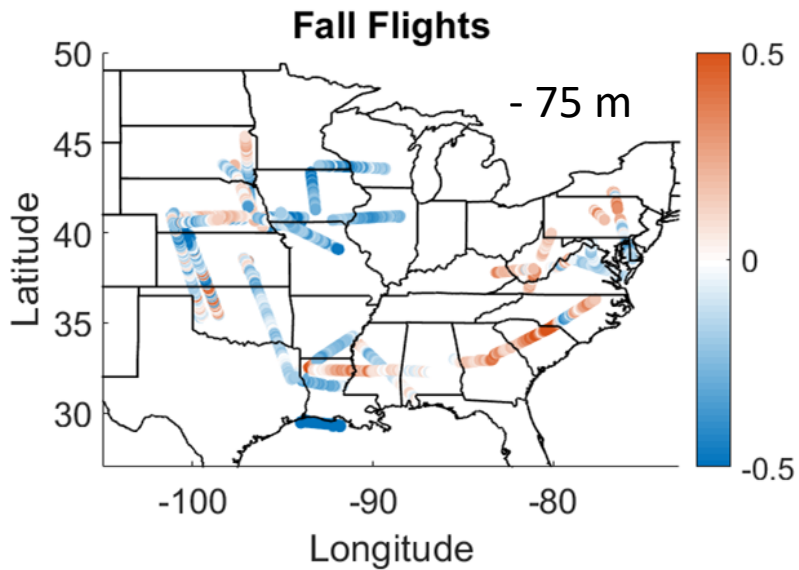
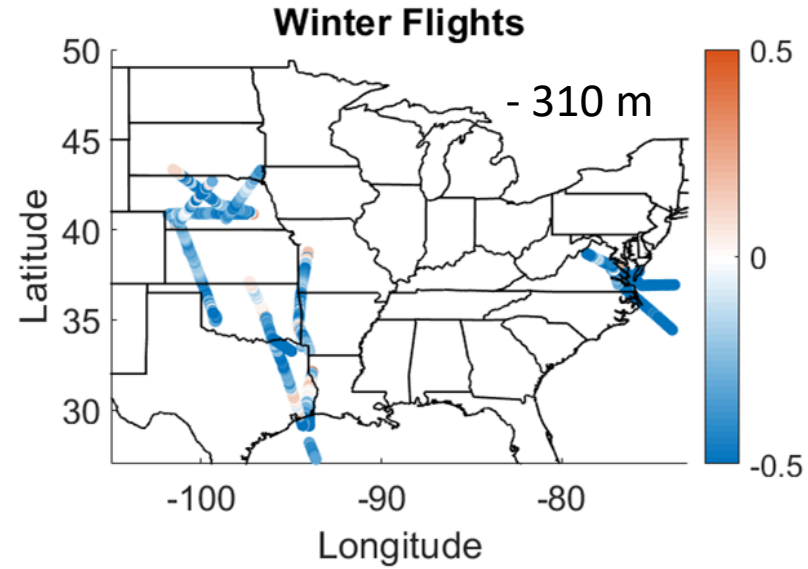
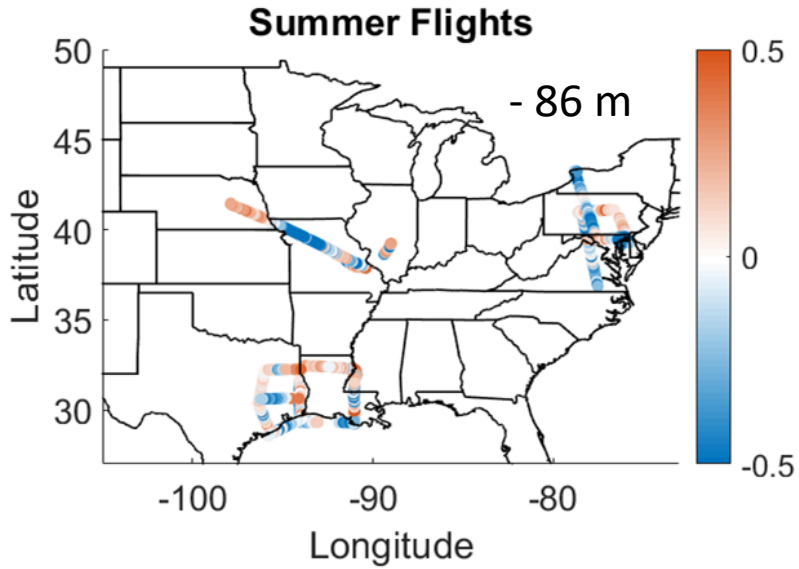


Subset of flight days with long, coherent ABL depth retrievals.

ABL depths in meters AGL.

Campbell et al, in prep.

WRF-CPL ABL depth differences



Model-data differences in km AGL.

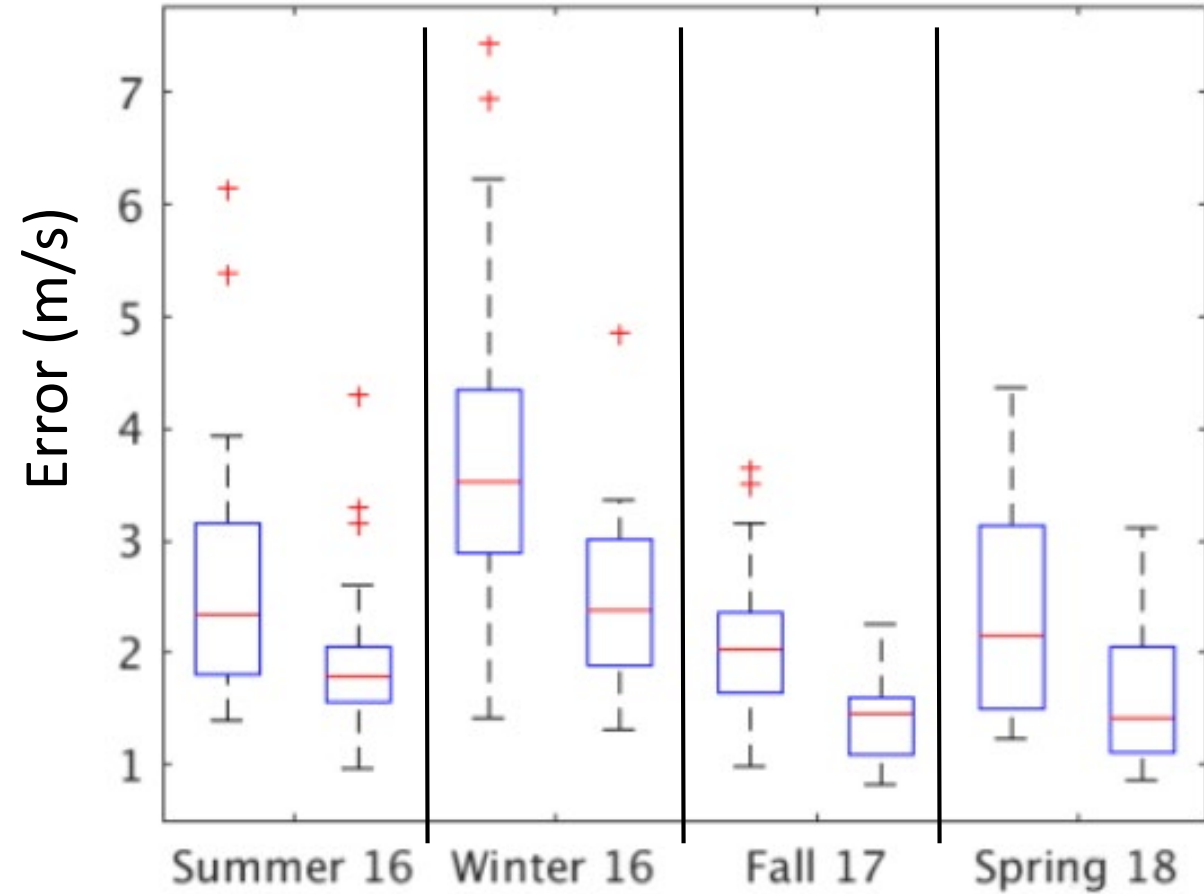
Seasonal mean differences shown on each figure.

WRF-MYNN-Noah ABL depth appears to have a systematic low bias with respect to these data.

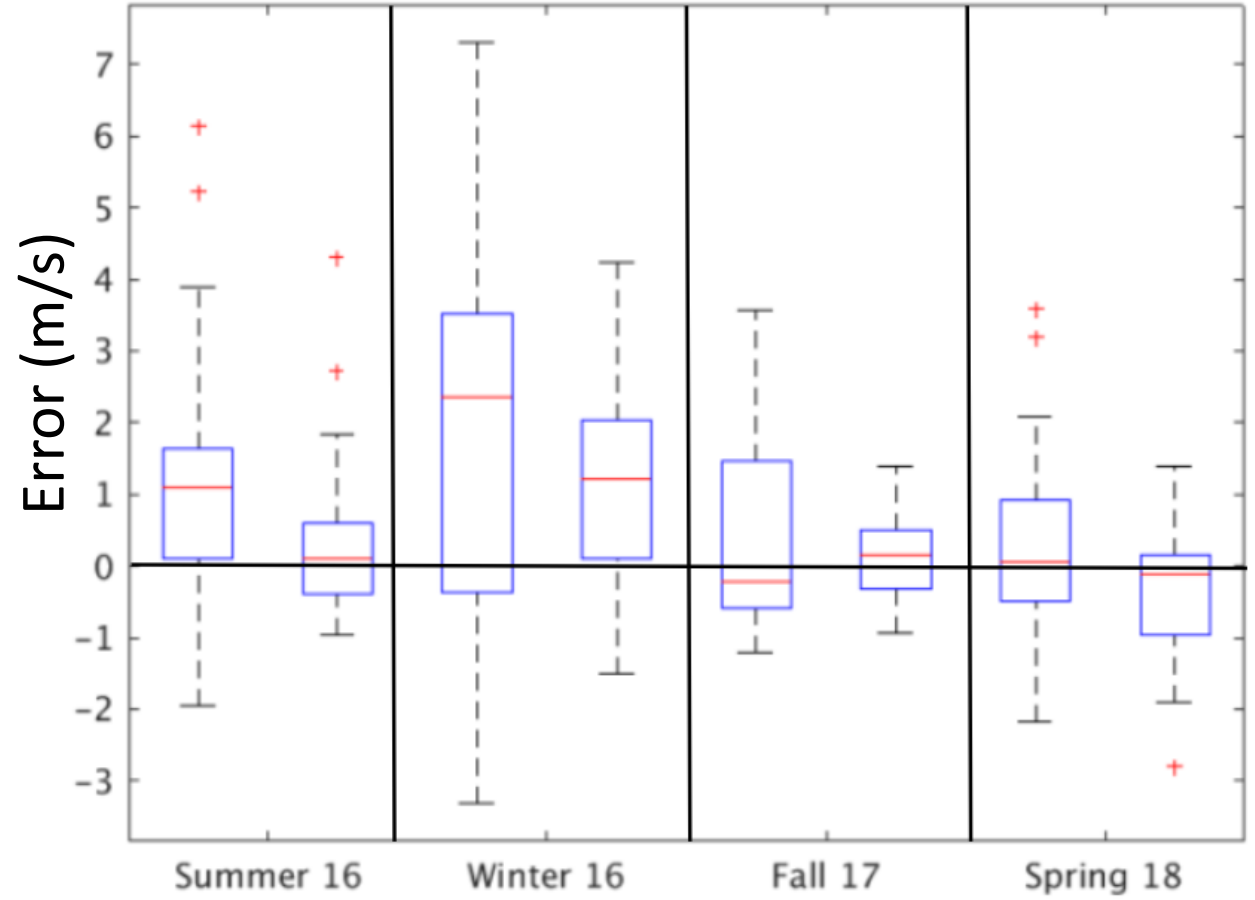
Campbell et al, in prep

First steps toward ABL wind evaluation

Absolute Wind Speed Error (Boundary layer)



Wind Speed Bias (Boundary layer)

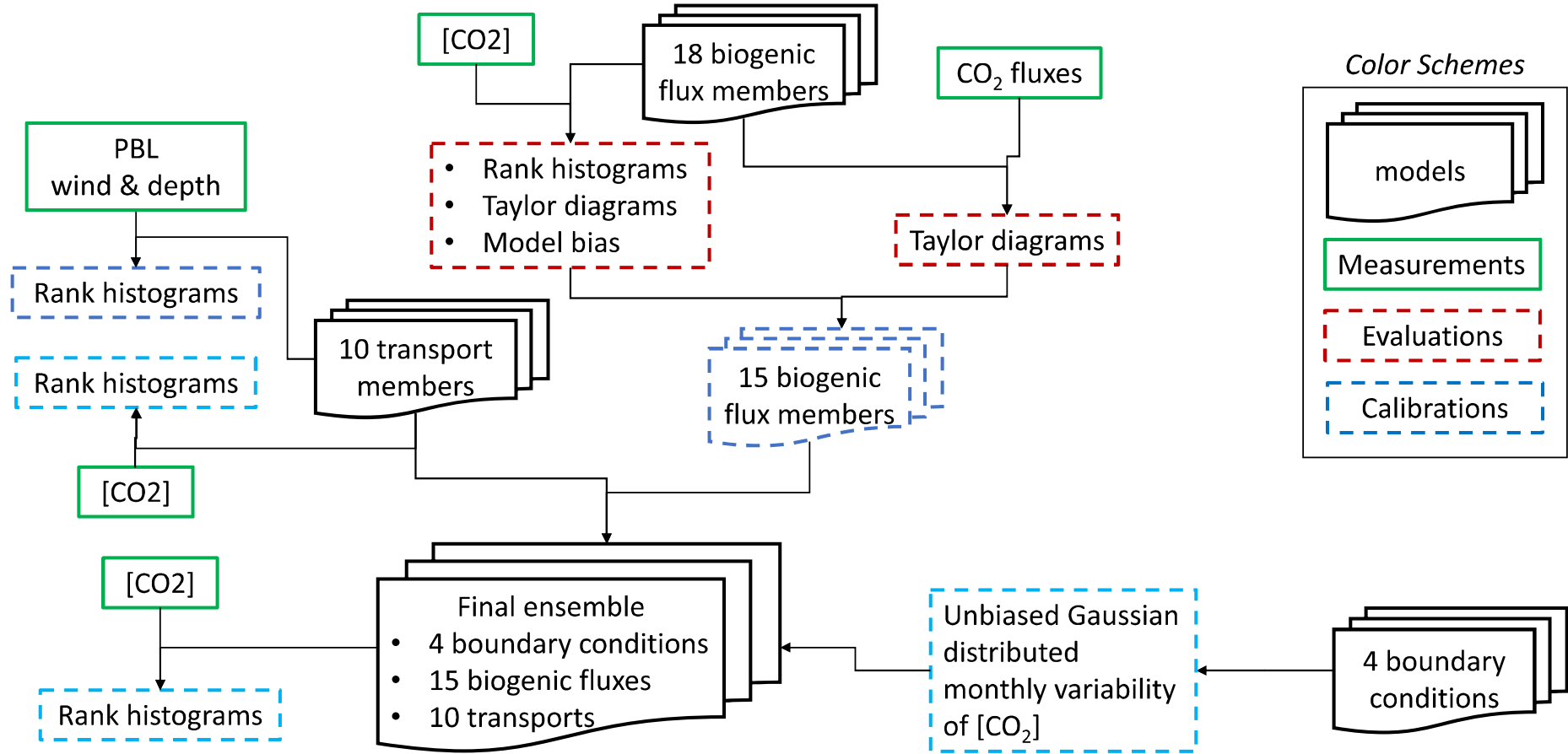


Penn State WRF baseline run: Random error (left) and bias (right), without (left set) and with (right set) nudging to ERA5. Barkley and Feng.

Work underway

- Protocol is under development for retrieval of atmospheric transport model column output, coincident with ACT lidar ABL depth retrievals and in situ sounding.
- Plan is to apply that protocol broadly – and conduct a multi-season, large-scale, weather-aware evaluation of the ABL properties (wind, depth) of the atmospheric transport models used for GHG inversion studies (and to perform coincident evaluation of their GHG fields).
- What follows depends in part on the findings, and the interest of the research community in improving *trace-gas relevant ABL properties of atmospheric reanalyses*.

WRF-based calibrated GHG ensemble modeling system



ABL depth, wind speed and wind direction data used to calibrate the transport ensemble following Diaz-Isaac et al., 2019

Figure 6. Flow chart of the summary of the ensemble evaluation and calibration processes.



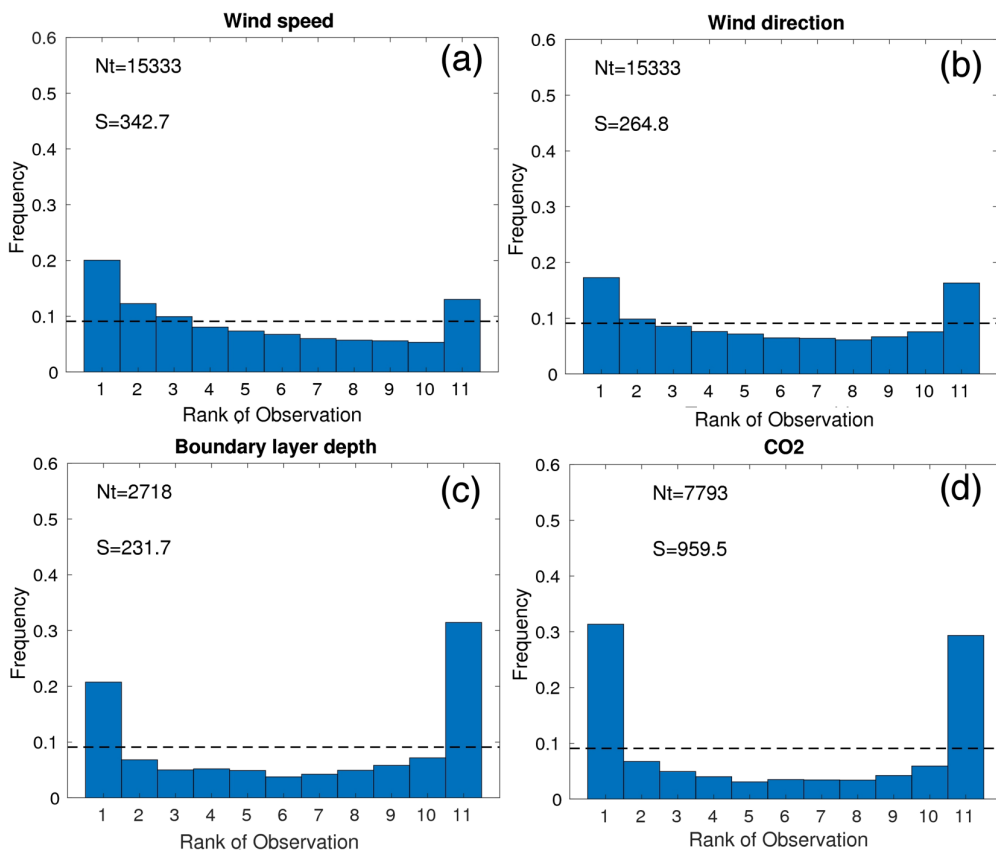


Figure 2. Rank histograms of the transport ensemble suite for 0 UTC (a) 925 hPa wind speed, (b) 925 hPa wind direction, (c) PBL depth, and (d) midday average PBL CO₂ mole fractions. Dashed lines denote the ideal values of the rank histograms. N_t denotes the total number of the observations used. S denotes the rank histogram score of the ensemble. The dashed line is the ideal frequency of a flat distribution.

This calibration was done with rawinsonde data averaged over seasons and the entire continent. Regional, seasonal biases are likely to persist.

But this is an important beginning!

WRF-based GHG ensemble modeling system calibration

Left: Calibration of ABL winds and depth.

Below: Calibration of ABL CO₂ mole fraction.

Feng et al, 2019a

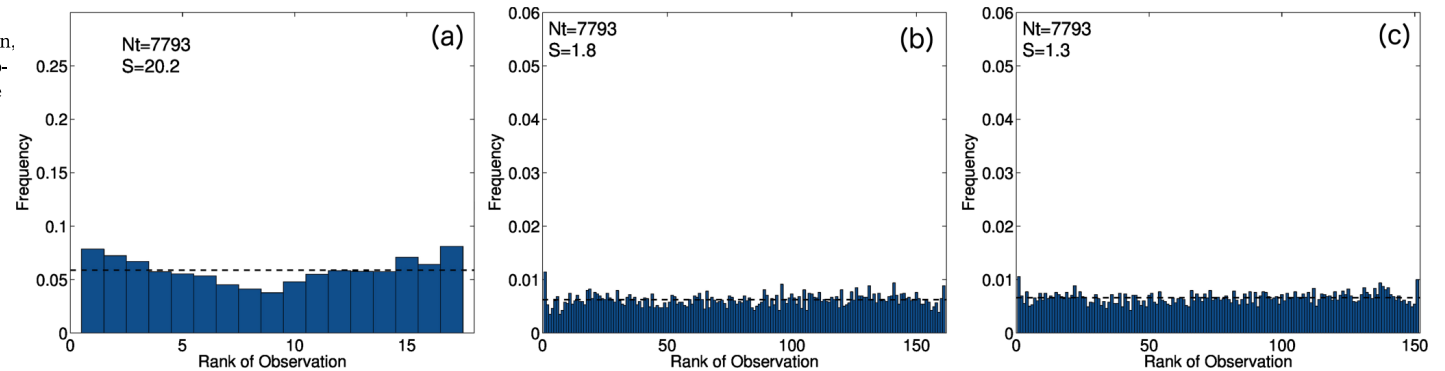


Figure 5. Rank histograms of (a) calibrated biogenic flux ensemble suite, (b) the combination of the calibrated biogenic flux and transport ensemble suites, and (c) the full ensemble with the inclusion of the uncertainties of transport, biogenic fluxes, and boundary conditions for the atmospheric CO₂ mole fractions. Dashed lines denote the ideal values of the rank histograms. N_t denotes the total number of the observations used from six NOAA CO₂ tower sites. The locations and information can be found in Figure 1a and Table 1. Data points represent individual hourly mean values, and the histograms are aggregated over all sites and daytime hours of the entire year. S denotes the rank histogram score of the ensemble.

Ongoing, anticipated and desired analyses

- Create a well-documented, quality-checked data base of ABL observations.
- Evaluate the ABL depth and winds in the models used for atmospheric GHG inversions.
 - Identify biases.
 - Identify less-biased transport models.
 - Improve inverse flux estimates by relying on the less-biased models.
- Use the ACT ABL depth and wind data to create better transport model ensembles. Apply these to atmospheric inversions.
- Develop improved ABL simulations to implement in atmospheric inversion systems.

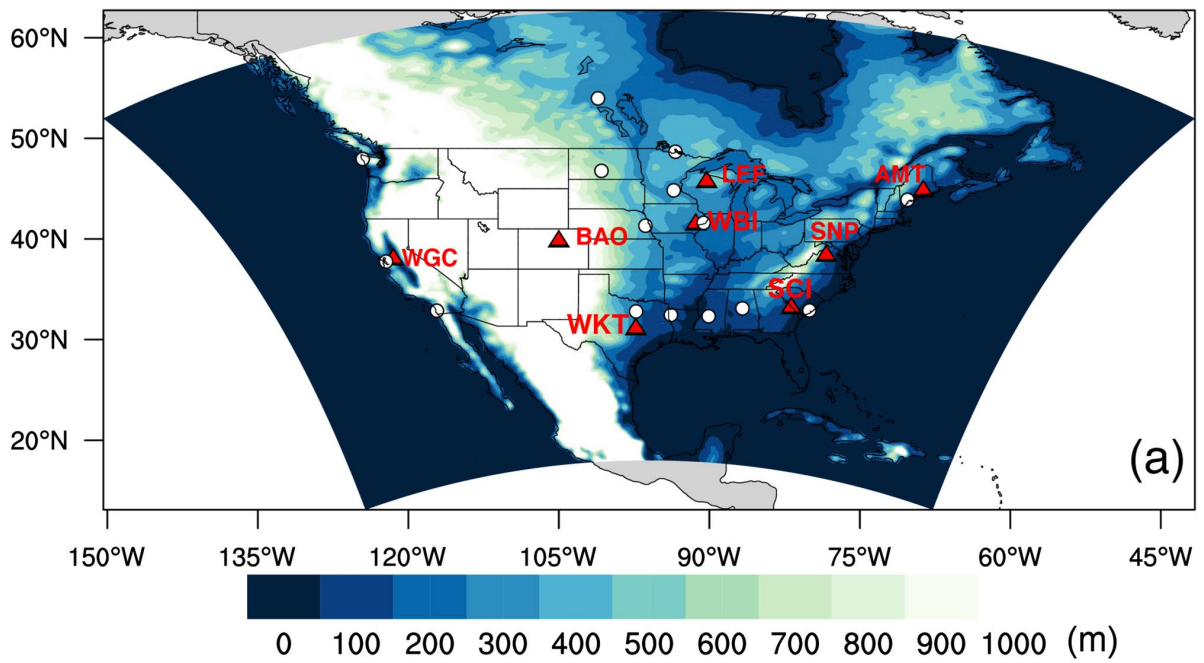
PLEASE JOIN THE EFFORT!



References

- Davis, K. J., D. H. Lenschow, S. P. Oncley, C. Kiemle, G. Ehret and A. Giez, 1997: The role of entrainment in surface-atmosphere interactions over the boreal forest. *J. Geophys. Res.*, 102, 29219-29230.
- Davis, K.J., N. Gamage, C. Hagelberg, D.H. Lenschow, C. Kiemle and P.P. Sullivan, 2000. An objective method for determining atmospheric structure from airborne lidar observations. *J. Atmos. Oceanic Tech.*, 17, 1455-1468.
- Díaz-Isaac, Liza I., Thomas Lauvaux, and Kenneth J. Davis. Impact of physical parameterizations and initial conditions on simulated atmospheric transport and CO₂ mole fractions in the US Midwest, *Atmos. Chem. Phys.*, 18, 14813–14835, 2018 <https://doi.org/10.5194/acp-18-14813-2018>
- Díaz-Isaac, L. I., Lauvaux, T., Bocquet, M., and Davis, K. J.: Calibration of a multi-physics ensemble for estimating the uncertainty of a greenhouse gas atmospheric transport model, *Atmos. Chem. Phys.*, 19, 5695-5718, <https://doi.org/10.5194/acp-19-5695-2019>, 2019.
- Feng, S., T. Lauvaux, K. Davis, K. Keller, Y. Zhou, C. Williams, A. Schuh, J. Liu, I. Baker, (2019a). Seasonal characteristics of model uncertainties from biogenic fluxes, transport, and large-scale boundary inflow in atmospheric CO₂ simulations over North America. *Journal of Geophysical Research: Atmospheres*, 124, 14,325–14,346. <https://doi.org/10.1029/2019JD031165>
- Feng, S., Lauvaux, T., Keller, K., Davis, K. J., Rayner, P., Oda, T., & Gurney, K. R. (2019b). A road map for improving the treatment of uncertainties in high-resolution regional carbon flux inverse estimates. *Geophysical Research Letters*, 46. <https://doi.org/10.1029/2019GL082987>
- Grabon, Jeffrey S., Kenneth J. Davis, Christoph Kiemle and Gerhard Ehret, 2010. Airborne Lidar Observations of the Transition Zone Between the Convective Boundary Layer and Free Atmosphere During the International H₂O Project (IHOP) in 2002. *Boundary-Layer Meteorol.*, 134, 61–83, DOI 10.1007/s10546-009-9431-1
- Kiemle, C. W. A. Brewer, G. Ehret, R. M. Hardesty A. Fix, C. Senff, M. Wirth, G. Poberaj, and M. A. Lemone, 2007. Latent Heat Flux Profiles from Collocated Airborne Water Vapor and Wind Lidars during IHOP_2002, *J. Atmos. Oceanic Tech.*, 24 , 627-639, DOI: 10.1175/JTECH1997.1
- Kiemle, C., G. Ehret, A. Giez, K. J. Davis, D. H. Lenschow and S. P. Oncley, 1997: Estimation of boundary-layer humidity fluxes and statistics from airborne DIAL. *J. Geophys. Res.*, 102, 29189-29204.
- Sarmiento, Daniel P., Kenneth J. Davis, Aijun Deng, Thomas Lauvaux, Alan Brewer, Michael Hardesty, 2017. A comprehensive assessment of land surface-atmosphere interactions in a WRF/Urban modeling system for Indianapolis, IN, *Elem Sci Anth*: 2017;5:23. DOI: <http://doi.org/10.1525/elementa.132>

Calibration data for the Penn State WRF GHG ensemble modeling system



Above: Rawinsonde stations and GHG mole fraction towers

Feng et al, 2019a



Below: CO₂ flux towers

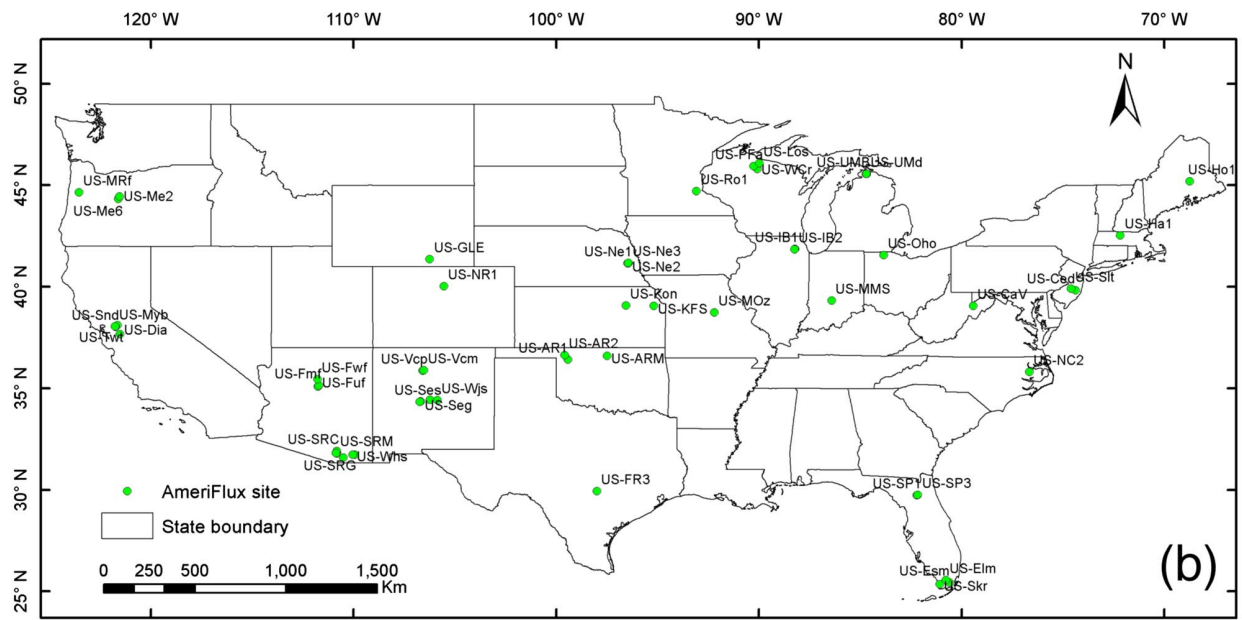


Figure 1. (a) The simulation domain and locations of the observation. Shaded contour is terrain height in meters. Red triangles denote the locations of the NOAA CO₂ towers used in this work, and the names of the towers are marked. The Information of these towers can be found in Table 1. White dots denote the locations of the NOAA rawinsonde stations. Note that we removed WGC and BAO from the model calibration procedure due to the local contamination. (b) The locations of the AmeriFlux towers. Information describing these towers can be found in Table S1.