Improving WRF Representation of Coastal, Marine, and Residual Boundary Layers and Quantifying the Effects on Ozone Prediction

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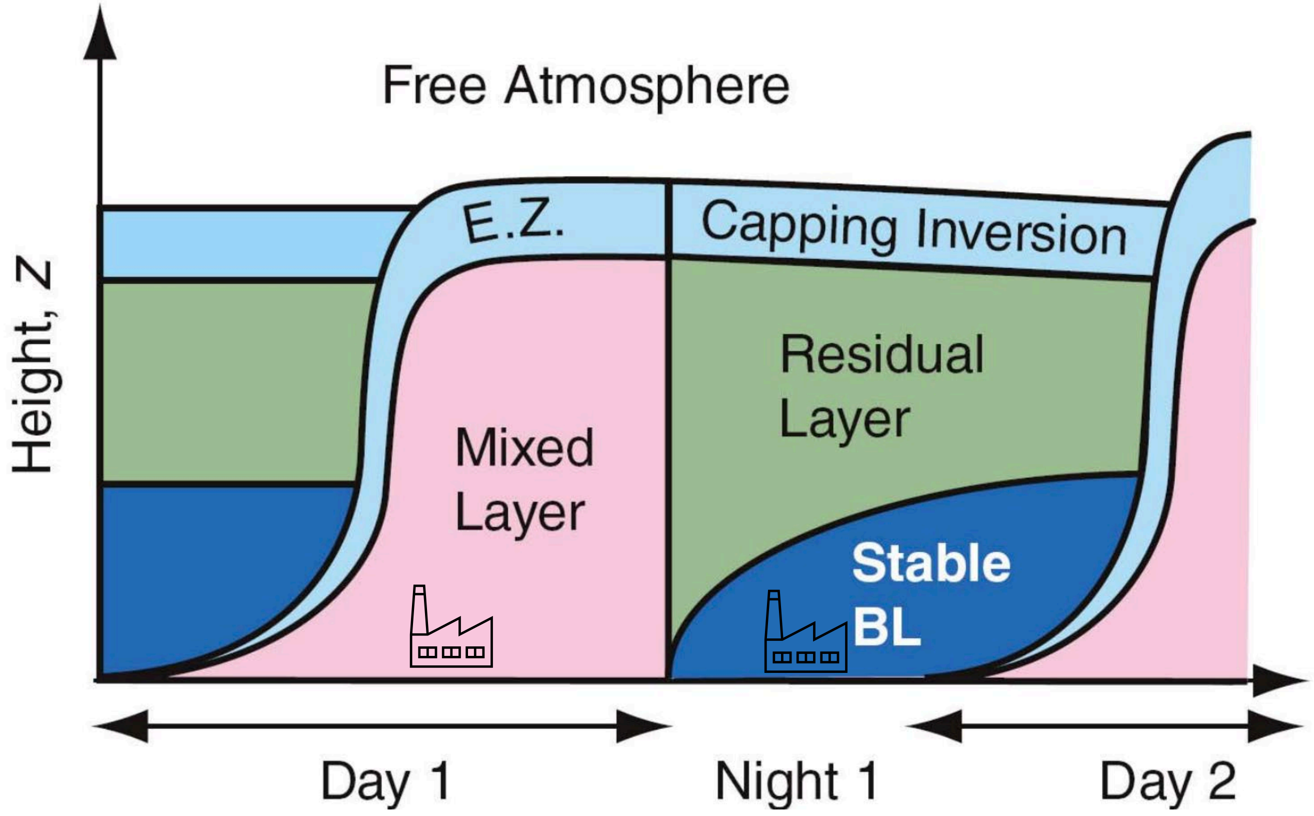
AQRP 24-021

Background: Planetary Boundary Layer (PBL)



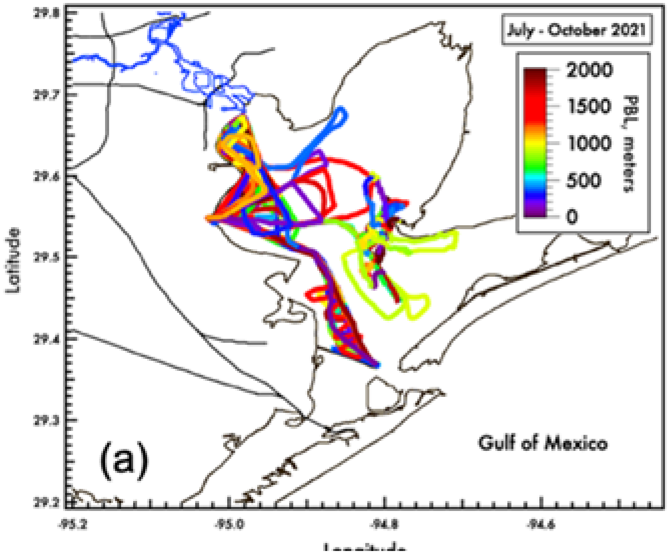
- Complex structure with diurnal changes
- Marine boundary layer observations non-existence till recently

TRACER-AQ Field Campaigns: 2021 - 2023

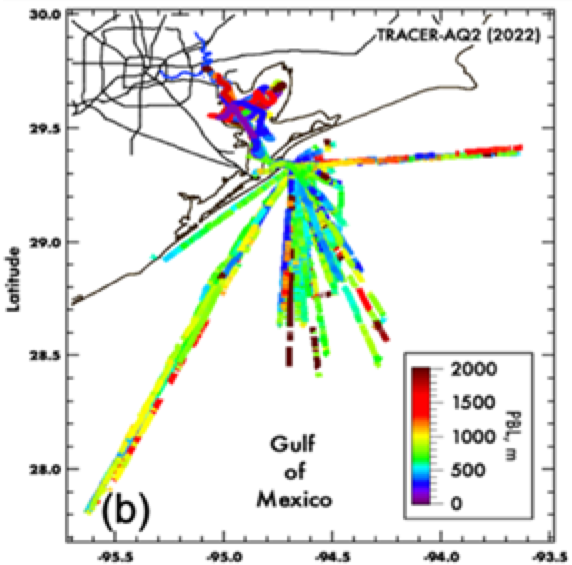
UH Pontoon

UH Osprey

July – Oct 2021

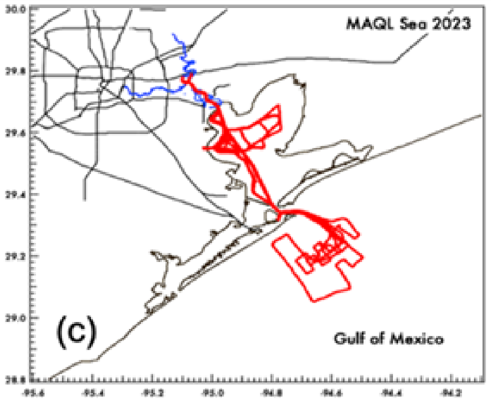


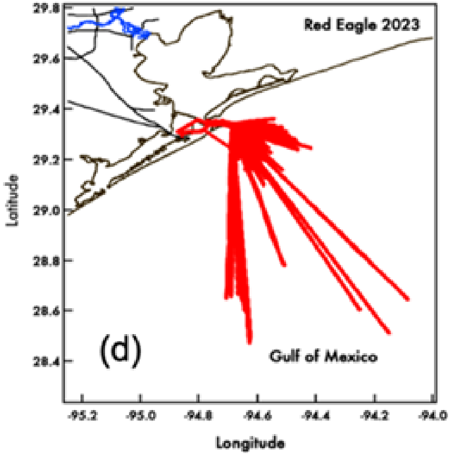
July – Oct 2022



Victory

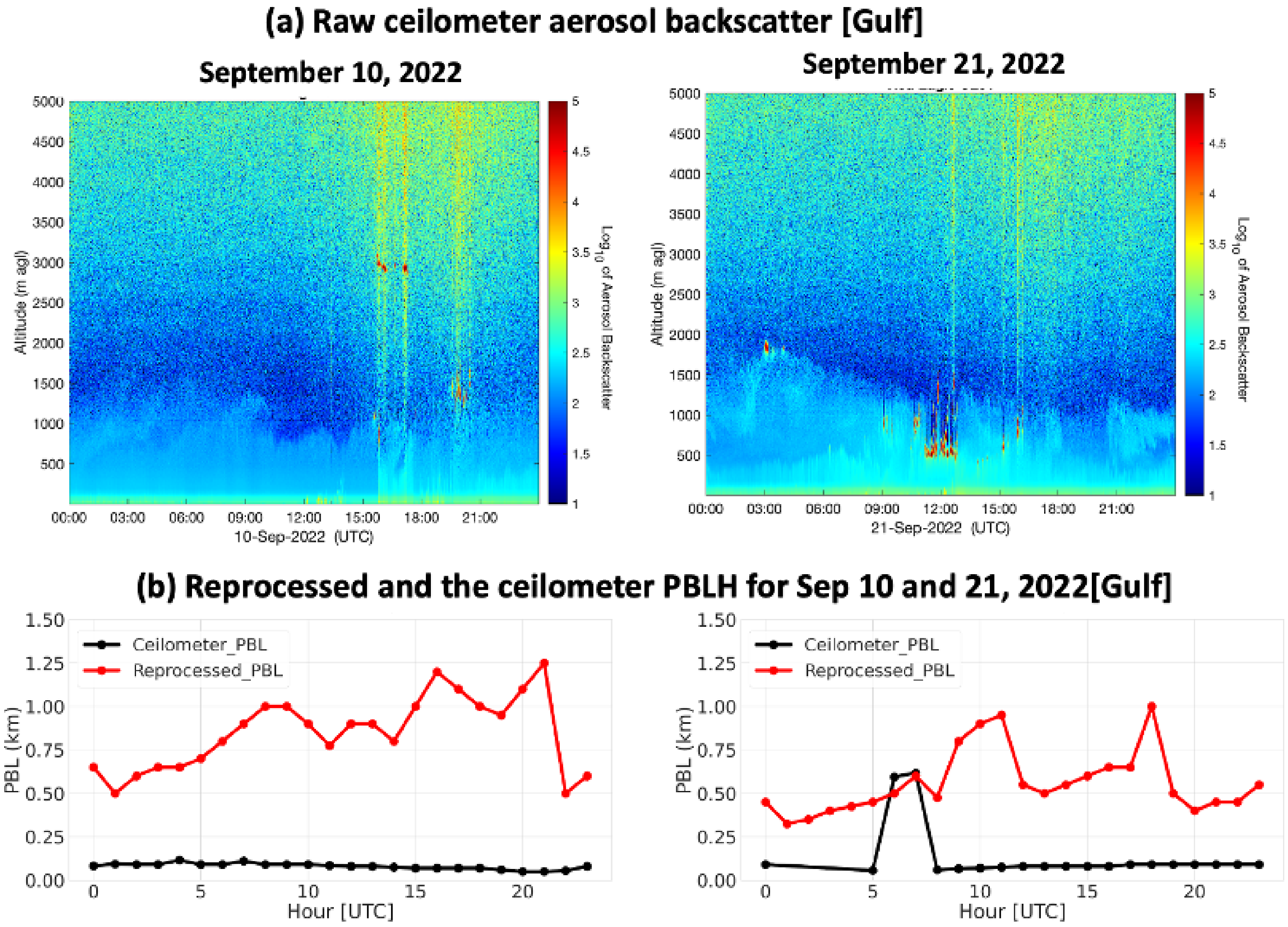
Apr – Oct 2023





PBLH derived from ceilometers

Aerosol Backscatter



Griggs et al., 2024

Objectives/Tasks

1. Marine PBL synopsis and model evaluation

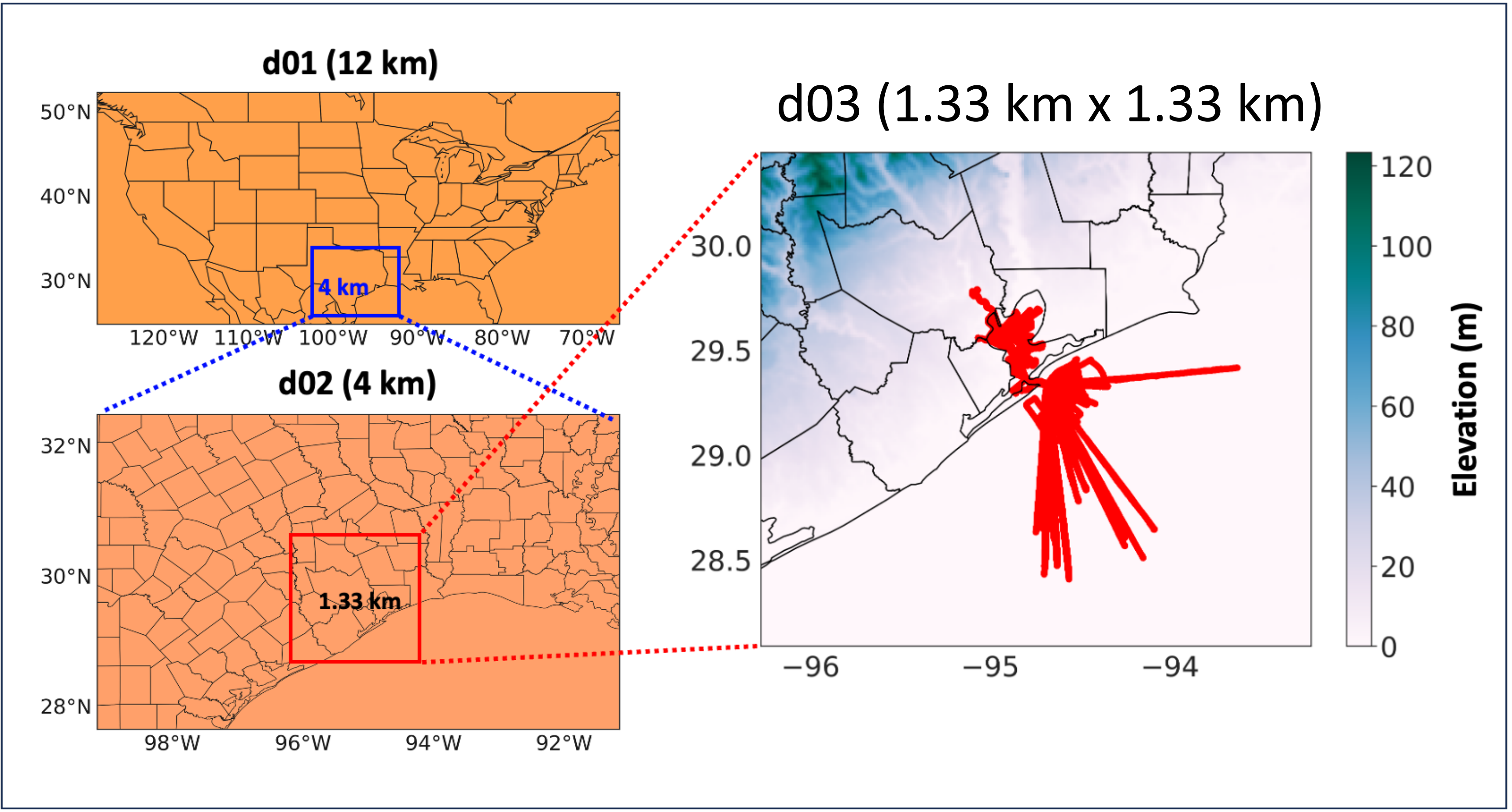
2. Improvements to marine PBL in WRF

3. Improvements to WRF representation of Residual Layer

4. Effect of improved PBL on CAMx ozone prediction and source attribution

WRF Model

WRF v4.6.0, 3-nested domains



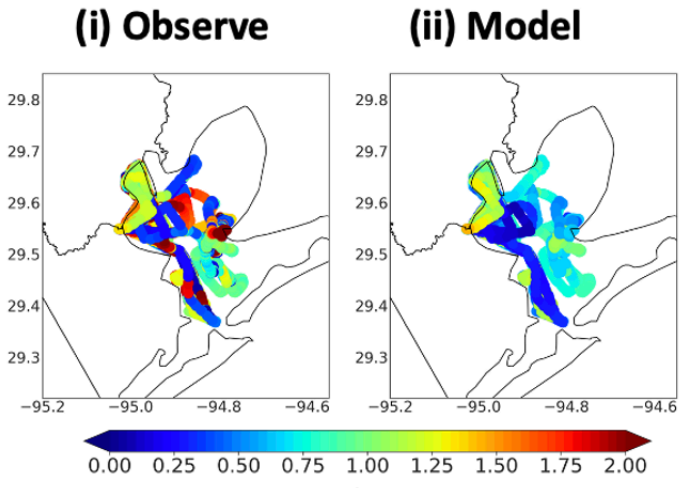
WRF Configuration

	Base
BC Meteorology	HRRR
Microphysics	2M
PBL Scheme	MYNN2.5
Cumulus Physics Scheme	New Tiedtke

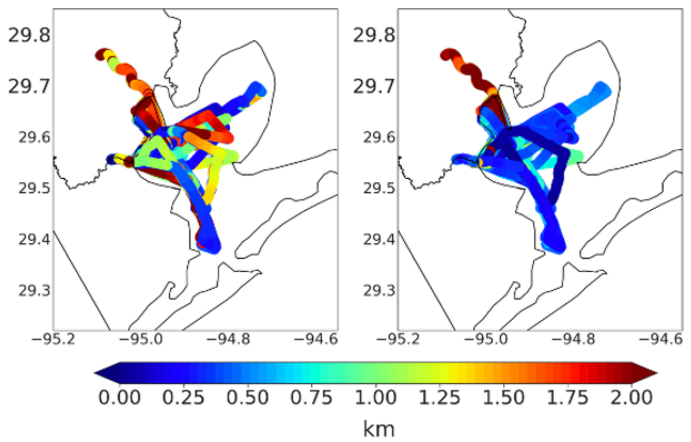
Liu et al., 2023

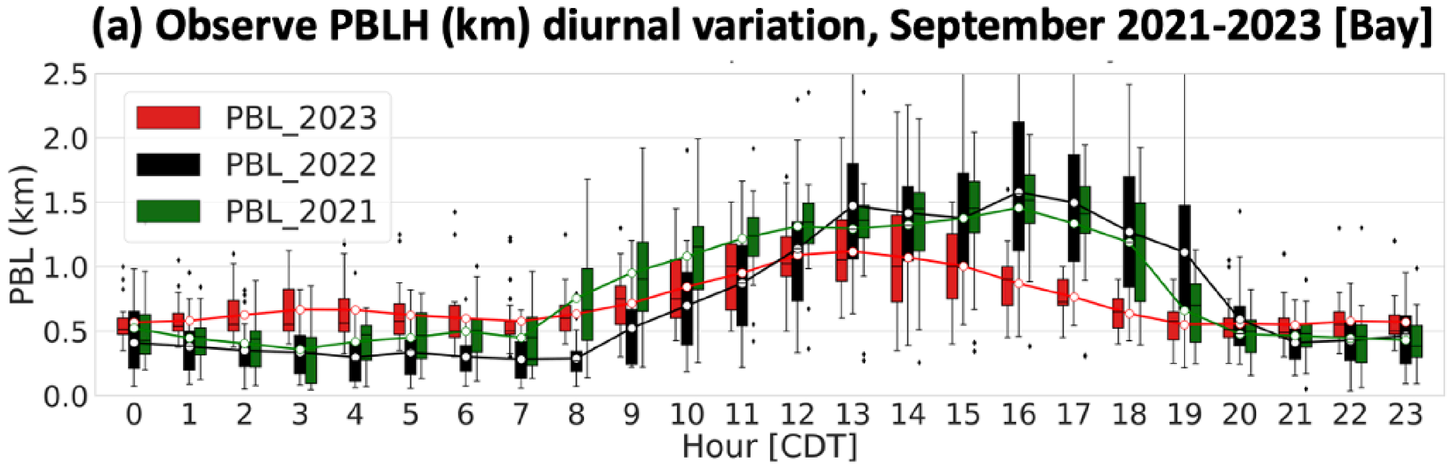
PBLH: Galveston Bay

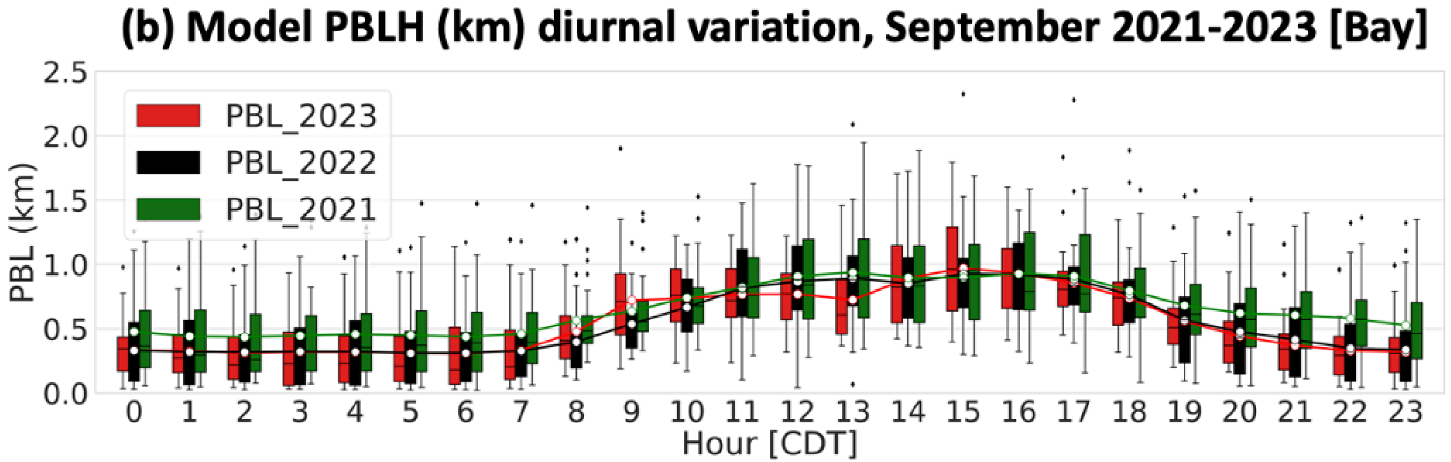
July-Sep 2021



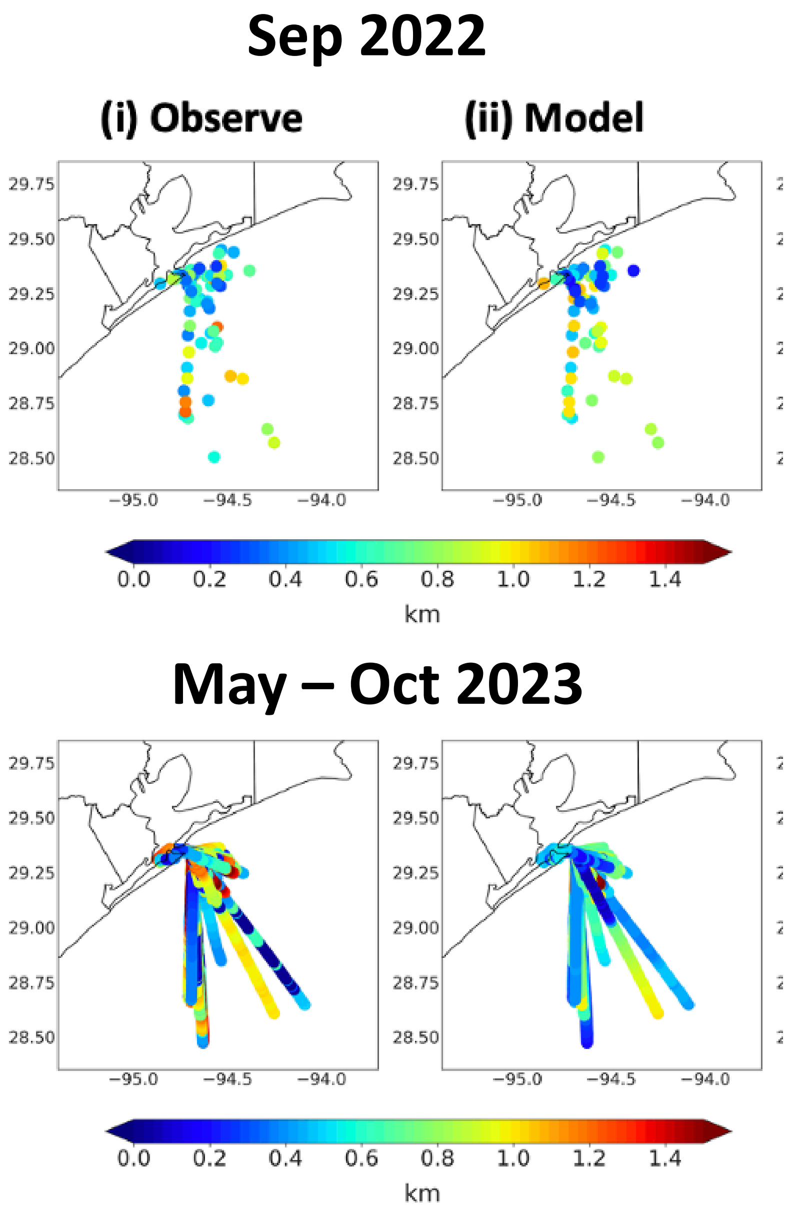
Aug – Sep 2022

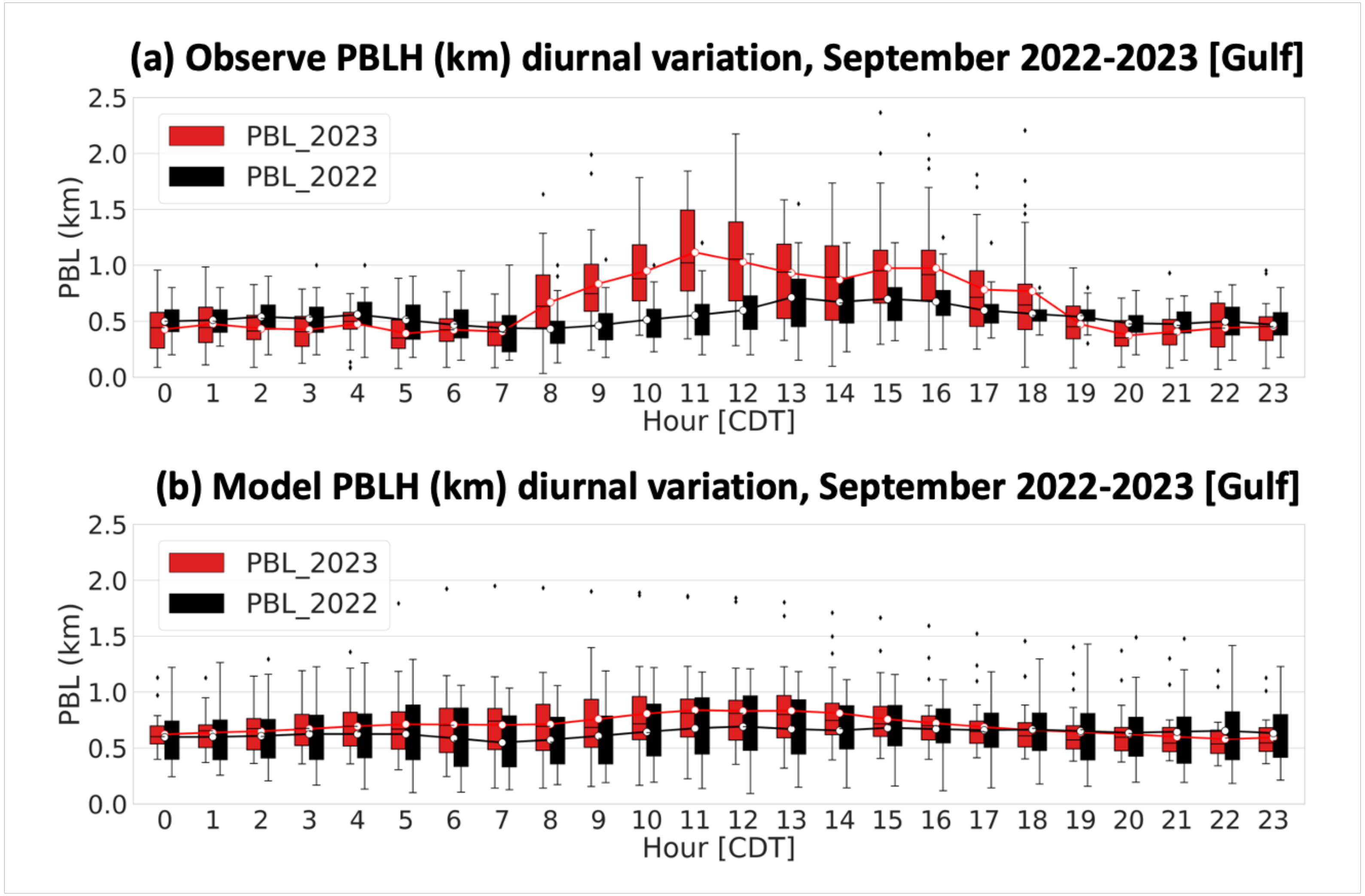






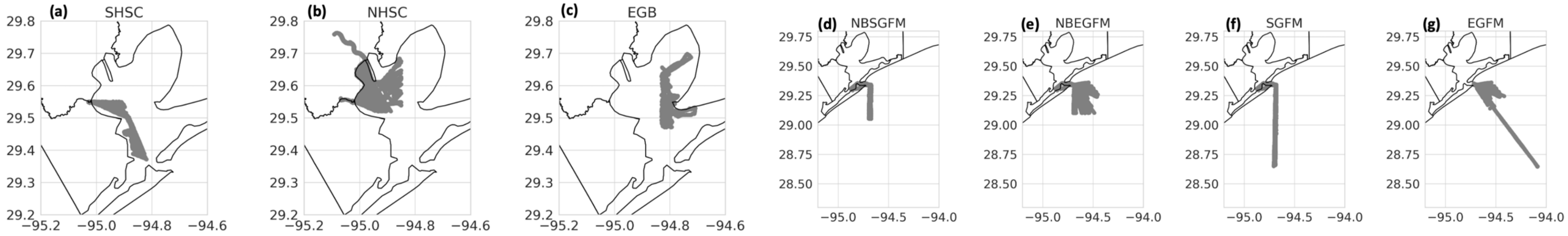
PBLH: Gulf of America



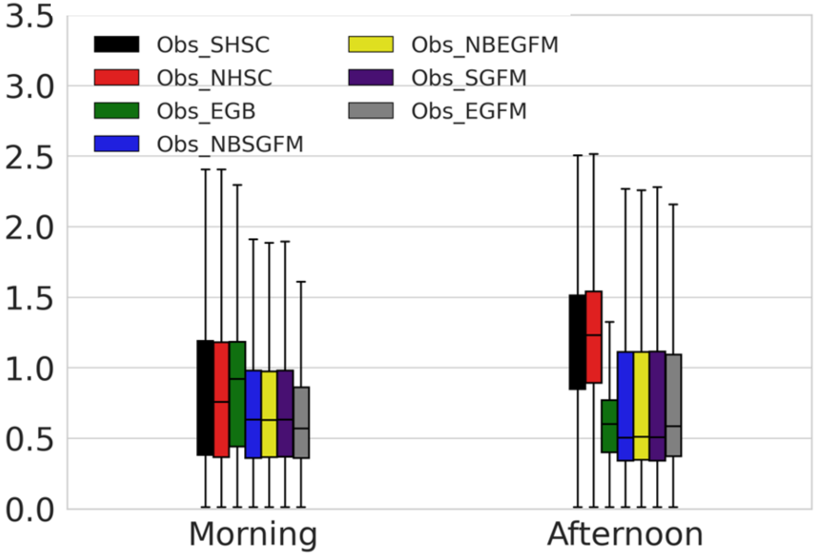


PBLH: Spatial Distributions

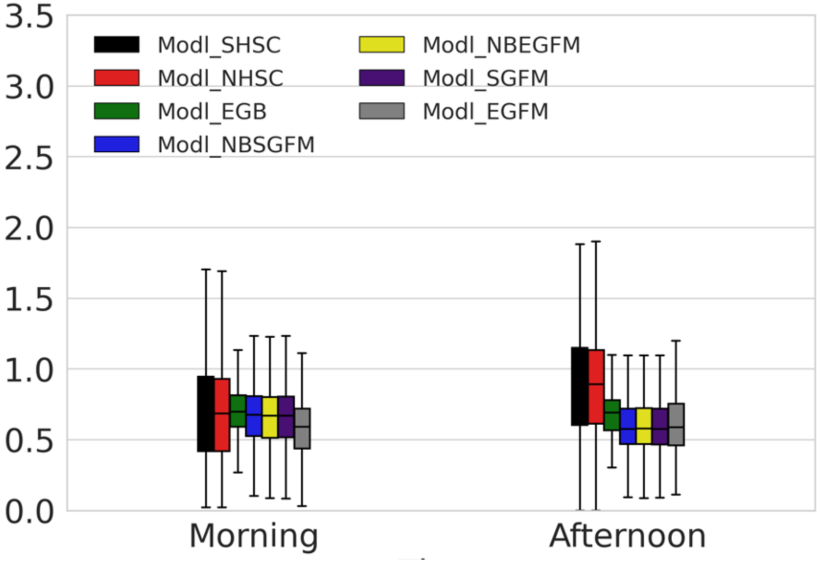
Six Regions



Observation



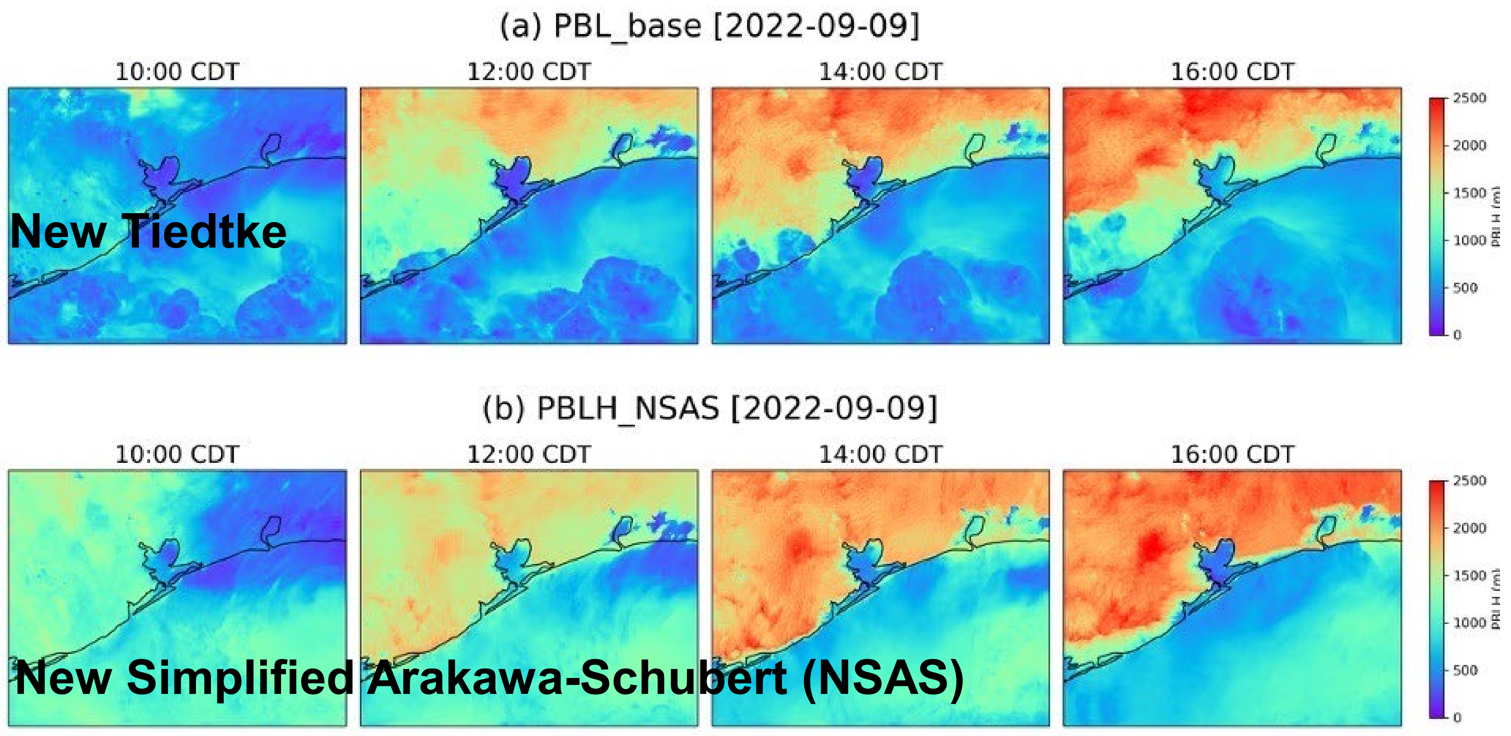
Model



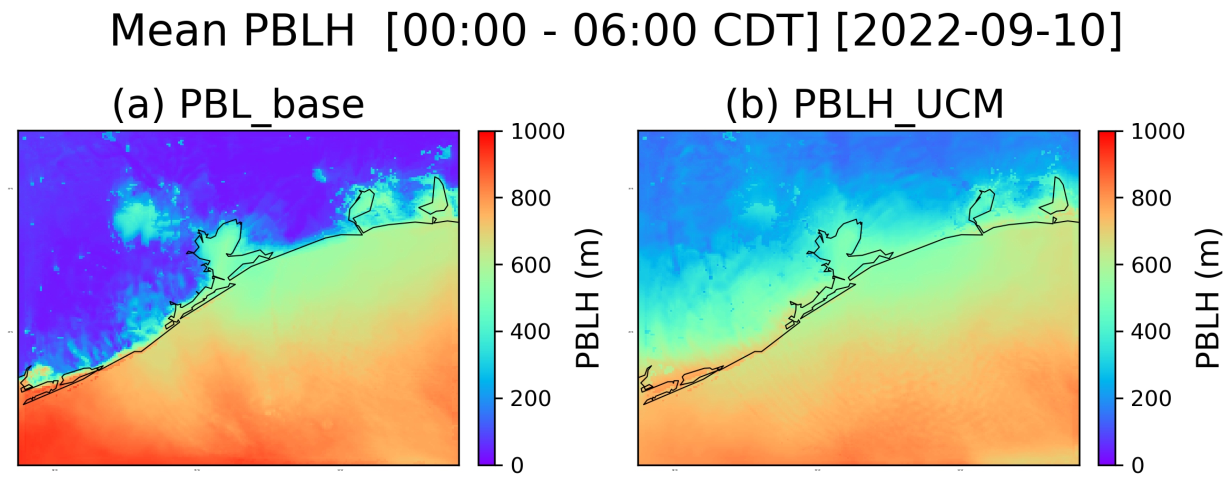
Physical Parameter Perturbations in MYNN PBL Scheme

Parameters/Constants	Description	Default Values	Perturbation Range	References
B1	Constant for Dissipation Rates	24	[12,36]	Nakanishi & Niino, (2009)
B2	Constant for Dissipation Rates	15	[7.5, 22.5]	Nakanishi & Niino, (2009)
α1	Constant for Turbulent length scale (L_T)	0.23	[0.2-0.3]	Yang et al. (2017)
Pr	Turbulent Prandtl Number	0.74	[0.7 – 2.0]	Pithan et al., (2015)
Z0	Surface roughness	0.0185	[0.01 – 0.03]	Yang et al. (2017)
C3	Closure Constant	0.33	[0.33 – 0.5]	Huang & Peng, (2017)
ALBD	Albedo	0.08	[0.06-0.09]	Liu et al. (2022)

PBL dependence on Cumulus physics



PBL dependence on urban canopy treatment



Additional Schemes Conducted as WRF Sensitivity

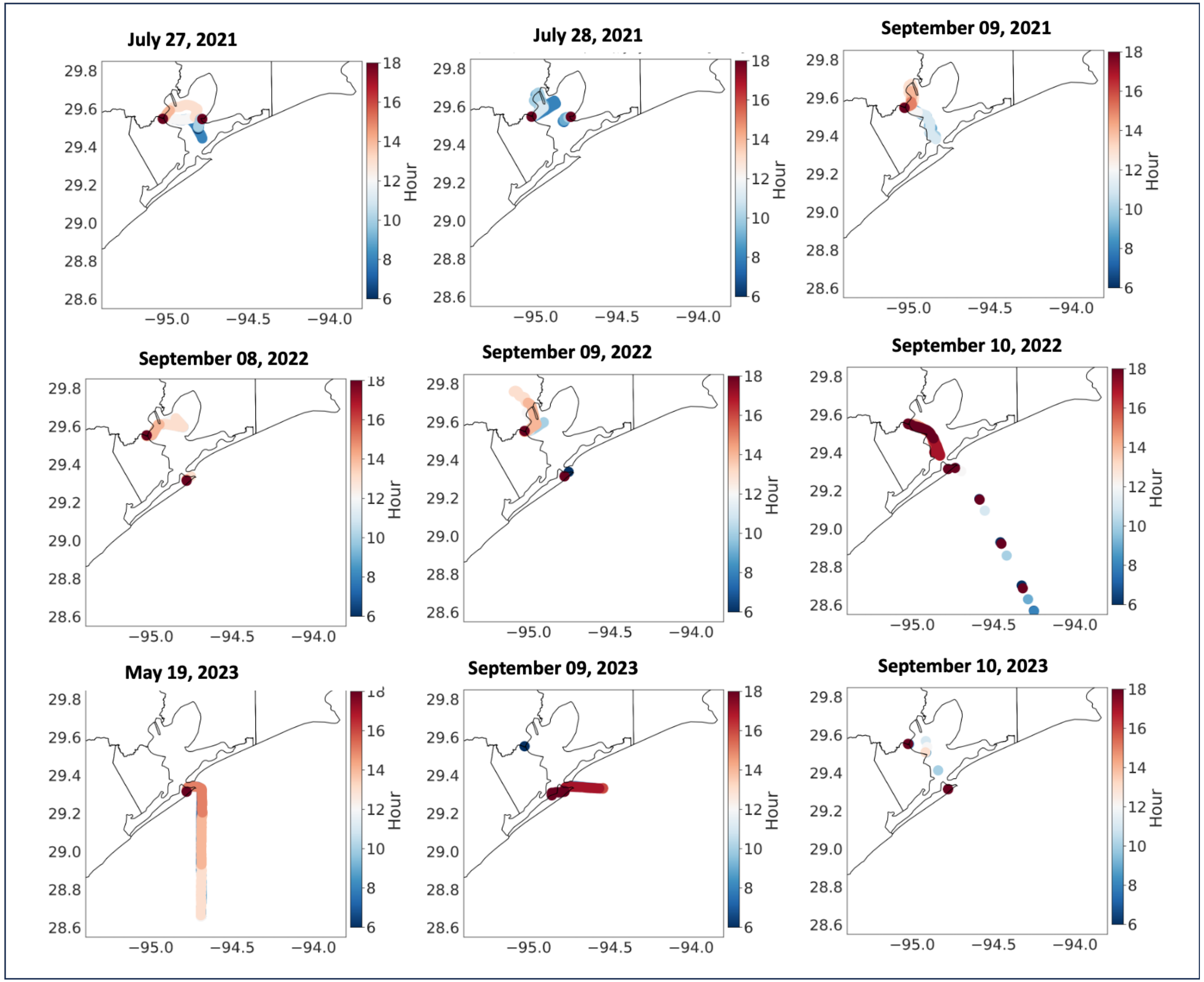
Schemes	Description	Base Model Setting	Customized Settings
MYNN	PBL scheme	2.5	3.0
UCM	Urban Canopy Model	off	on
Cumulus physics	Switched to different schemes	New Tiedtke	New Simplified Arakawa-Schubert (NSAS)
1-D ocean mixed layer model	Ocean physics	off	on

25 Perturbation Simulations, each conducted for 9 Case Days

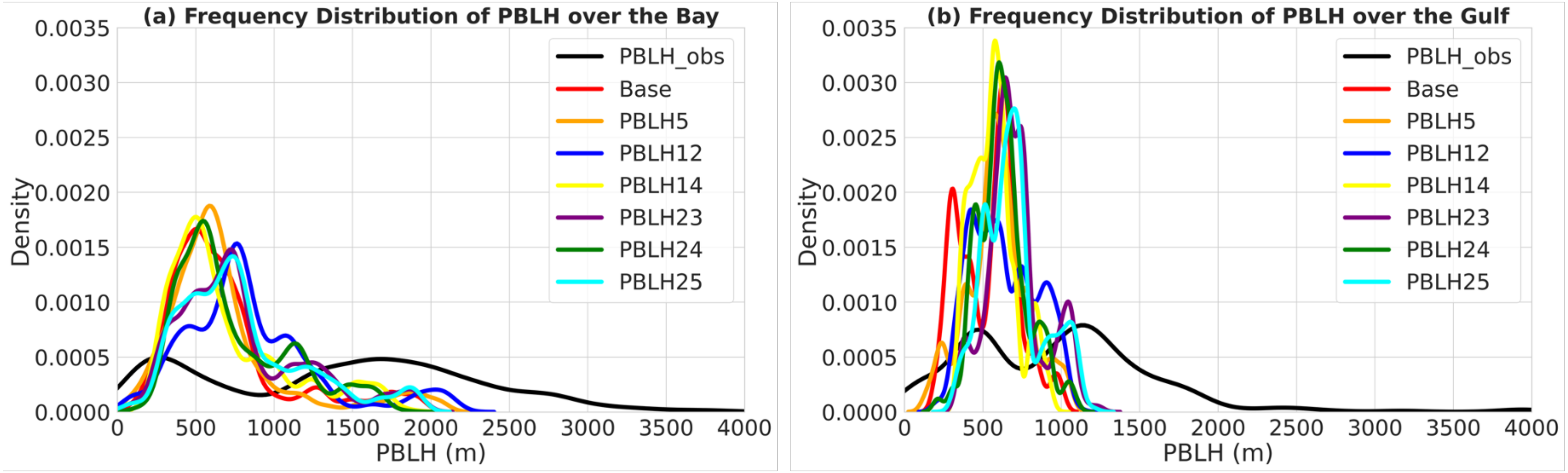
2021: Jul 27, Jul 28, Sep 9

2022: Sep 8, Sep 9, Sep 10

2023: May 19, Sep 9, Sep 10



Four Perturbation Simulations Outperformed the Base

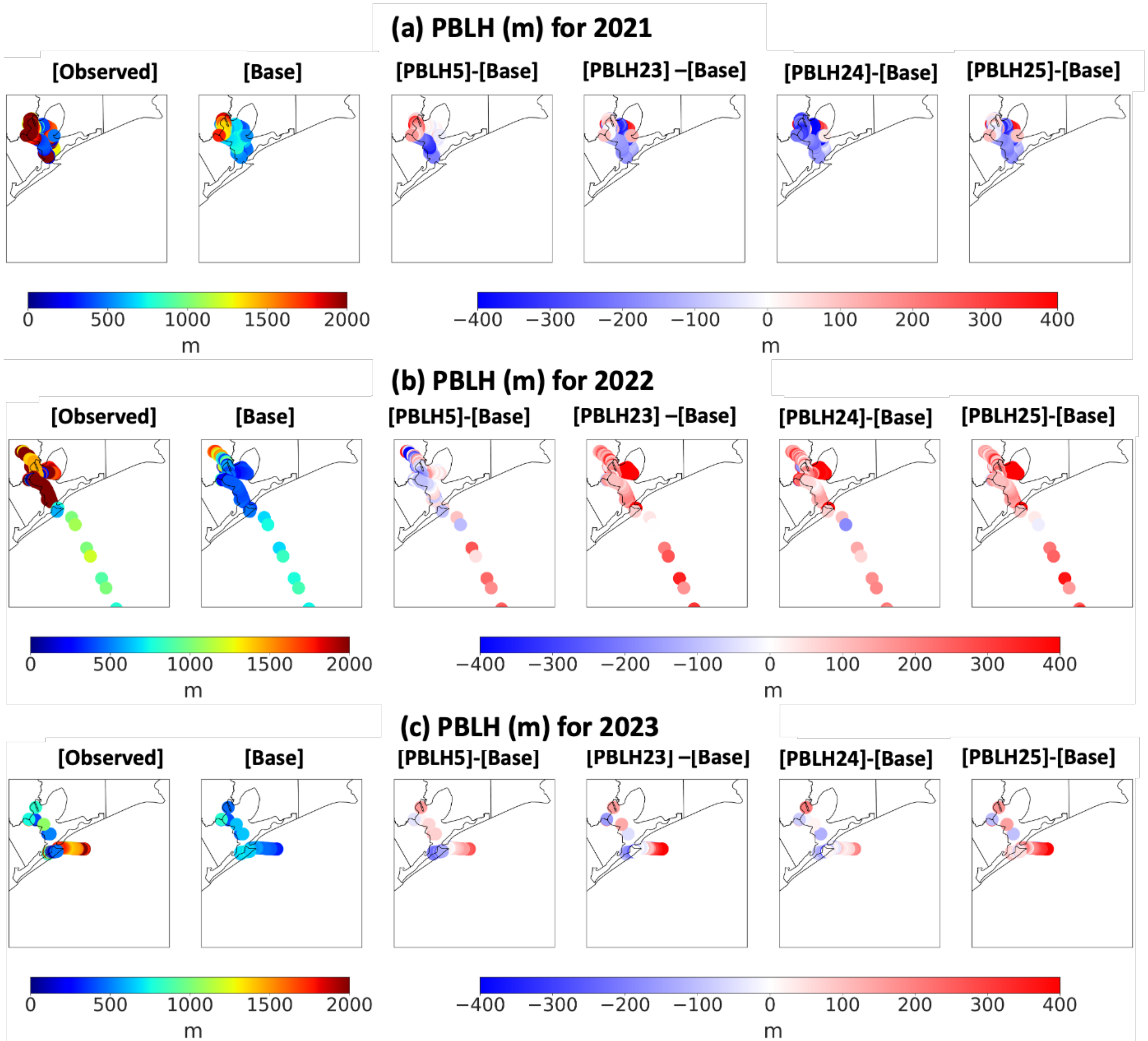


PBLH5: Closure constant C3 in MYNN2

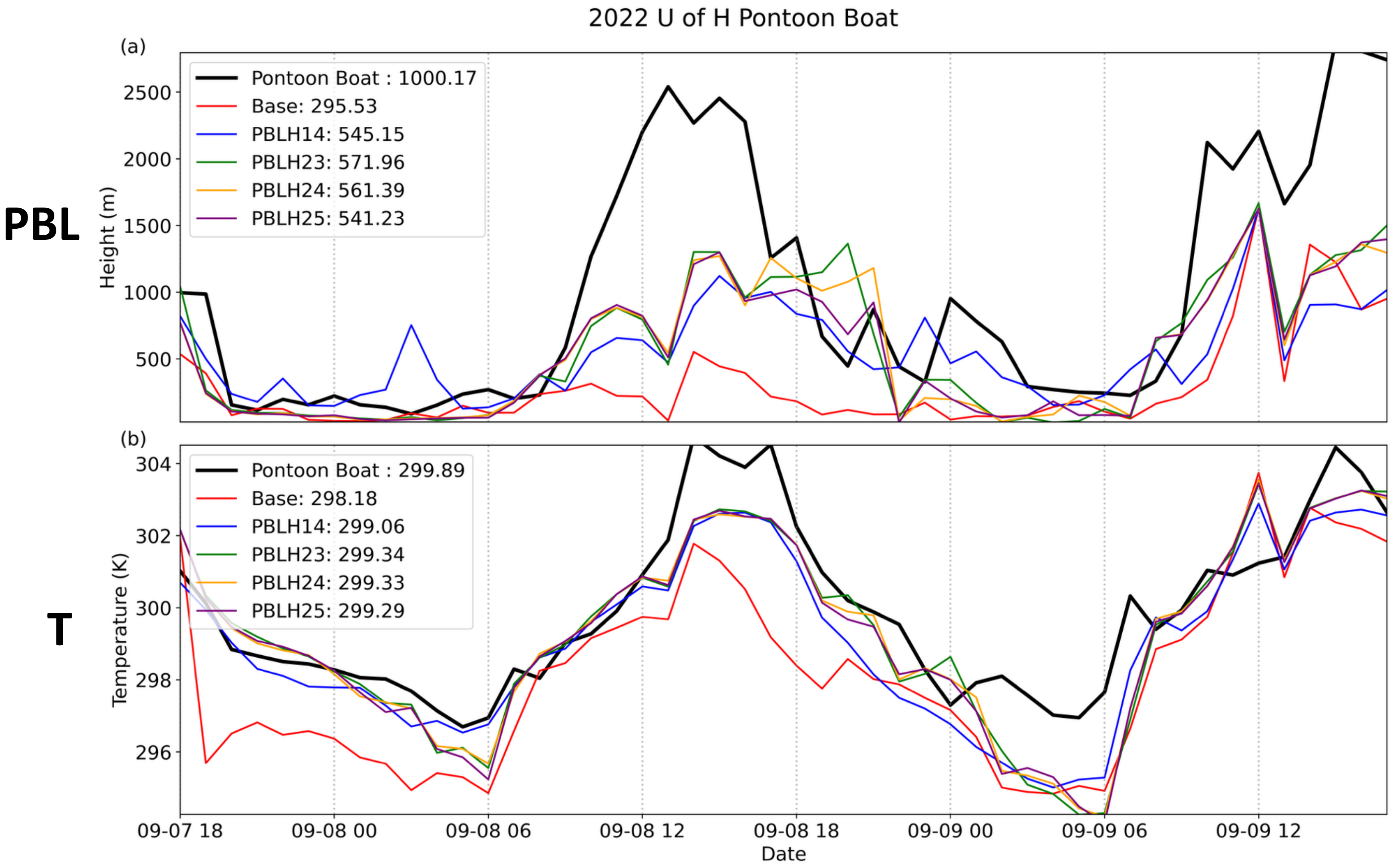
PBLH23: NSAS cumulus scheme + 1-D ocean model

PBLH24: NSAS + 1-D ocean model + Urban Canopy Model

PBLH25: NSAS + 1-D ocean model + Roughness Length



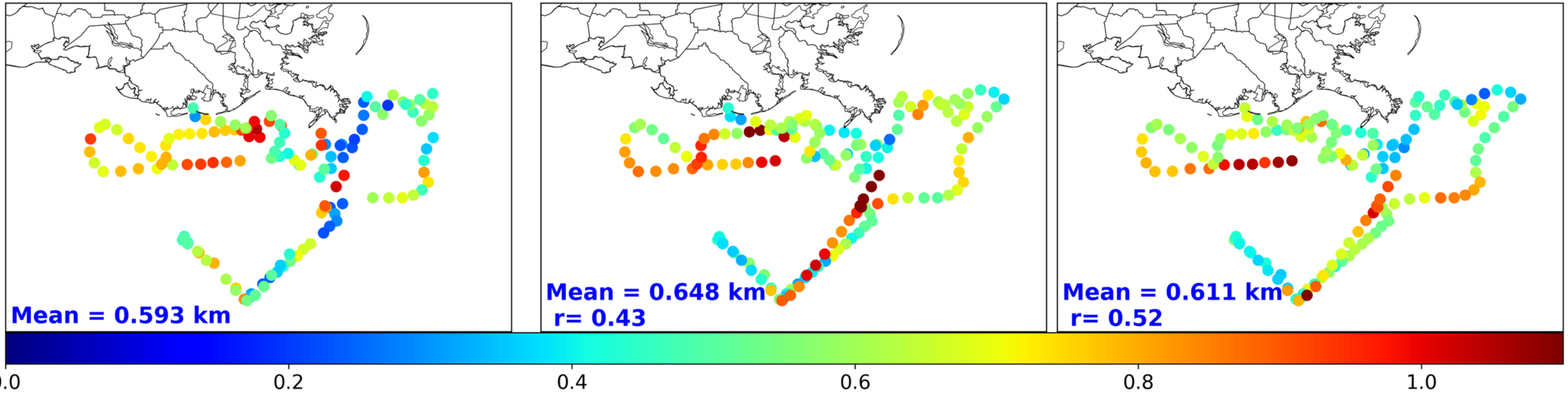
PBLH23 - 25 outperformed PBLH5 over Galveston Bay.

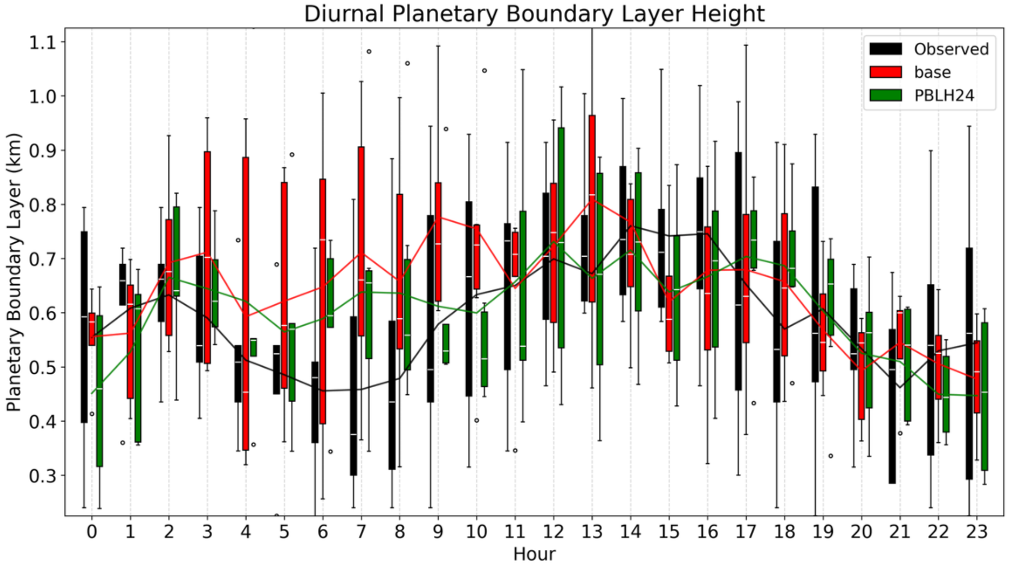


PBL
T
2022 U of H Pontoon Boat
(a)
Pontoon Boat : 1000.17
Base: 295.53
PBLH14: 545.15
PBLH23: 571.96
PBLH24: 561.39
PBLH25: 541.23
Height (m)
2500
2000
1500
1000
500
(b)
Pontoon Boat : 299.89
Base: 298.18
PBLH14: 299.06
PBLH23: 299.34
PBLH24: 299.33
PBLH25: 299.29
Temperature (K)
304
302
300
298
296
09-07 18
09-08 00
09-08 06
09-08 12
09-08 18
09-09 00
09-09 06
09-09 12
Date

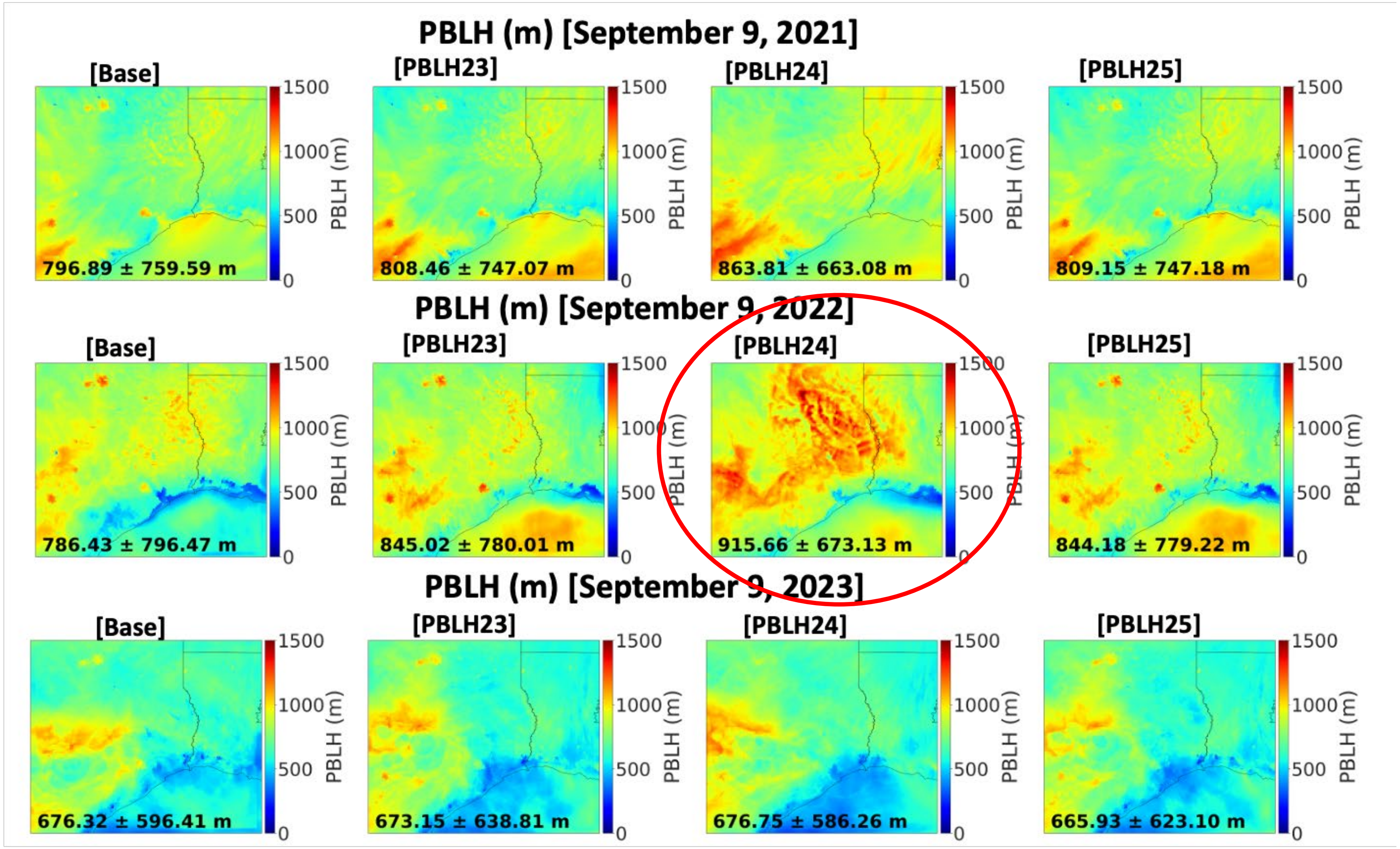
Validation by SCOAPE-19 PBLH Observations

Observation **Base** **PBLH24**



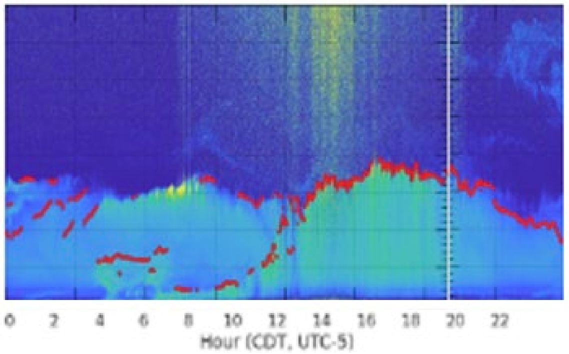


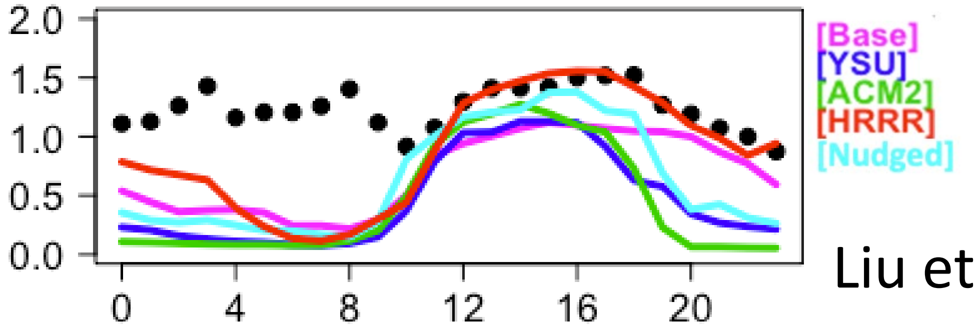
Effects on 4km-Resolution WRF



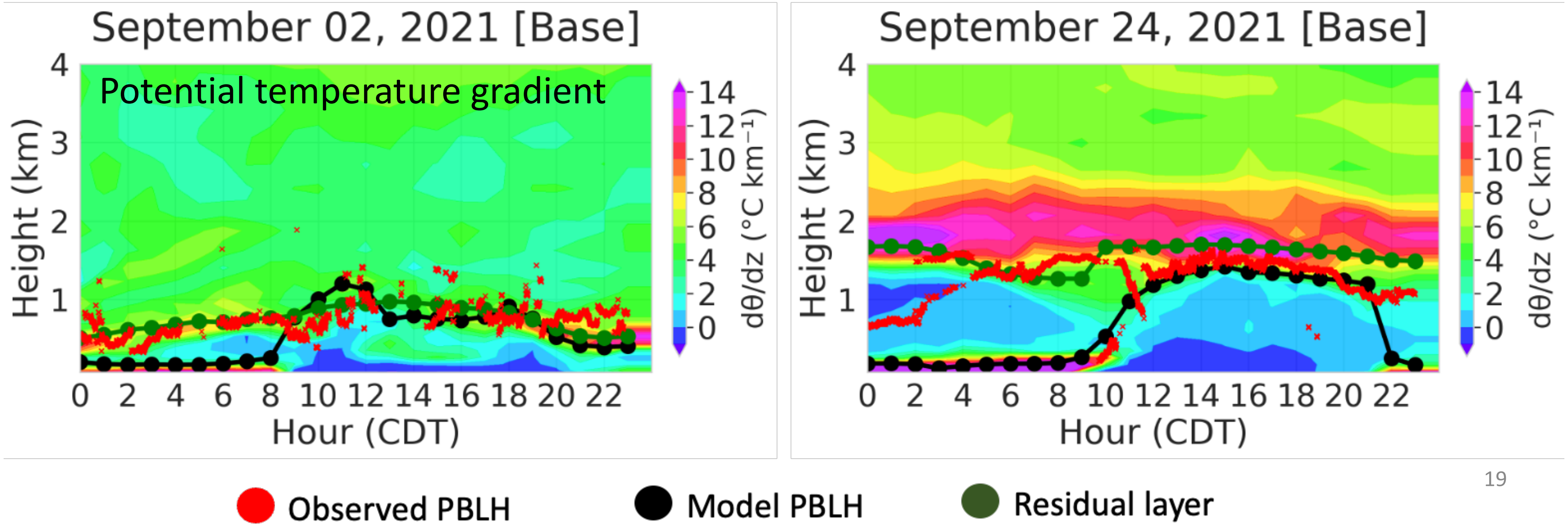
Lack of Residual Layer Representation in WRF

Ceilometer derived PBL at La Porte (Sep 8, 2021)





Liu et al., 2023



Residual Layer Diagnosis Methods

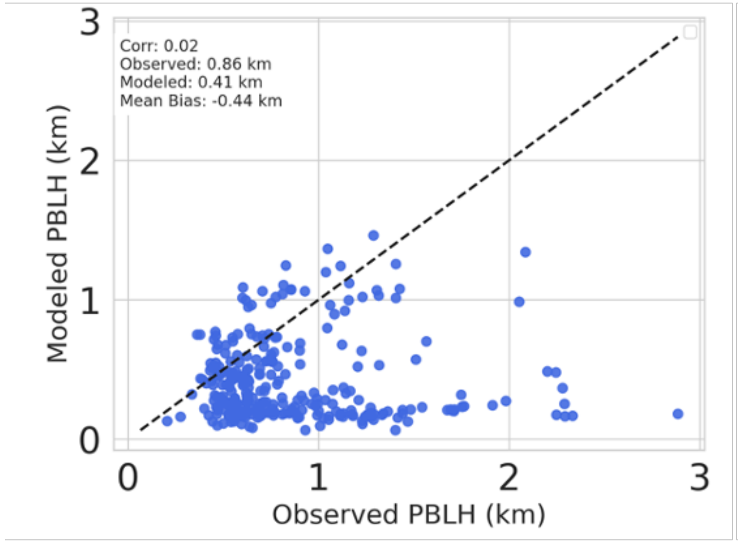
Empirical method

RL is calculated using the vertical gradient of potential temperature (∂θ/∂z), which identifies strong capping inversions

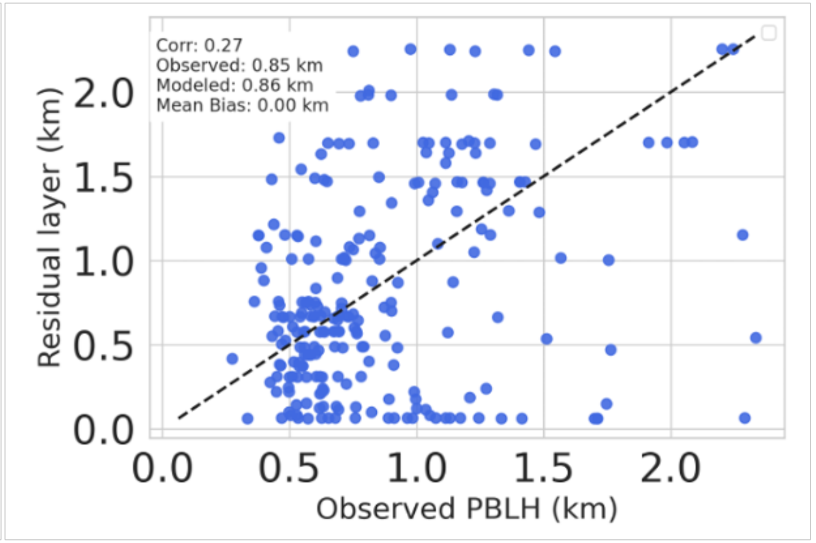
Semi-theoretical method

RL is calculated using dynamic and thermodynamic parameters, including **vertical profiles of wind speed**, vertical velocity, potential temperature, turbulent kinetic energy (TKE), and their gradients, to assess the balance between mechanical and buoyant turbulence

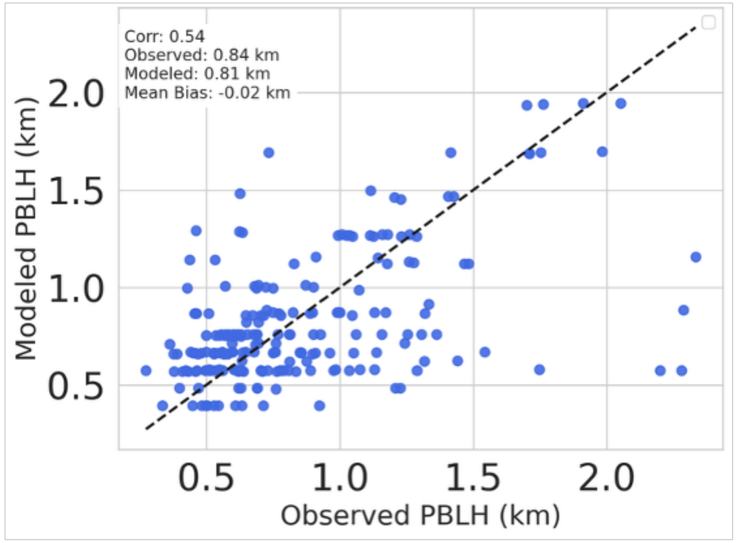
Base Model-Observe



Empirical method-Observe



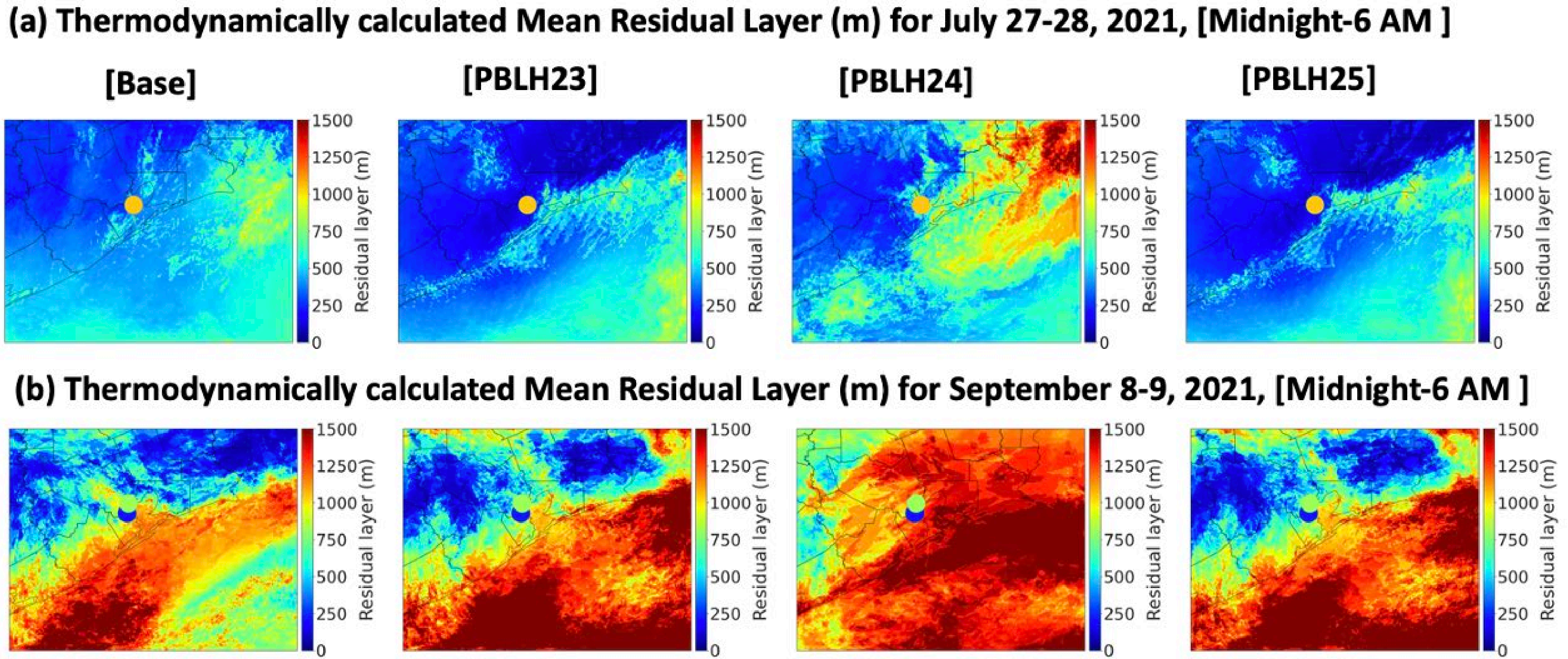
Theoretical method-Observe



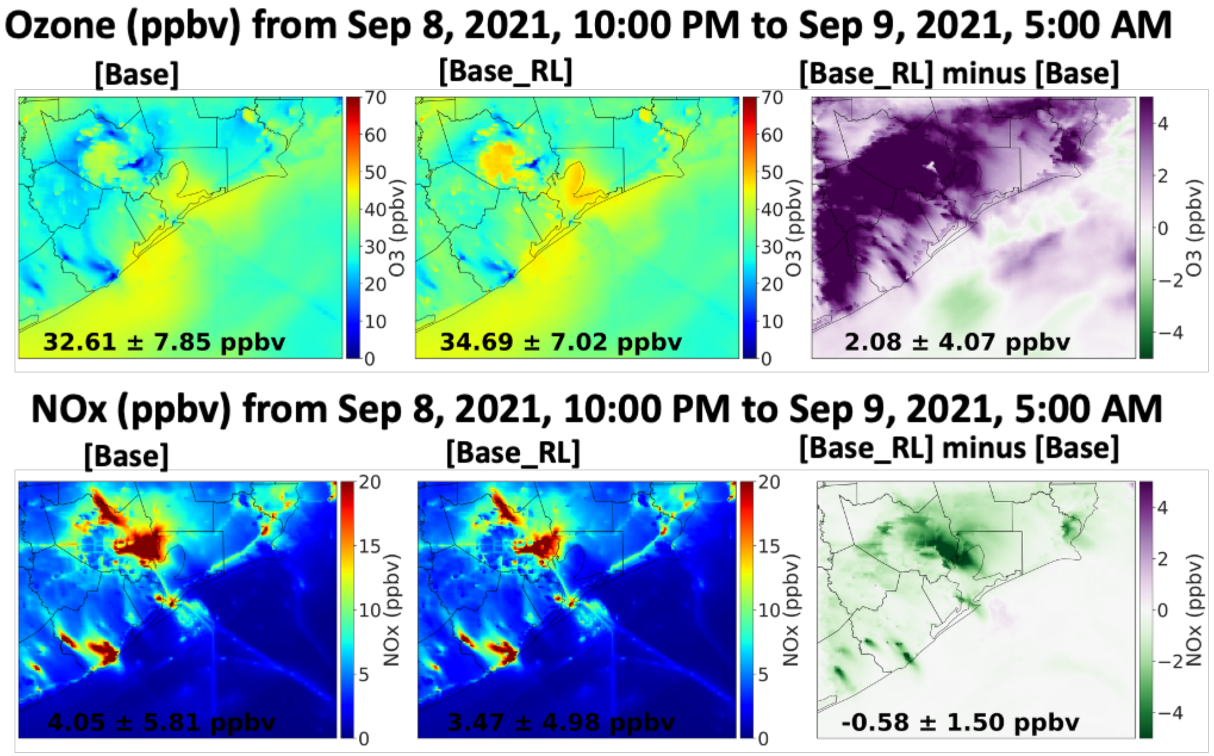
PBL Perturbations Changed RL Height

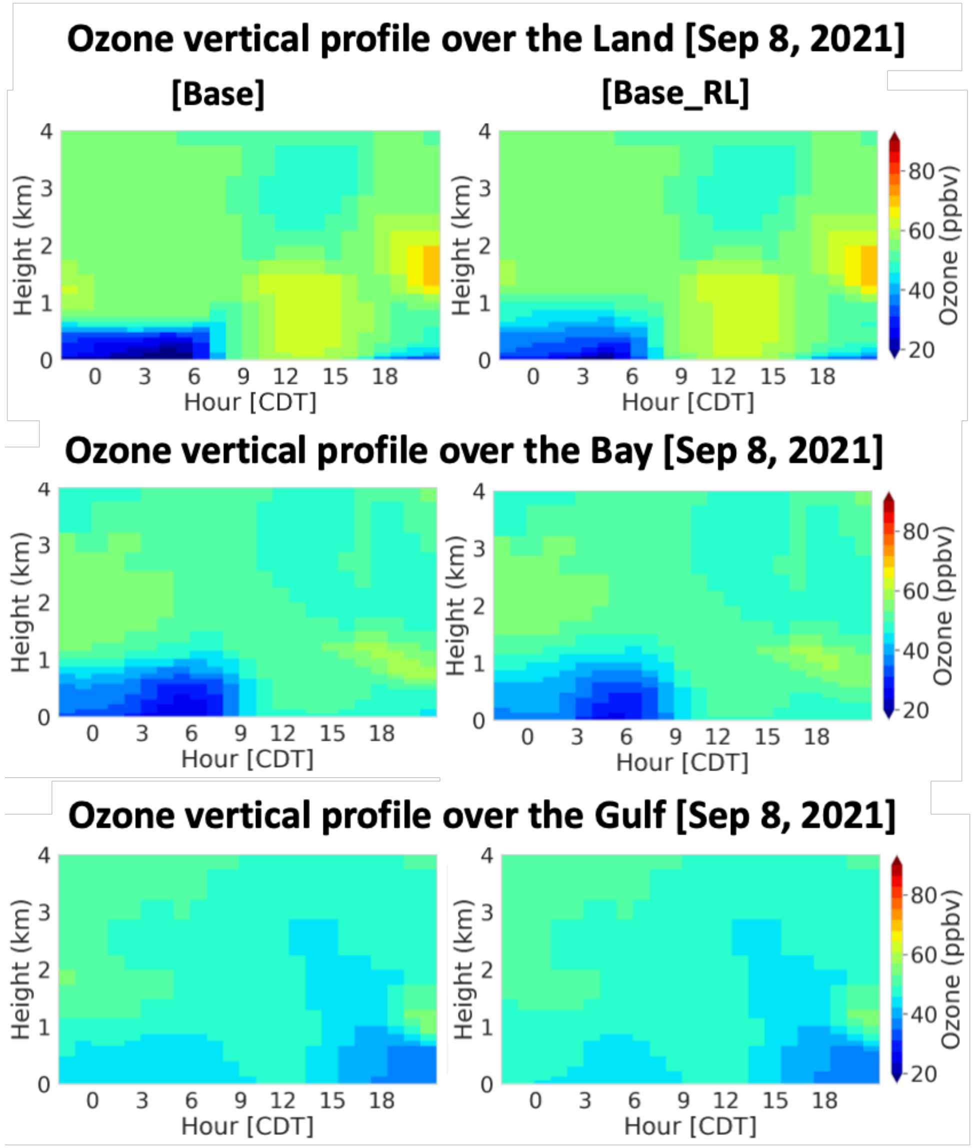
July 27-28, 2021

Sep 8-9, 2021



Residual Layer Effects

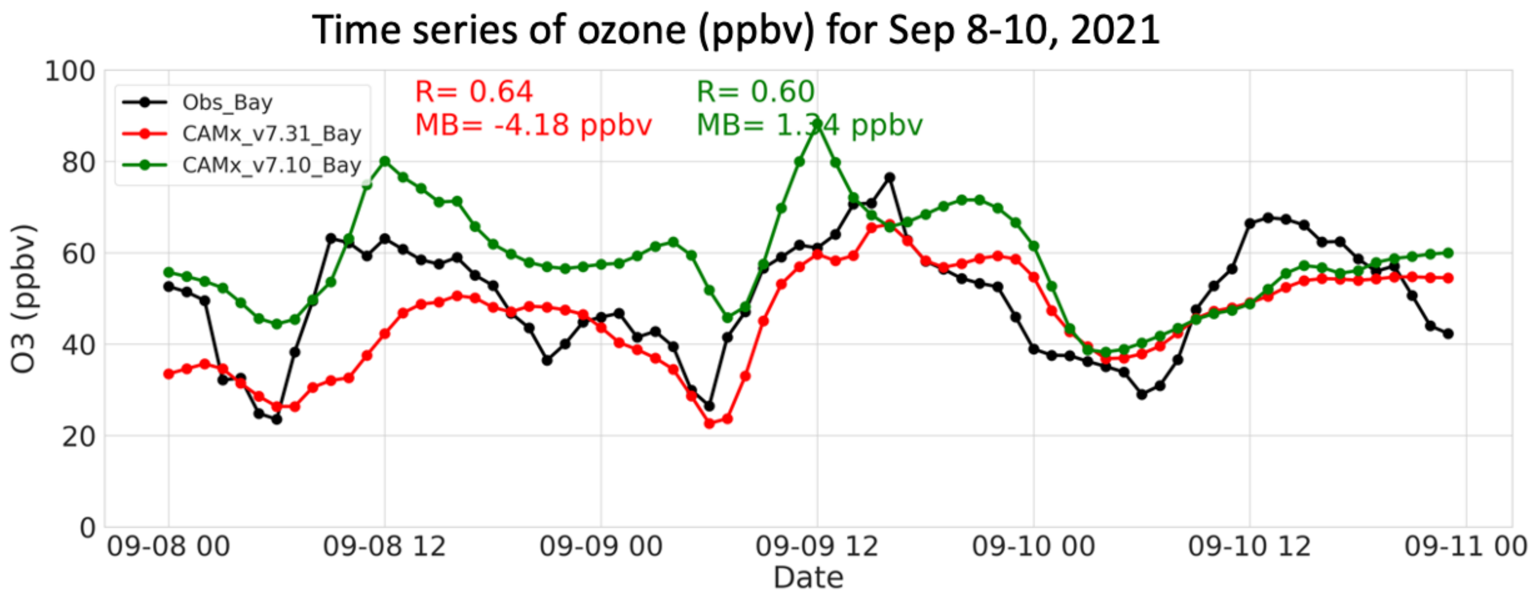




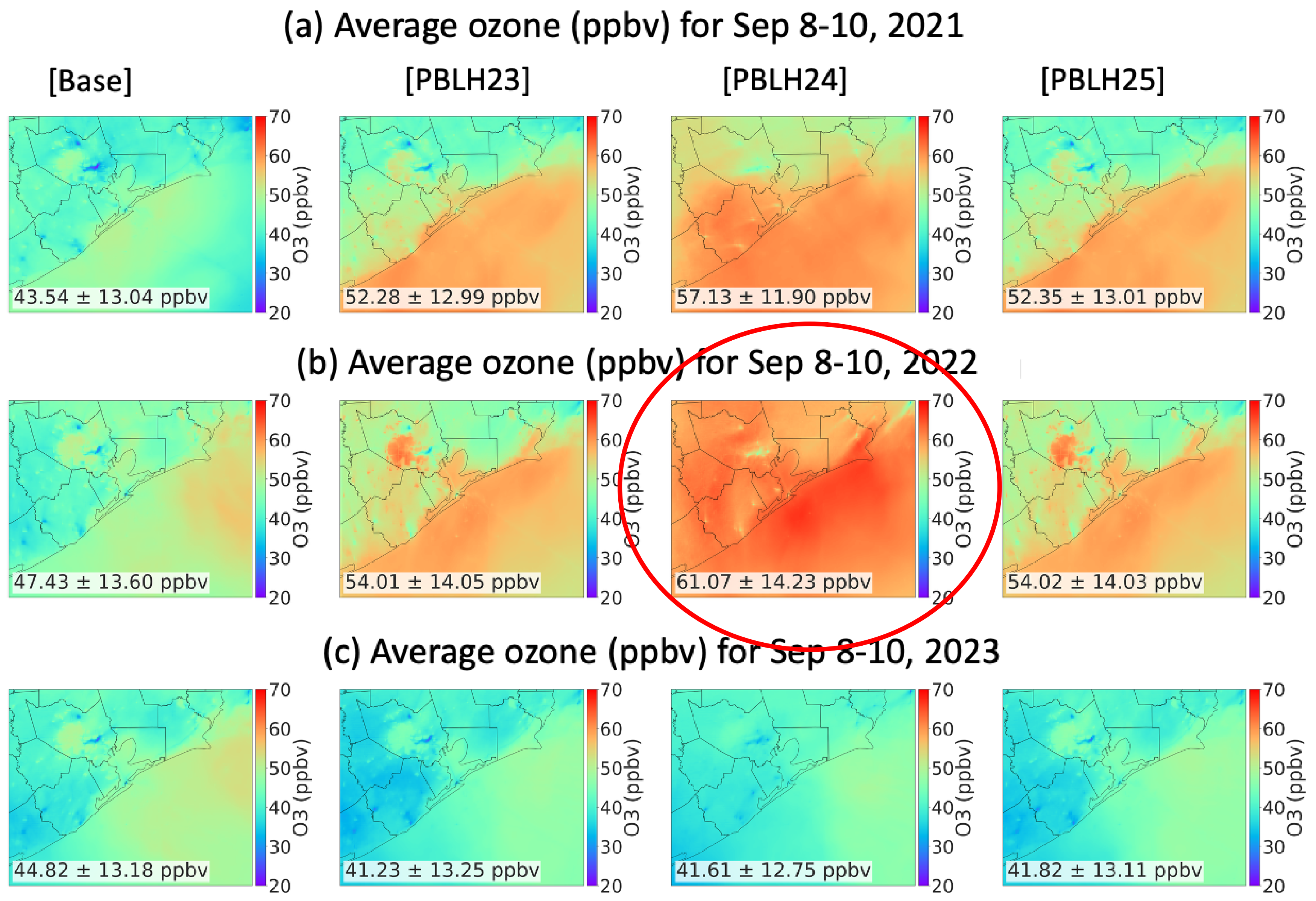
Effects of Improved PBL on Ozone Prediction in CAMx

CAMx Model Specifics

(1) v7.3.1, driven by WRF v4.6.0 base and perturbation runs
(2) Chemical boundary conditions from GEOS-Chem;
(3) Anthropogenic emissions: SIP 2019 Emissions in Texas, regridded from 4 km to 1.33 km in d03 domain



CAMx v7.3.1 base (this work) improves upon CAMx v7.10 (Li et al., 2023)



2021:
O_3 increases by 8 – 14 ppbv

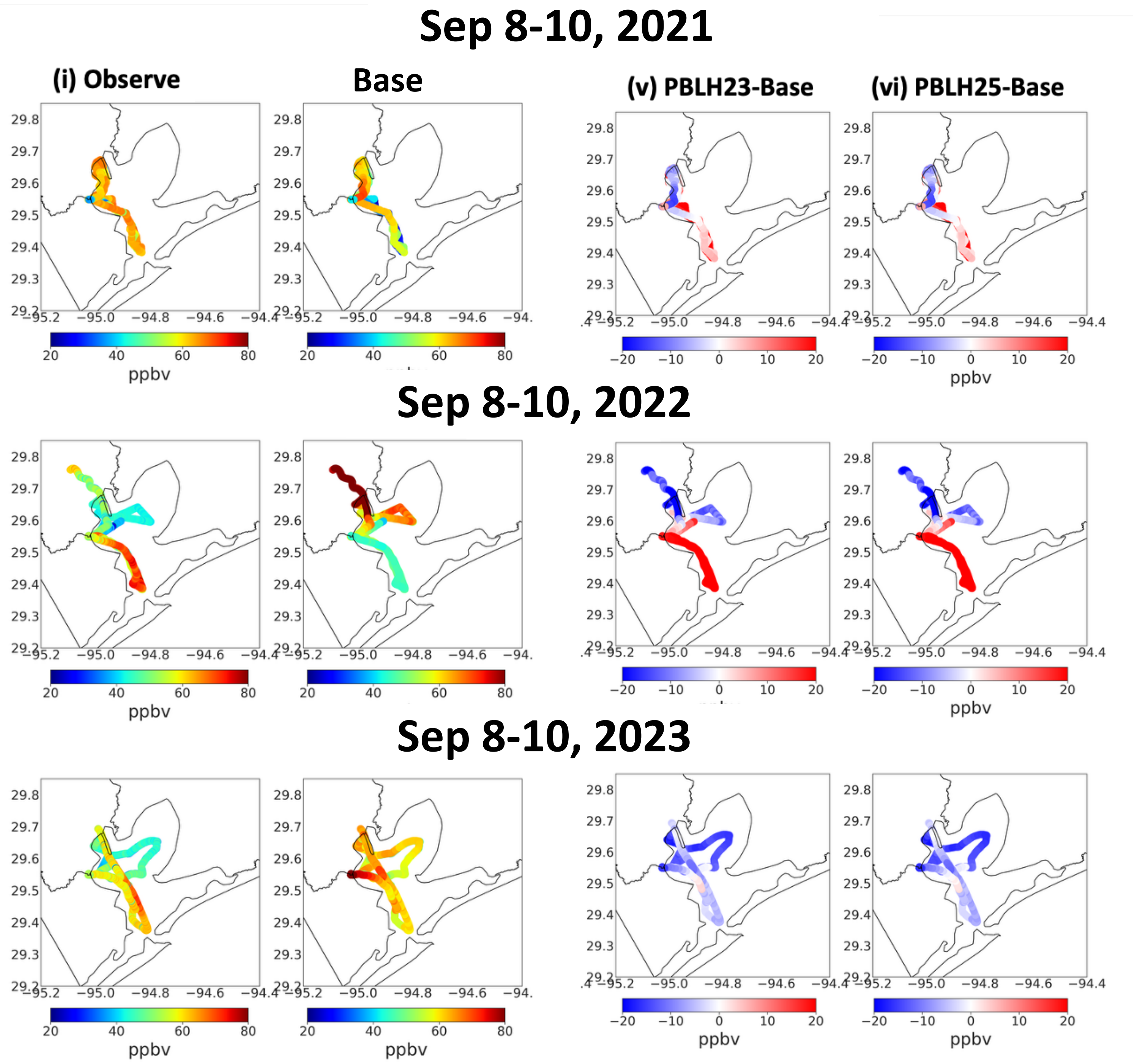
2022:
O_3 increases by 7 – 14 ppbv

2023:
O_3 decreases by 2 ppbv

Galveston Bay

Perturbation runs match better with boat observations.

Mode biases reduced by +/-15 ppbv with higher correlations.

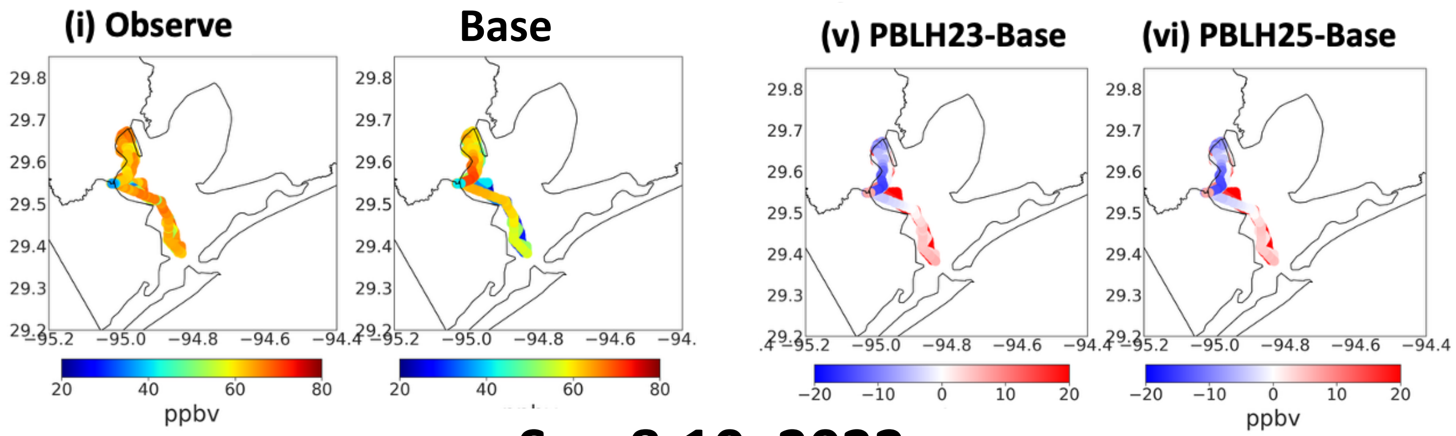


Galveston Bay

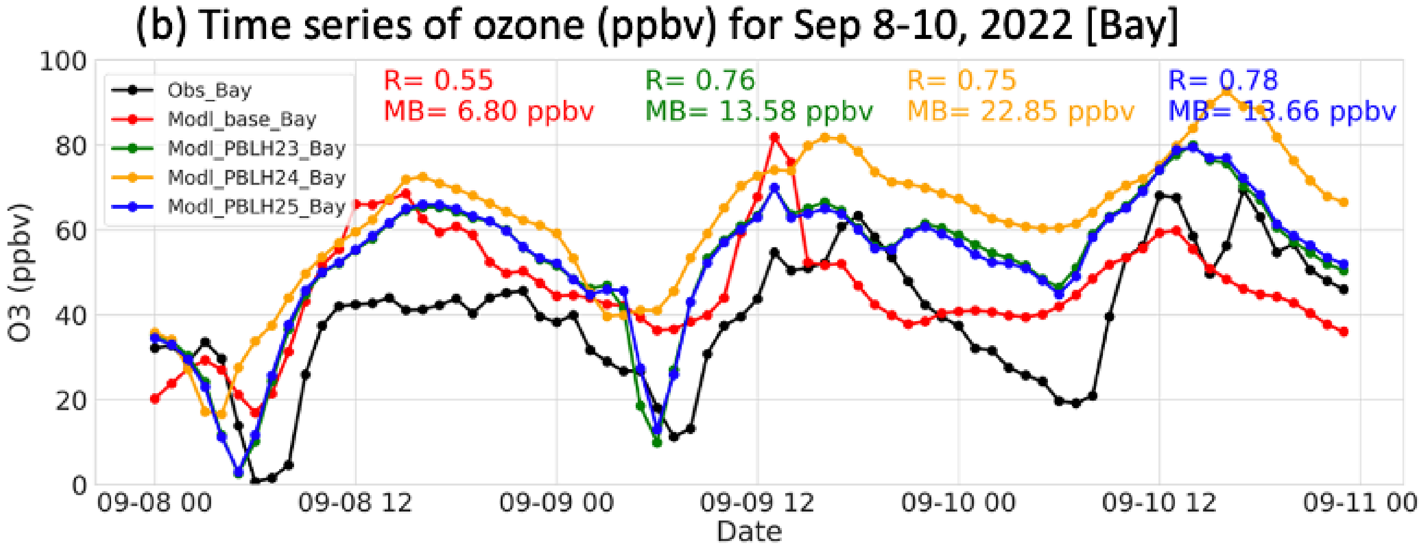
Perturbation runs match better with boat observations.

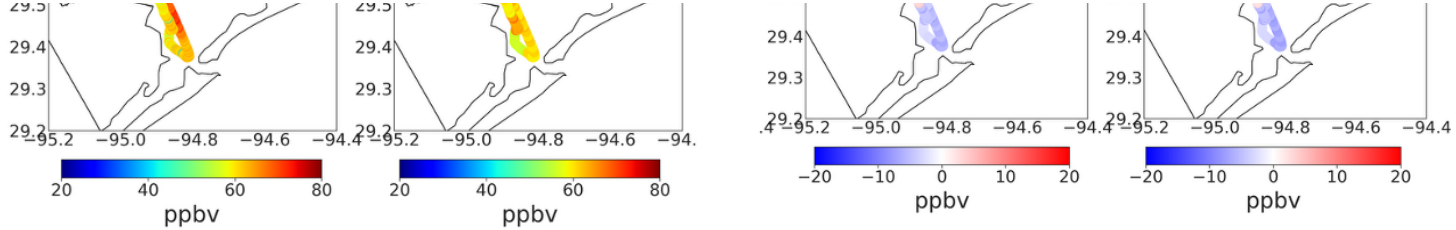
Mode biases reduced by +/-15 ppbv with higher correlations.

Sep 8-10, 2021



Sep 8-10, 2022

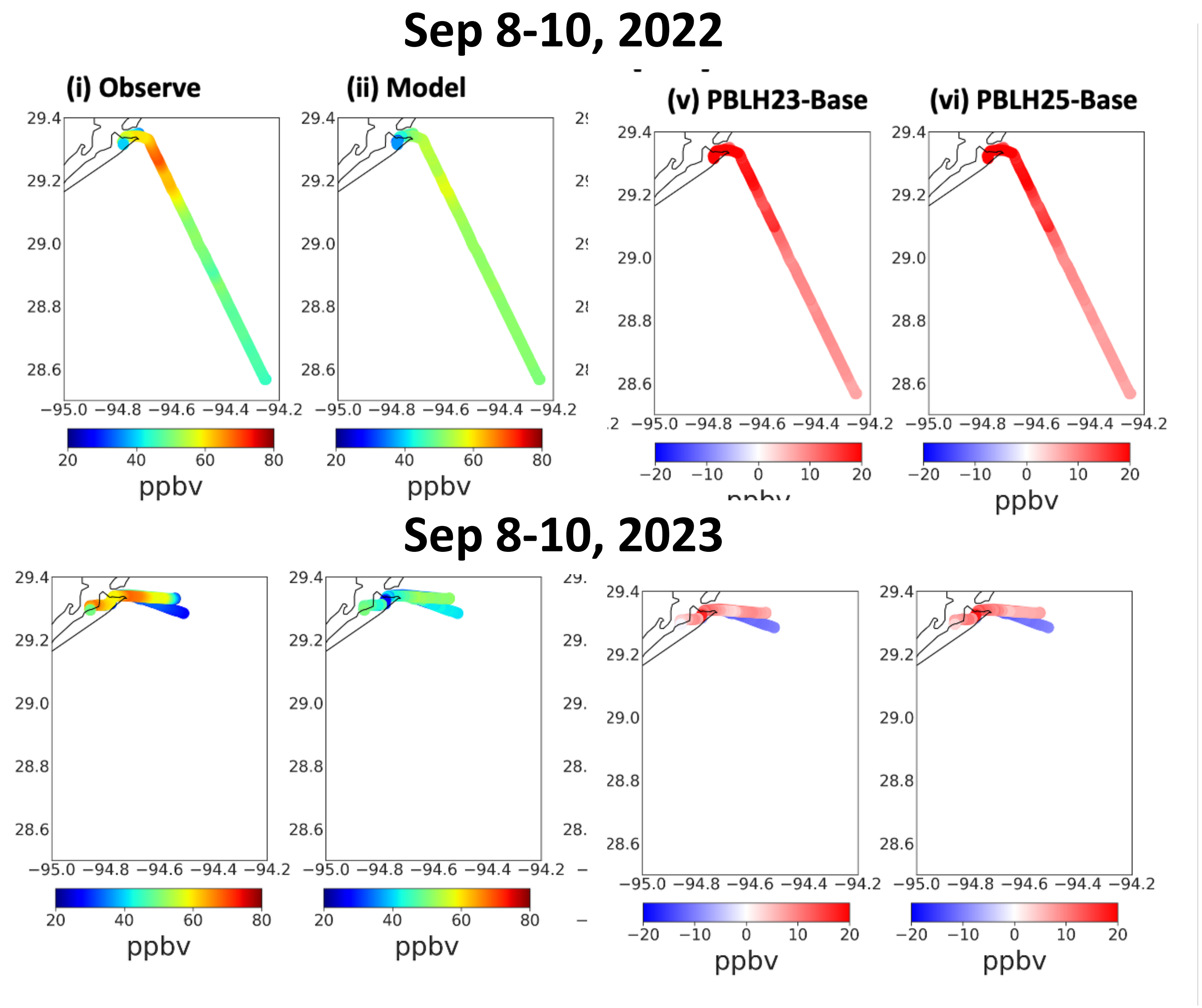




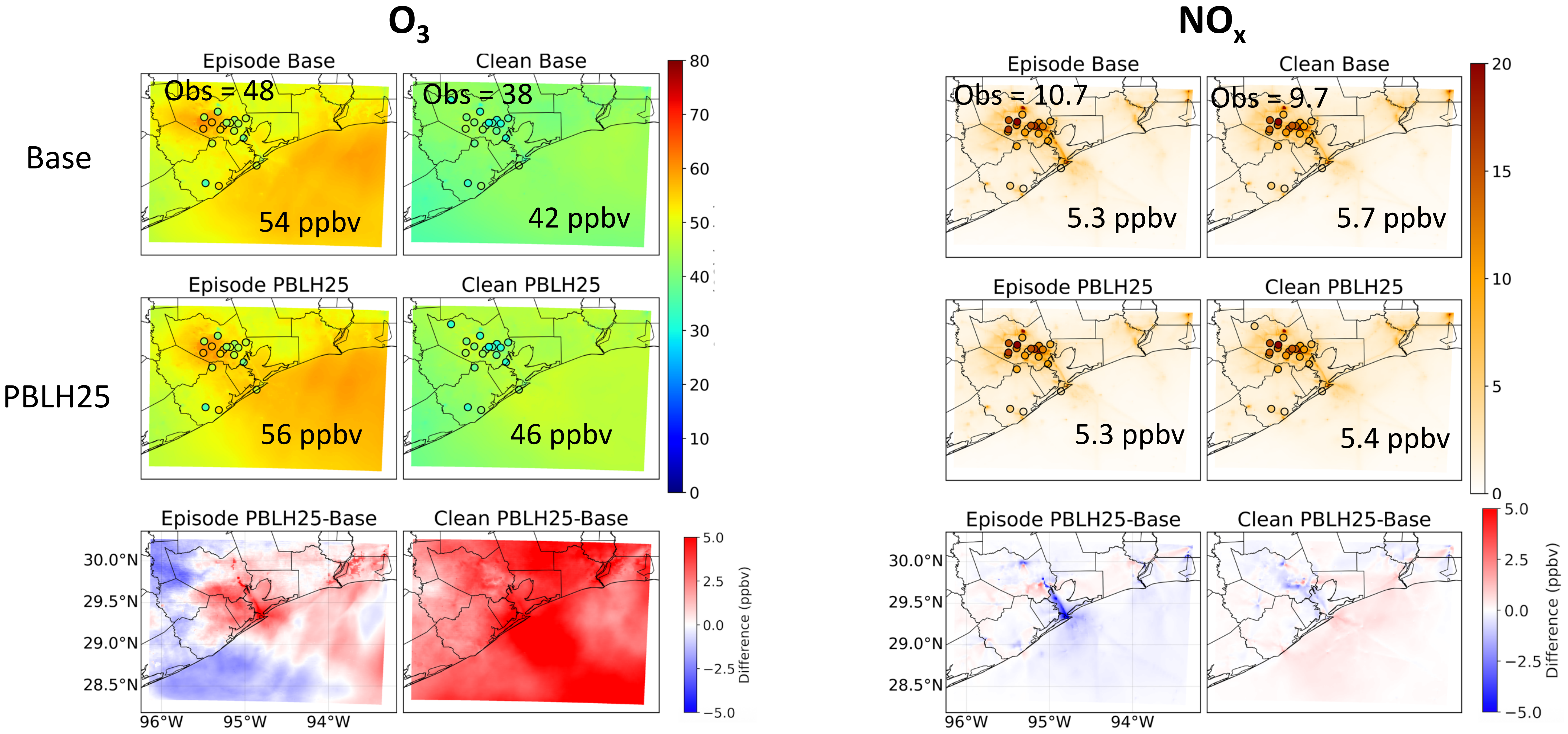
Gulf of America

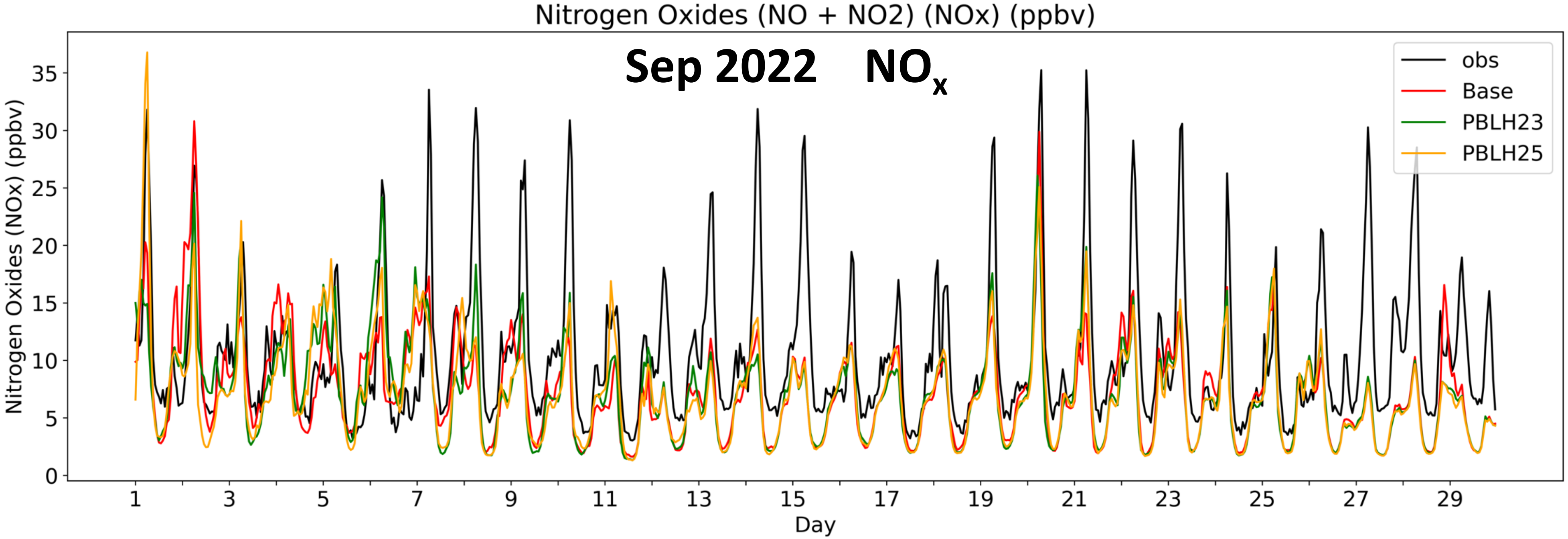
Perturbation runs match better with boat observations.

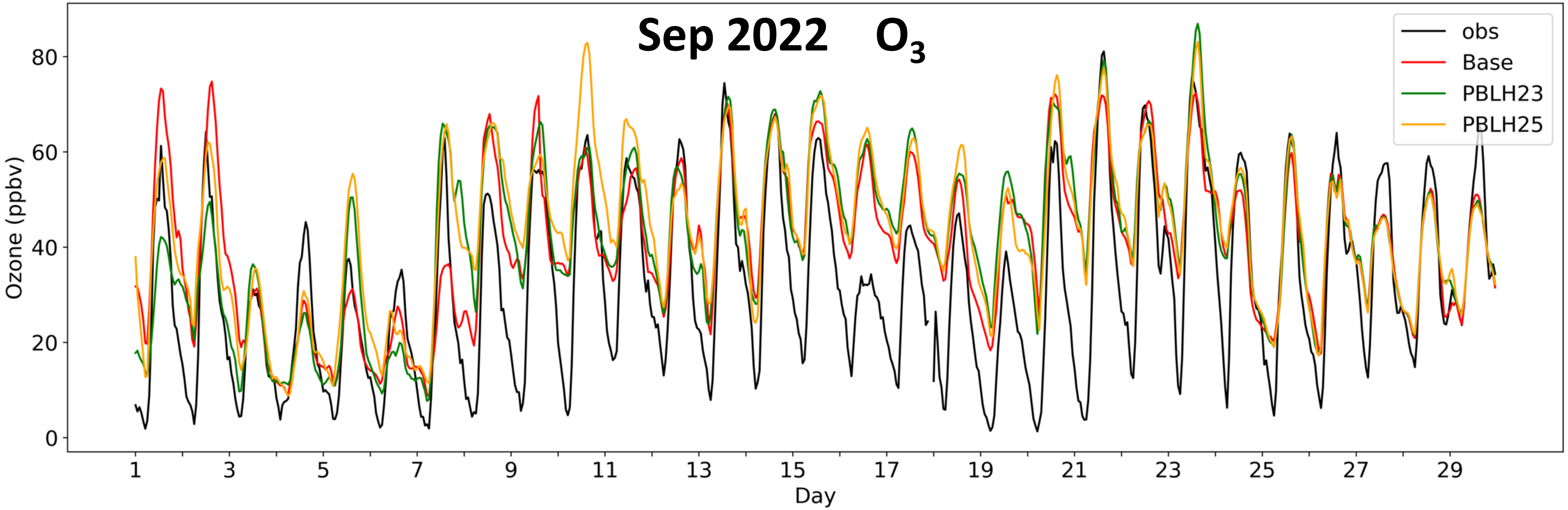
Mode biases reduced by +/- 5 ppbv with higher correlations.



Compared to Surface Monitors on land: Sep 2022




Nitrogen Oxides (NO + NO2) (NOx) (ppbv)
Sep 2022 NOx
obs
Base
PBLH23
PBLH25
Nitrogen Oxides (NOx) (ppbv)
0
5
10
15
20
25
30
35
1
3
5
7
9
11
13
15
17
19
21
23
25
27
29
Day


Sep 2022 O3
obs
Base
PBLH23
PBLH25
Ozone (ppbv)
0
20
40
60
80
1
3
5
7
9
11
13
15
17
19
21
23
25
27
29
Day

Regional vs. Local Contributions to Ozone: Base

Sep 8-10, 2021 **Sep 8-10, 2022** **Sep 8-10, 2023**

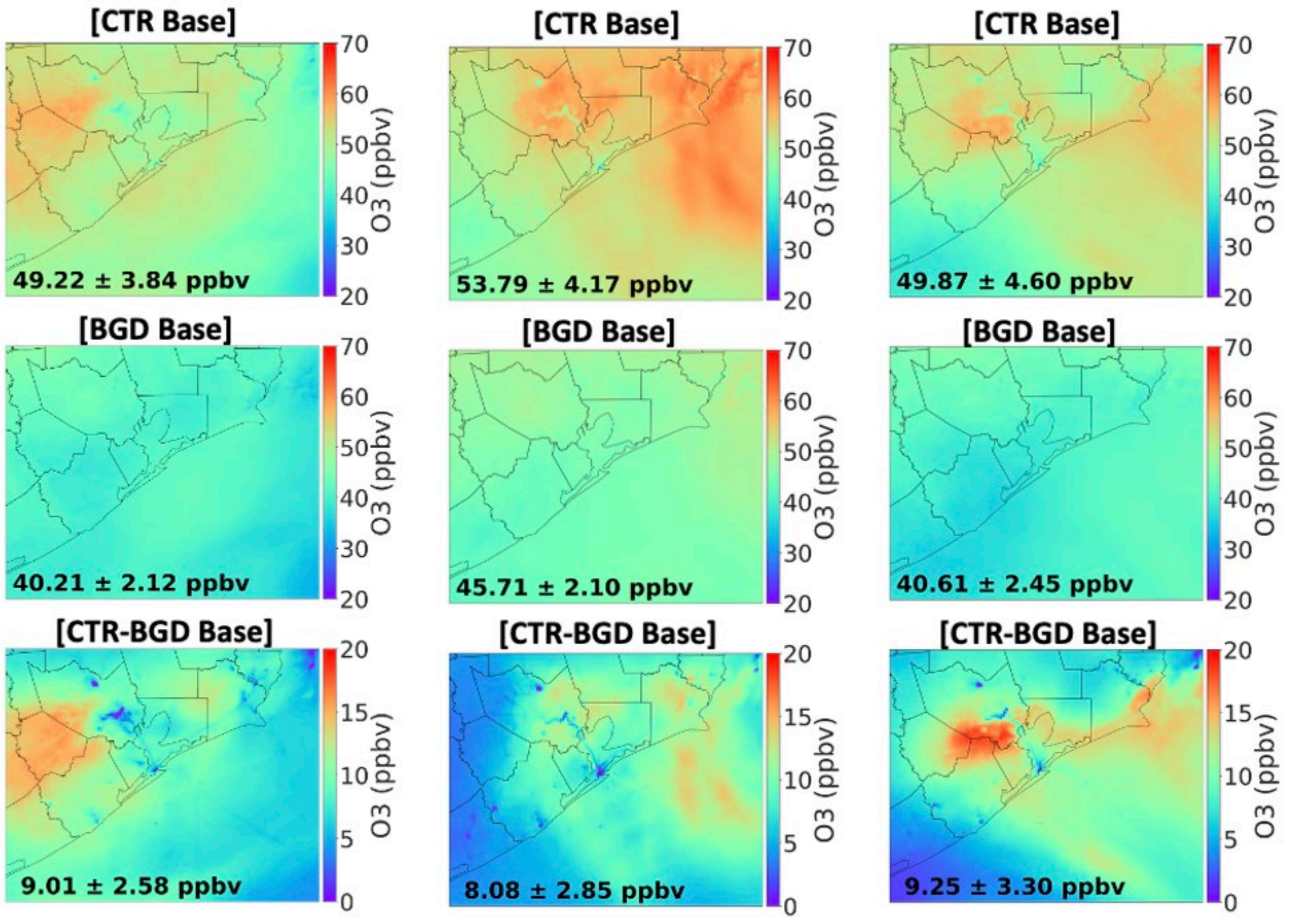
Total Ozone

50-54 ppbv

Regional BG Ozone
41 - 46 ppbv

Locally-produced Ozone

8-9 ppbv



Regional vs. Local Contributions to Ozone: PBLH25

Sep 8-10, 2021 | Sep 8-10, 2022 | Sep 8-10, 2023

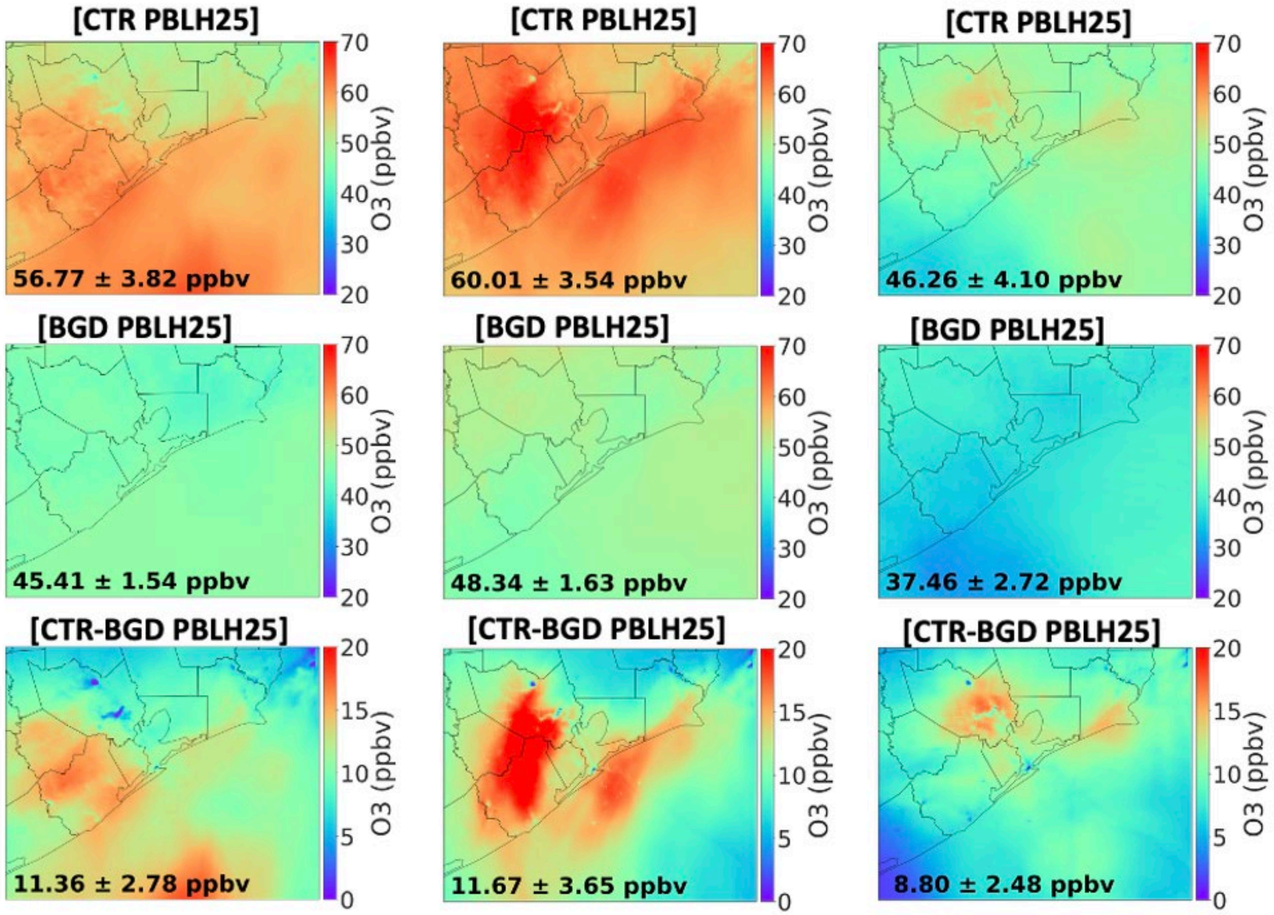
Total Ozone

46-60 ppbv

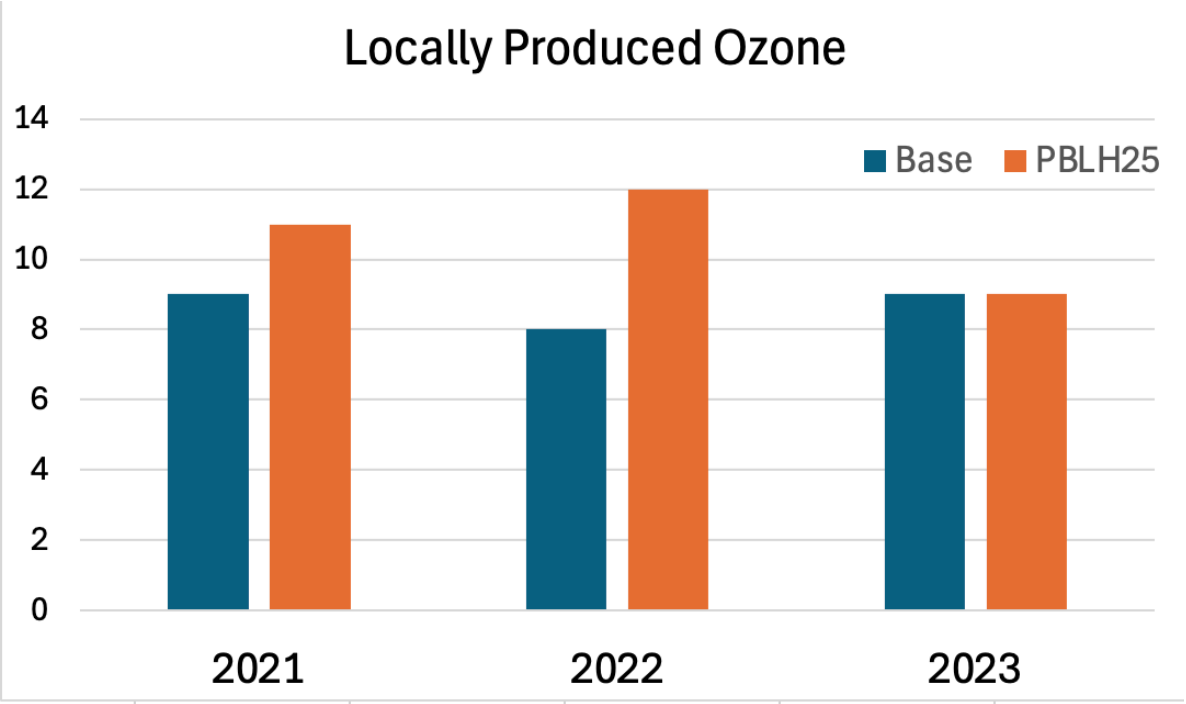
Regional BG Ozone
37 - 48 ppbv

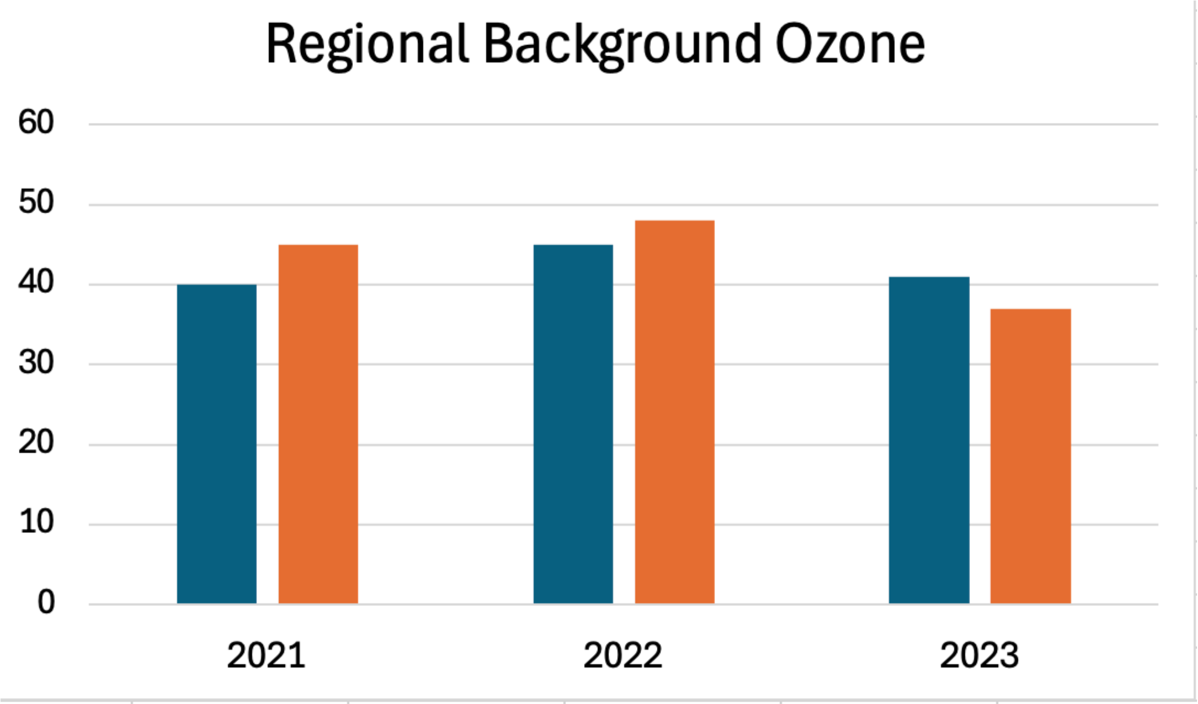
Locally-produced Ozone

9 – 12 ppbv

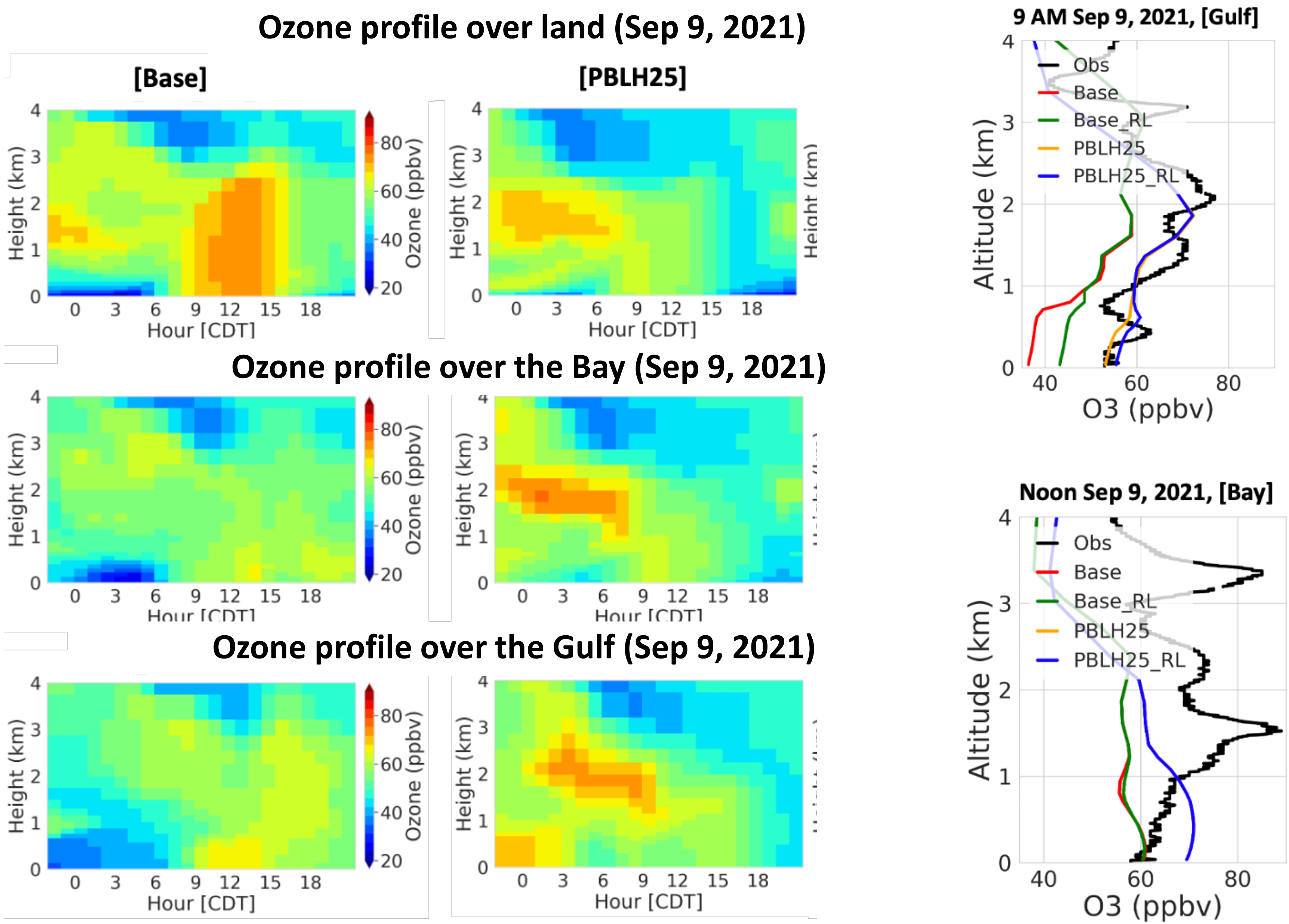


Regional vs. Local Contributions to Ozone





Effects on Ozone Vertical Profiles



Summary

- Marine PBL is higher in Galveston Bay than in the Gulf. WRF v4.6.0 base model underestimates marine PBL, especially over Galveston Bay in the afternoon

- Three new settings in combination (PBLH25) were found to robustly improve marine PBL prediction (by 400 – 500 m): higher surface roughness, 1-D ocean mixed layer model, and NSAS cumulus scheme

- Implemented the diagnosis of RL in WRF. The improved PBL simulations resulted in higher RL in the model.

- Improved PBL resulted in better ozone prediction at offshore locations, reducing model biases by up to 15– 20 ppbv along ship tracks and increasing monthly-mean ozone by 5 ppbv.

- Ozone prediction at surface monitors does not change significantly, but locally-produced ozone became 30-40% higher on high-ozone days with the improved PBL due to enhanced vertical transport of ozone

Suggestions on Future Work

- PBL modeling improvement
- Effects of PBL improvements on ‘top-down’ emissions and vertical transport of pollutants
- Differences between Galveston Bay and the Gulf of America in terms of physical and chemical characteristics and the model representation of such differences
- Residual layer product is a diagnostic tool and does not affect vertical mixing between surface layer, residual layer, and the free troposphere. This requires more work on the CAMx side.
- Urban canopy model gives mixed results and need further investigation.

Acknowledgement

- TRACER-AQ 2021 – 2023 field team
- Jeremiah Johnson (Ramboll Americas) for help with marine emissions
- AQRP
- TCEQ

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