A comprehensive evaluation of the Eta-CMAQ forecast model performance for O_3, its related precursors, and meteorological parameters during the 2004 ICARTT study

Shaocai Yu[$,] Rohit Mathur[+], Kenneth Schere[+], Daiwen Kang[$],
Brian Eder[+], Jonathan Pleim[+], Tanya Otte[+]

Atmospheric Sciences Modeling Division
NERL, U.S. EPA, RTP, NC 27711.

[$] On assignment from Science and Technology Corporation
[+] On assignment from Air Resources Laboratory, NOAA

Introduction

O_3 forecast

- **Necessary**
  - **O_3: a secondary pollutant,**
    - **Adversely affects human health**
    - **produced by pollution from natural and human activities**
  - **Warn the public:**
    - **unhealthy air**
    - **voluntarily reduce emission-producing activities**

- **Forecasting methods (EPA, 1999):**
  - **Persistence, climatology, regression equation etc.**
  - **3-D air quality models:**
    - **Spatial and temporal distributions of O_3 and its precursors**
    - **Understand chemical-physical processes controlling O_3 formation**

Objective

❶ **Evaluate Eta-CMAQ model performance on the spatial and temporal variations of O_3 with AIRNOW Obs over the eastern US**

❷ **Comprehensively examine the ability of Eta-CMAQ in representing chemical-physical processes for O_3 formation with 2004 ICARTT data**

International Consortium for Atmospheric Research on Transport and Transformation (ICARTT)

Model Description

- **Eta-CMAQ model suite: (R. Mathur et al. Talk (9/26))**
  - **Eta** forecast model provides meteorological fields for **CMAQ** (Otte et al., 2005)
  - CB-4 (version 4.2): photochemical processes

- **ICARTT Period: July 1 to August 15, 2004**

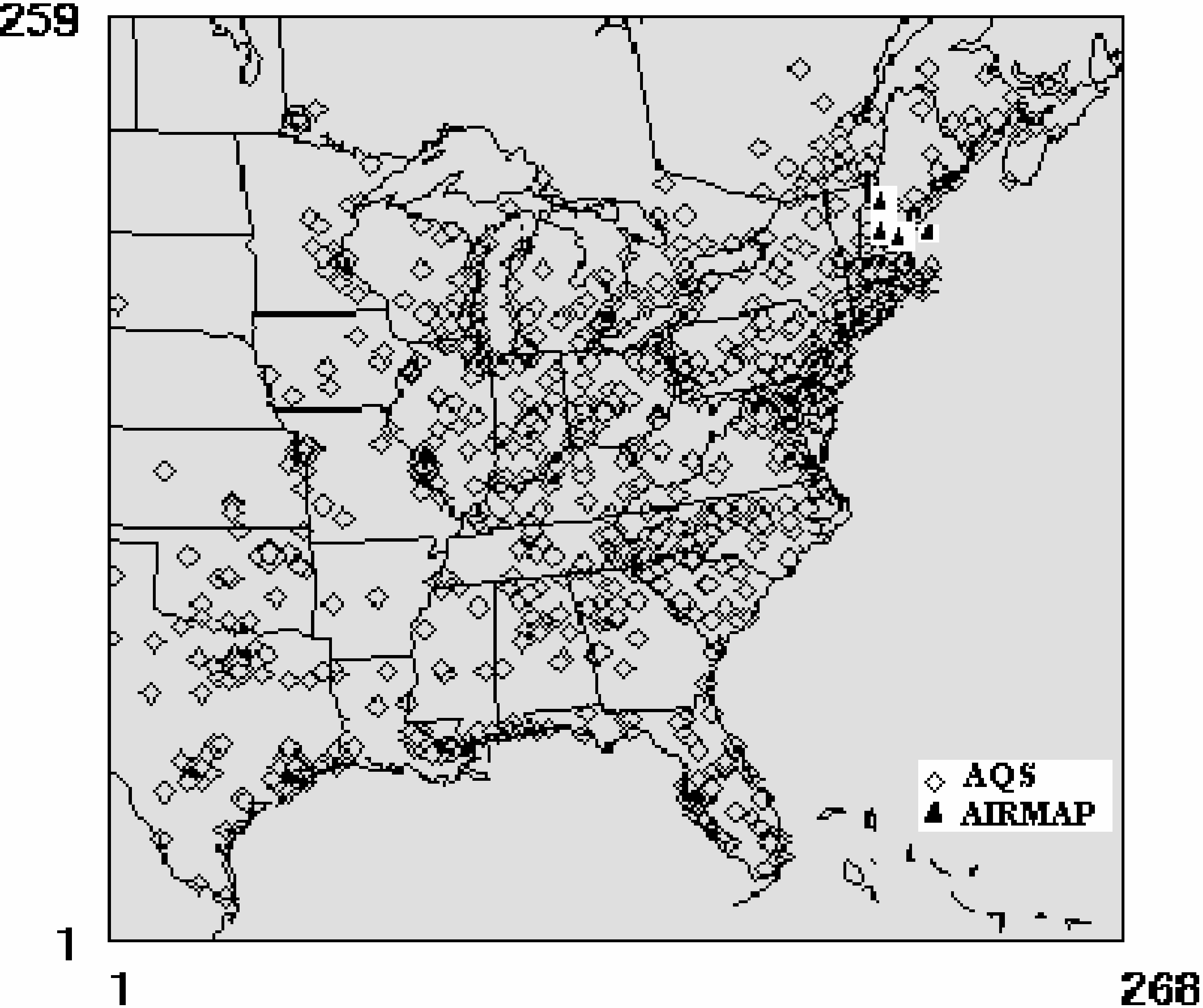
- **Using results: 12 UTC run and**
  target period for next day forecast (04 UTC to 03 UTC)

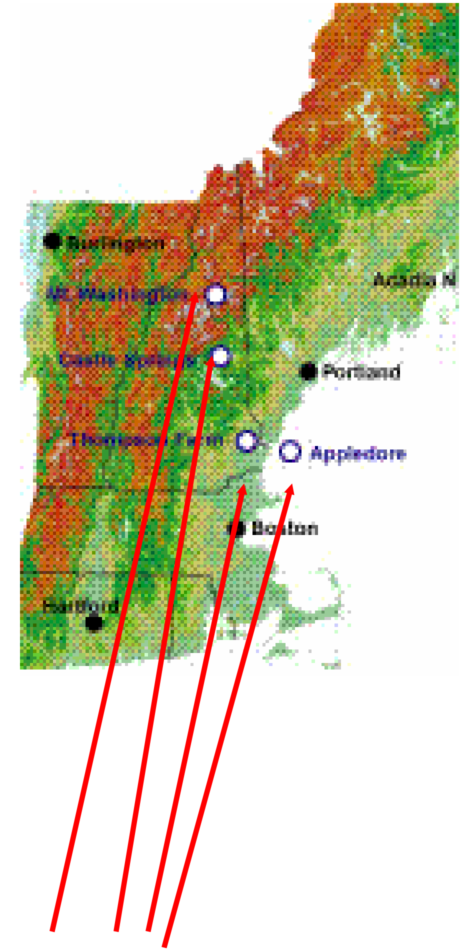
❖Observations

- EPA AIRNOW network:
  - ⇨ Hourly O_3 at 614 sites in E US.

- 2004 ICARTT Data (See Fig.)
  - ⇨ Vertical profiles (O_3, CO, NO, NO_2, HNO_3, SO_2, RH, T, WS, WD) from aircraft (P-3 and DC-8), ozonesonde, Lidar.
  - ⇨ Ground data over the ocean on Ron Brown ship
  - ⇨ Ground Data at Four AIRMAP sites

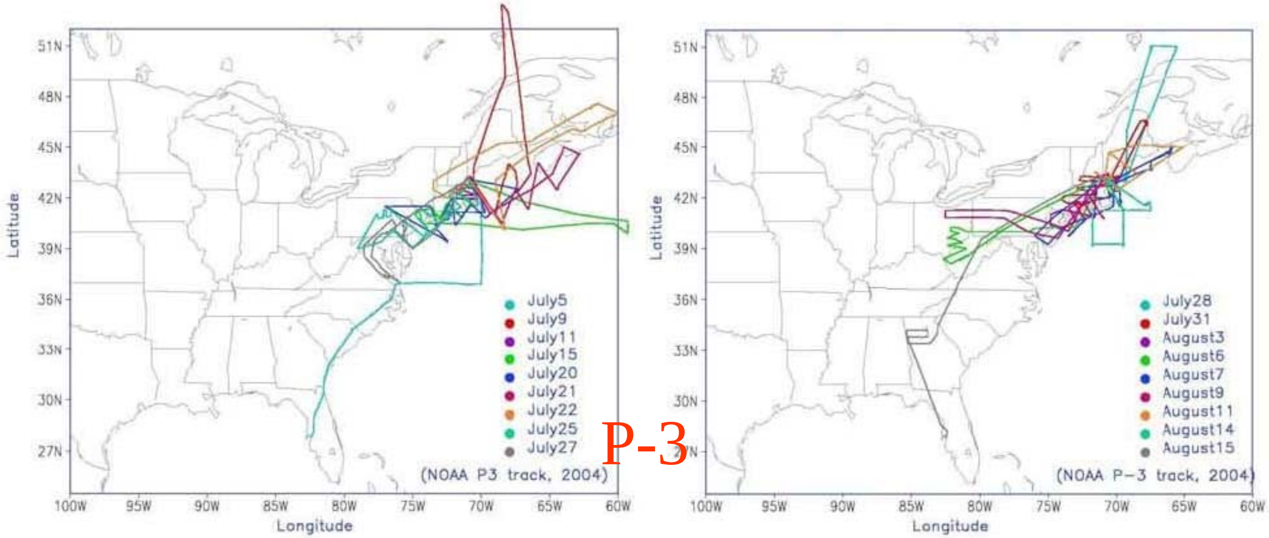
Site names	Variables
THOMPSON FARM (TF)(NH)	O3, NO, CO, JNO2, NOy, SO2, T, RH, wind speed, dir.
CASTLE SPRINGS (CS) (NH)	O3, NO, CO, JNO2, NOy, SO2, T, RH, wind speed, dir.
MOUNT WASHINGTON (MWO) (NH)	O3, NO, CO, SO2, JNO2
APPLEDORE ISLAND (IS) (ME)	O3, CO



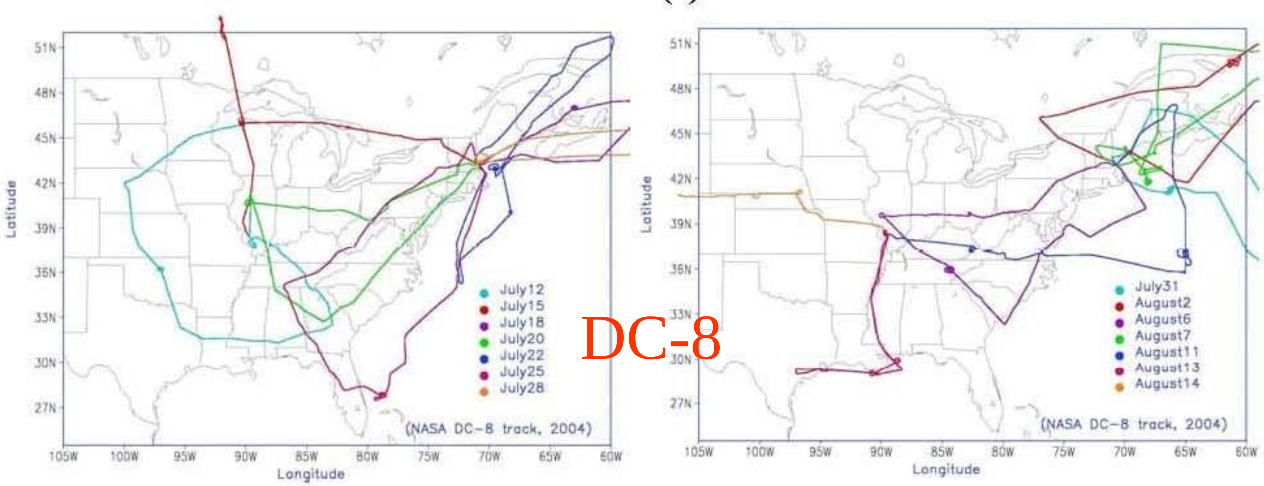


AIRMAP sites

Model domain and site (AIRNOW, AIRMAP) locations



(a)

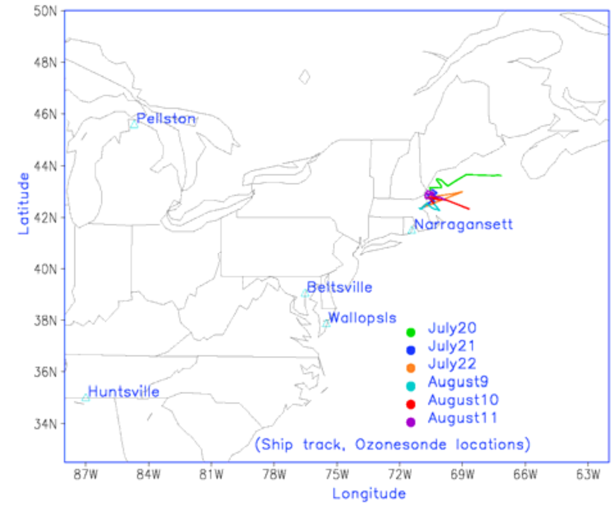


(b)

Tracks of (a) P-3, (b) DC-8,

(c) Ship, ozonesonde sites

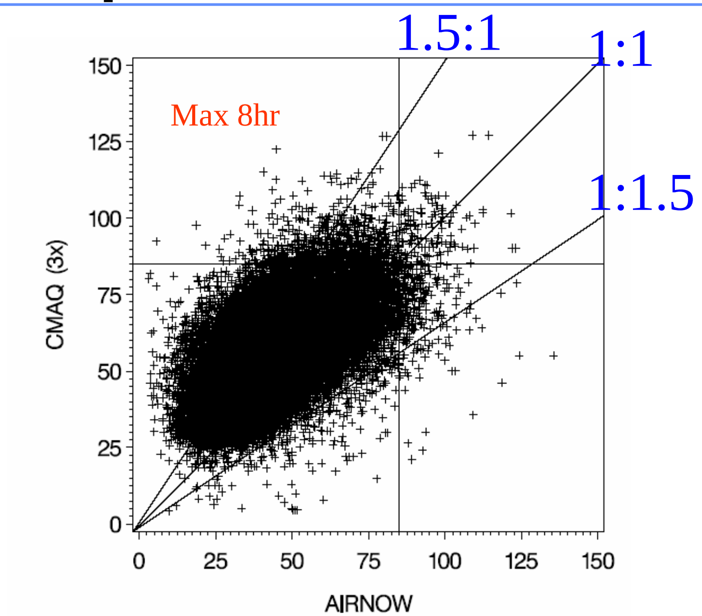
- P-3: Northeast;
- DC-8: Eastern US.
- Ship: mid-Atlantic Ocean

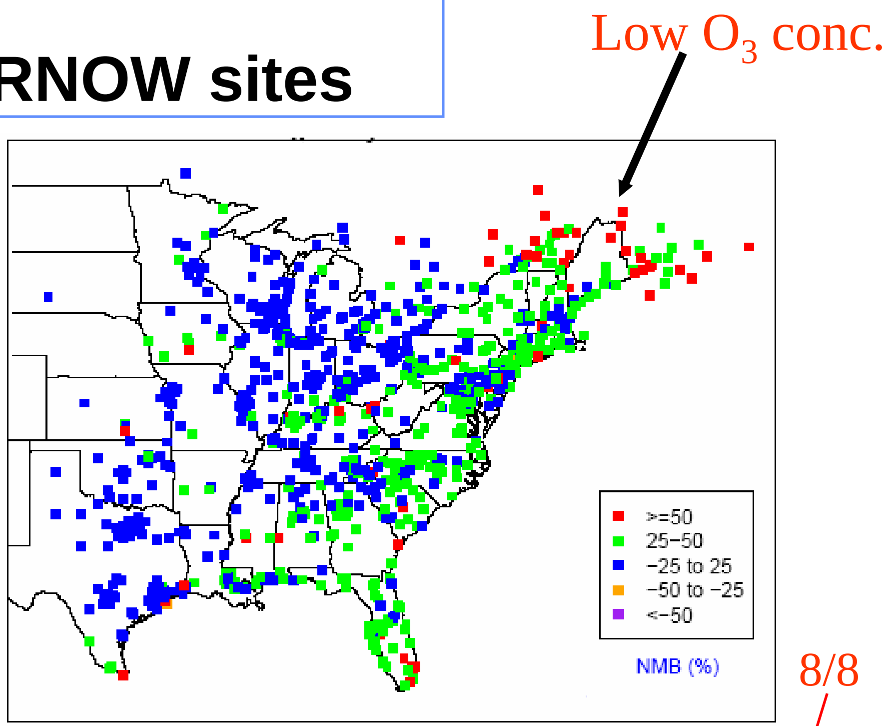


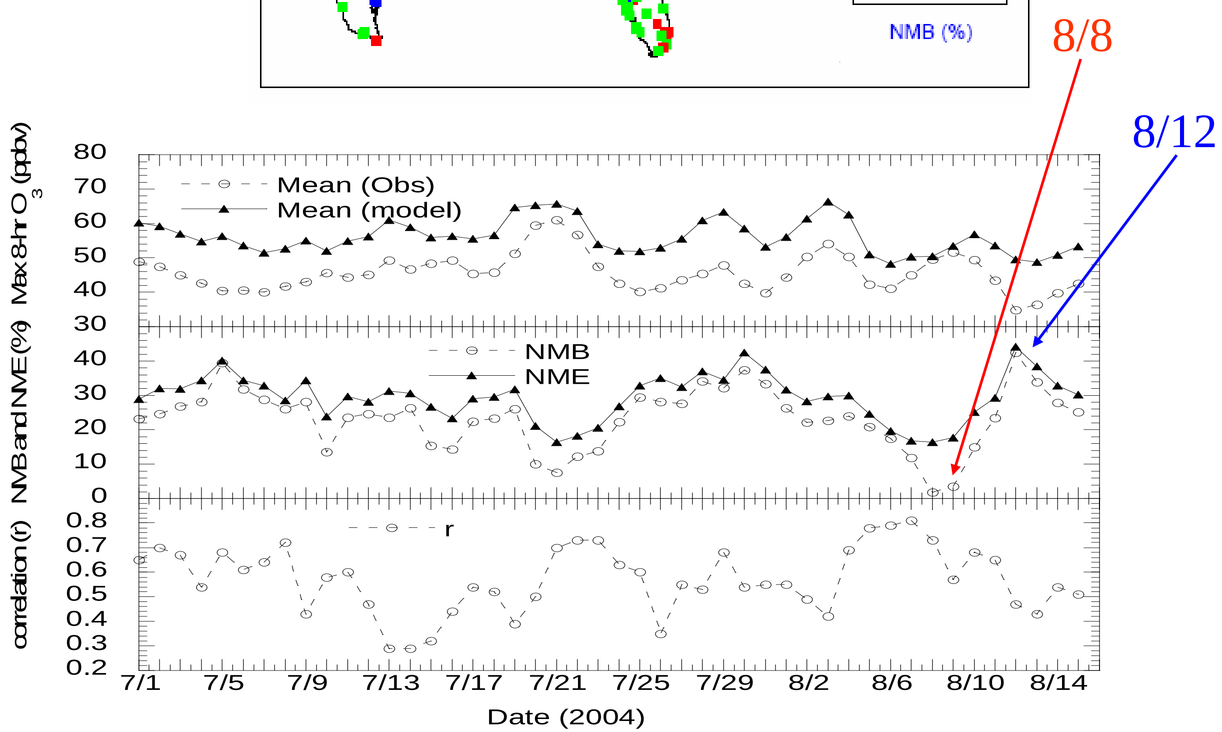
(c)

❖Results

1. Operational evaluation at AIRNOW sites





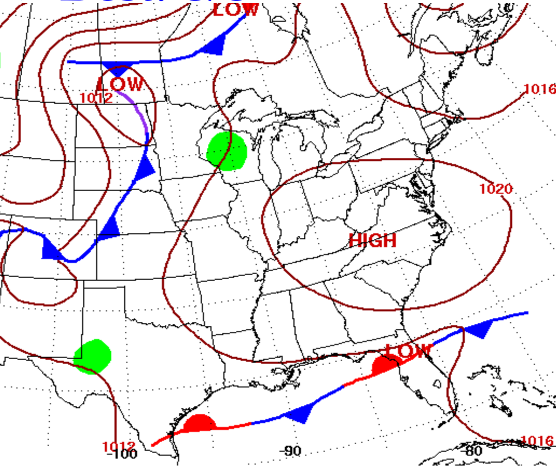


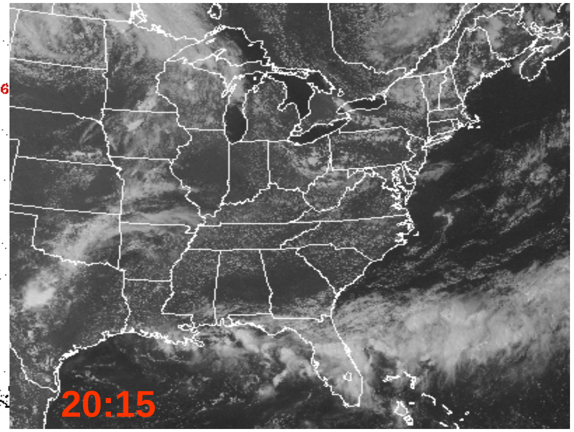
- ➢Best: 8/8
- ➢Worst:8/12

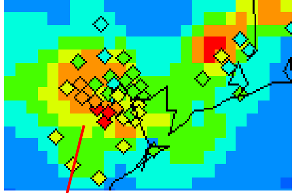
❖Results

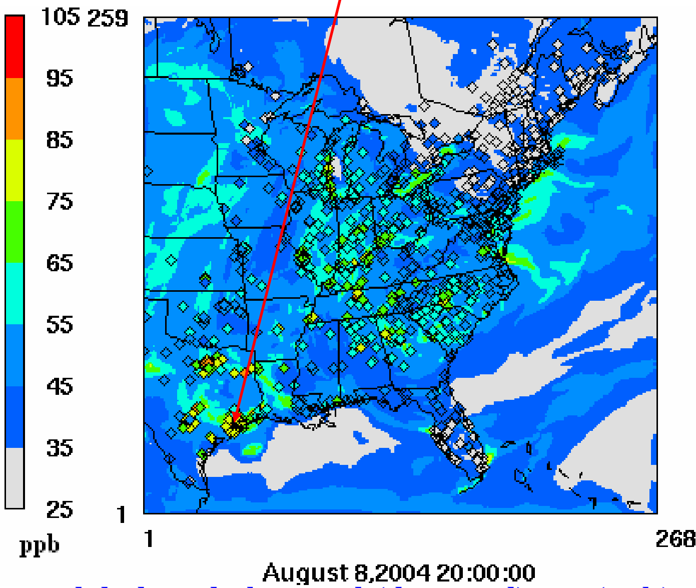
1. Operational evaluation at AIRNOW sites

➢Best: 8/8



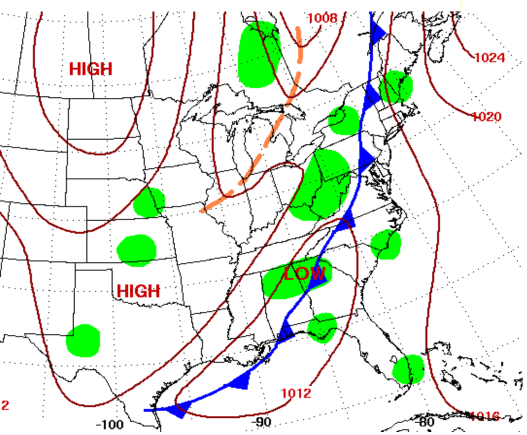


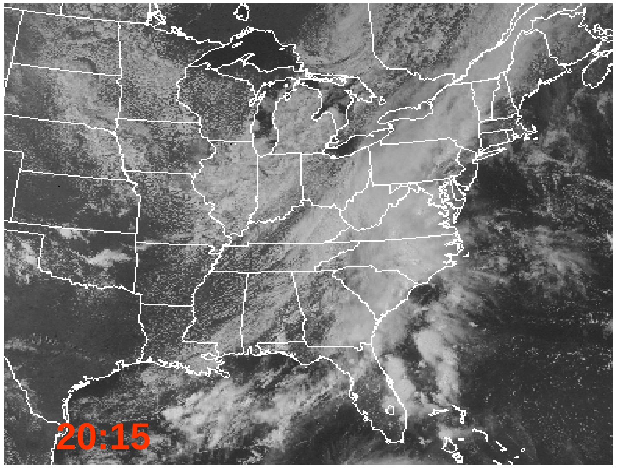


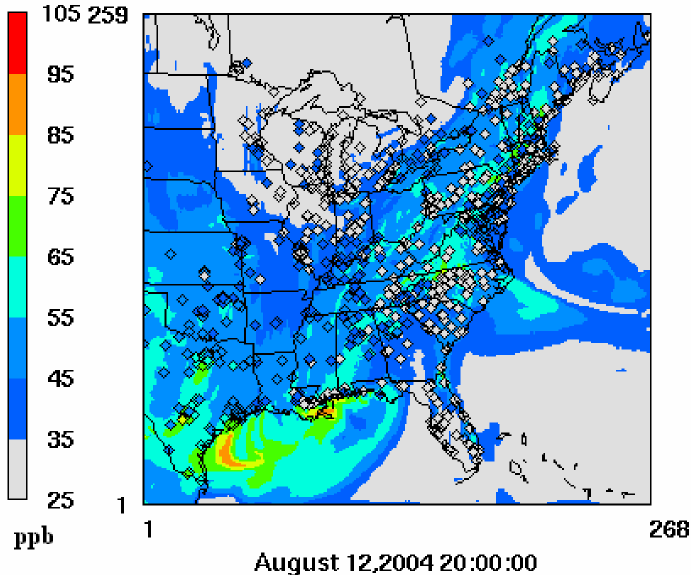


Modeled and observed (diamond) O_3 (ppb)

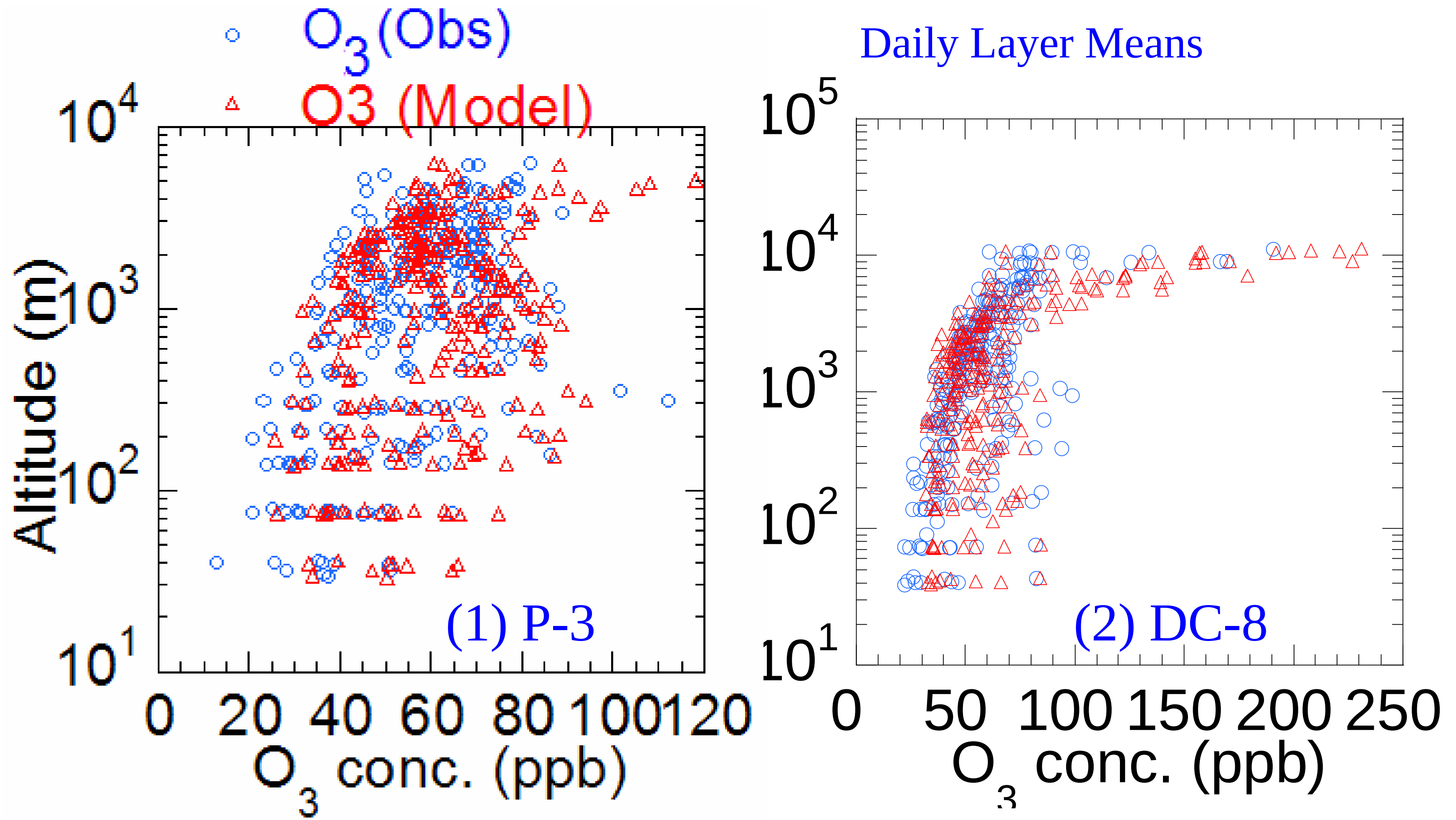
➢Worst: 8/12: Cloud and precipitation effect







❖ Results: O_3 Vertical profiles (7/1-8/15)



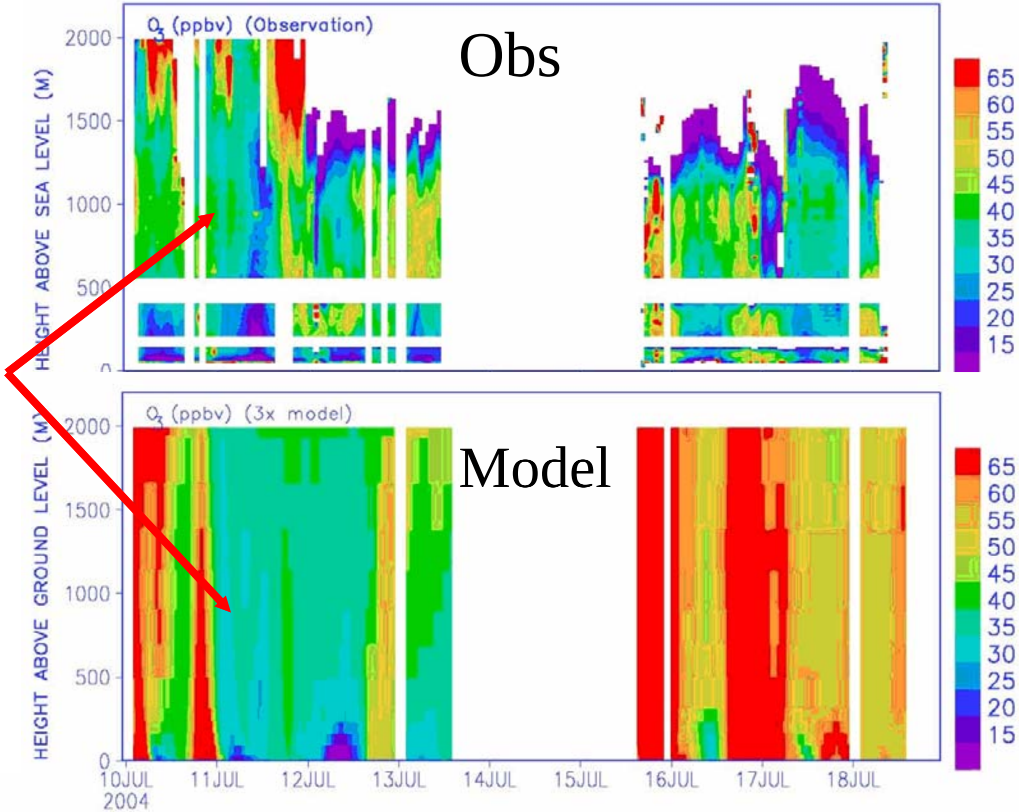
•Model reproduced vertical structure and pattern of obs at low altitude and more uniform but

•Overpredicted Obs at high altitudes

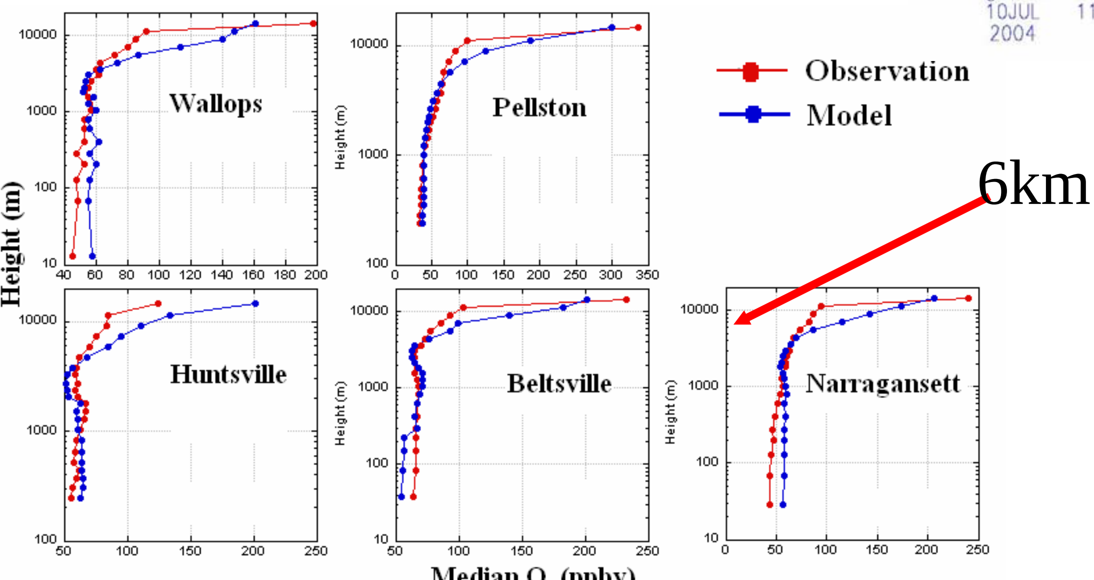
❖ Results: O_3 Vertical profiles

- ➢Lidar: Model reproduced obs at low altitude and more uniform

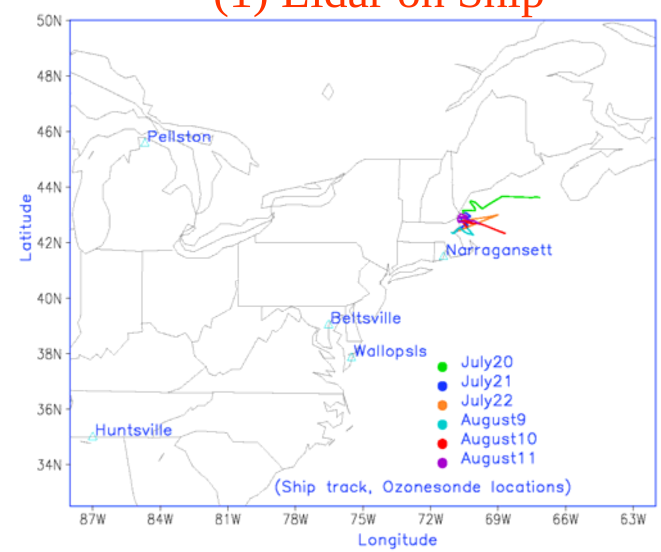
- ➢Ozonesonde: Over predictions above 6 km:
  - Impact from GFS derived LBC and coarse model resolution in FT



(1) Lidar on Ship



(2) July-August Median Profiles (Ozonesonde)



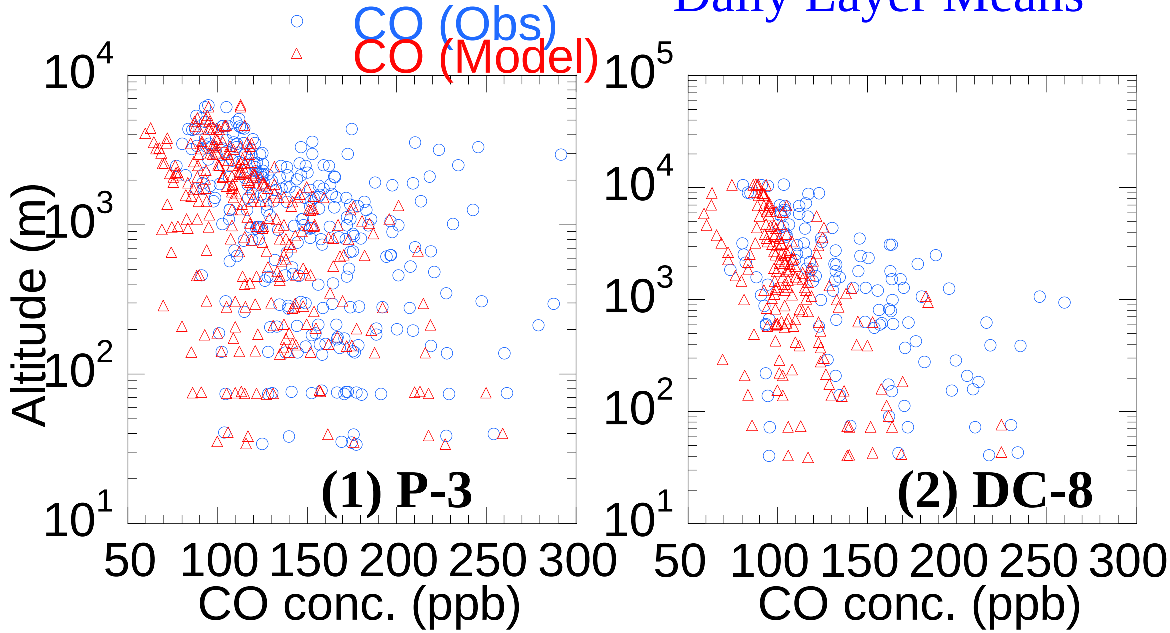
❖ *Results*: CO and HNO_3 Vertical profiles (7/1-8/15)

Daily Layer Means

CO:

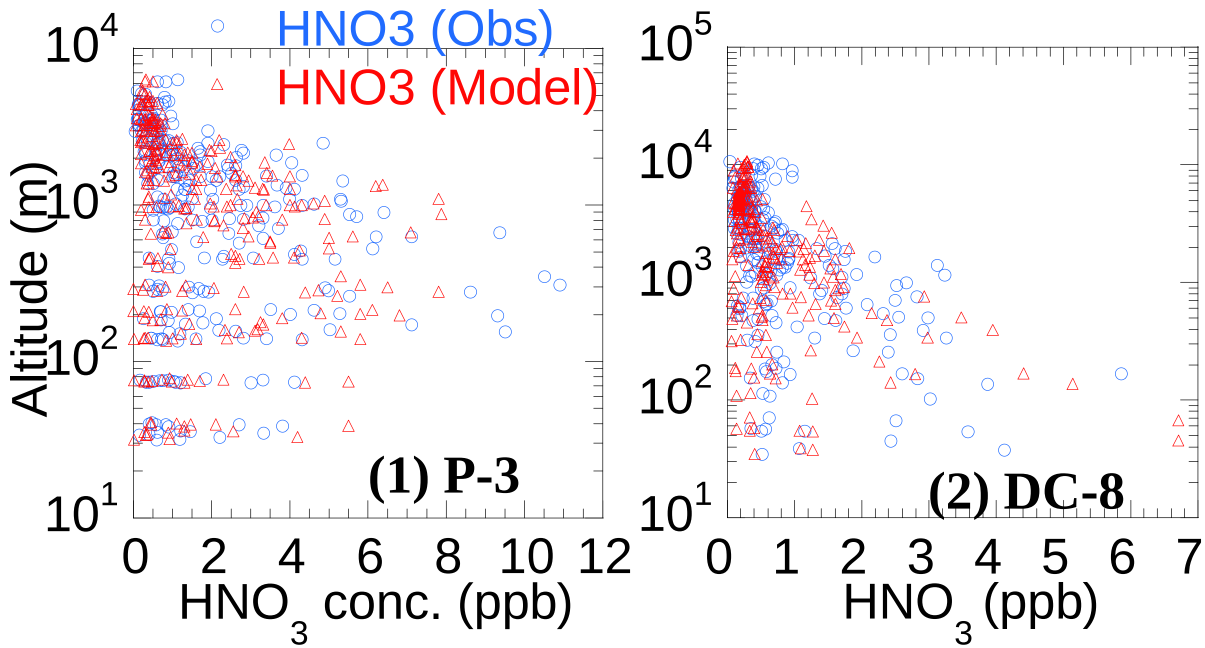
➢ Consistent Underpredictions.

⇨ partly due to inadequate representation of biomass burning effects from outside the domain



HNO_3:

➢ Good performance relative to P3 obs

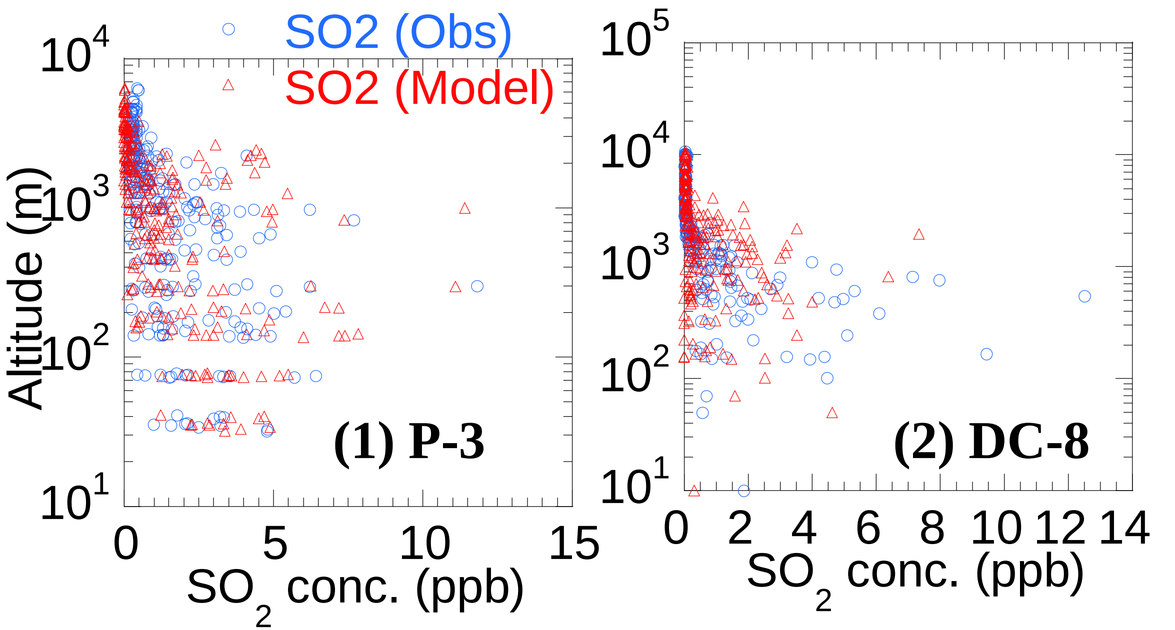


Results: SO_2, NO, HCHO vertical profiles

Daily Layer Means

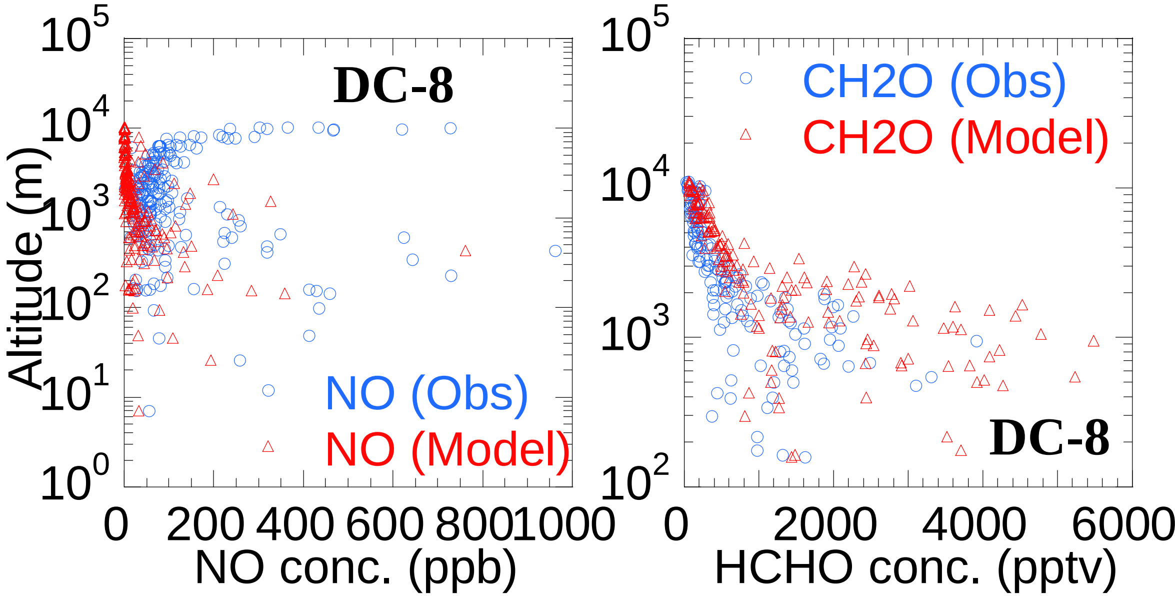
SO_2:

- Close to obs at high altitude
- Higher than obs at low altitude relative to P3 obs



NO:

- Under predictions of NO at h>3000 m
  - ⇨ Aircraft and lightning NO emissions are not in inventory

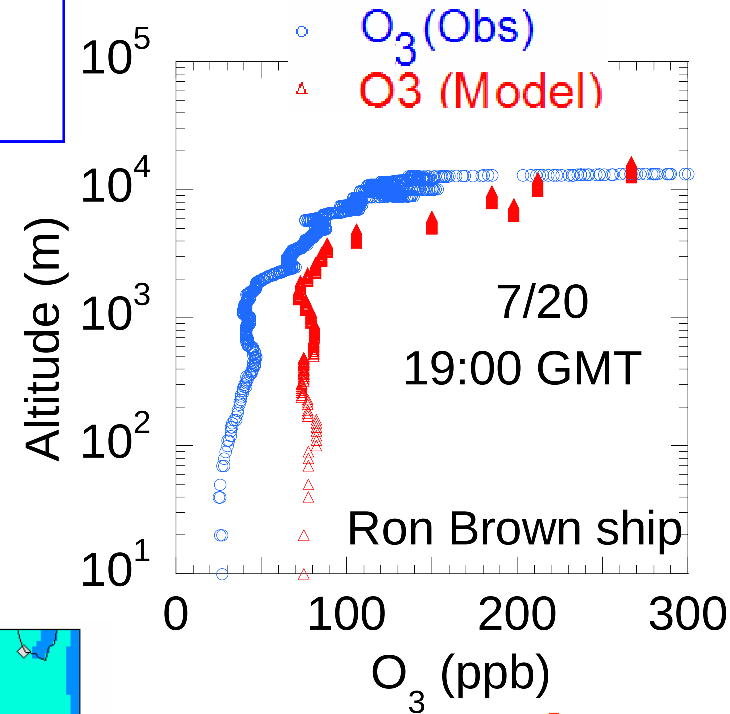


HCHO:

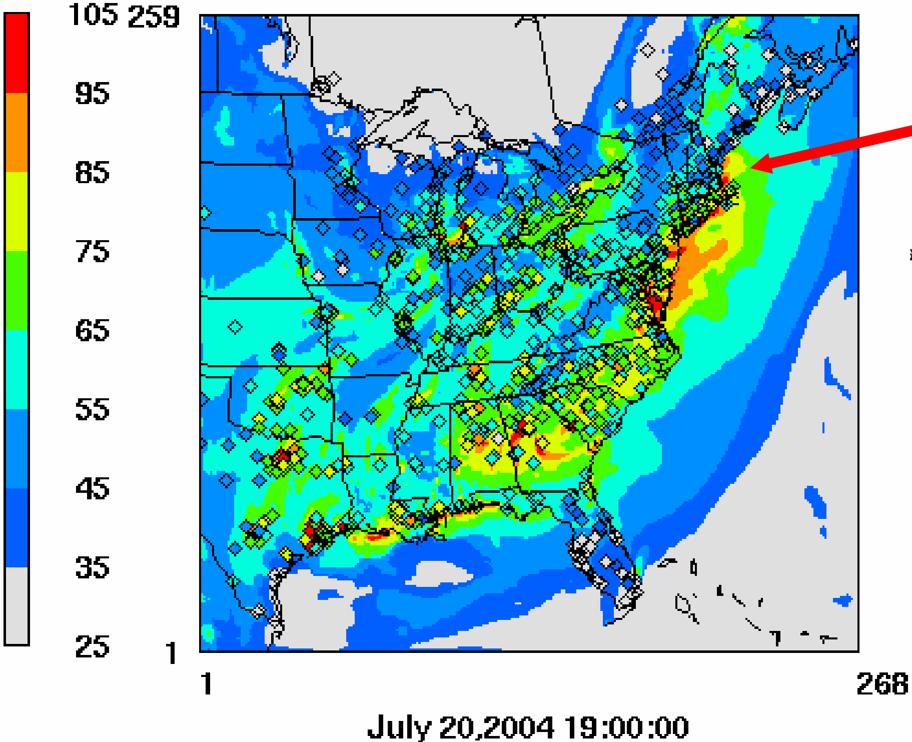
- Close to obs at high altitude but higher than Obs at lower altitude

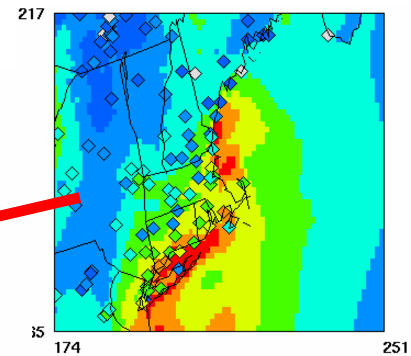
❖ <u>*Results*</u>: ***Case of 7/20 for overprediction over ocean***

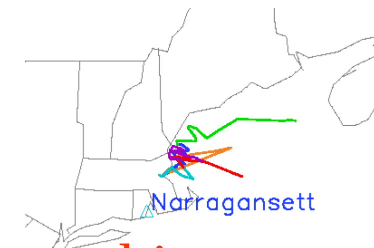
- ➢ Model overpredicted 30 ppb from the surface to 8 km over the ocean outside of Maine due to
  - ⇨ Incorrect PBL ??
  - ⇨ Incorrect dry deposition ??
- ➢ Need more work



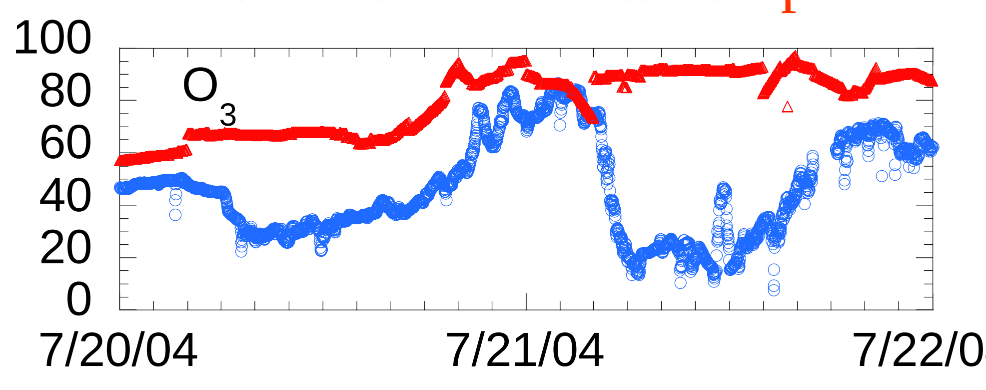
Ozonesonde







Surface on Brown ship

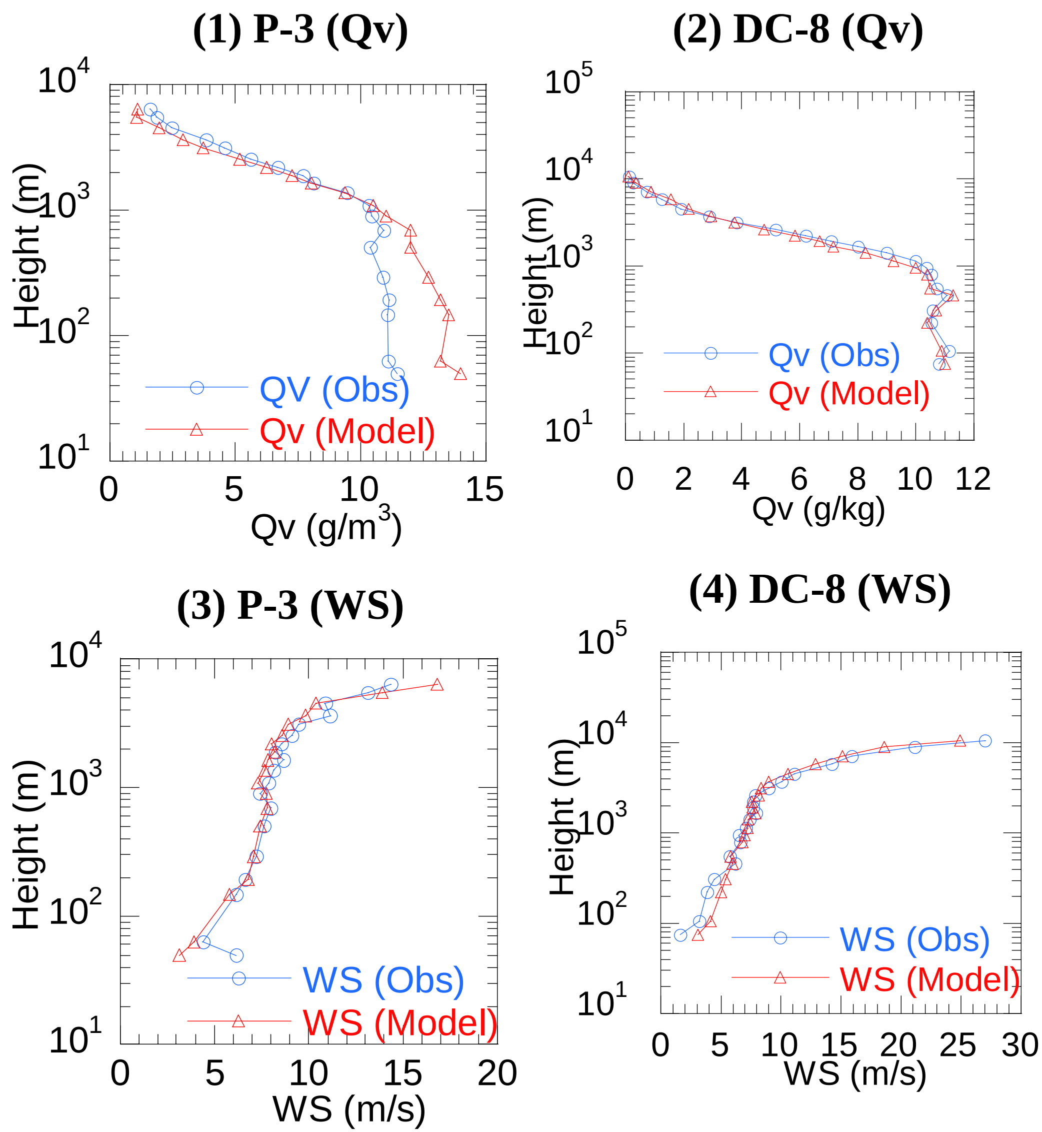


Results: *Meteorological vertical profiles*

Water vapor (Q_v) and WS:

- Model reproduced vertical structure well
  - ⇨relative to DC-8 obs.
- Over predicted Qv at low altitudes
  - ⇨ relative to P-3 Obs

Very good for T, P, WD (not shown)

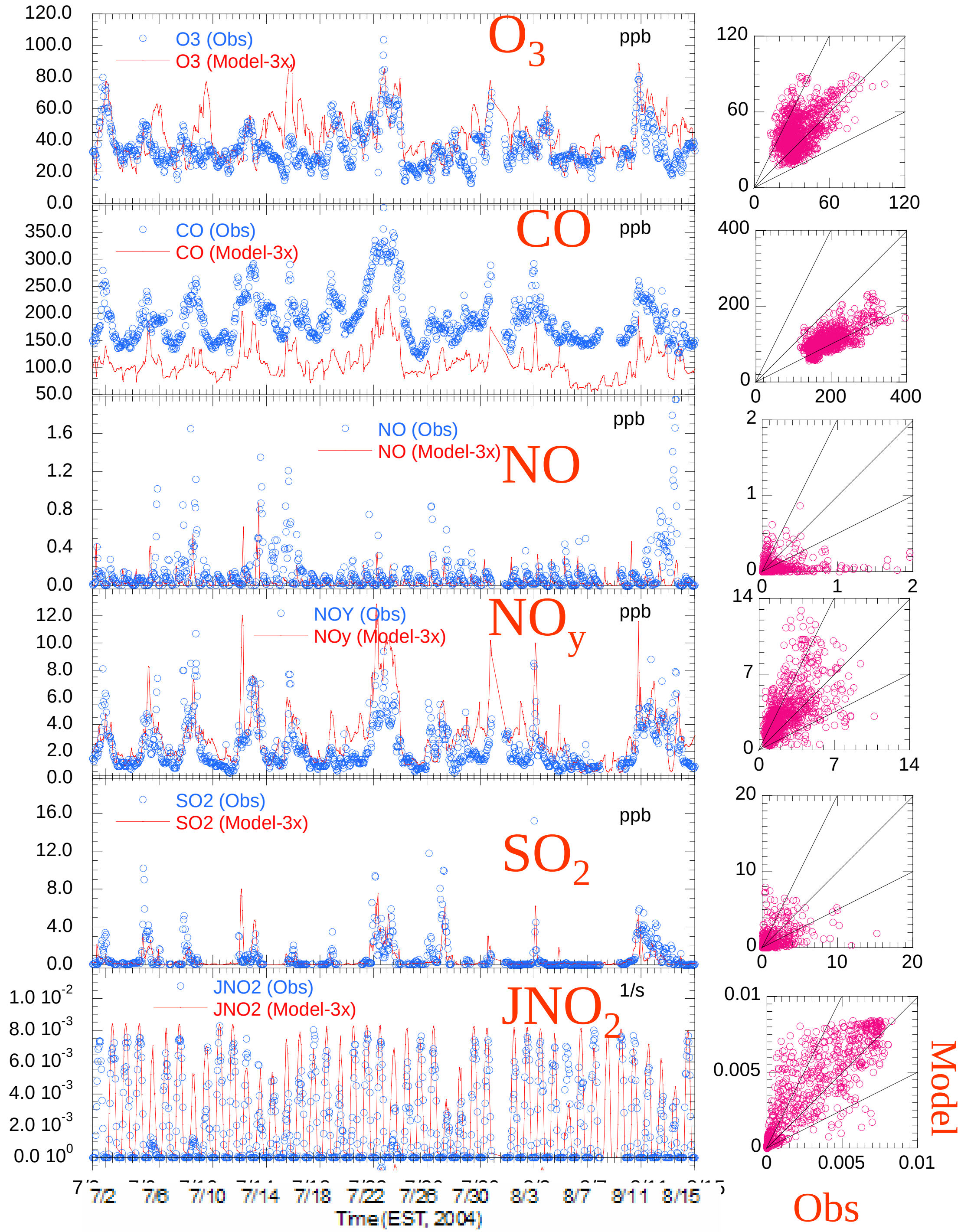


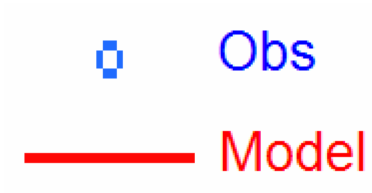
Layer means from July 1-August 15, 2004

❖ *Results*

3. Time-series evaluation at AIRMAP sites

Castle Springs (CS)





❖ Results

3. Time-series at AIRMAP sites

❖ Hanna et al. (2001):

- 50% uncertainty in JNO_2
  - 40 ppbv (or 20%) uncertainty in max O_3
- Model reproduces
  - 43-53% of observed JNO2 within a factor of 1.5

➢ Priority: more accurate determination of JNO_2 in model

Parameters	Mean (ppb) Obs	Mean (ppb) Model	r	% within a factor of 1.5
Castle Springs (N=1047)				
O_3	35.17	43.63	0.493	66.6
NO	0.14	0.05	0.222	12.1
CO	188.84	108.78	0.706	19.3
NO_Y	2.27	3.14	0.587	43.6
SO_2	1.16	0.87	0.388	29.6
JNO_2 (1/S)	3.18×10^{-3}	4.07×10^{-3}	0.820	49.6
Isle of Schoals (N=1078)				
O_3	36.68	52.31	0.541	56.9
CO	171.70	121.15	0.610	60.9
NO	0.76	0.18	0.448	0.8
Mount Washington (N=1076)				
O_3	45.87	45.85	0.554	87.7
NO	3.64	0.01	-0.054	8.9
CO	152.43	95.19	0.301	46.7
NO_Y	4.04	2.23	-0.060	20.6
SO_2	0.74	0.30	-0.001	19.0
JNO_2 (1/s)	3.59×10^{-3}	4.43×10^{-3}	0.768	43.1
Thompson Farm (N=1067)				
O_3	28.80	41.68	0.751	48.1
NO	0.33	0.29	0.436	31.3
CO	173.07	154.66	0.593	77.7
NO_Y	3.93	7.26	0.321	28.8
SO_2	1.22	1.63	0.084	14.3
JNO_2 (1/s)	3.19×10^{-3}	3.90×10^{-3}	0.865	53.8

❖ *Results* (diagnostic evaluation)

✓ NO_x-sensitive regimes: $[O_3]/[NO_x]$, O_3 production efficiency: $[NO_z]/[O_3]$

- **NO_x-sensitive regimes: $[O_3]/[NO_x]$**
  - ⇨ Arnold et al., 2003:
    - $[O_3]/[NO_x]$<14: VOC-sensitive
      >46: NO_x-sensitive

Statistical summary of number of hours(The values in parentheses are the percentages (%))

	Castle Springs		MWO		Thompson Farm	
O_3/NO_x	Obs	Model	Obs	Model	Obs	Model
0-14	32 (7)	18 (4)	13 (4)	0 (0)	181 (38)	105 (22)
15-25	34 (7)	19 (4)	3 (1)	0 (0)	51 (11)	72 (15)
26-45	94 (20)	18 (4)	16 (5)	2 (1)	59 (12)	125 (26)
>46	312 (66)	417 (88)	285 (90)	315 (99)	188 (39)	177 (37)

⇨ Both model and obs: CS and MWO sites are mainly under strongly NO_x-sensitive conditions (>66%)

❖ *Results*

O_3 production efficiency: ε_N

O_3-NO_z slope

❖Parrish et al., 1993 :

- O_3-NO_z slope:
  ⇨upper limit of ε_N

❖ε_N :

- Obs: 8.5 to 10.7
- Model: 5.2 to 6.7

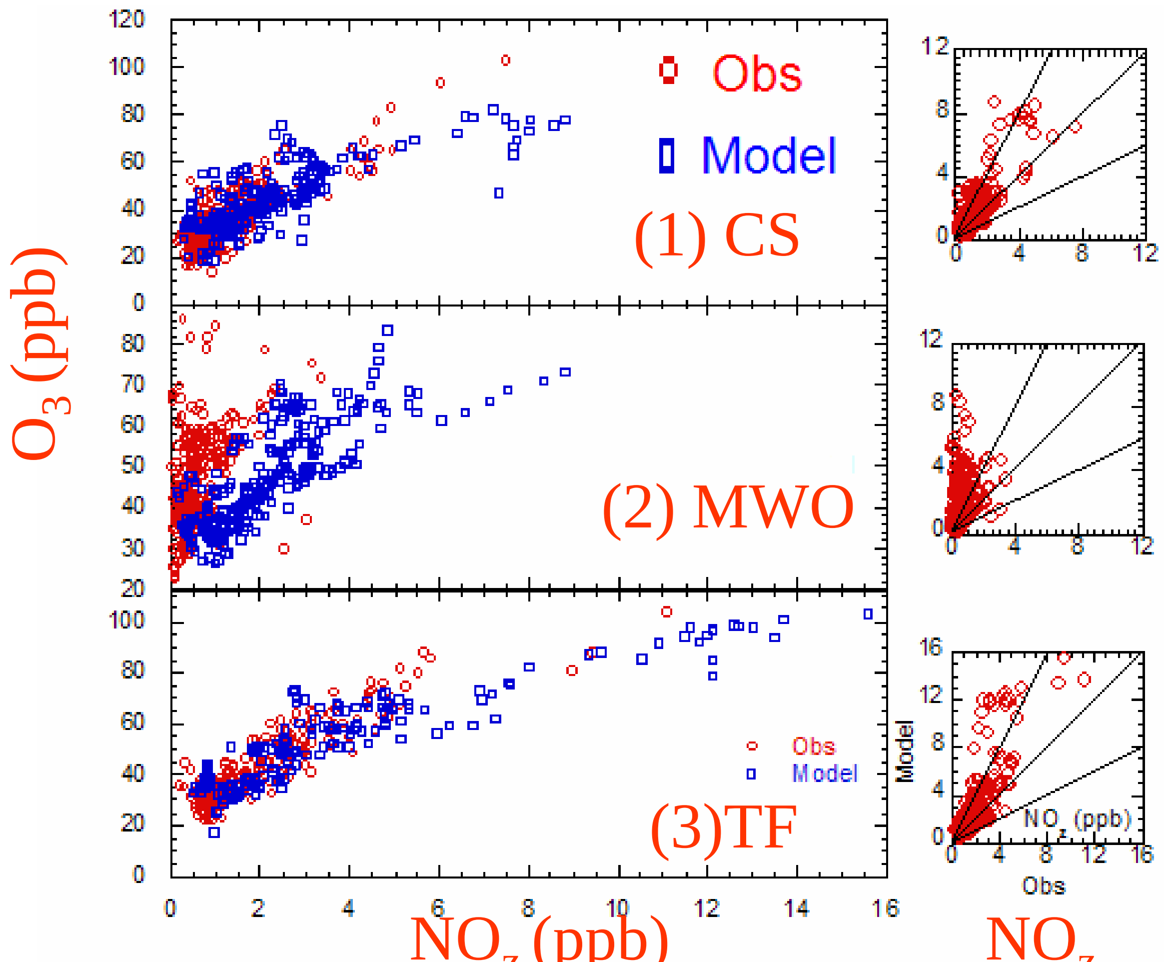
❖At rural sites in E US

(Olszyna et al., 1994):

ε_N : 5 to 10

The observational data with [O3]/[NOx]>46 (aged air masses)

Sites	Regression equations
CS (N=312)	Obs: $[O_3]=10.7[NO_z]+22.8$, $r^2=0.70$
	Model: $[O_3]=6.4[NO_z]+30.1$, $r^2=0.61$
MWO (N=285)	Obs: $[O_3]=9.5[NO_z]+41.5$, $r^2=0.18$
	Model: $[O_3]=6.7[NO_z]+32.4$, $r^2=0.61$
TF (N=188)	Obs: $[O_3]=8.5[NO_z]+26.4$, $r^2=0.80$
	Model: $[O_3]=5.2[NO_z]+34.0$, $r^2=0.83$



Conclusions

- At AIRNOW sites, model was **able to reproduce the daily variations of** observed max 8-hr O_3 and reproduced majority (73%) of observed max 8-hr O_3 within factor of 1.5 with NMB=22%.
  - ⇨ Poor performance for cloudy days

- Model reproduced the O_3 vertical profiles from aircraft, lidar, and zonosonde at low altitude well but tended to overpredict in high altitude>6km
  - ⇨ **attributed to GFS derived LBCs combined with coarse vertical model resolution in FT**

- Model under predicted CO consistently (by ~30%) from surface to high altitude
  - ⇨ partly due to inadequate representation of biomass burning effects from outside the domain

- Model under predicted NO consistently at the high altitude
  - ⇨ Aircraft and lightning NO emissions are not in the inventory

- The modeled upper limits (5.2 to 6.7) of ε_N estimated by O3-NO_z slopes are 40% lower than the observations (8.5 to 10.7)

Future research needed

- For real time forecast of O_3, key is the prognostic model forecasts of meteorological fields:
  - Cold front patterns,
  - cloud cover
  - wind fields
- Improve photochemical mechanism and emission
- Improve model's convective cloud scheme for vertical transport
- Improve the model performance for JNO_2, especially during the cloudy periods
- **More evaluation using process analyses for the 2004 ICARTT data is underway**

Disclaimer

The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. This work constitutes a contribution to the NOAA Air Quality Program. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views.

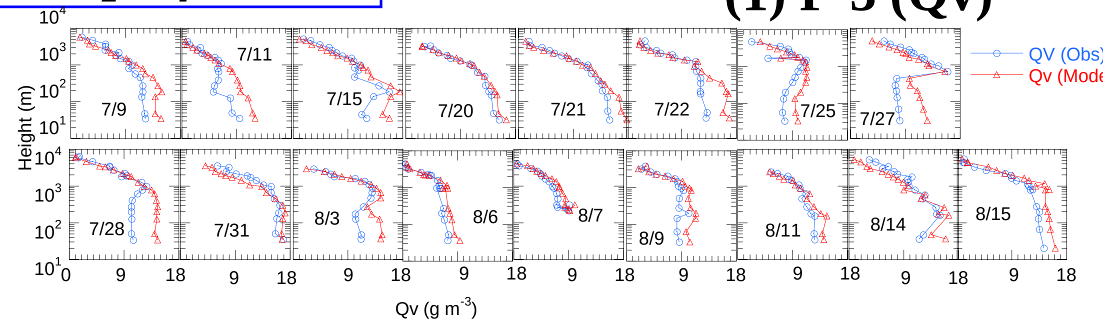
Results: Meteorological vertical profiles

Water vapor (Qv) and WS:

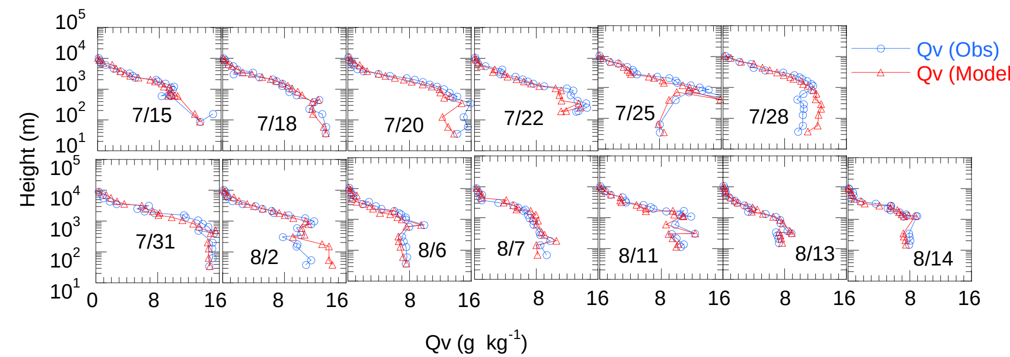
➢ Very good performance.

Very good for T, P, WD (not shown)

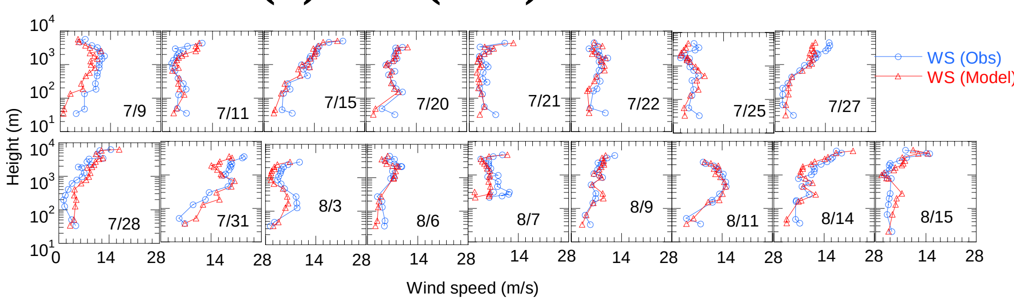
(1) P-3 (Qv)

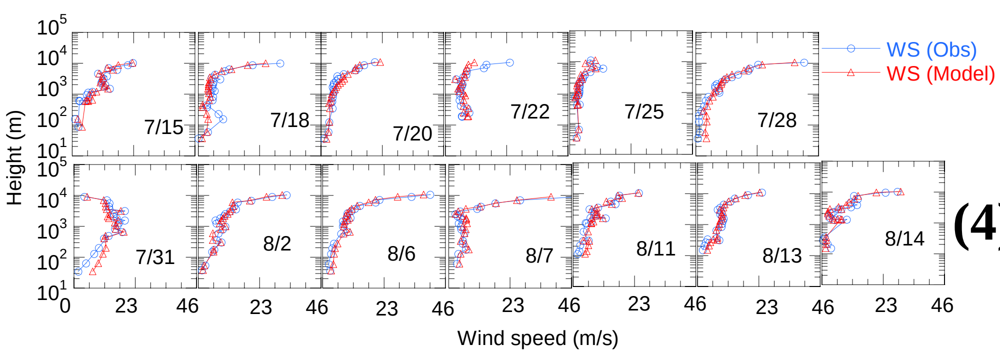


(2) DC-8 (Qv)



(3) P-3 (WS)



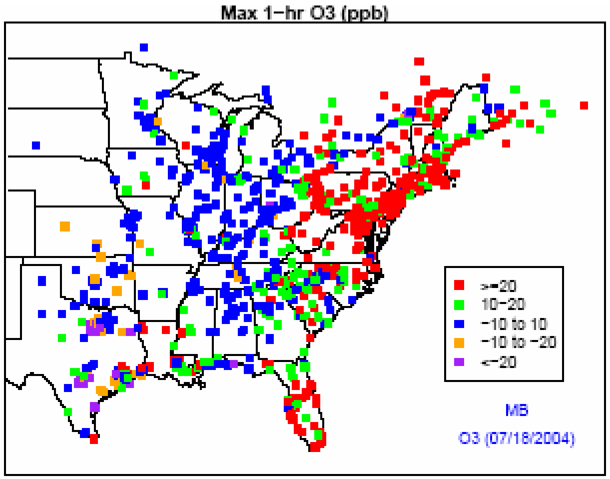


(4) DC-8 (WS)

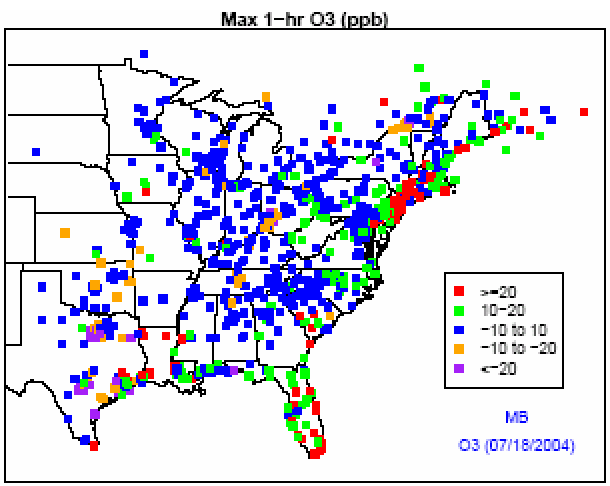
Surface O_3 Model Performance: Bias

Impacts of model enhancements to cloud mixing and photolysis effects

Base

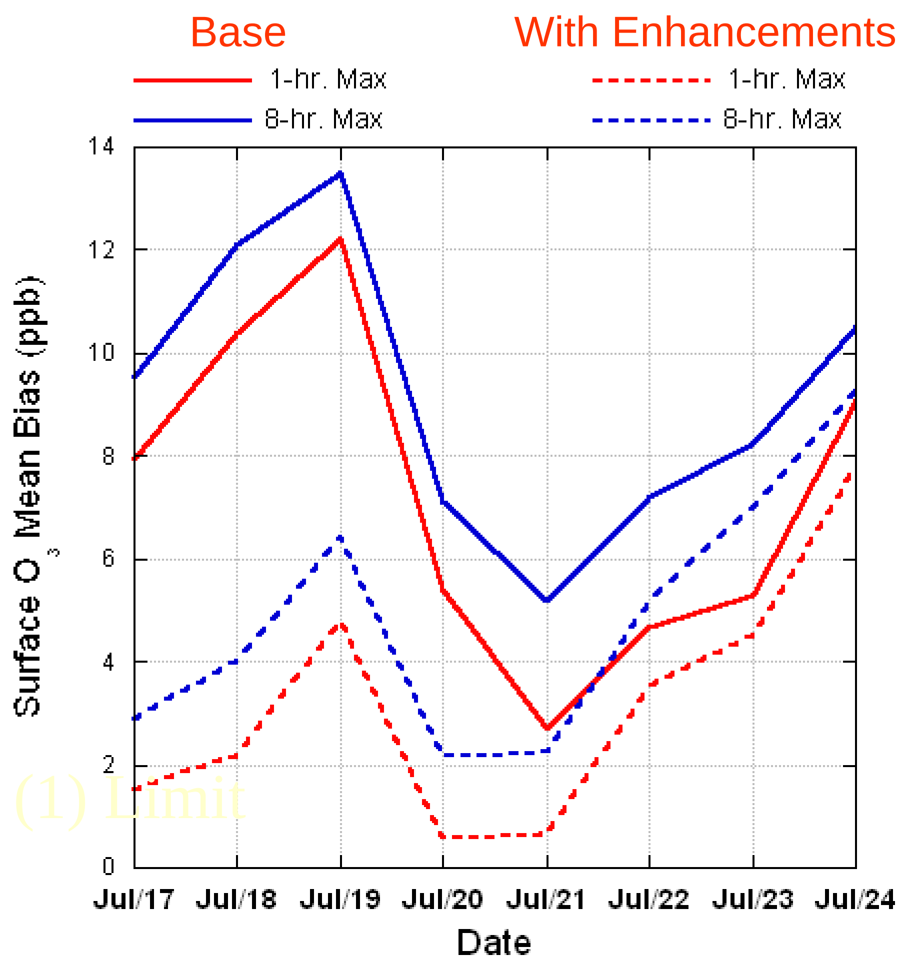


With Enhancements



(1) Limit cloud-top to below the GSF tropopause to reduce downdarft transport.

(2) Use modeled and clear sky radiation field to estimate below-cloud photolysis attenuation factors

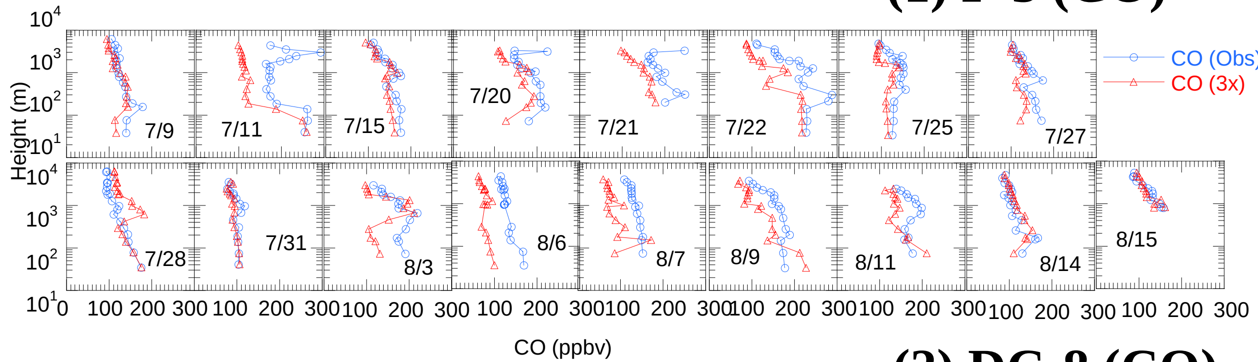


Results: *CO and HNO3 Vertical profiles*

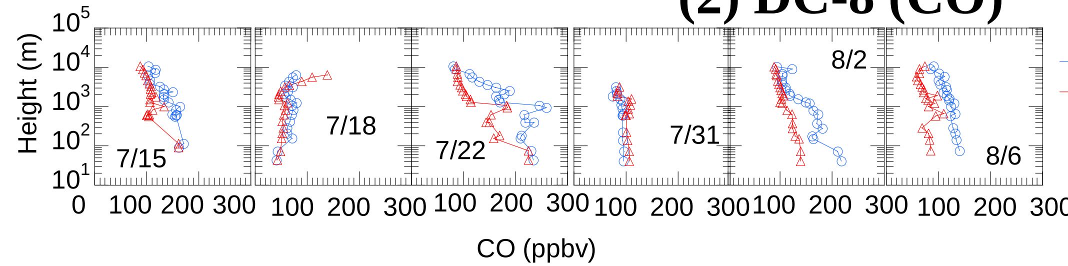
CO:

- Consistent Underpredictions.
  - partly due to inadequate representation of biomass burning effects from outside the domain

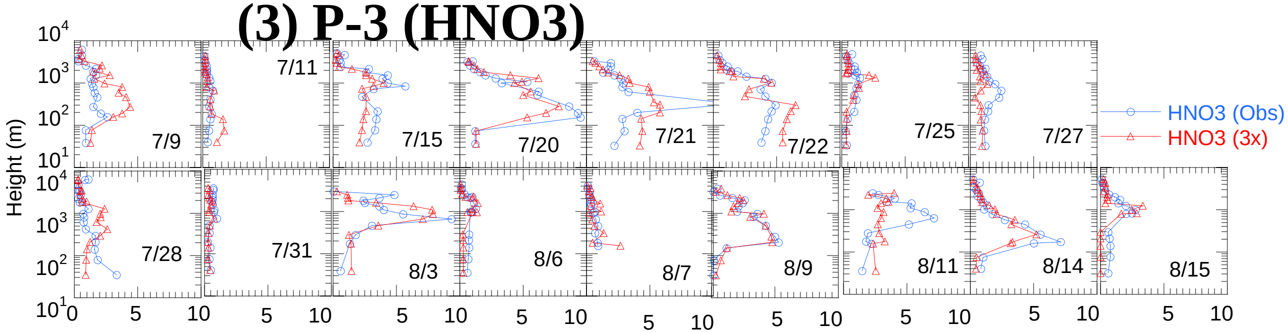
(1) P-3 (CO)



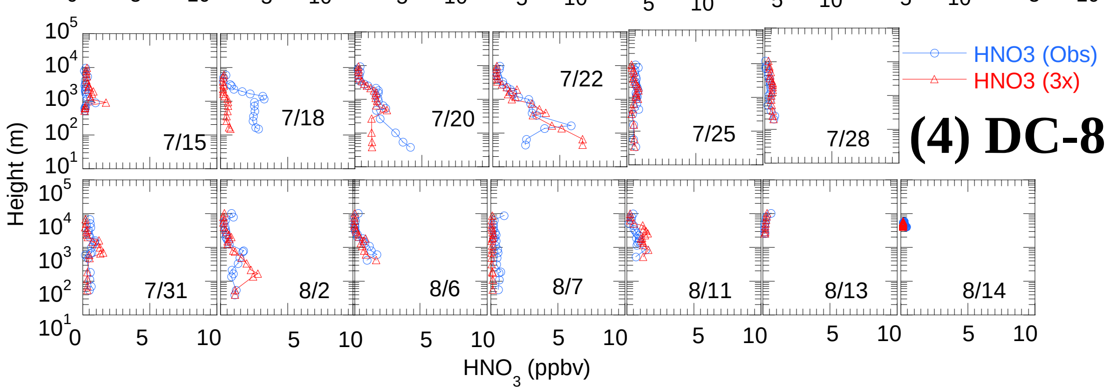
(2) DC-8 (CO)



(3) P-3 (HNO3)



(4) DC-8 (HNO3)



HNO3:

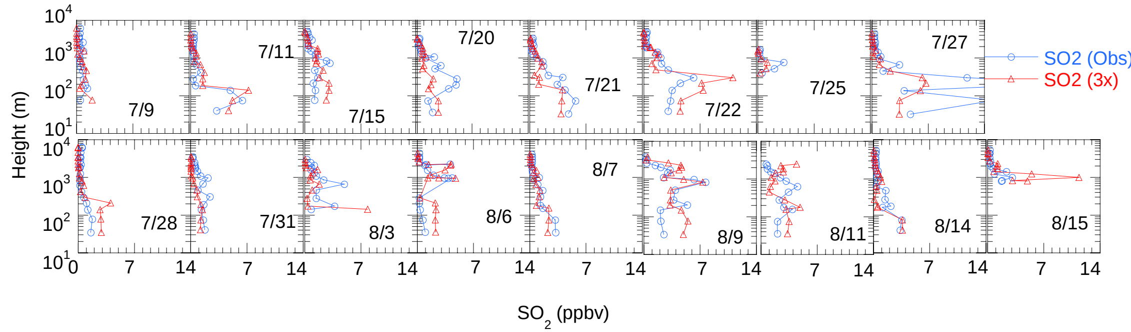
- Good performance
  - Except
    - P3: 7/9, 8/11
    - DC-8: 7/18

Results: SO2, NO, HCHO vertical profiles

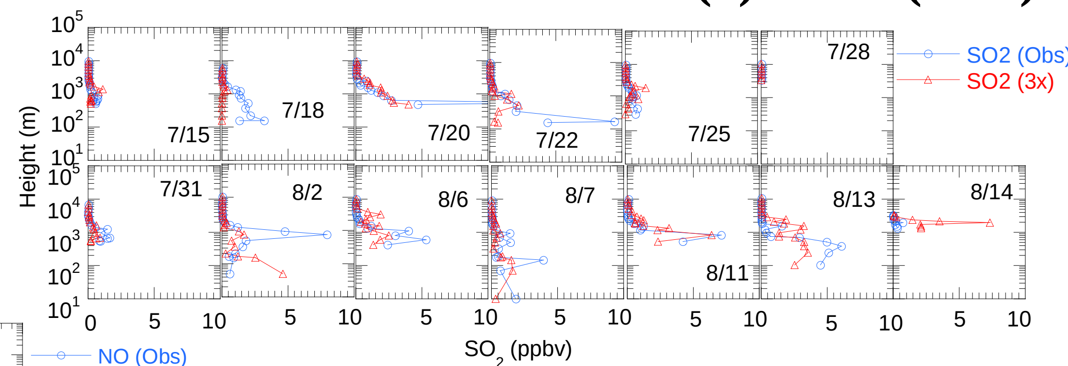
SO2:

- ➢Close to obs at high altitude
- ➢Higher than obs at low altitude most of time.

(1) P-3 (SO2)



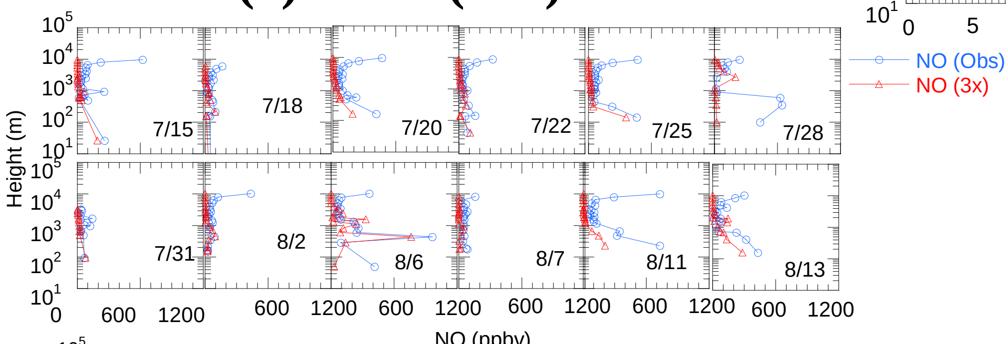
(2) DC-8 (SO2)



NO:

- ➢Under predictions of NO at h>3000 m
  - Aircraft and lightning NO emissions are not in inventory

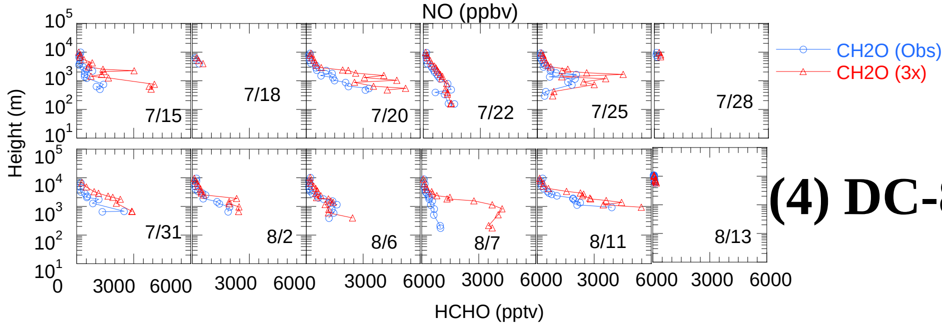
(3) DC-8 (NO)



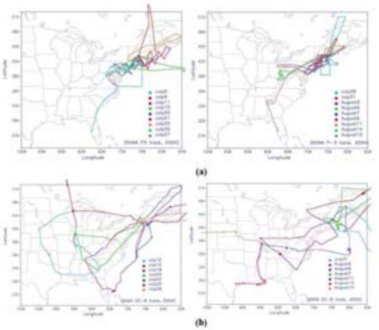
HCHO:

- ➢Close to obs except 8/7

(4) DC-8 (HCHO)

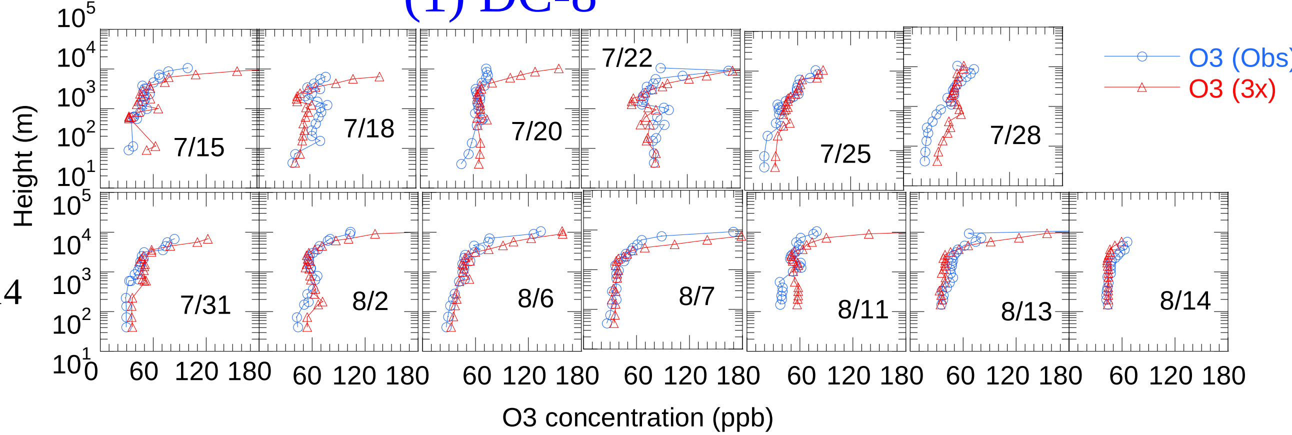


❖ Results: O3 Vertical profiles



- •Model reproduced obs at low altitude and more uniform
- • Except: DC-8: 7/28, 8/11
  P-3: 7/9, 7/15, 7/20-22, 7/28, 8/14

(1) DC-8



(2) P-3