Paths to improved atmospheric transport reanalysis for urban GHG studies

Kenneth J. Davis[1], Nikolay Balashov[1], Zachary R. Barkley[1], Aijun Deng[1,2], Liza I. Diaz-Isaac[1,3], Brian R. Gaudet[1], Thomas Lauvaux[1,4], Natasha L. Miles[1], Scott J. Richardson[1], Daniel P. Sarmiento[1,5]

[1]The Pennsylvania State University, [2]Utopus Insights, [3]Scripps Institute of Oceanography, [4]LSCE, France, [5]SAIC

CO2USA, Salt Lake City, Utah, 25 October, 2018.

INFLUX motivation

- Develop the methods needed to quantify greenhouse gas (GHG) emissions from cities
- Provide the scientific basis to support GHG emissions mitigation efforts
  - Assertion: Inventory assessments alone are insufficient. Independent evaluation from the atmosphere is needed.
  - National Research Council / Pacala et al., (2010); Ogle et al., Env. Res. Lett. (2015); Alvarez et al., Science, (2018); European Research Commission / Bergamaschi et al., (2018).

INFLUX goals

Indianapolis Flux Experiment (INFLUX) – influx.psu.edu

- Goals
  - Develop and assess methods of quantifying GHG emissions at the *urban scale*.
  - Determine whole-city emissions of CO_2 and CH_4
  - Measure emissions of CO_2 and CH_4 at 1 km^2 spatial and weekly temporal resolution
  - Distinguish biogenic vs. anthropogenic sources of CO_2
  - Quantify and reduce uncertainty in urban emissions estimates

Davis et al., Elementa, 2017

Challenges

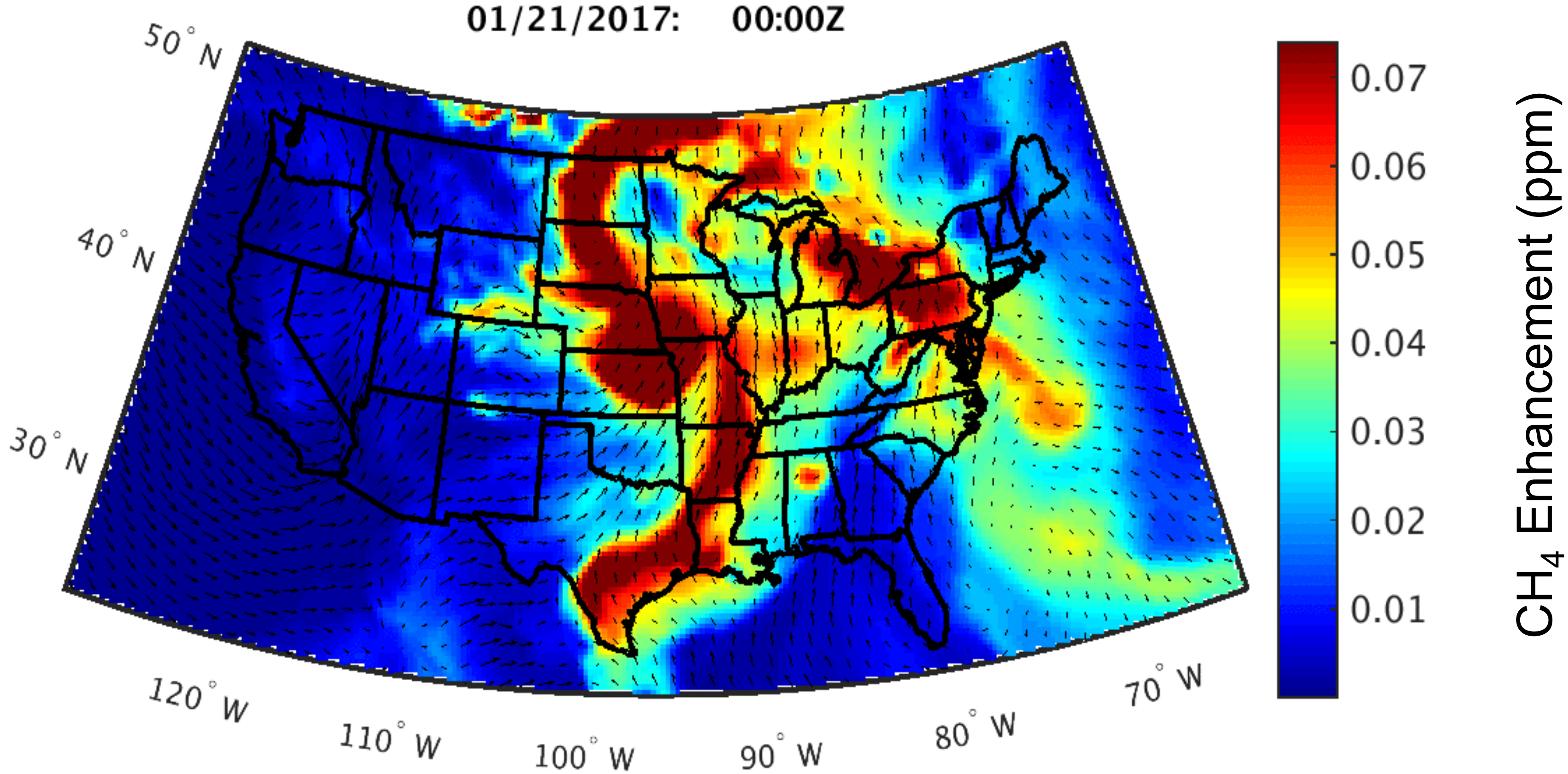
- GHGs are long-lived. The impact of urban emissions on atmospheric mole fractions is modest.
  - GHG measurements must be made with high accuracy and precision, and placed carefully.*
  - *Atmospheric transport must be known to high fidelity.*
  - GHG background conditions must be well known.

*Richardson et al., (2017); Miles et al., (2017); Wu et al., (2017); Gaudet et al., (2017).

Mesoscale atmospheric models are powerful tools for urban GHG studies

- They allow us to:
  - Interpolate sparse meteorological data through space and time using our understanding of atmospheric physics. *Reanalysis.*
  - Quantify our best understanding of the relationship between GHG fluxes and atmospheric mole fractions.`

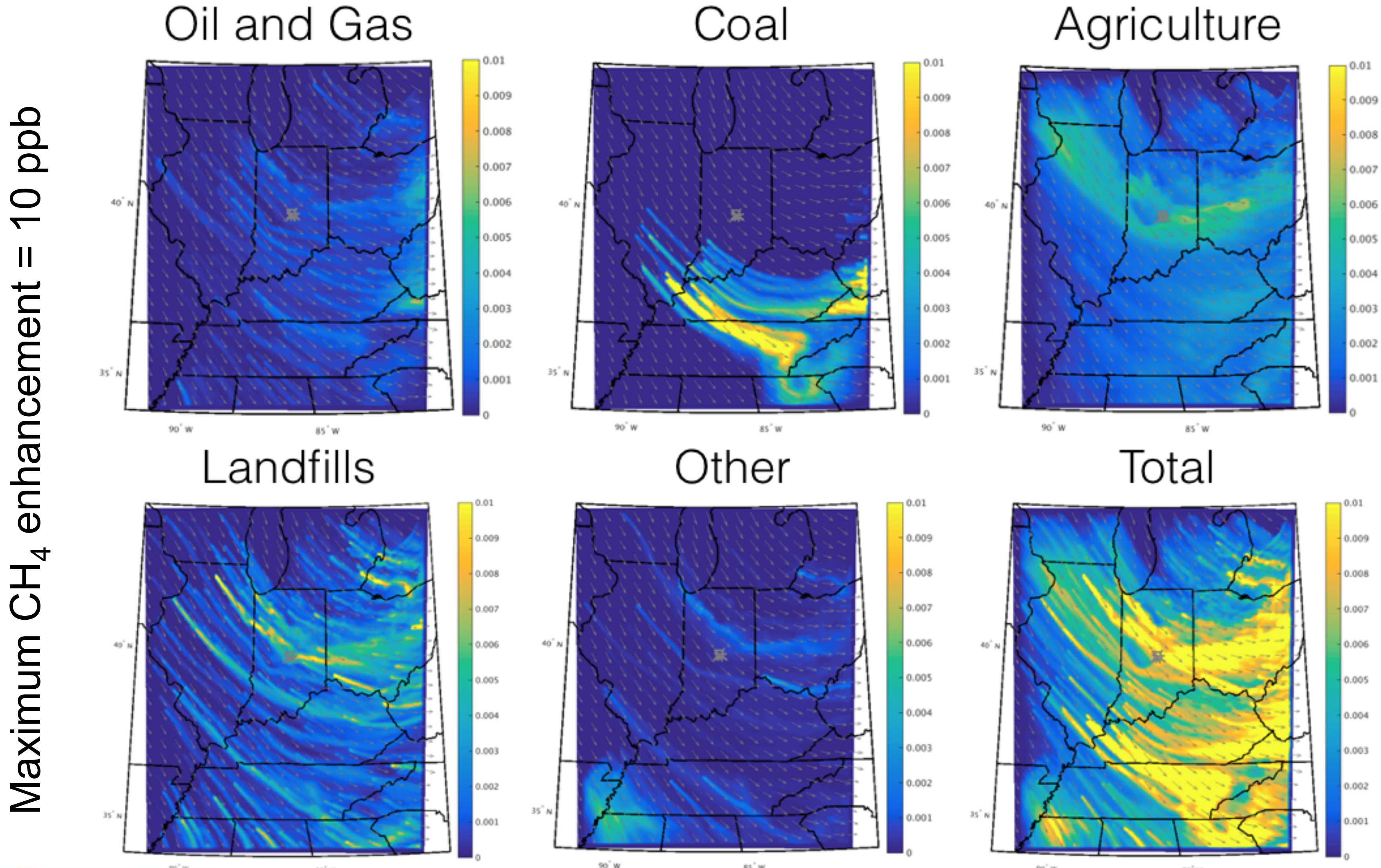
"Forward" simulation of a day of anthropogenic methane advection.



WRF-Chem boundary layer CH_4 with EPA 2012 gridded emissions inventory

Barkley and Balashov

"Forward" simulation of the methane background for Indianapolis

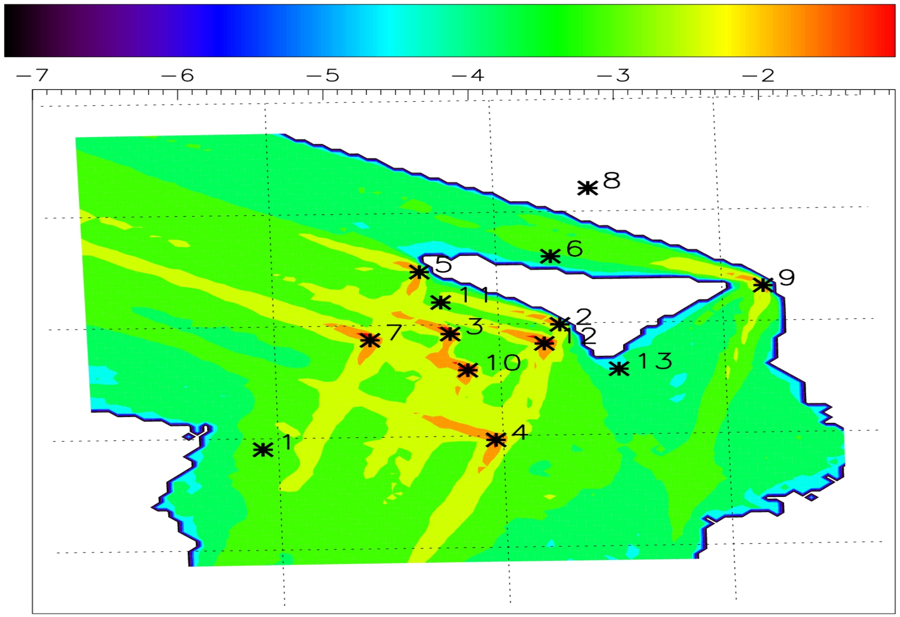


03/13/2013, 19Z WRF-Chem at 350 meters

Balashov

PennState

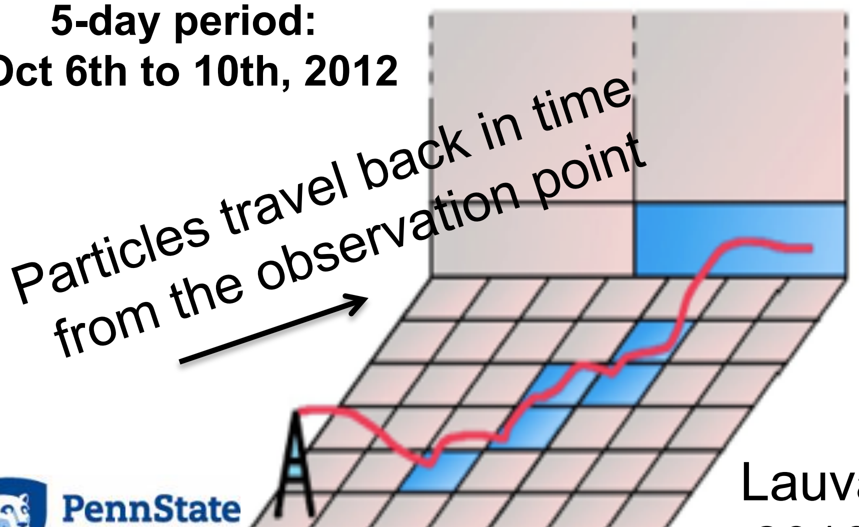
Influence functions: Relationship between GHG fluxes and atmospheric mole fractions at observation points

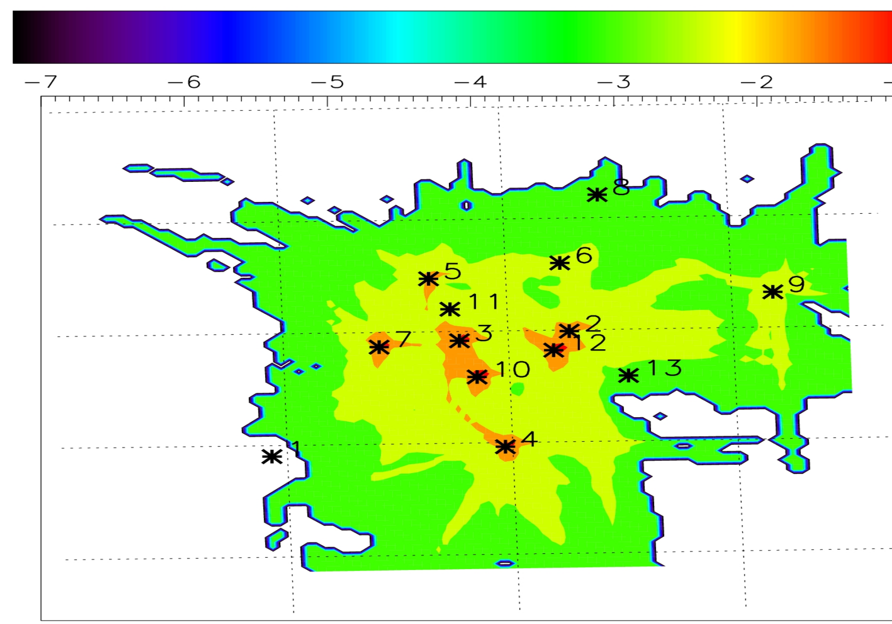


Averaged 1 km resolution INFLUX tower surface influence functions (in log (ppm / (gC km^{-2} h^{-1})) averaged over 5 days and 55 days.

WRF-LPDM.

5-day period:
Oct 6th to 10th, 2012





Lauvaux et al, 2016, JGR-A

55-day period
Oct 6th to Nov 29th, 2012

PennState

Mesoscale models can be used to simulate transport across hundreds of kilometers at high resolution for months to years

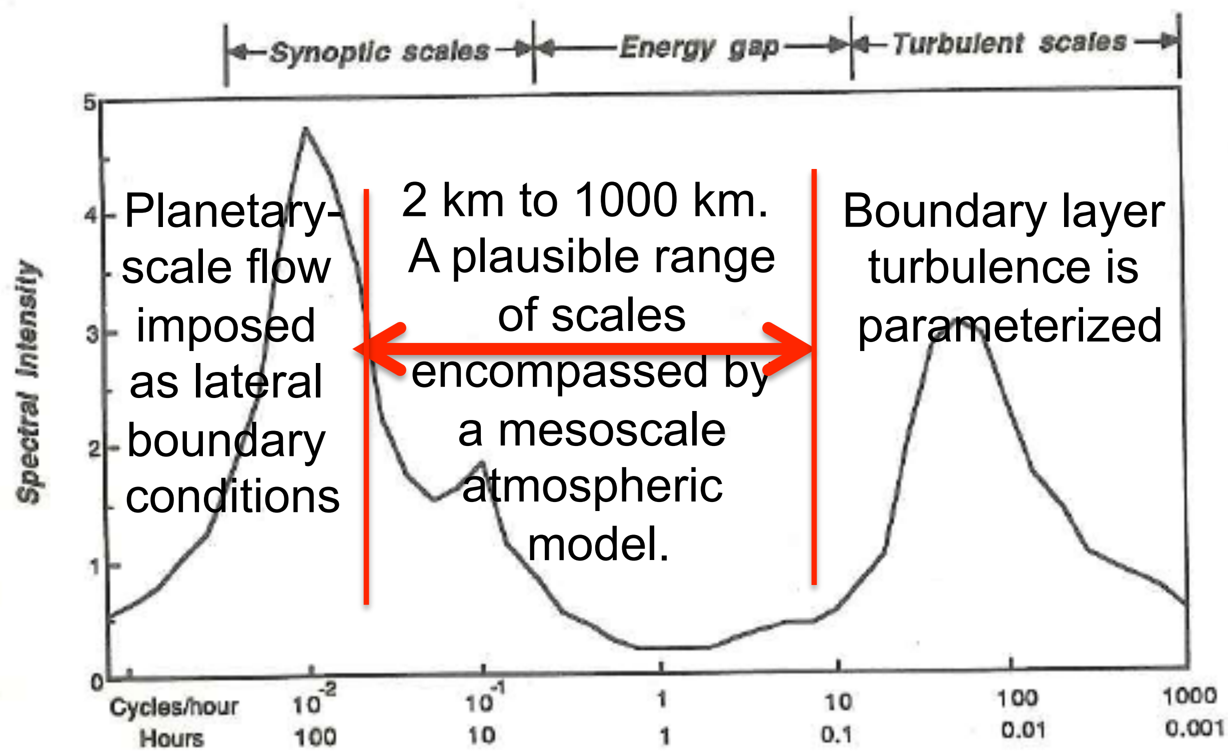


Fig. 2.2 Schematic spectrum of wind speed near the ground estimated from a study of Van der Hoven (1957).

The serpent in the garden:

Limited computing capacity and incomplete knowledge forces us to approximate (parameterize) turbulence and other importance processes.

Stull, 1988

Sources of divergence in mesoscale atmospheric simulations

- Physical parameterizations of:
  - Land surface energy and momentum fluxes
  - Atmospheric boundary layer turbulence
  - Convective cloud development
  - Cloud microphysics
  - Atmospheric radiation
- Model resolution, domain, nesting, numerics
- Large-scale atmospheric initial and boundary conditions

WRF* is not a single atmospheric model

- It has multiple options for nearly all of those potential causes of divergence.
- It is a modeling system that can be configured hundreds of different ways.

- Don't blame WRF. All mesoscale models have this problem – they just might not allow all these options to be explored.

*Weather Research and Forecast model, maintained at NCAR. The prior version, MM5, was known as the Penn State / NCAR Mesoscale Model.

Do they matter – all these subtleties of atmospheric transport modeling? For urban GHG studies?

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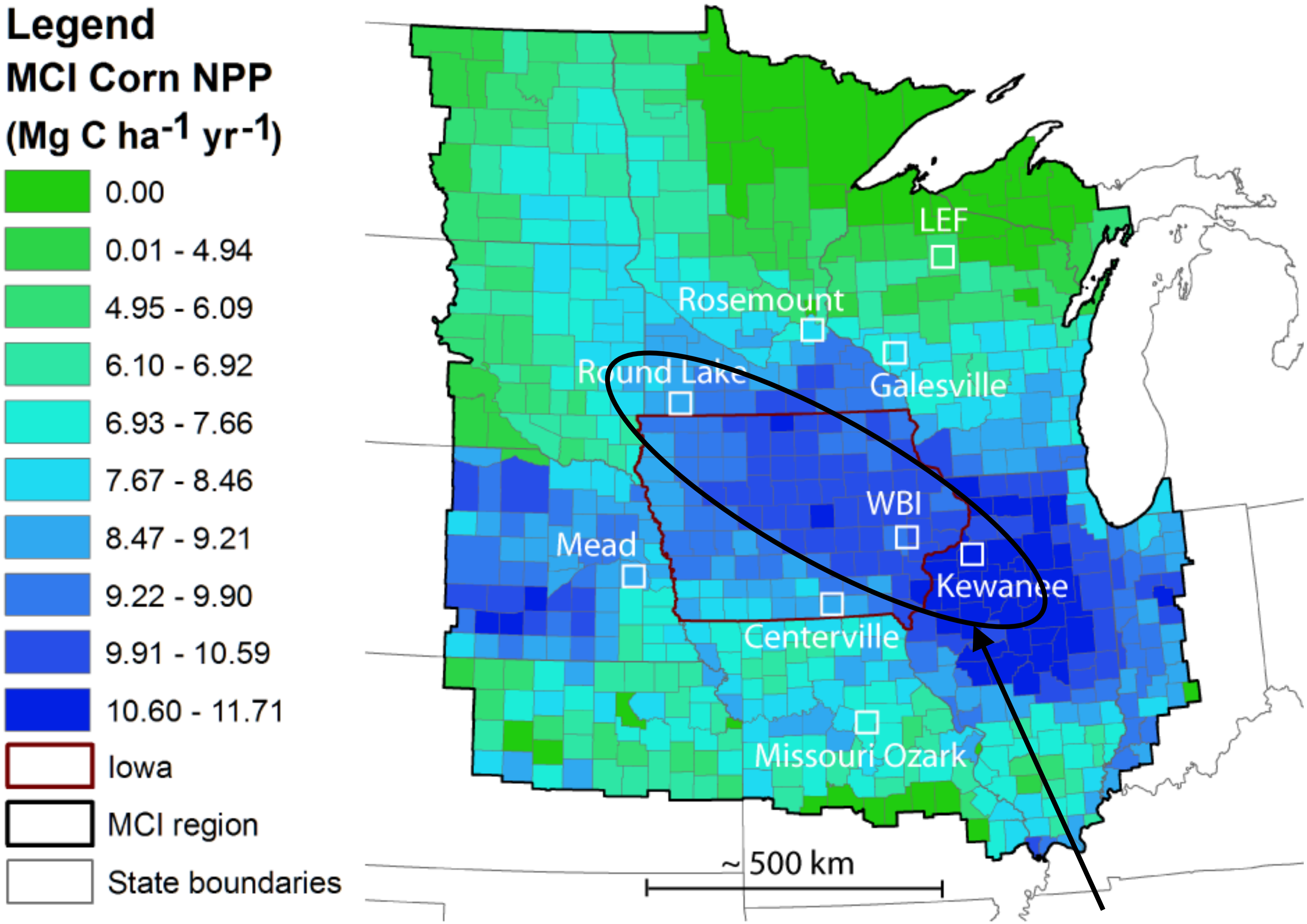
First, "regional" studies.

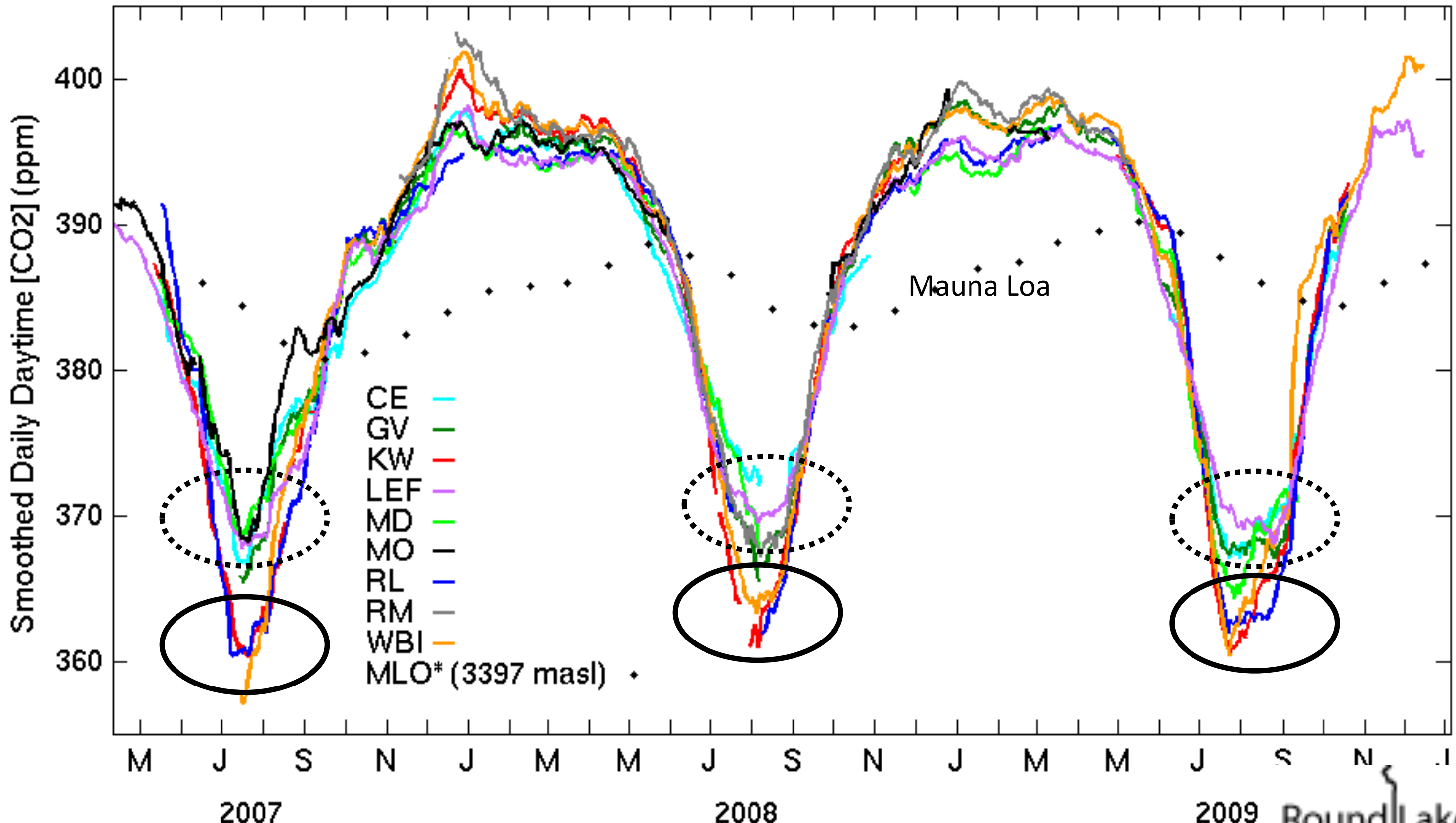
MidContinent Intensive Tower-Based CO_2 Observation Network:
Highest density regional CO_2 monitoring network ever deployed

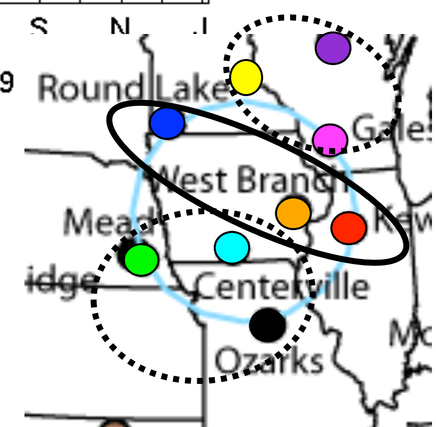


Miles et al, 2012, JGR-B

Corn-dominated sites

Dramatic regional CO_2 gradients provide *a test-bed for atmospheric GHG modeling* and flux estimation.



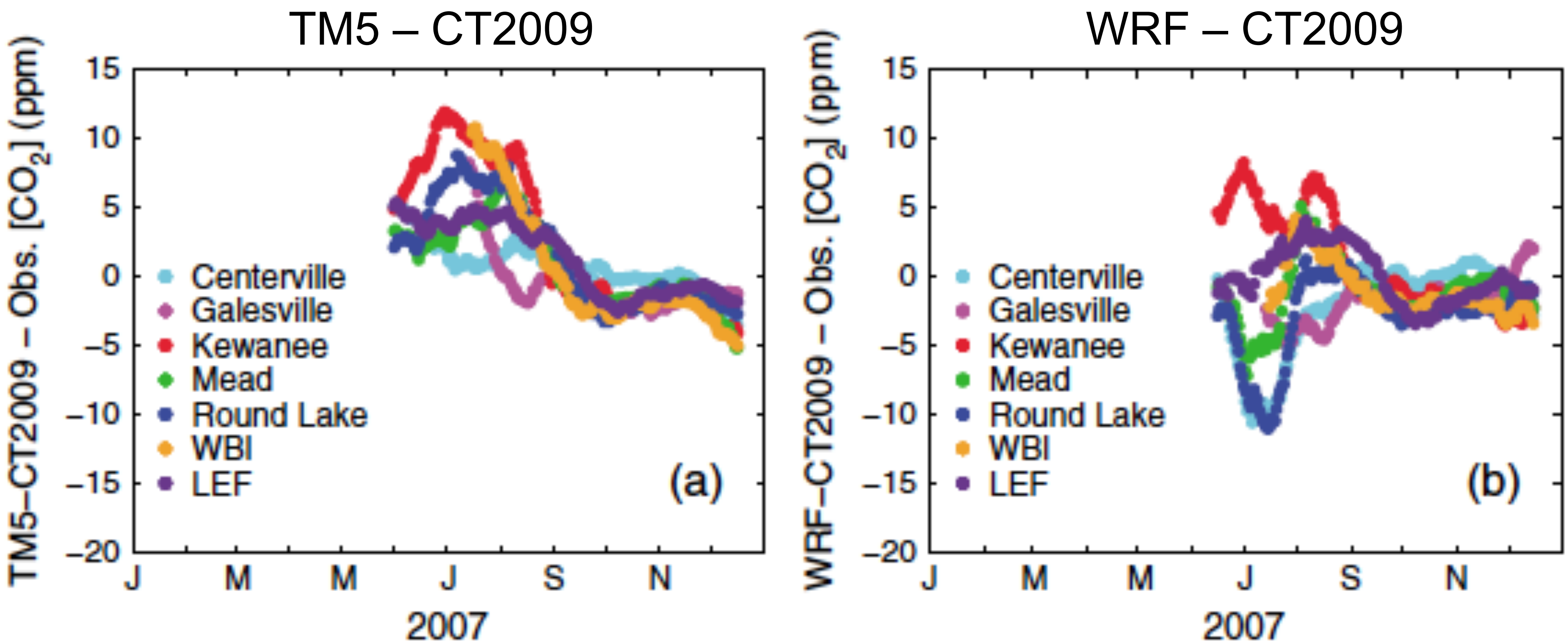


MCI 31 day running mean daily daytime average CO2

- Large differences in seasonal drawdown, despite nearness of stations.
- Differences tied to density of corn.

Miles et al, 2012, JGR-B

Comparison – TM5 and WRF
How much does atmospheric transport matter for simulating atmospheric CO_2?



Identical CO_2 fluxes and lateral boundary conditions.

Midsummer, monthly-averaged ABL CO_2 differs by as much as 15 ppm due only to atmospheric transport.

Diaz-Isaac et al, 2014, JGR-A.

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Maybe this is just a problem with global transport models? (TM5)

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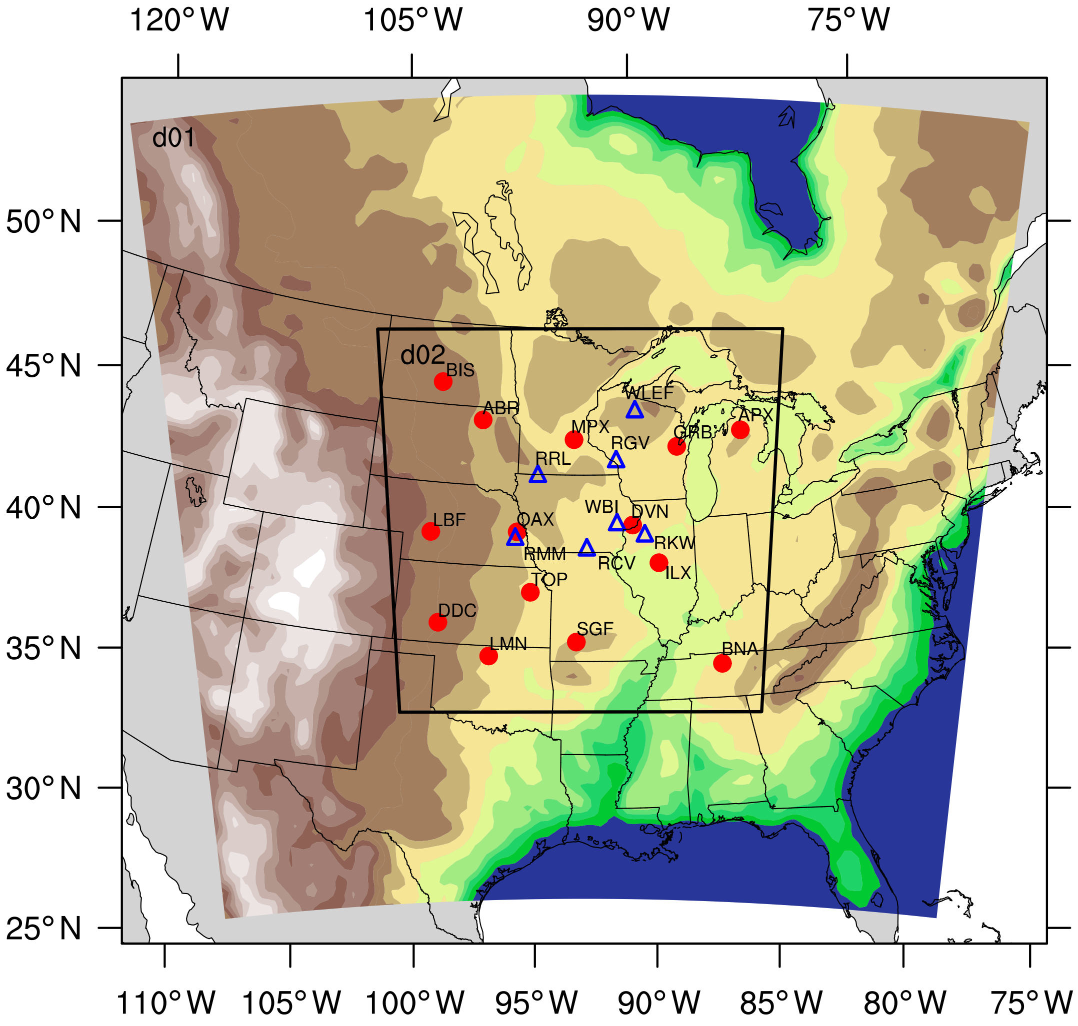
Evaluation of WRF-Chem CO_2 simulations in the upper Midwest, summer



Evaluation of *mid-afternoon* CO_2, *ABL depth, and ABL winds*.

Blue are tower-based CO_2 observation points (PSU, NOAA).

Red are rawinsonde stations (NOAA).

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

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
38	NARR	Thermal dif.	MYJ	No CP	WSM 5-class
39	NARR	Thermal dif.	MYNN	No CP	WSM 5-class
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

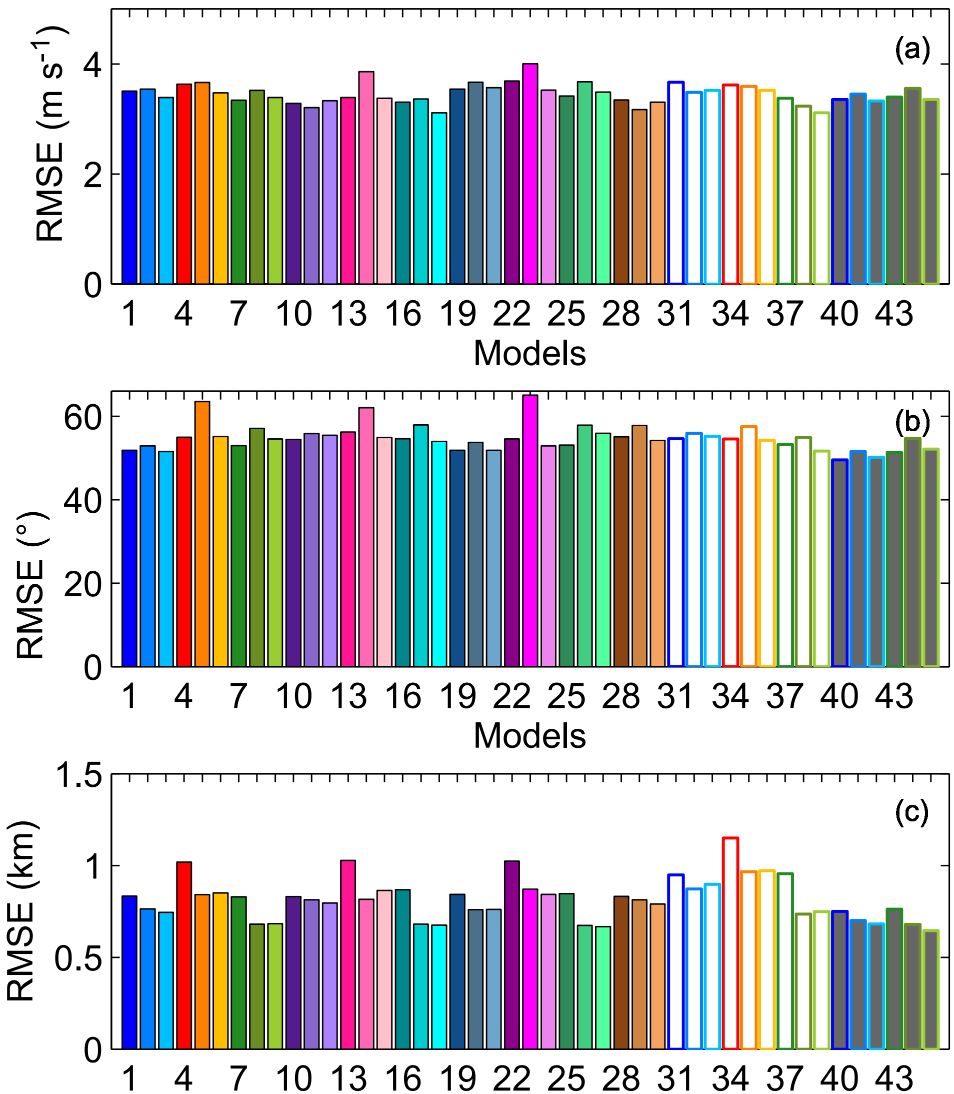
45-member transport ensemble

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.

Diaz-Isaac et al, ACP, 2018

Random errors are significant for *all* model configurations



Afternoon conditions, daily comparison.

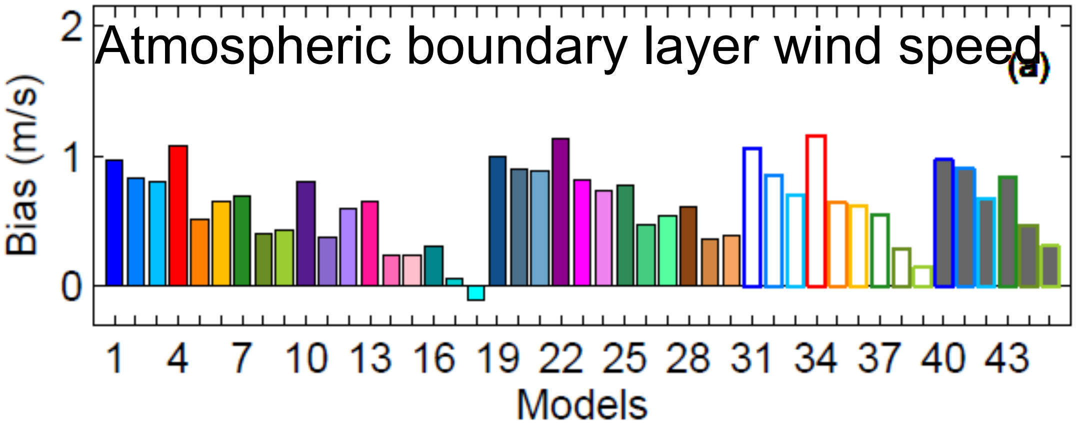
ABL wind (a) RMSE ~ 3 m/s.

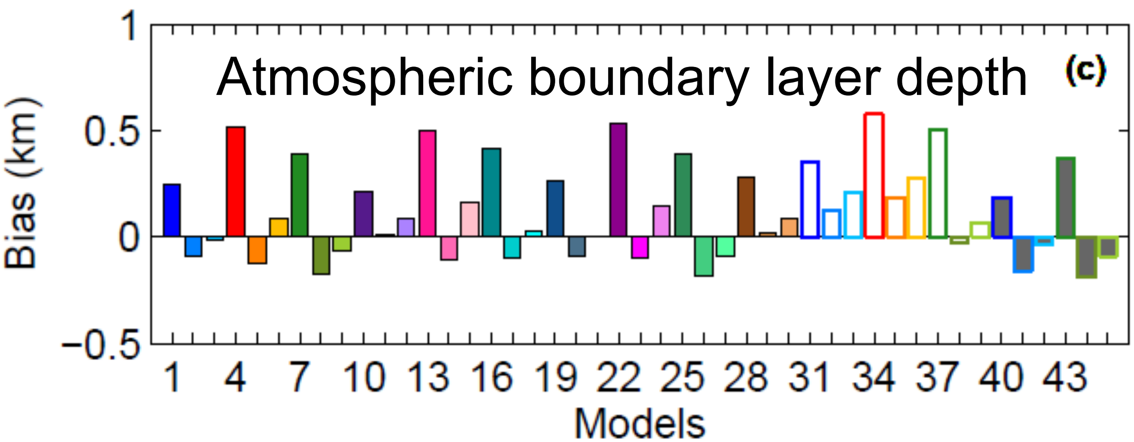
ABL wind direction (b) RMSE ~ 50 degrees.

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

Diaz-Isaac et al, ACP, 2018

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.

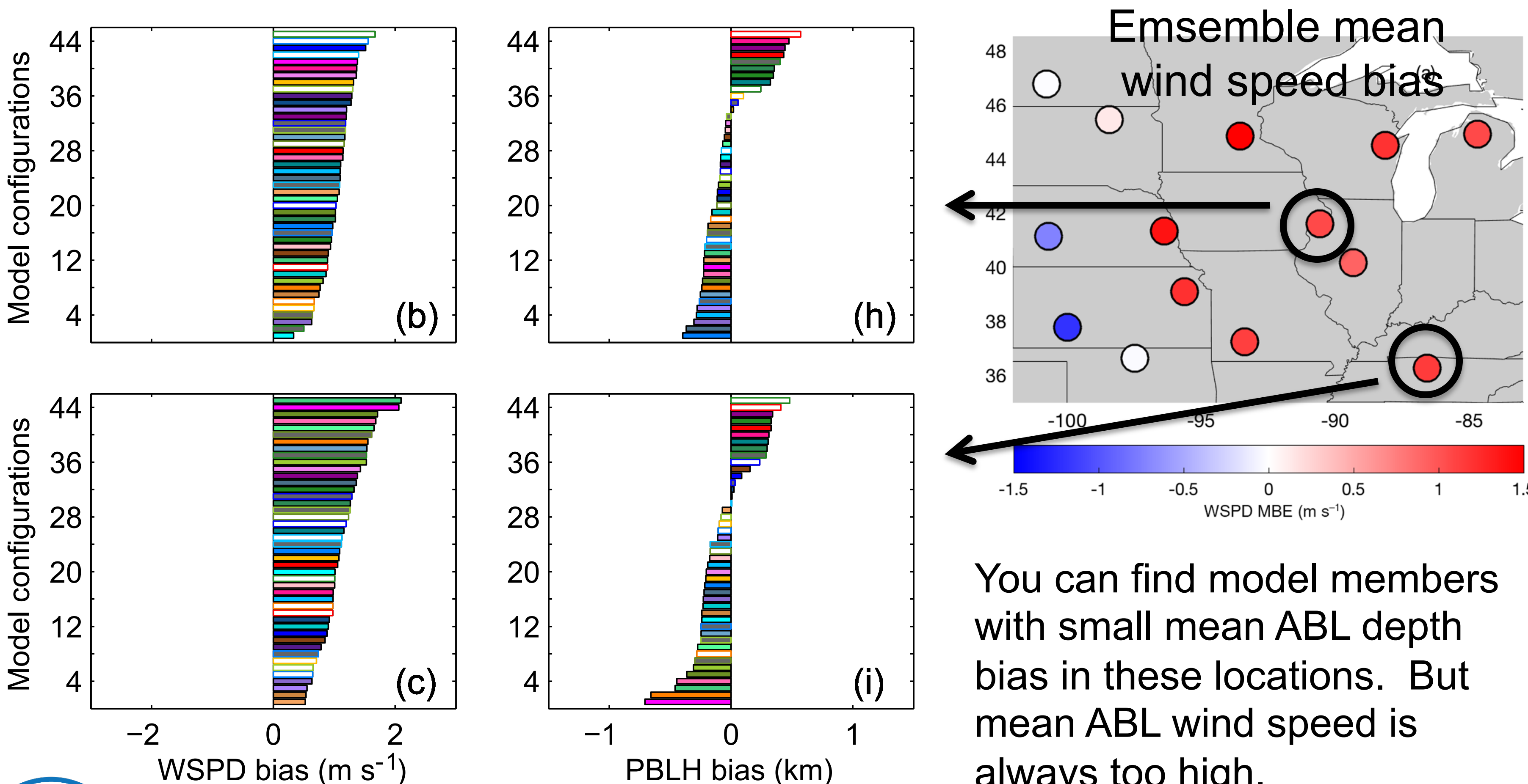
MYNN with thermal diffusion LSM appears to minimize both biases.

YSU-RUC appears to maximize biases.

No cumulus parameterization increases biases.

Diaz-Isaac et al, ACP, 2018

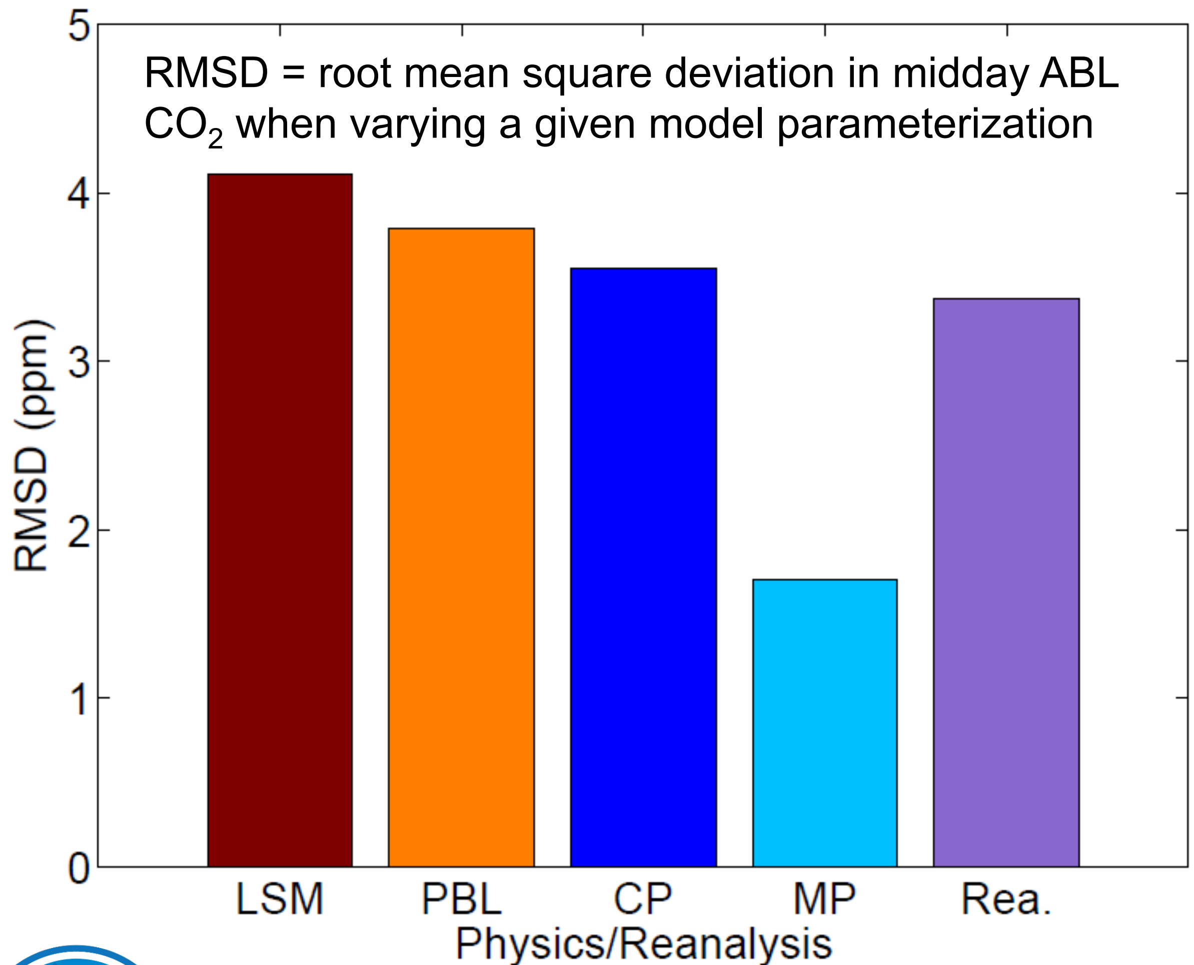
Biases have spatial structure and some locations are always biased



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.

Diaz-Isaac et al, ACP, 2018

ABL CO_2 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)

Diaz-Isaac et al, ACP, 2018

Take-aways – Diaz-Isaac 14, 18

- No single model configuration works everywhere all the time – but you can minimize biases by choosing carefully.
- Nearly every component of the model configuration has a significant impact on CO_2.
- The variability in simulated CO_2 is quite significant.

Do they matter – all these subtleties of atmospheric transport modeling? For urban GHG studies?

Yes!

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No.

Do similar results hold true for urban atmospheric transport?

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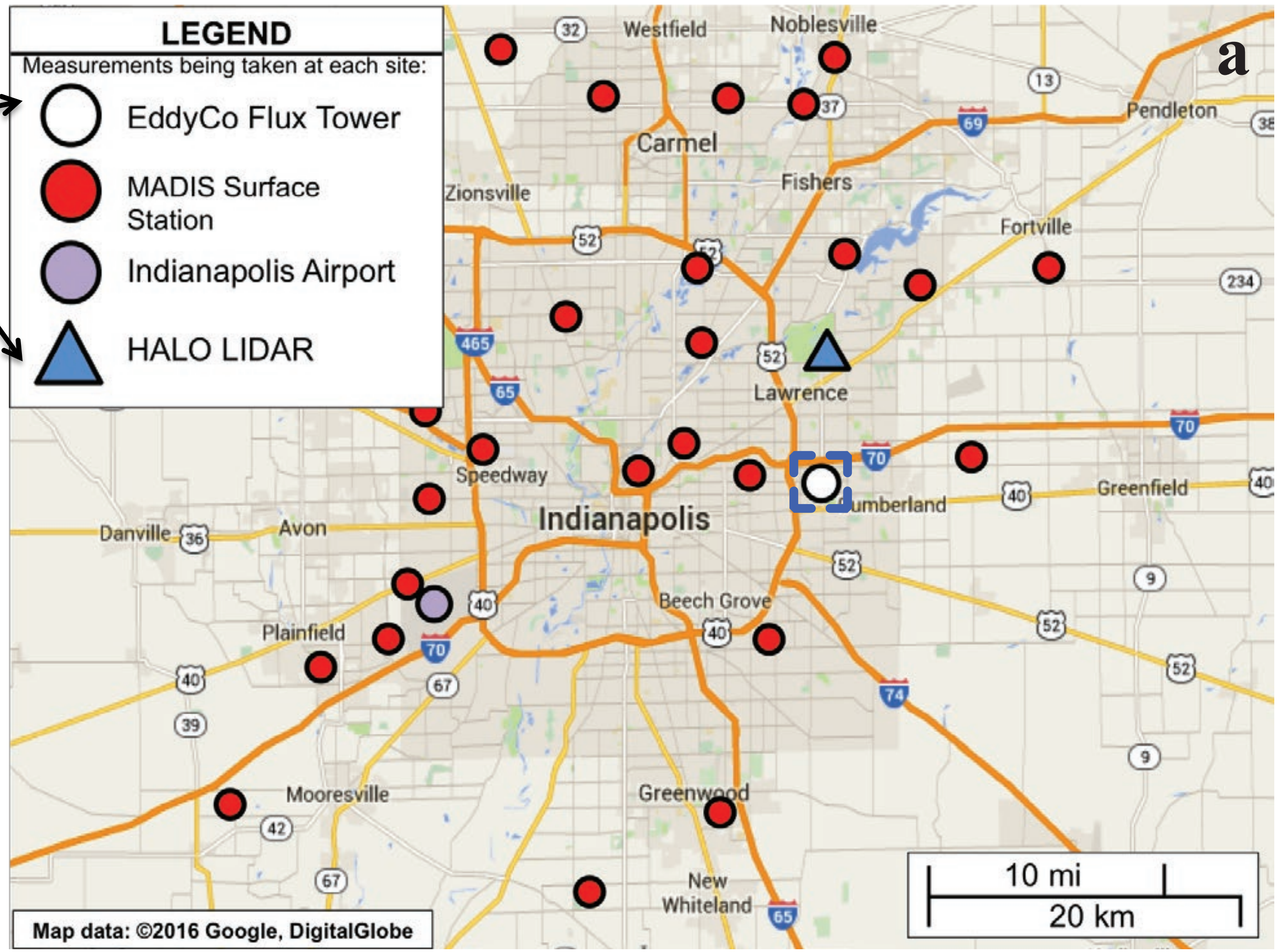
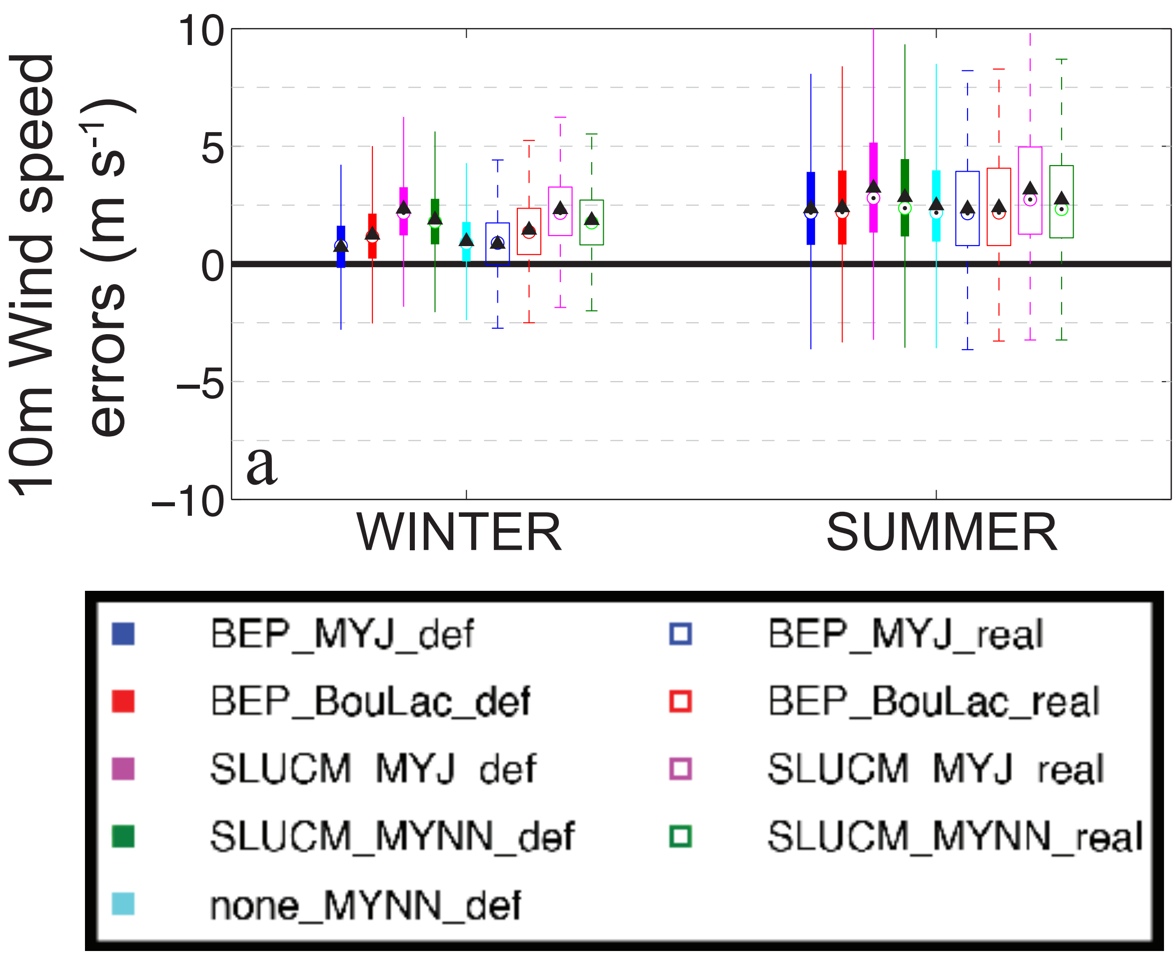
Meteorological evaluation data for WRF-Chem in Indianpolis

INFLUX



Sarmiento et al, Elementa, 2017

Wind speed: Random errors are large, WRF-Chem is too windy



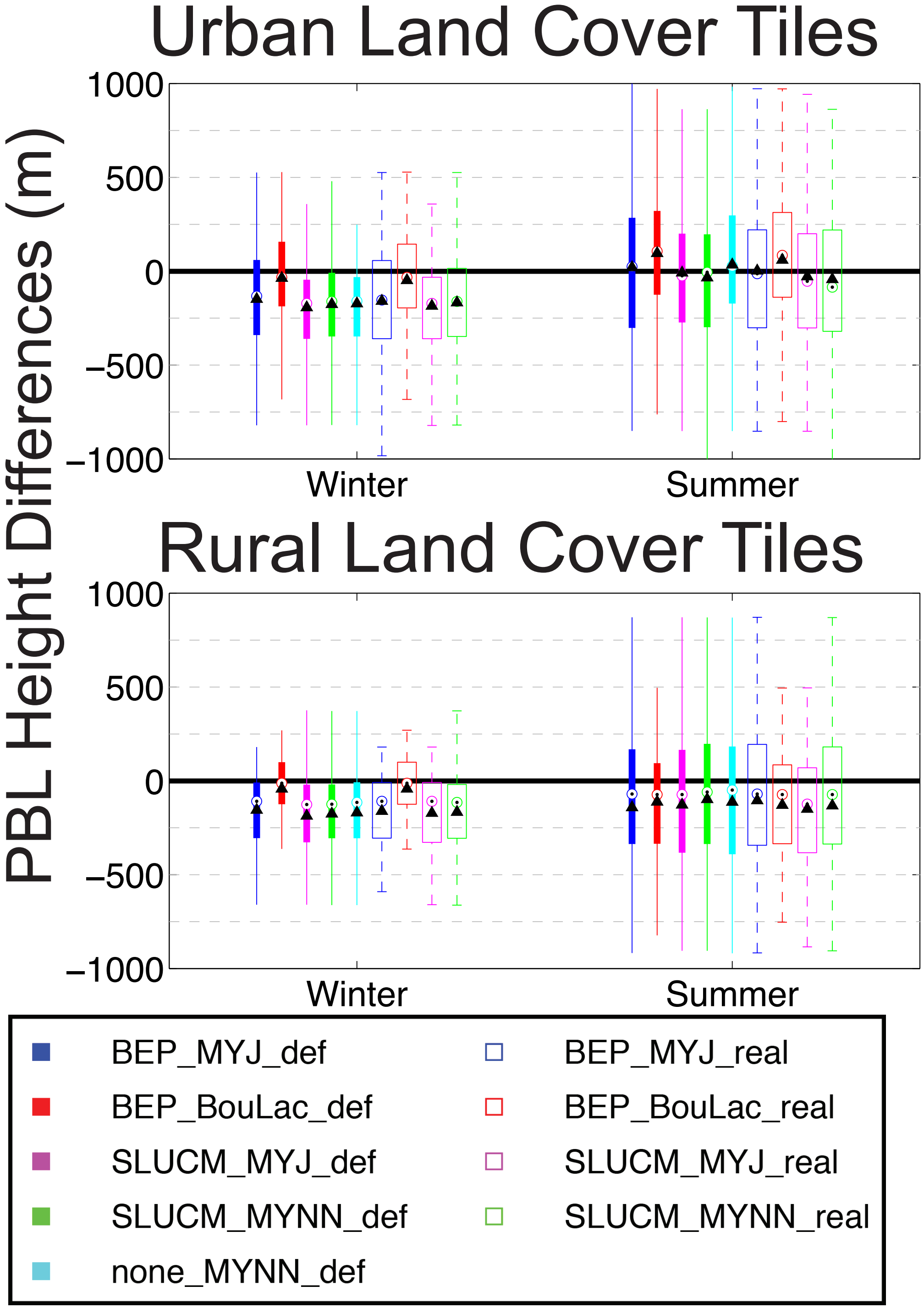
No configuration removes 10-m wind speed bias.

WRF-Chem ensemble run for Indianapolis, one summer and one winter month.

Land cover, LSM and ABL model varied *within the city*.

Random errors and biases shown – midday conditions.

Sarmiento et al, Elementa, 2017



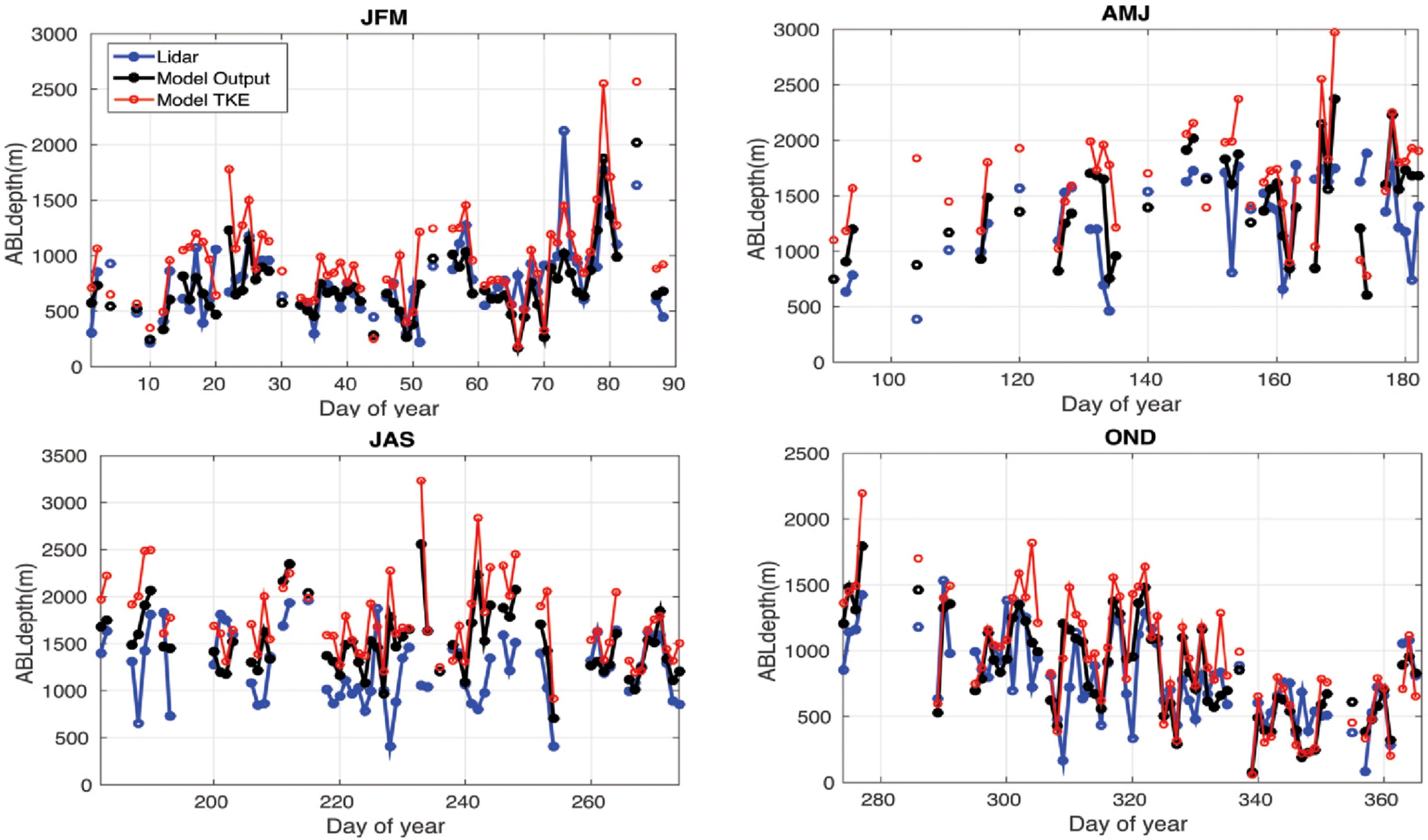
All configurations show large random errors, and similar biases in ABL depth.

Bias varies based on location (within, outside the city).

The background meteorological simulation is more important to urban conditions than the setup of the urban land surface and boundary layer model?

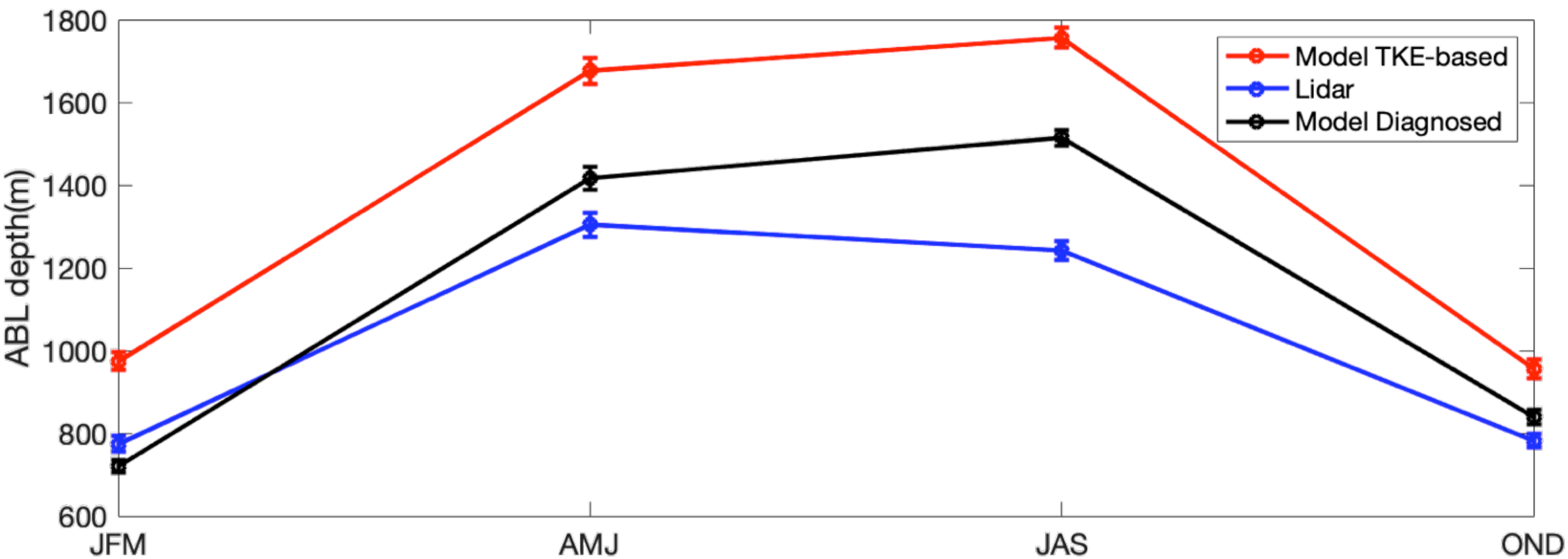
Sarmiento et al, Elementa, 2017

Full-year evaluation of ABL depth and winds using the INFLUX/NOAA Doppler lidar and our default WRF configuration (MYNN-NOAH)



Pan et al, in preparation

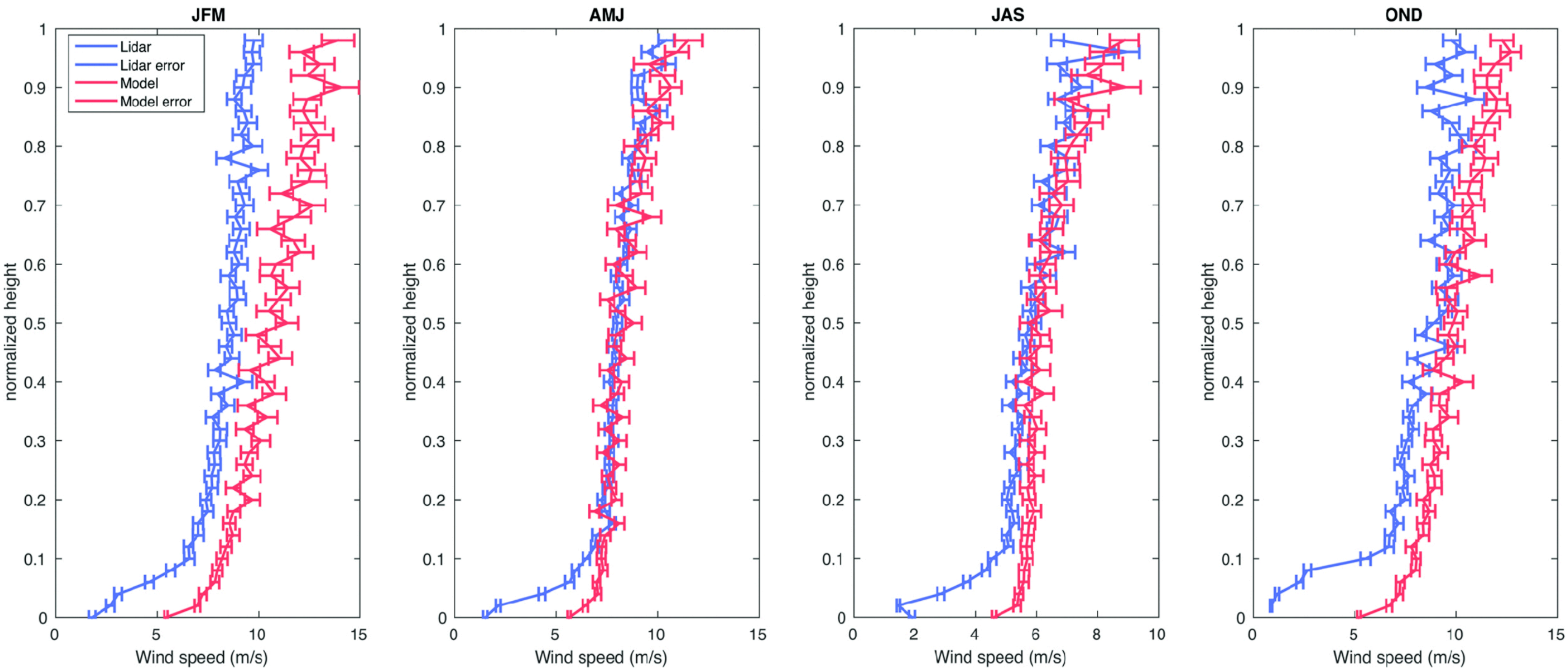
Seasonal mean biases in midday ABL depth.



Winter is less biased than summer.
TKE-depth is greater than model-diagnosed ABL depth.

Pan et al, in preparation

Seasonal mean biases in midday ABL wind speed.



Always too windy near the ground.
Winter ABL winds too high. Summer ABL winds about right.

Pan et al, in preparation

Seasonal mean biases in midday ABL wind speed.

ME of wind speed and direction between lidar and model

	Count		Wind Speed (m/s)			Wind Direction (degree)		
	Model	Lidar	Model	Lidar	Difference	Model	Lidar	Difference
JFM	7656	10367	10.5±0.07	8.0±0.04	2.5±0.11	231±1	222±1	9±2
AMJ	6260	9604	8.4±0.05	7.9±0.04	0.5±0.09	212±1	202±1	10±2
JAS	9709	14439	6.4±0.04	5.7±0.03	0.7±0.07	218±1	210±1	8±2
OND	7973	10691	9.7±0.06	8.1±0.05	1.7±0.11	241±1	230±1	11±2

Pan et al, in preparation

So…can we do anything about this state of affairs?

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Yes!

Paths to improved atmospheric transport simulations

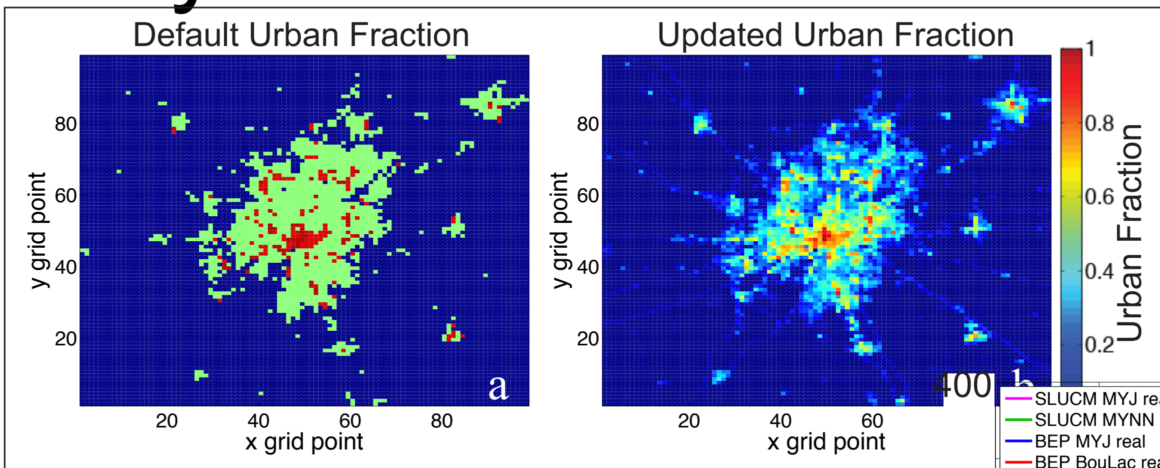
- Fix the models – identify causes of errors and eliminate them.
- Add meteorological observations and assimilate them – kick the model in the right direction.
- Quantify the uncertainty caused by atmospheric transport.
- Embrace calibrated transport model ensembles.

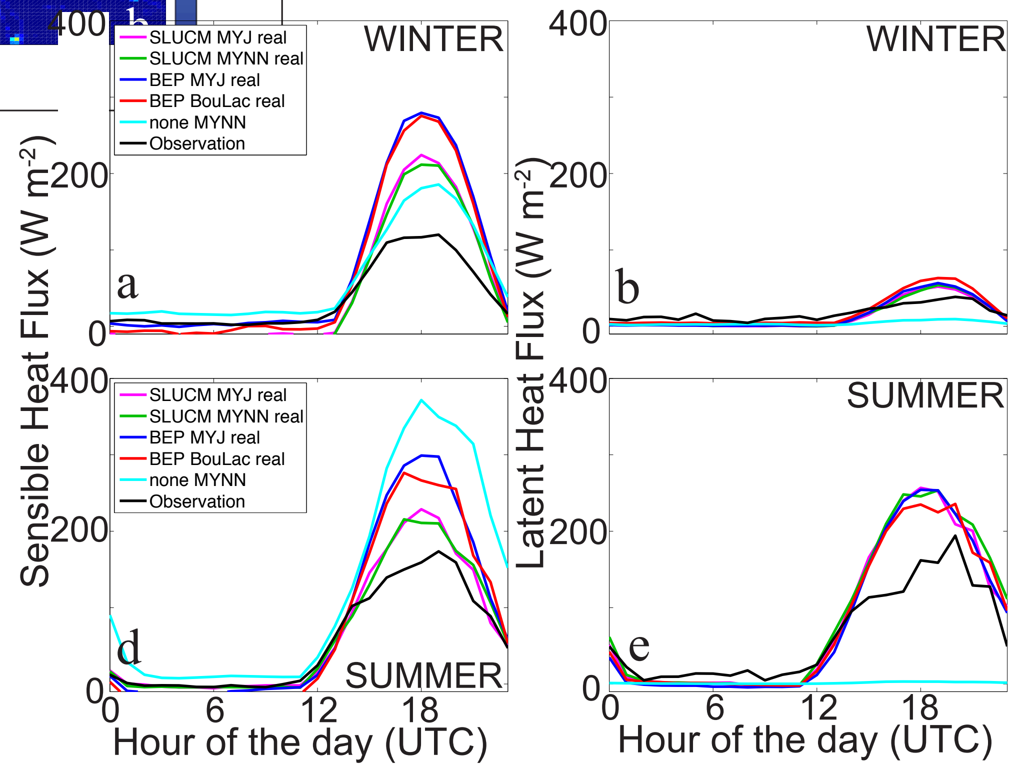
So…can we do anything about this state of affairs?

Yes!

Fix.

Urban land cover in WRF leads to systematic biases in surface fluxes





WRF makes Indy a (bumpy) parking lot by default.

Urban sensible heat fluxes are greatly overestimated.

May help explain overestimate in ABL depth.

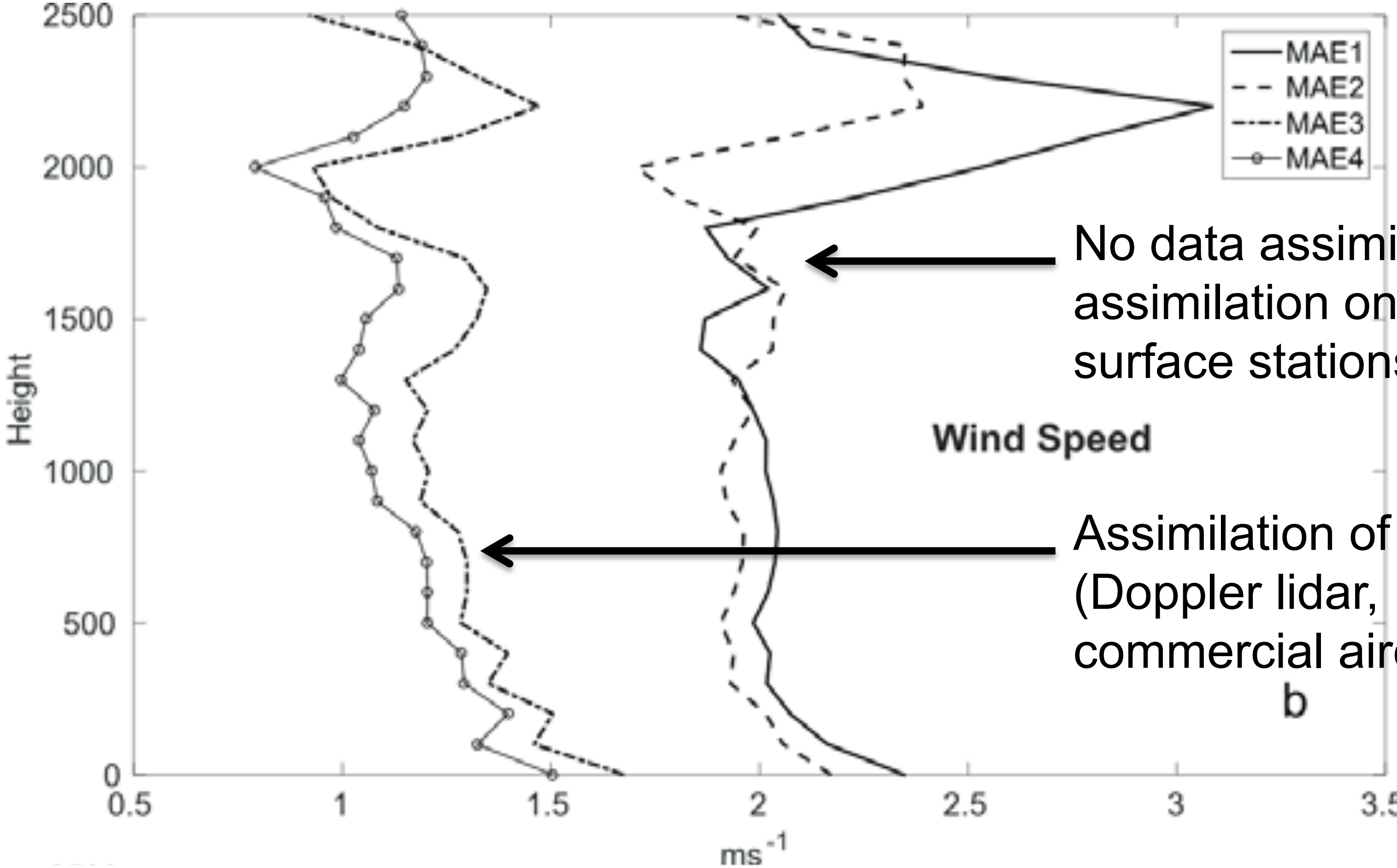
Sarmiento et al, Elementa, 2017

So…can we do anything about this state of affairs?

Yes!

Fix. Kick.

Meteorological data assimilation greatly reduces random errors



No data assimilation, and assimilation only of surface stations.

Assimilation of ABL winds (Doppler lidar, commercial aircraft).

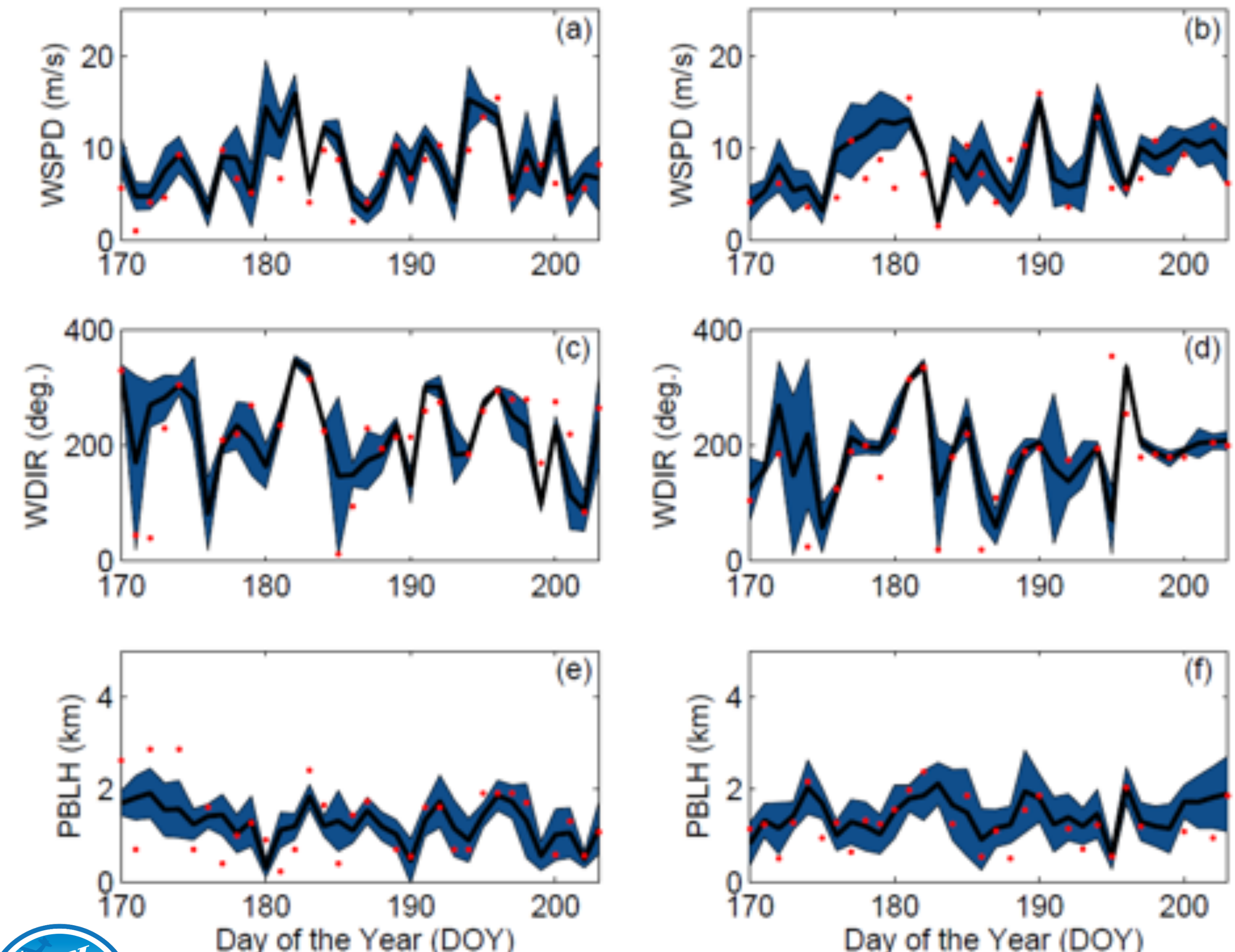
Deng et al, Elementa, 2017

So…can we do anything about this state of affairs?

Yes!

Fix. Kick. Quantify with calibrated ensembles.

How do you calibrate an atmospheric transport model ensemble?



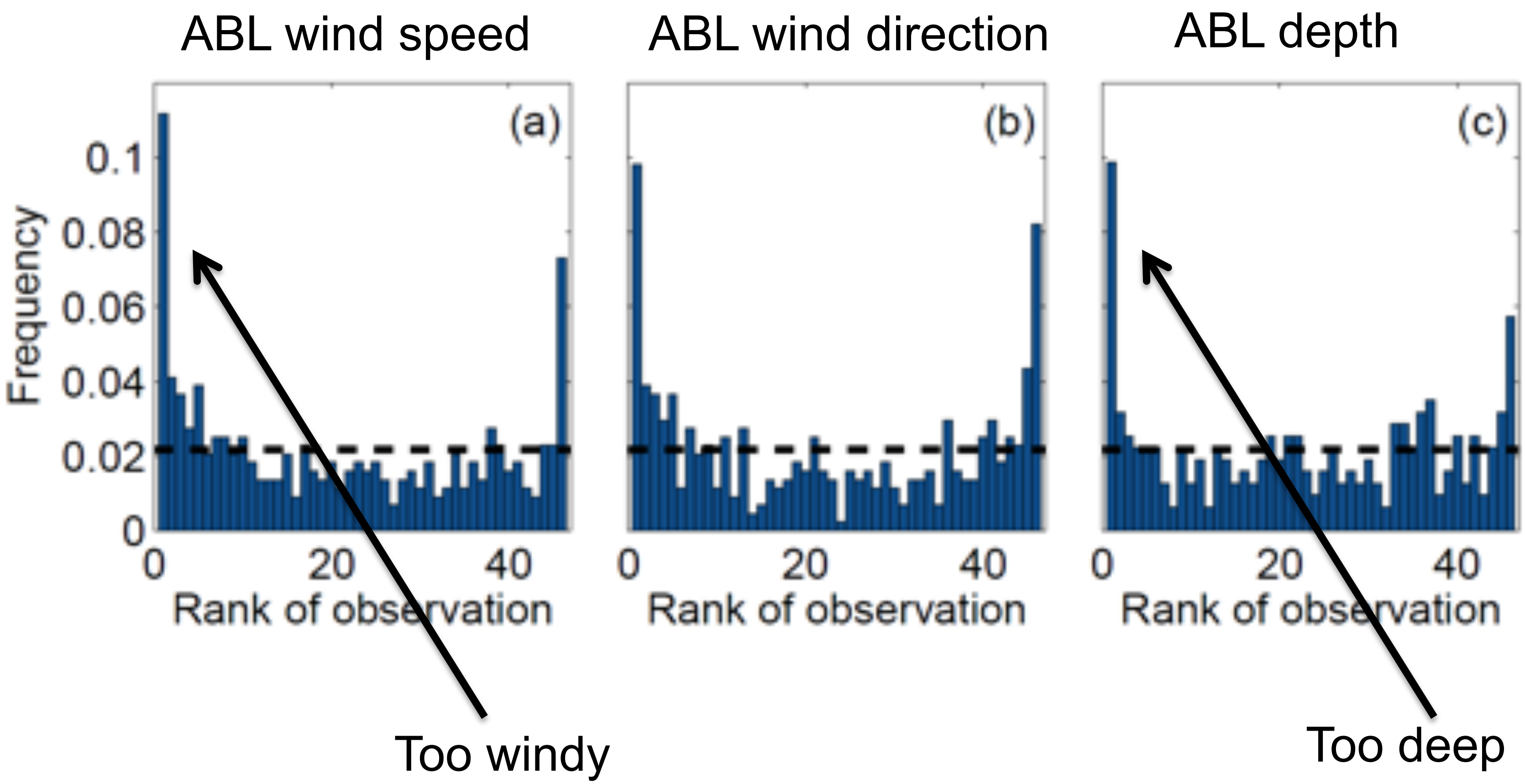
Construct a "rank histogram."

Rank the observation with respect to its location among the members of the ensemble.

The ensemble should encompass the observations (sufficient spread), but not have too much spread.

Diaz-Isaac et al, submitted to ACP

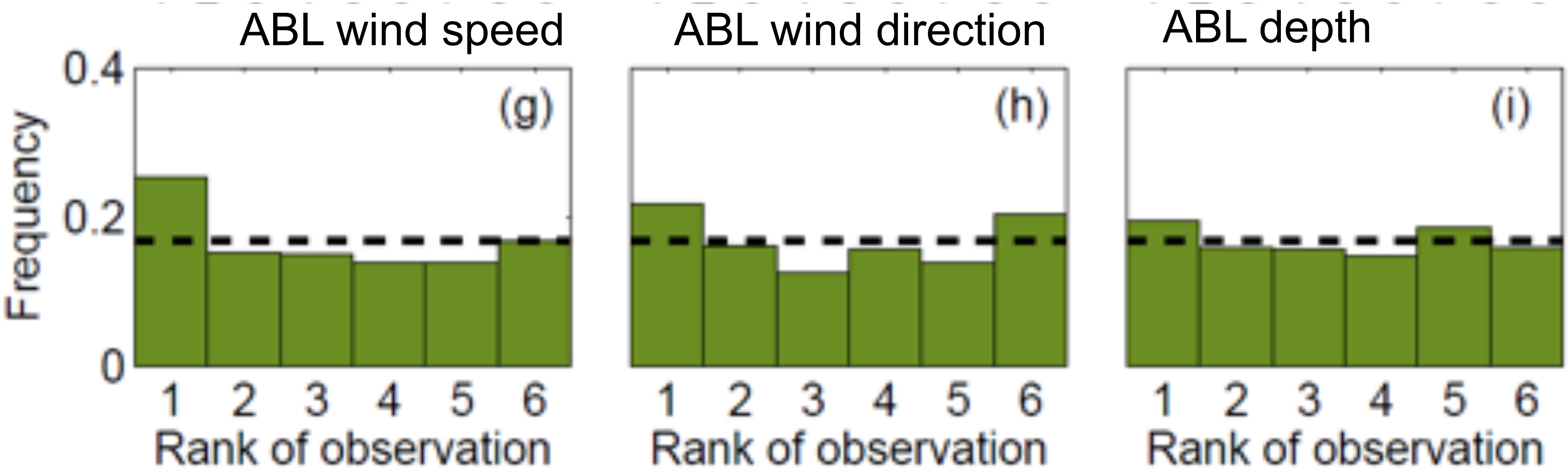
That 45-member ensemble is "under-dispersive"



We can improve the ensemble by throwing out biased members.

Diaz-Isaac et al, submitted to ACP

Pruned 5-member ensemble

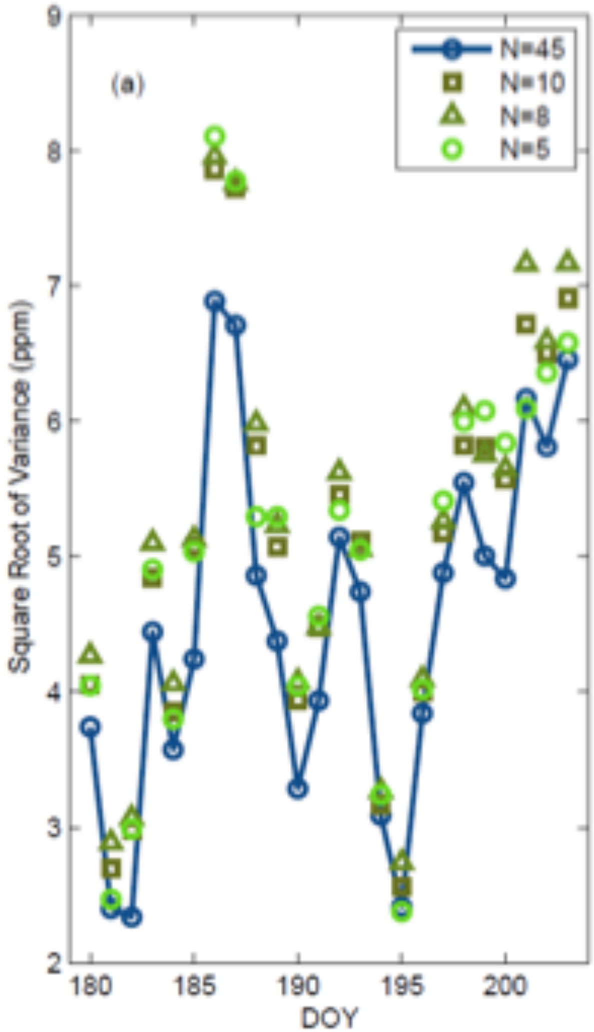


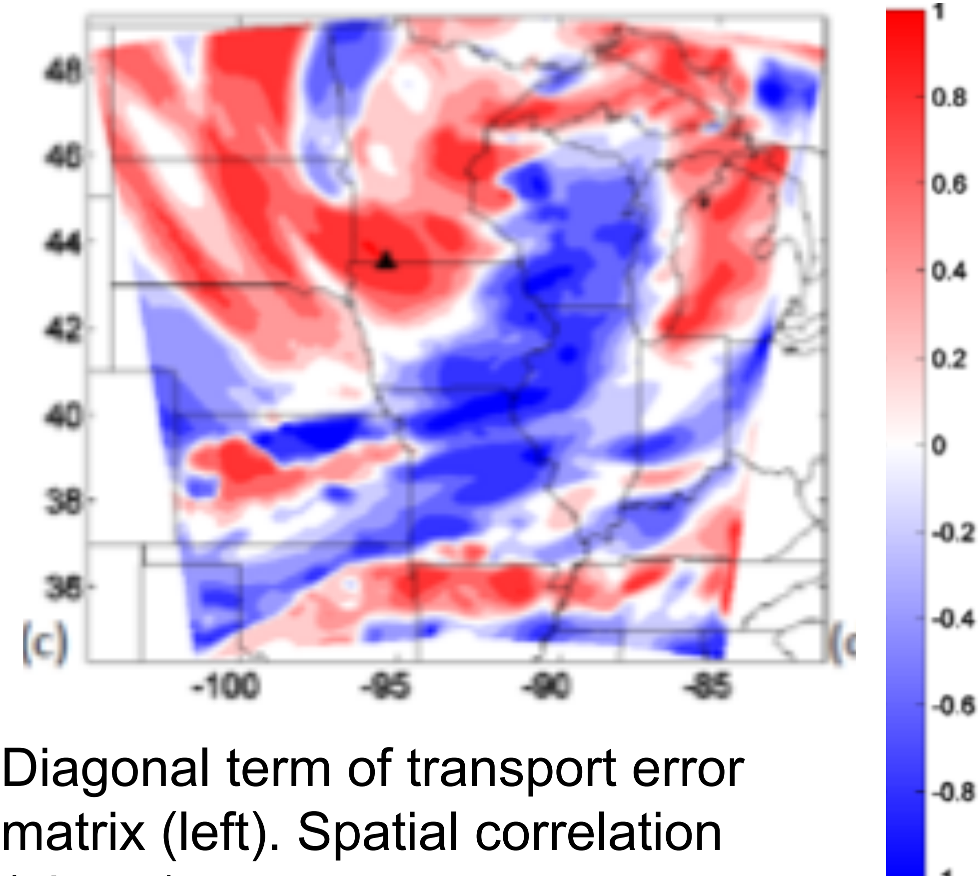
Still some trouble with ABL winds, but much improved.
Modest biases.
Spread among models is a good representation of atmospheric model transport uncertainty.

N	Sub-ensemble	Wind Speed			Wind Direction			PBLH		
		δ	Bias m/s	σ m/s	δ	Bias Deg.	σ Deg.	δ	Bias m	σ m
10	[5 14 17 26 31 33 34 35 37 45]	5.6	0.6	3.6	4.1	-0.8	57.9	2.1	83.2	823.7
8	[5 14 15 17 33 34 37 38]	5.7	0.5	3.5	3.7	-0.4	58.1	2.5	99.3	828.3
5	[16 17 23 33 35]	5	0.5	3.6	3.4	-0.7	59	0.6	76.2	810.7

Diaz-Isaac et al, submitted to ACP

We can use the ensemble to quantify complex CO_2 error structures.





Diagonal term of transport error matrix (left). Spatial correlation (above).

We should do this for cities!

Diaz-Isaac et al, submitted to ACP

Conclusions

- Mesoscale atmospheric transport models are powerful tools for urban GHG studies, but they are modeling systems full of complex, significant errors.
- *Quantifying these uncertainties is critically important*
- Local boundary layer observations (Doppler lidar, instrumented commercial aircraft, surface flux measurements) have proven invaluable in assessing model performance at Indianapolis.
- Paths forward:
  - Identify model shortcomings and correct them.
  - Choose the best model configurations for your site and season.
  - Assimilate boundary layer observations.
  - Employ *calibrated* ensembles to quantify the remaining uncertainty.

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