Evaluation of model performance in air quality forecasting during scientific campaigns.




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Pictures by Frank Flocke (NCAR) and Cameron McNaughton (UHawaii)

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Outline

- Improving ozone modeling through systematic data analysis.
  - ICARTT
  - MILAGRO
- Analyzing the effect of model resolution on model performance.
- 4D Var approach to recovery of Asia emissions during Trace-P.

- Correlation among observations
  - What is high ozone correlated to?
- Correlation among model and observations
  - How well does the model perform?
- Correlation between model bias of species
  - What errors in precursors generate bias of ozone?
- Vertical profile
- Horizontal interpolation of model bias
  - How does model error distribute geographically?

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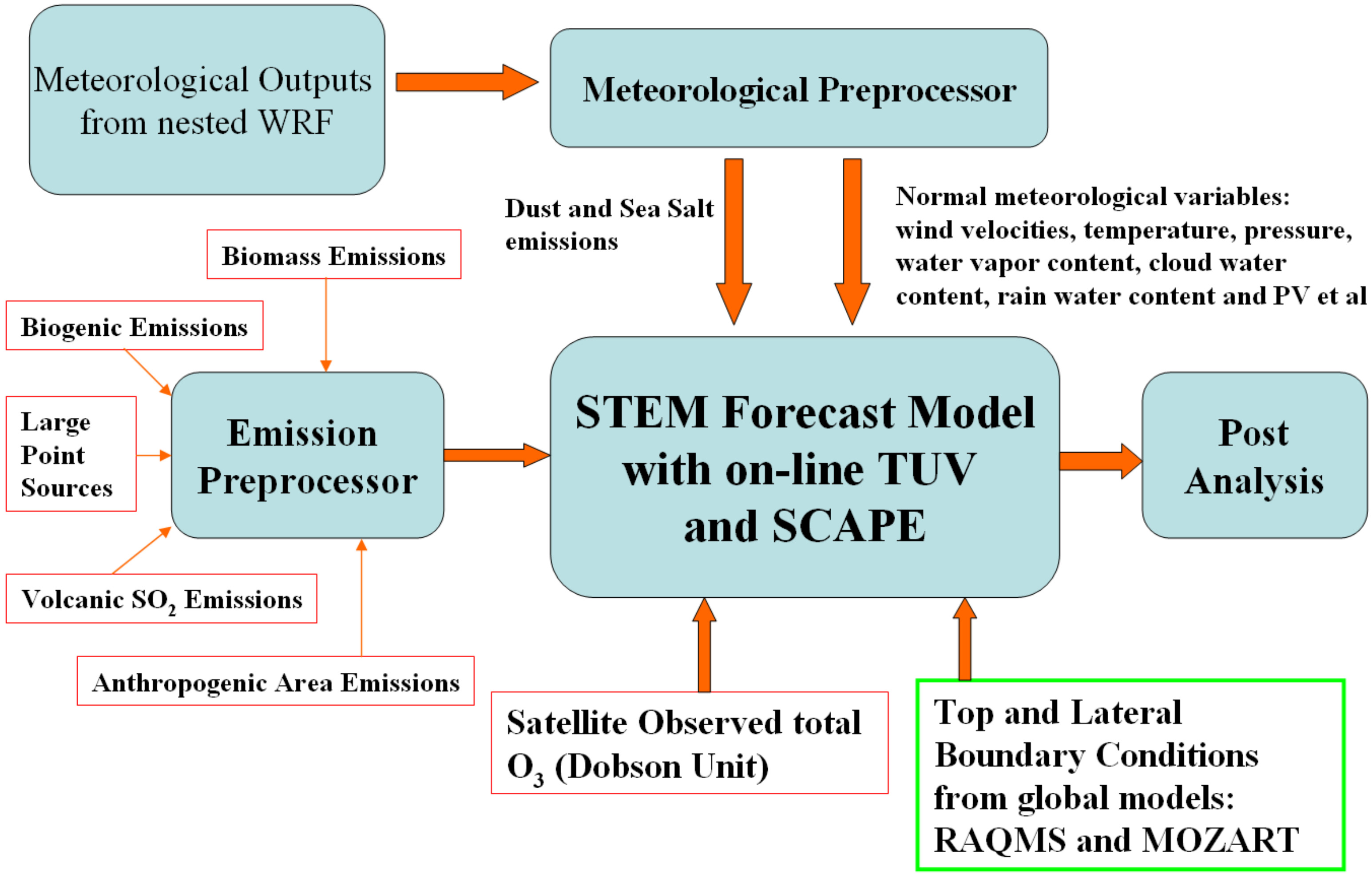
U. of Iowa STEM (Sulfur Transport and dEposition Model) Model Data Flow Chart



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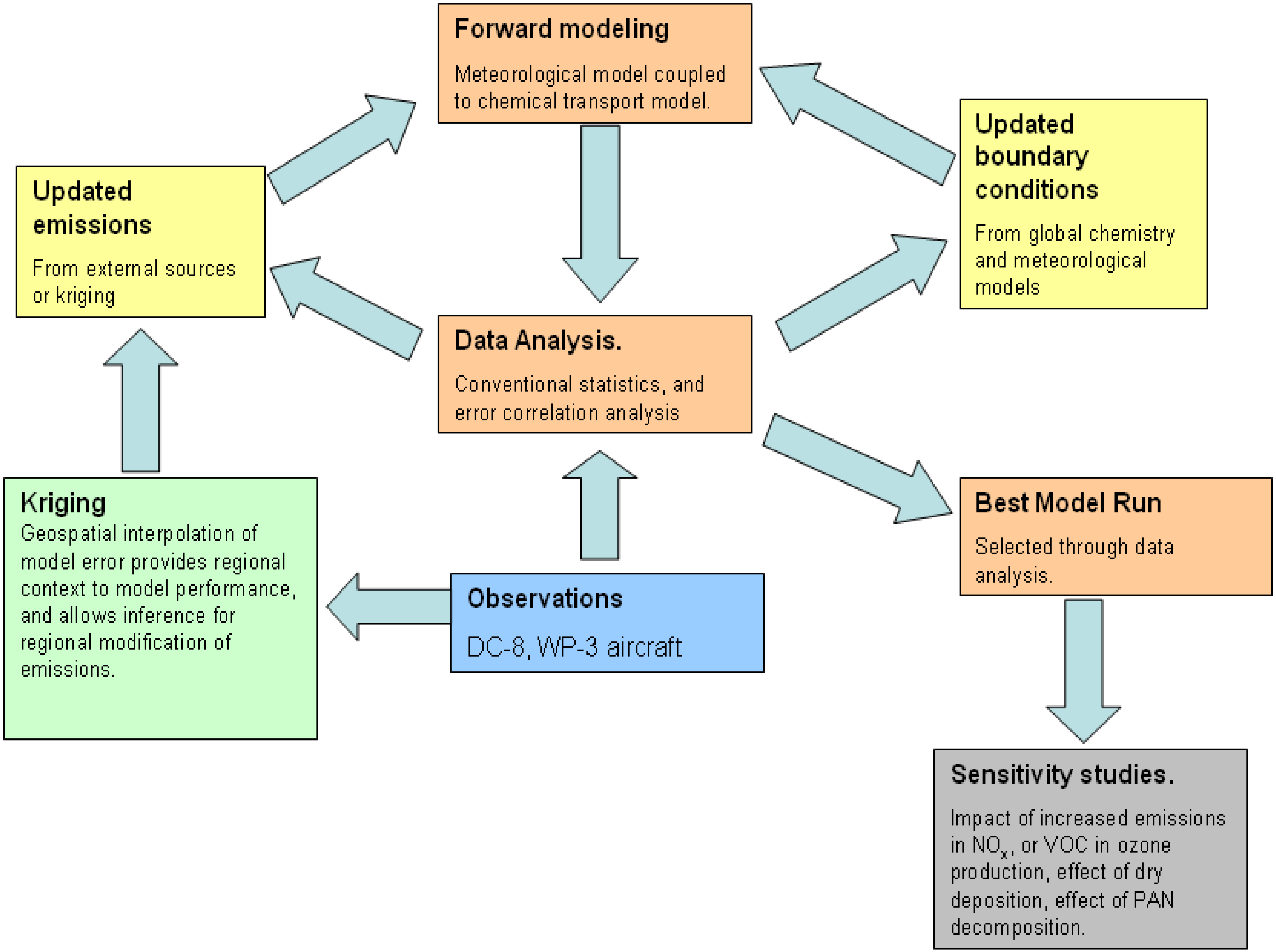
Analysis framework



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ICARTT campaign: July-August 2004 (Mena- Carrasco et al., 2007, JGR)

Figure 1 Flight tracks and altitude range for ICARTT. In red: 0-1km, Yellow: 1-4km, Green: 4-8km, Blue: 8-12km. Left: DC-8 Right: WP-3.

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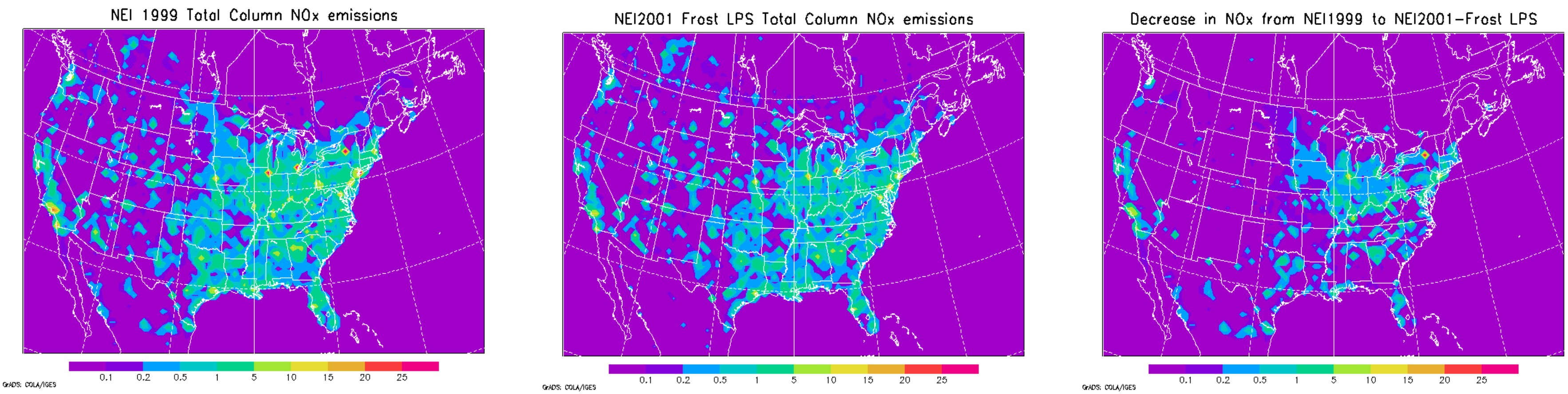

Figure 2 Total Column NO_x emissions Left: NEI 1999. Center NEI 2001-Frost LPS emissions. Right: Decrease in NO_x emissions from NEI 1999 to NEI 2001- Frost LPS. Scale in tonnes/km_2/year.

- Forecast presented positive surface ozone bias associated with bias of precursors, and of dry deposition seasonality.
- Updated 2001 NEI and large point sources showed improvement, but recurring bias in the SE and the Ohio River Valley
- New run with 60% reductions of area NO_x decreased bias [Frost et al., 2006]

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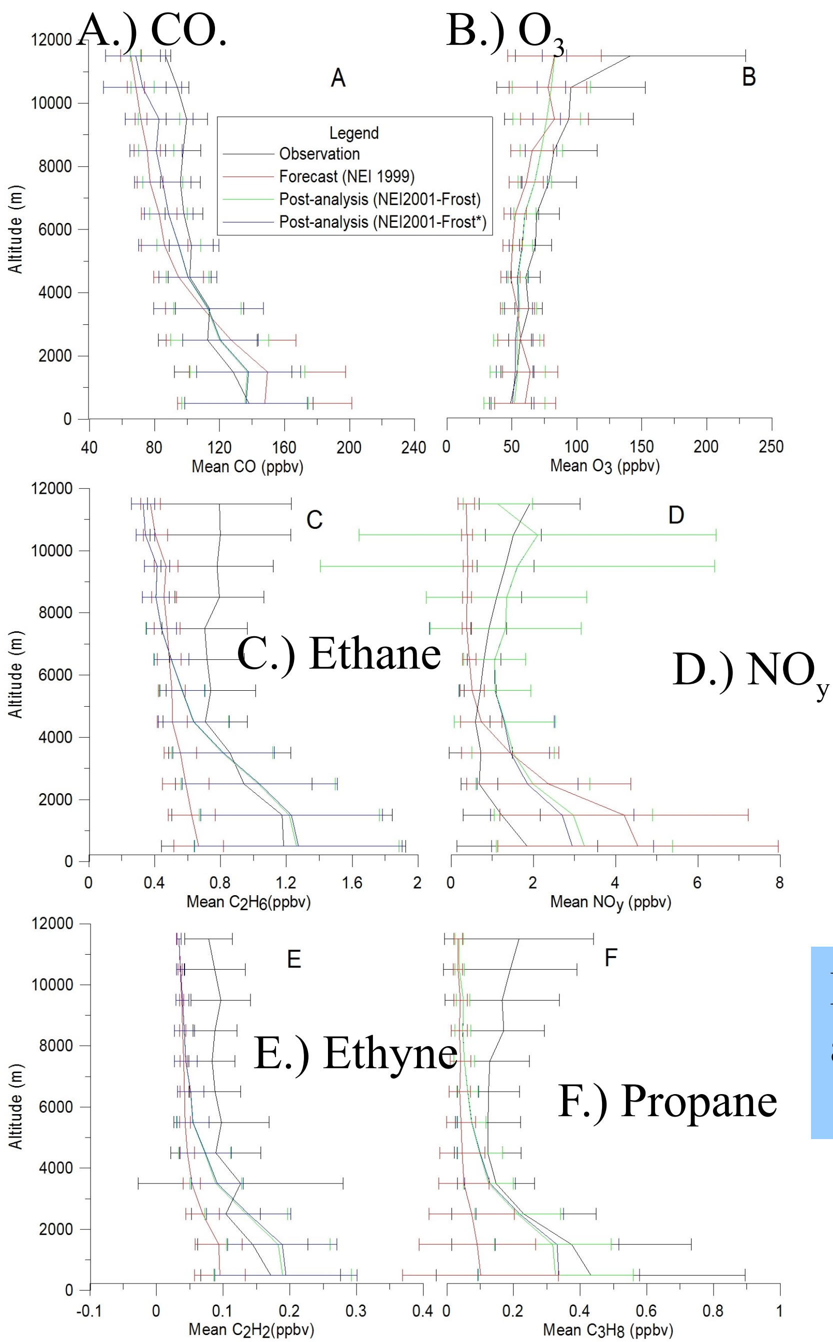
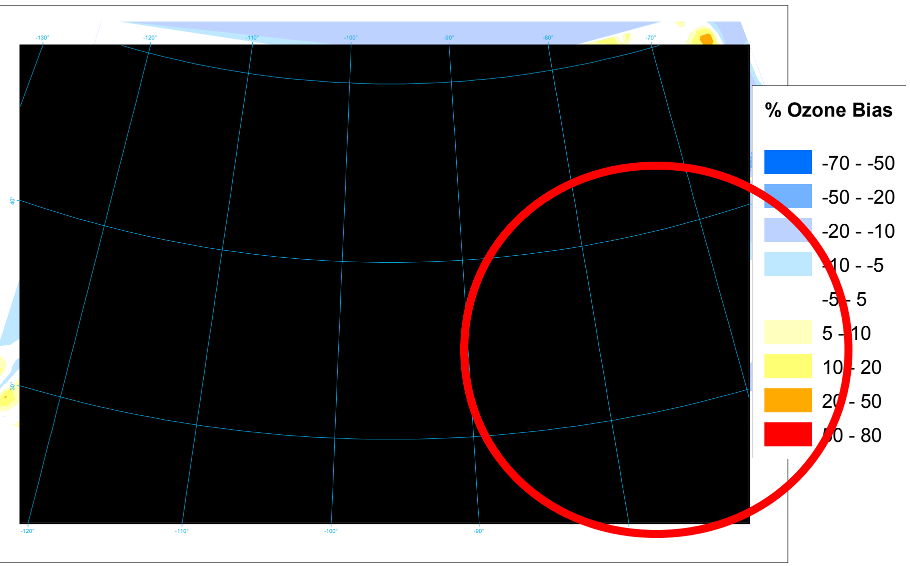


Ozone upper troposphere negative bias corrected by boundary conditions

Surface bias corrected by correcting NO_y and dry deposition rates

Figure 3: Observed and 60km-simulated O3, CO, and NOy vertical profiles and standard deviations for all DC-8 flights..

Model bias: Forecast, NEI1999



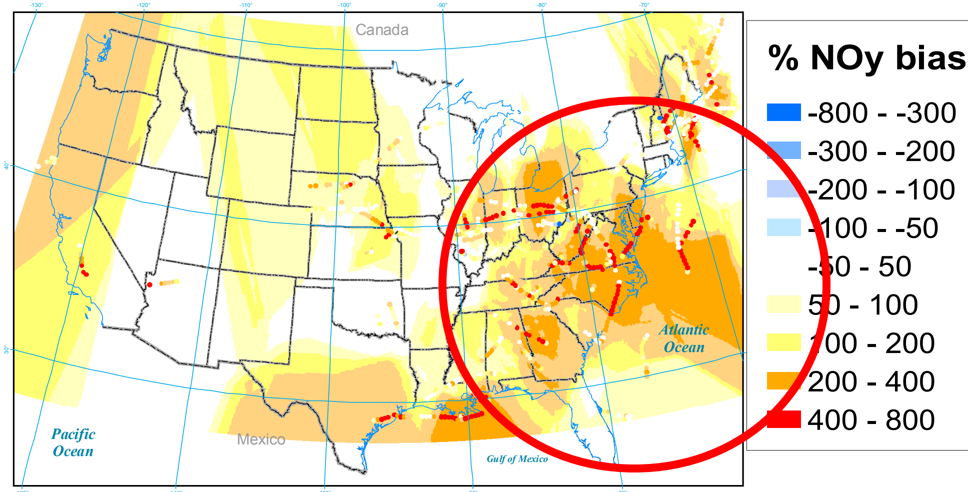


Figure 4. Interpolated percent bias (modeled-observed) for alt<4000m, DC-8 platform,Left: O_3 (n=1208) Right: NO_y (n=902). Wrong dry deposition rates.

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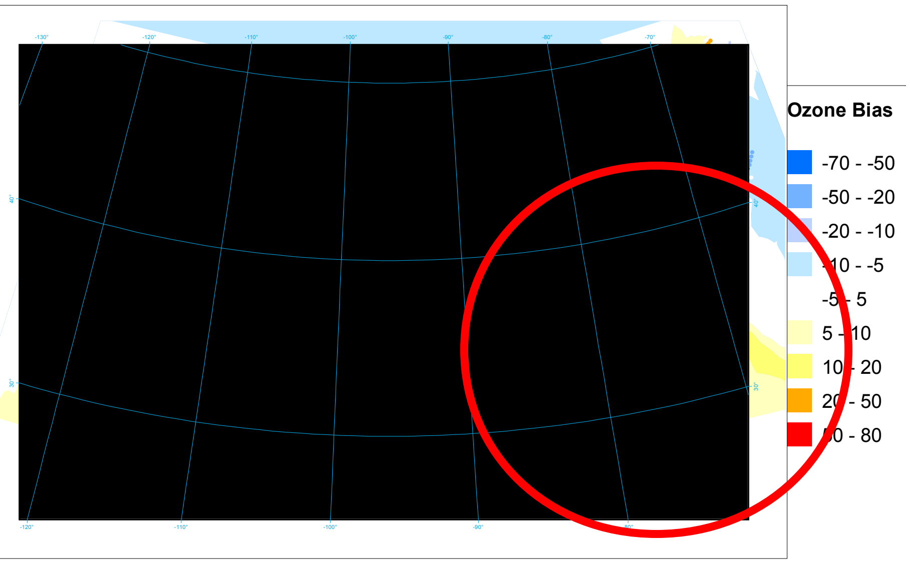
Model bias: NEI2001-Frost LPS



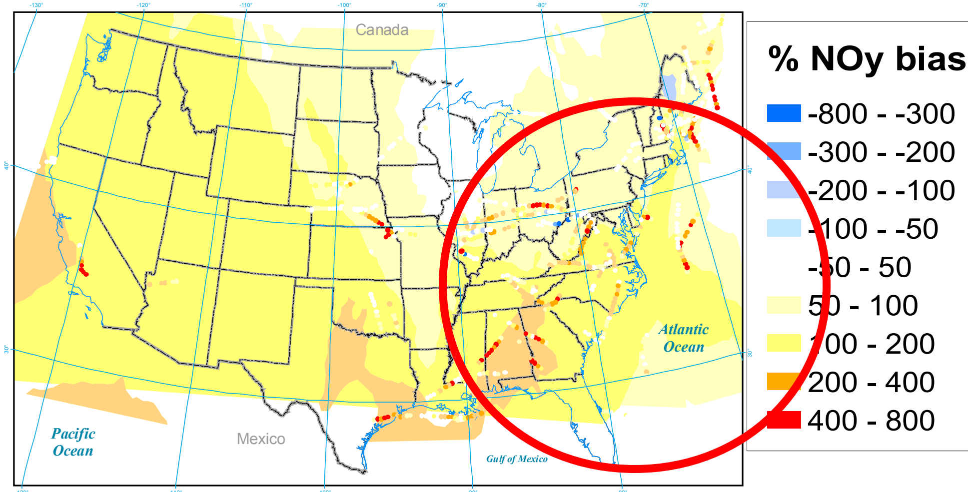


Figure 5. Interpolated percent bias (modeled-observed) for alt<4000m, DC-8 platform,Left: O_3 (n=1208) Right: NO_y (n=902). Post-analysis. Adjusted dry deposition rates, NEI2001- Frost Large Point Sources.

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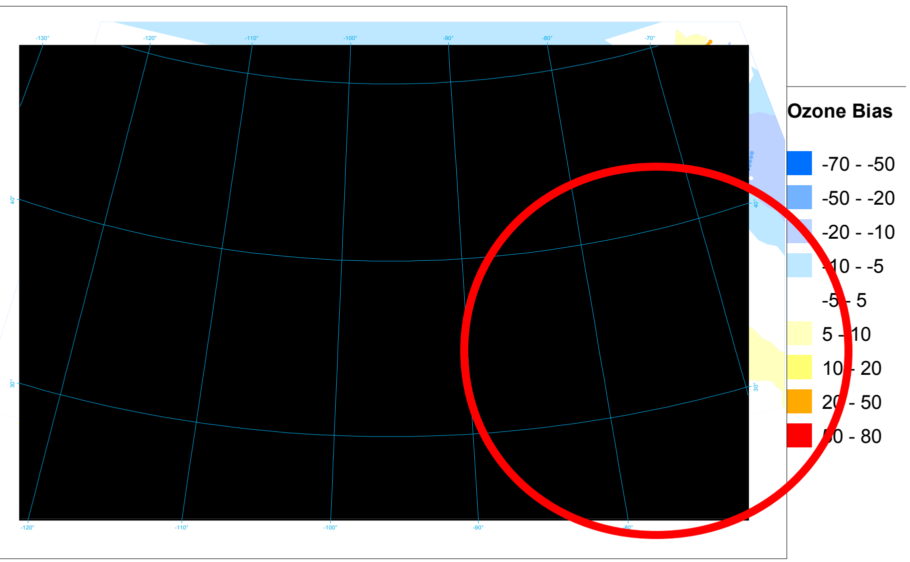
Model bias: NEI2001-FrostLPS*



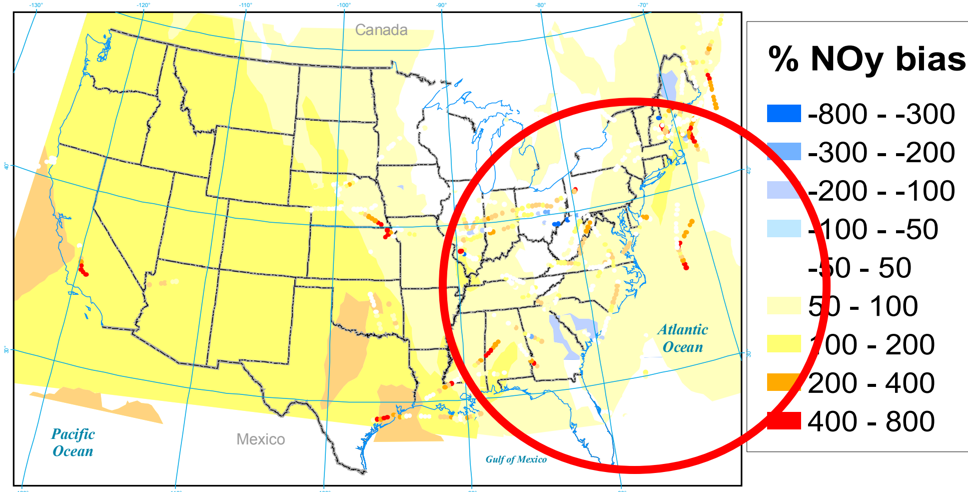


Figure 6. Interpolated percent bias (modeled-observed) for alt<4000m, DC-8 platform,Left: O_3 (n=1208) Right: NO_y (n=902). Post-analysis. Adjusted dry deposition rates, NEI2001- Frost Large Point Sources. Reduced area sources of NO_x by 60% for SE states.

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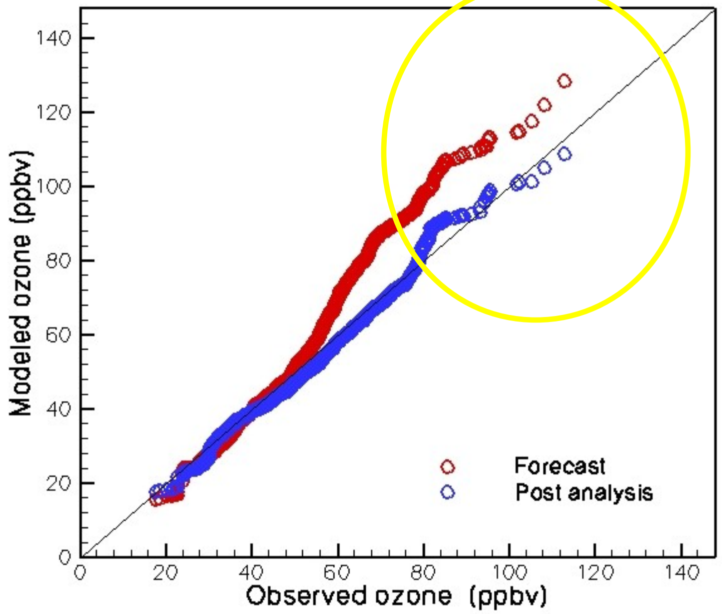
Quantile Quantile plots document improvement



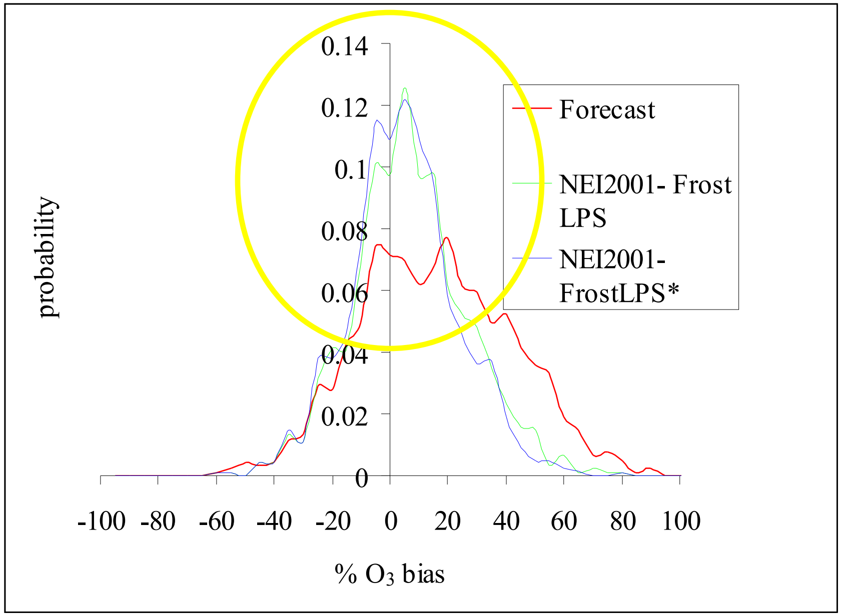


Figure 7 Left: Quantile-quantile plot of modeled ozone with observed ozone for DC-8 platform, data points collected at altitude less than 4000m, STEM-2K3, Forecast: NEI 1999, Post Analysis: NEI2001-Frost LPS*. MOZART-NCAR boundary conditions Right: Probability distribution of % ozone bias for Forecast (NEI 1999) and post analysis runs (NEI2001-FrostLPS and NEI2001-FrostLPS*) for DC-8 measurements under 4000m.

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Model performance statistics for selected species. Modeled vs. Observed data, DC-8 Platform.0-4km range. Frost LPS: NEI2001-FrostLPS. Frost LPS*: NEI2001-Frost LPS-Modified

Table 3. Model Performance Statistics for Selected Species[a]

	O_3				CO				NO_y			
	Forecast	Frost LPS	Frost LPS*	Obs	Forecast	Frost LPS	Frost LPS*	Obs	Forecast	Frost LPS	Frost LPS*	Obs
					0–1 km							
Mean modeled, ppbv	60.12	51.82	50.36	48.92	148	136	136	138	4.16	3.24	2.95	1.85
Mean bias, ppbv	11.21	2.90	1.45	–	9.75	−2.48	−1.84	–	2.70	1.40	1.11	–
S.D./mean modeled	0.39	0.34	0.33	0.33	0.36	0.29	0.27	0.28	0.77	0.66	0.67	0.92
R	0.71	0.70	0.72	–	0.61	0.68	0.68	–	0.59	0.59	0.56	–
					1–4 km							
Mean modeled, ppbv	58.97	54.68	53.32	57.34	131	127	125	119	2.76	2.26	2.09	0.93
Mean bias, ppbv	1.63	−2.66	−4.02	–	11.37	5.20	5.82	–	1.83	1.36	1.19	–
S.D./mean modeled	0.31	0.26	0.25	0.20	0.14	0.11	0.11	0.26	0.87	0.74	0.72	0.88
R	0.40	0.48	0.50	–	0.49	0.65	0.65	–	0.49	0.52	0.51	–
					4–12 km							
Mean modeled, ppbv	63.71	67.97	67.89	80.20	79	85	85	98	0.46	1.43	1.43	1.05
Mean bias, ppbv	−16.49	−12.23	−12.31	–	−19.37	−12.64	−12.60	–	−0.59	0.43	0.42	–
S.D./mean modeled	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.20	1.25	1.37	1.37	0.60
R	0.56	0.47	0.47	–	0.06	0.33	0.33	–	−0.13	0.10	0.10	–

[a]Modeled versus observed data, DC-8 platform. 0–12 km range. Frost LPS: NEI2001-FrostLPS. Frost LPS*: NEI2001-Frost LPS*. Modified area NO_x emissions. SD, standard deviation.

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MILAGRO 2006

MIRAGE-Mex
NASA DC-8

MIRAGE-Mex
NSF C-130, KingAir

MAX-Mex
DOE G-1, KingAir

MCMA-2006
CENICA

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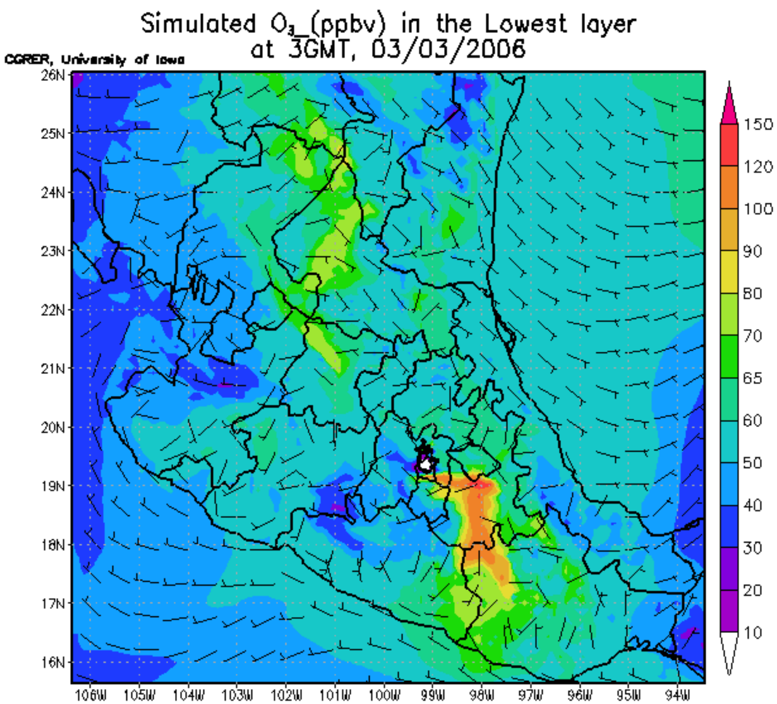
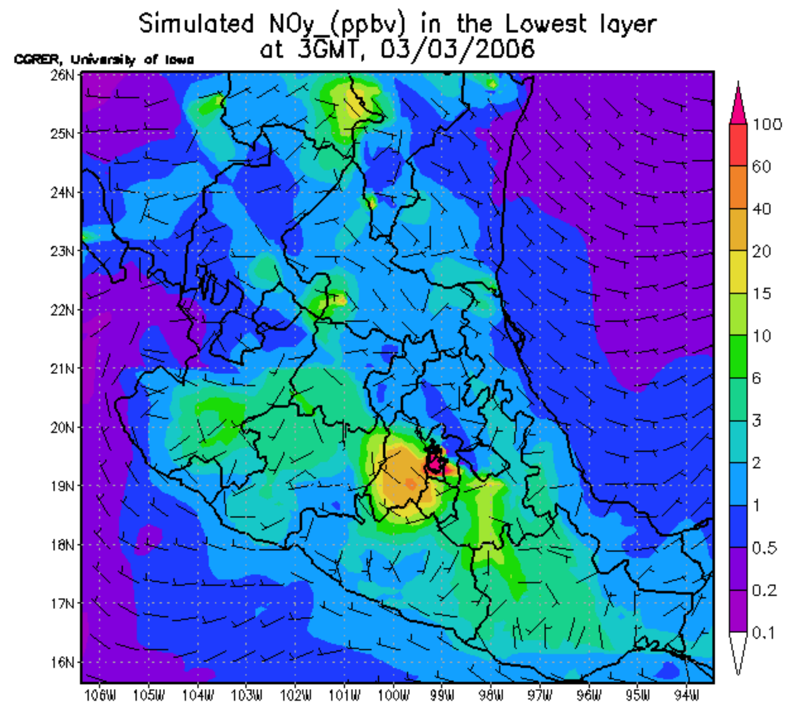
Air quality forecast during campaign March 04-07, 2006





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Model statistical performance from comparison of C-130 1m averaged observations to interpolated model output (12km STEM)

F run: Forecast, base emissions. **RAQMS BC and biomass burning**

G run: Post-analysis, **MOZART NCAR BC**, base emissions.

I run: MOZART NCAR BC reduced emissions of NO_x ,VOC.

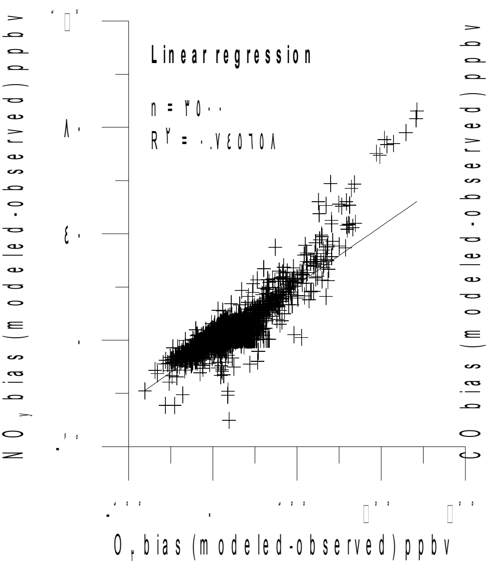
Table 1. Model performance statistics for selected species during MILAGRO, C-130 Platform. 0-6km range, flights 1-13. F: RAQMS BC, Base emissions. G: MOZART BC, base emissions. I: MOZART BC, reduced MC emissions(50% NO_x 60-70% VOC reduction).

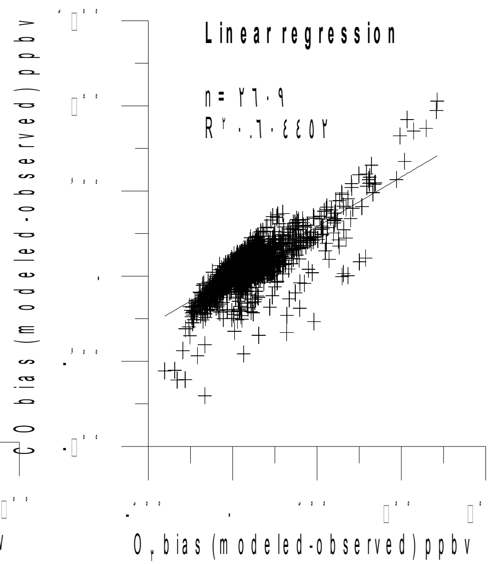
	Obs	F	G	I	Obs	F	G	I	Obs	F	G	I	Obs	F	G	I
Mean	58.73	74.23	71.70	66.12	146.86	179.65	188.66	184.72	1.84	4.22	4.22	1.98	0.27	1.29	1.24	0.34
SD/mean	0.33	0.45	0.44	0.29	0.58	0.57	0.48	0.46	1.77	2.28	2.20	1.84	2.00	2.72	2.68	2.68
R		0.54	0.60	0.58		0.60	0.66	0.67		0.70	0.75	0.75		0.58	0.63	0.64
%Bias		26.40	17.47	10.31		22.33	28.47	25.78		128.80	128.67	7.45		380.97	361.60	26.43
	NO_x				NO				NO_2				NO_y			
	Obs	F	G	I	Obs	F	G	I	Obs	F	G	I	Obs	F	G	I
Mean	0.82	0.52	0.52	0.51	0.16	0.12	0.12	0.12	0.65	0.42	0.39	0.38	2.99	5.15	5.06	3.57
SD/mean	4.40	3.32	3.23	2.70	2.87	3.75	3.77	3.75	2.85	3.14	3.09	2.73	1.53	1.78	1.71	1.45
R		0.62	0.63	0.70		0.45	0.45	0.55		0.66	0.65	0.71		0.61	0.66	0.63
Bias		-36	-37	-38		220	219	210		-36	-39	-41		72	69	19

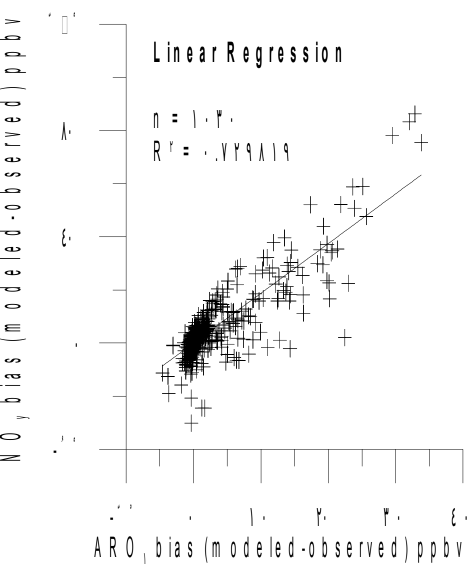
O_3 bias is highly correlated to errors of its precursors.

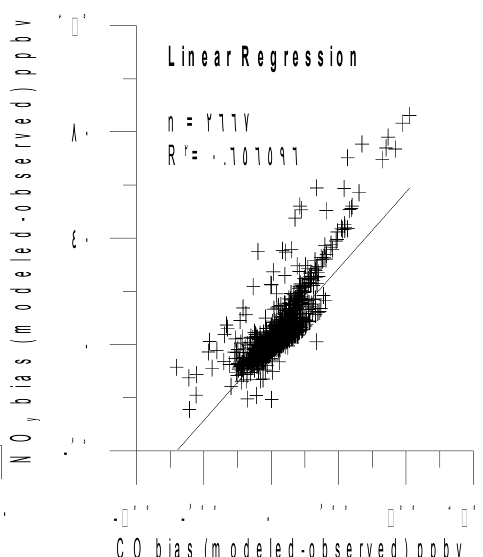
Ozone error correlated to NO_y, CO error.

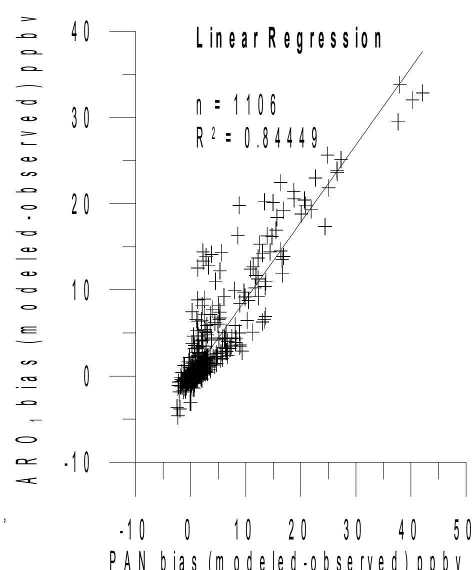
NO_y error correlated to C_3H_8 and ARO_1 errors

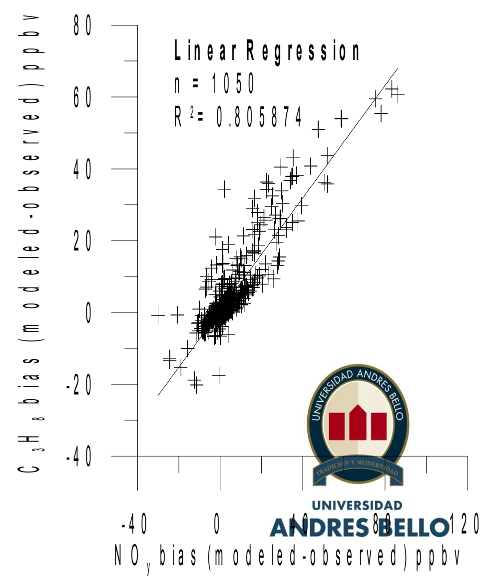












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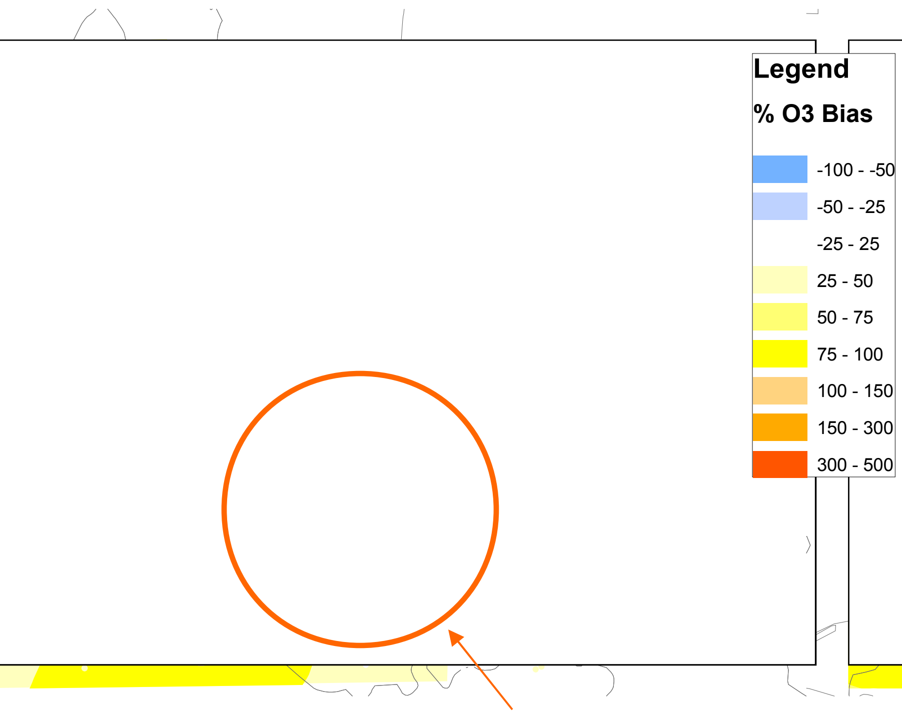
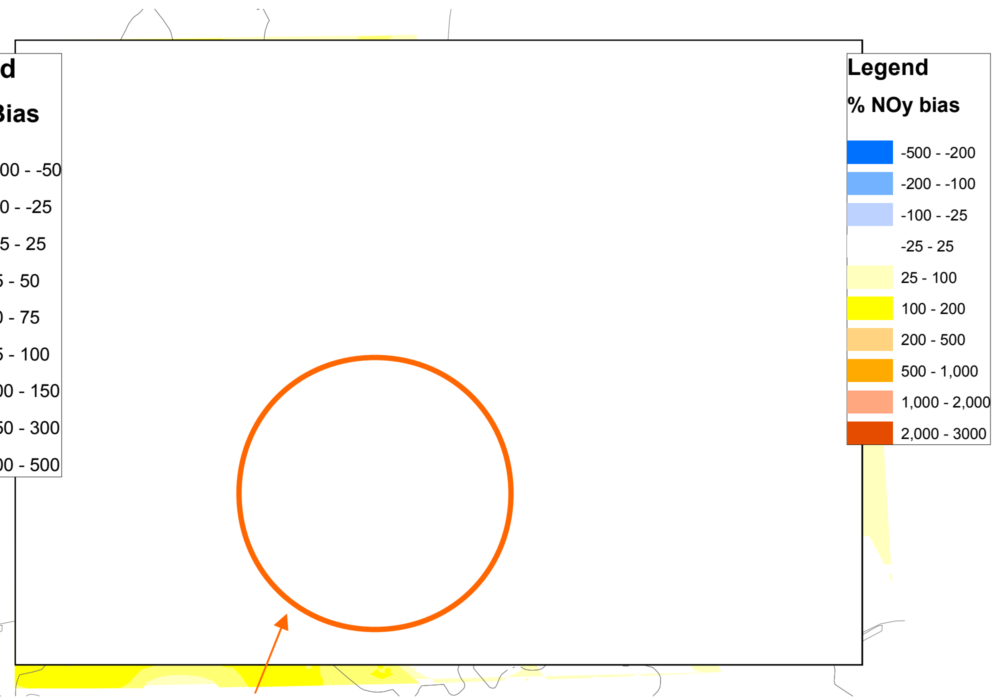
Model bias: Forecast

Figure 8. Interpolated model % bias (modeled-observed) extracted along C-130 flight tracks for MILAGRO. Forecast Model, RAQMS BC, base emissions. 12km STEM, n=5200. Altitude less than 5km ASL.





Correlation among model errors also has geographical structure.

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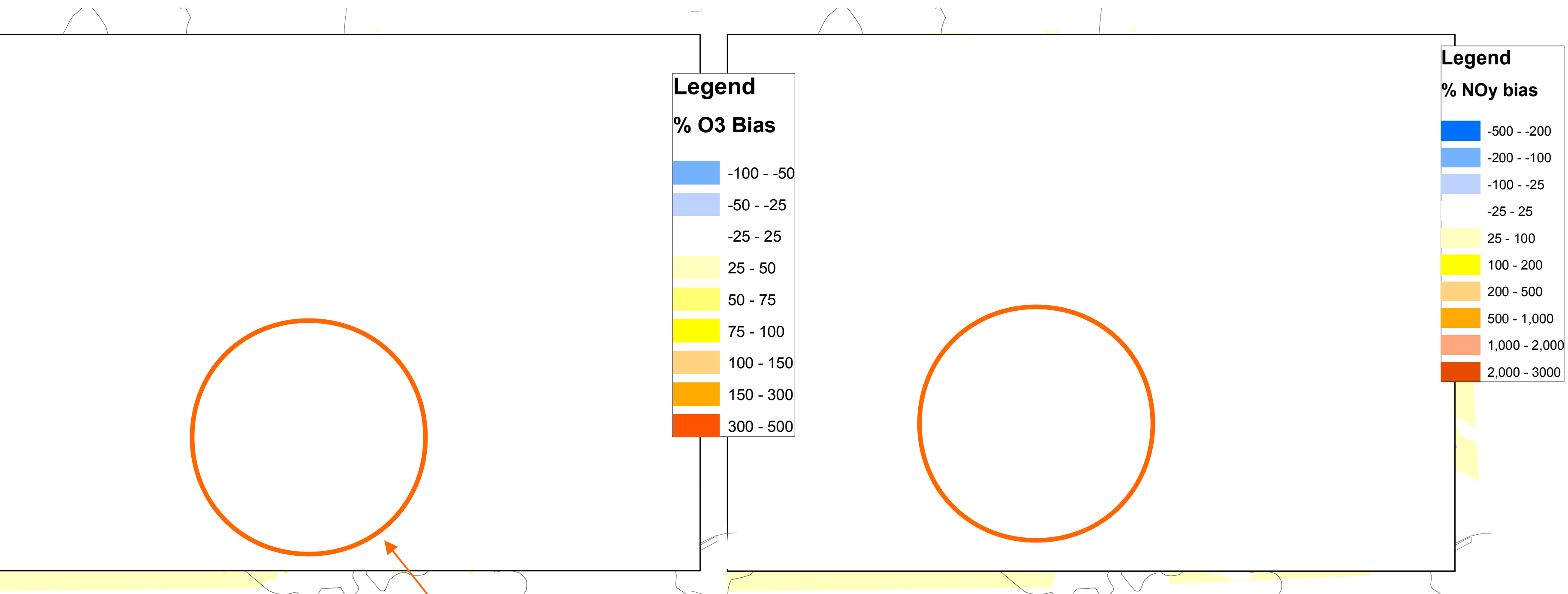
Model bias: Post-analysis

Figure 9. Interpolated model % bias (modeled-observed) extracted along C-130 flight tracks for MILAGRO. Post-analysis run, MOZART BC, reduced MC emissions. . 12km STEM, n=5200, altitude<5km ASL.



Reducing NO_y and VOC bias decreases regional O_3 bias

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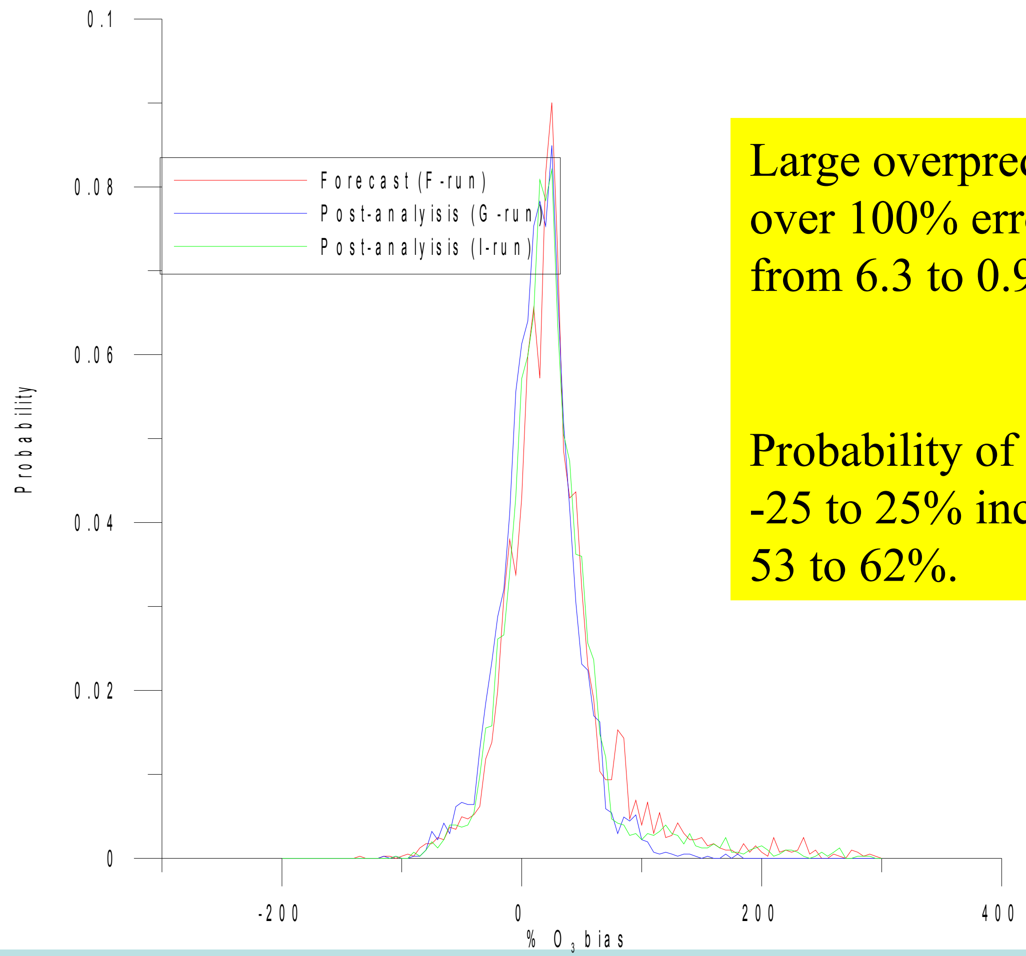
Probability distribution of % ozone bias



Large overpredictions of over 100% error reduced from 6.3 to 0.9%.

Probability of error from -25 to 25% increases from 53 to 62%.

Figure 10 Probability distribution of percent ozone bias for MILAGRO forecast and post analysis runs, based on values extracted along C-130 flight tracks, all altitude ranges.

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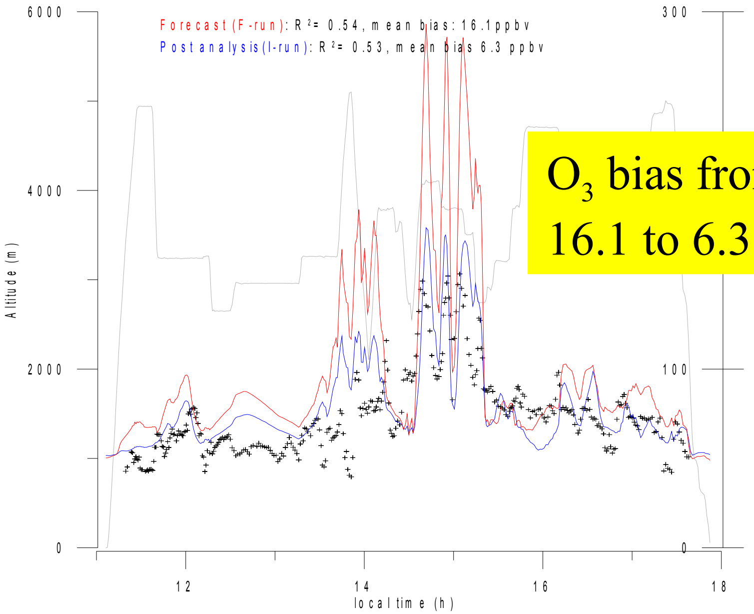
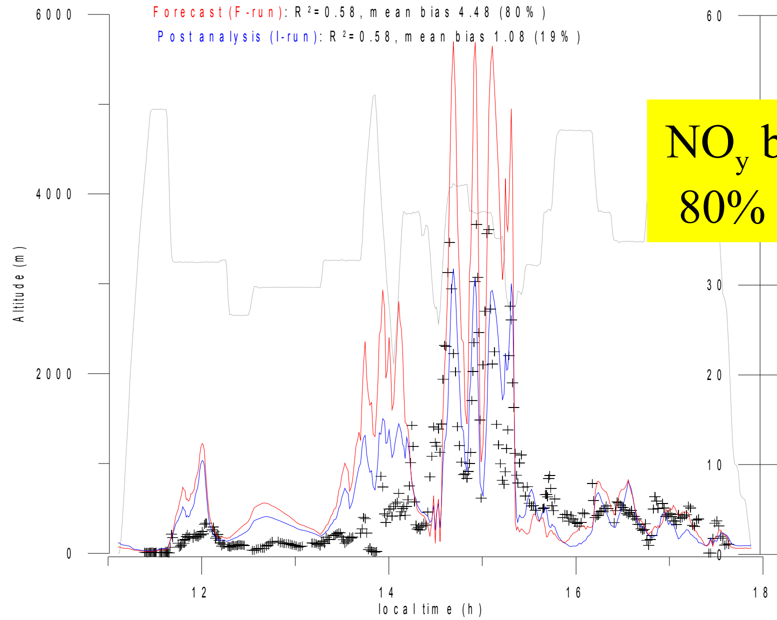
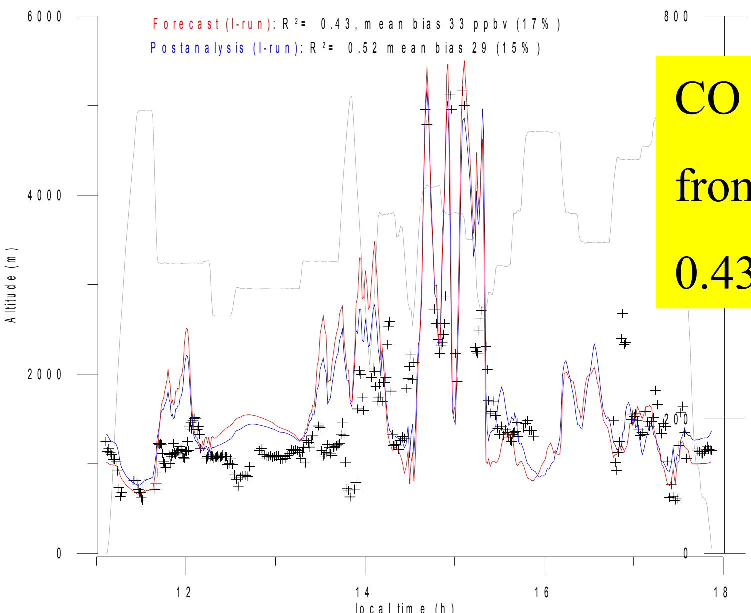
C-130 flight March 08, 2006



O_3 bias from 16.1 to 6.3



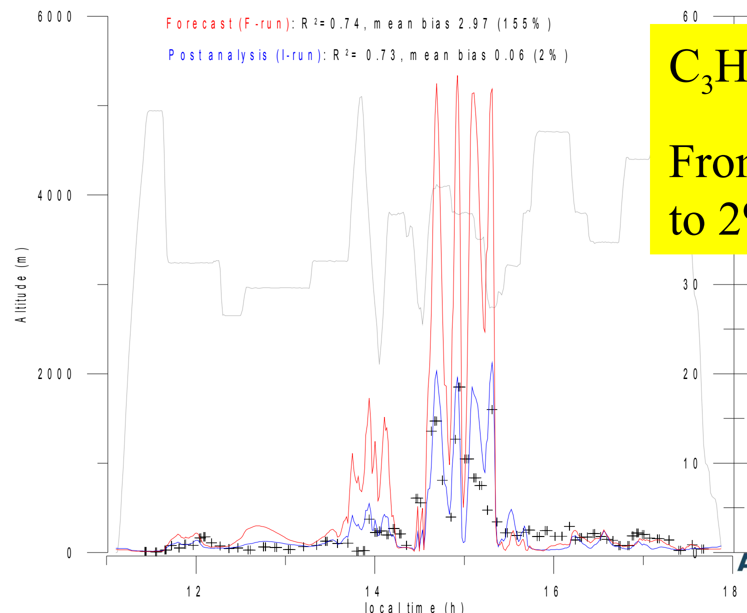
NO_y bias from 80% to 19%



CO R^2

from

0.43 to 0.52



C_3H_8 bias

From 155 to 2%

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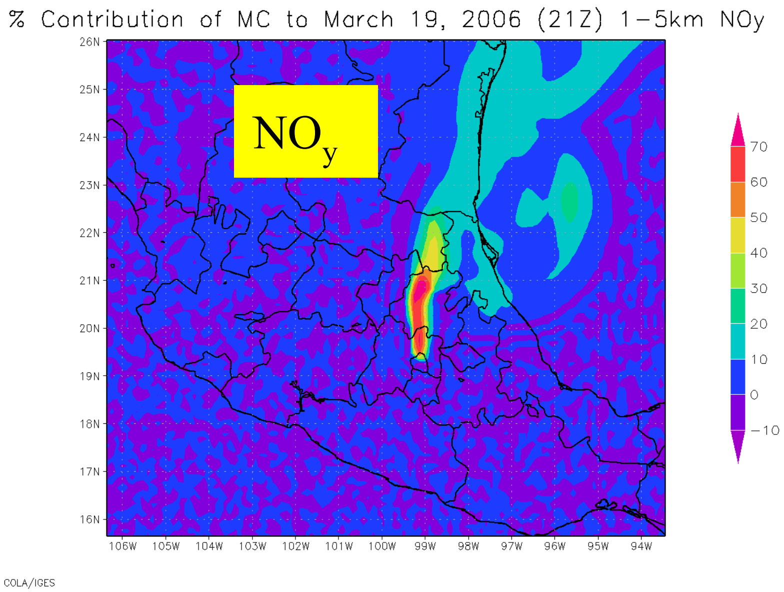
Contribución del DF pluma sobre Golfo de México (Mena-Carrasco et al., 2009, ACP)



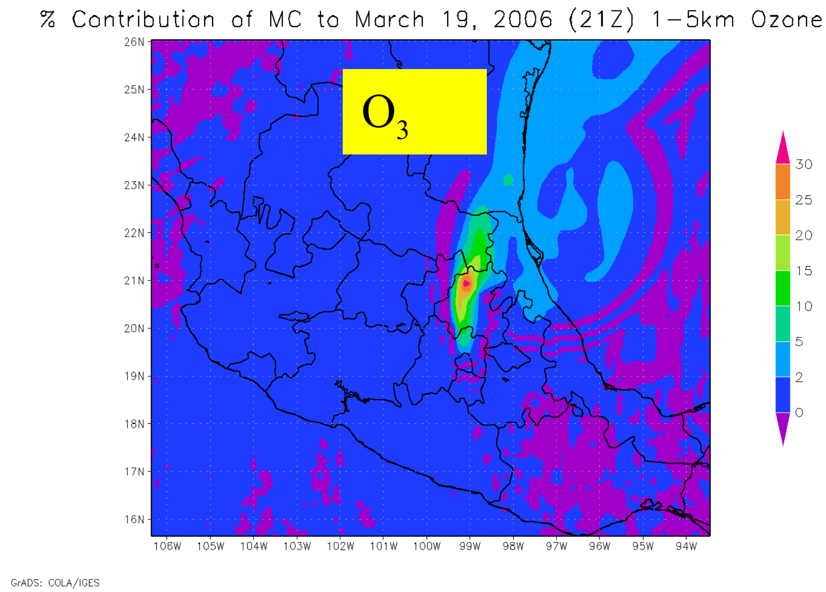


Figura 3. Contribución promedio del DF a ozono y NO_y para 12hrs , Marzo 19, 2006, rango 1-5km altura.

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Interpolación espacial de observaciones a lo largo de vuelo C-130

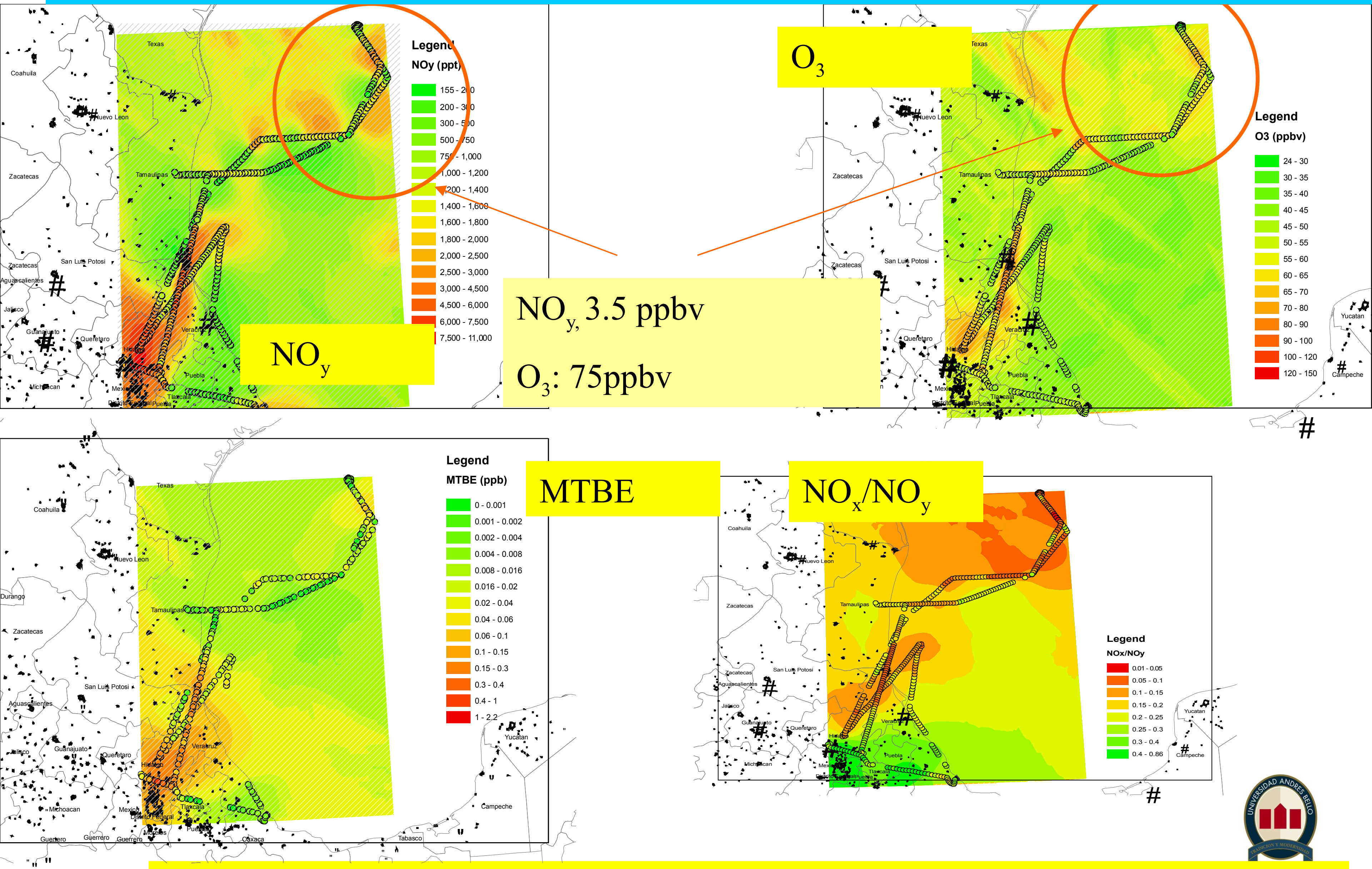
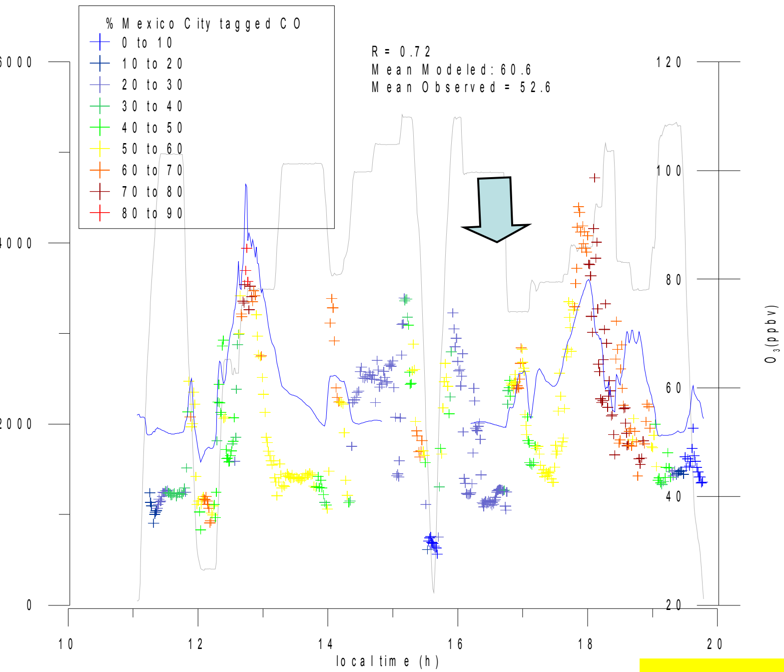


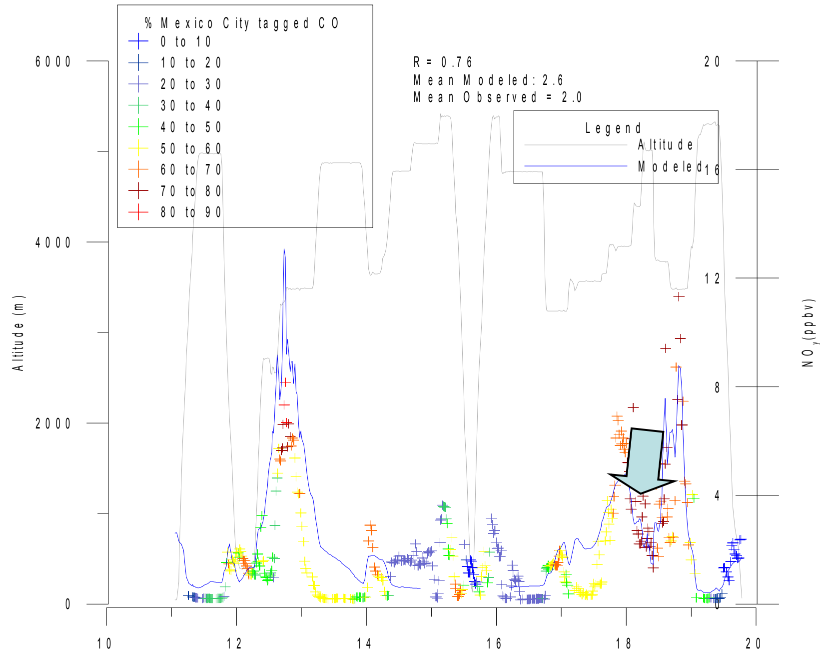
Figura 4. Interpolación de observaciones mediante kriging.

Contribución de DF a datos muestreados

O_3

NO_y





55% de CO viene de DF

Figura 5. Serie de tiempos de valores extraídos a lo largo de vuelo de C-130. Línea azul representa valores modelados. Línea gris representa altura de muestreo. Cruces representan valores observados, colorados de acuerdo a contribución de Ciudad de México a CO.

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Mexico National Emissions Inventory

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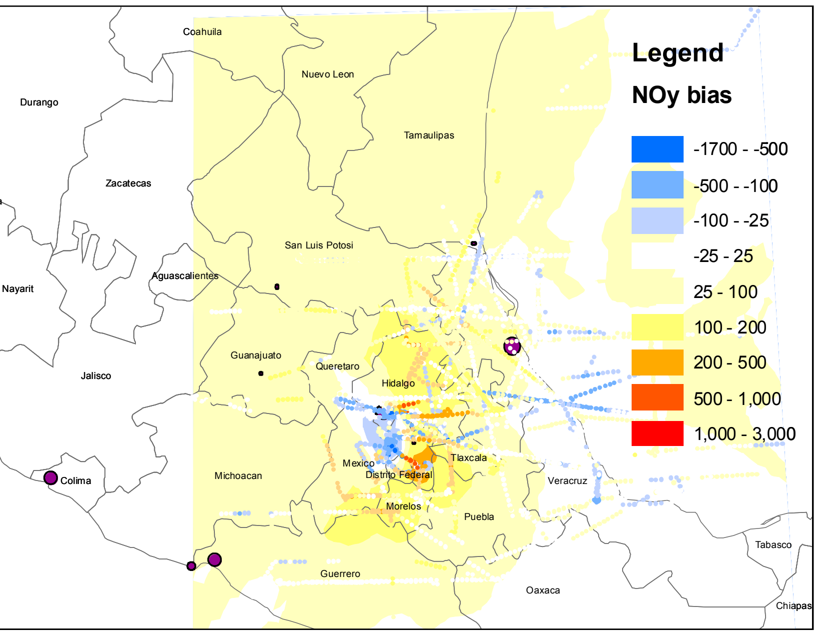
Model performance

Shows great promise in plume placement of regional pollution outside of Mexico City, especially associated to SO_2 and PM



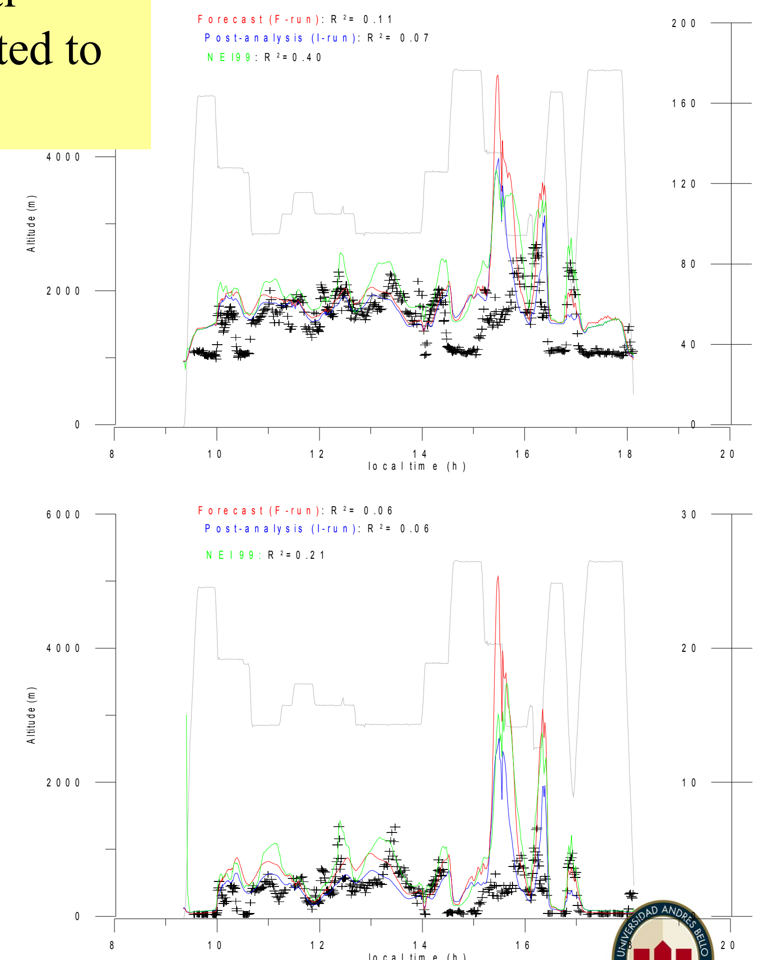
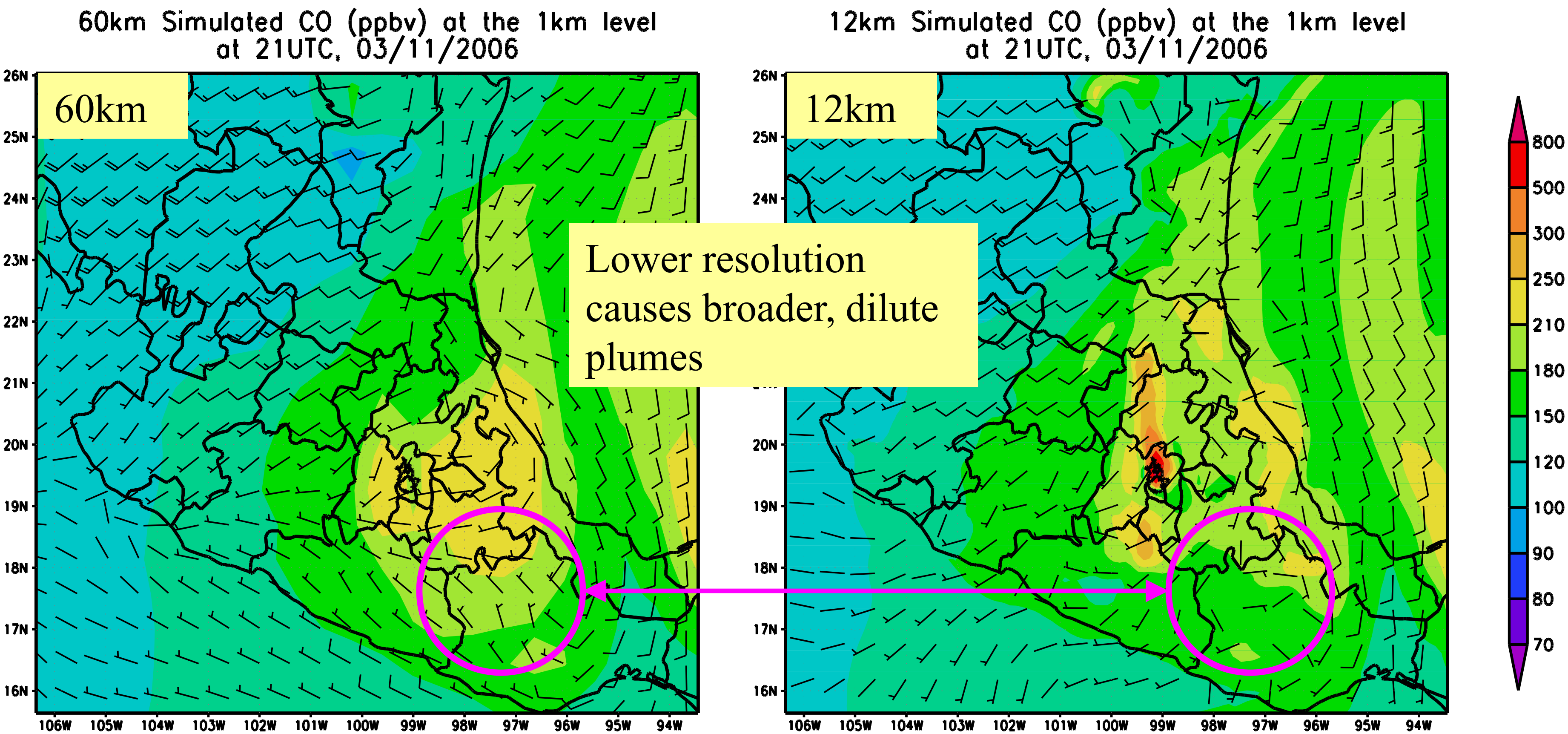


Figure 5. Interpolated model % bias (modeled-observed) extracted along C-130 flight tracks for MILAGRO. Mexico National Emissions Inventory

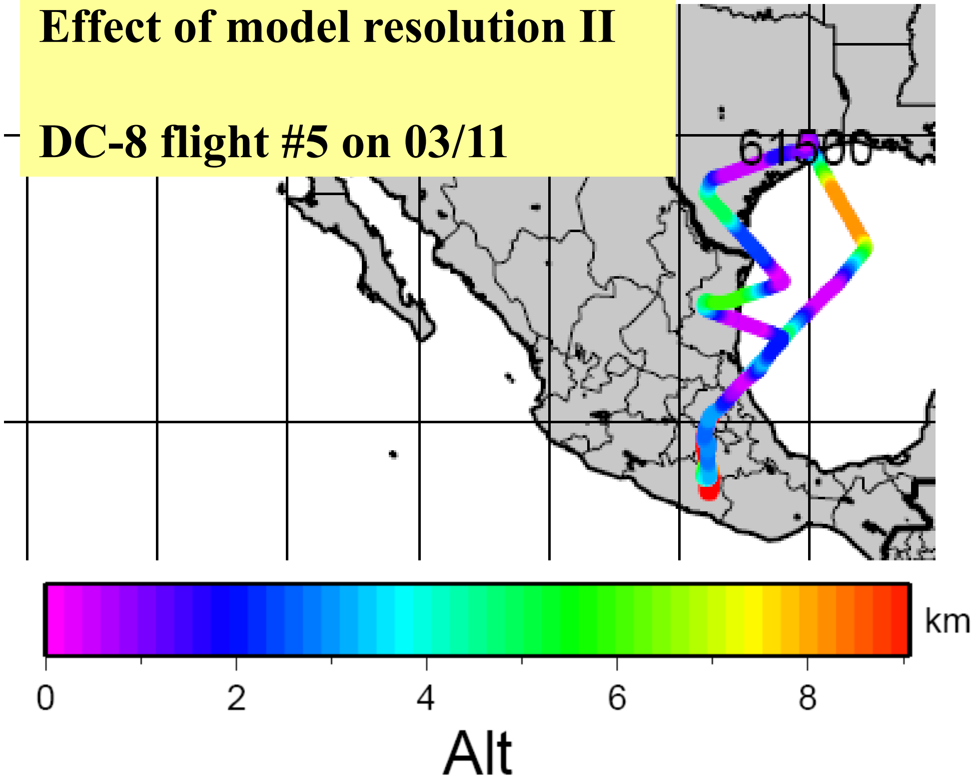
Effect of Model Resolution.

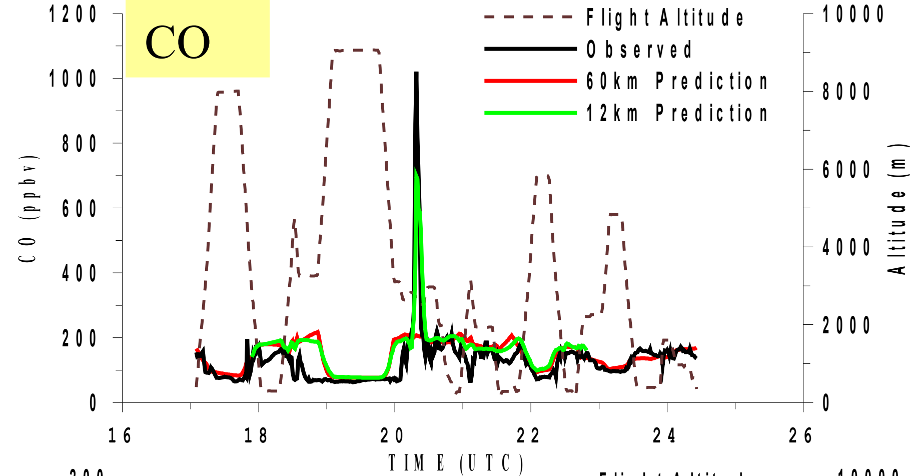


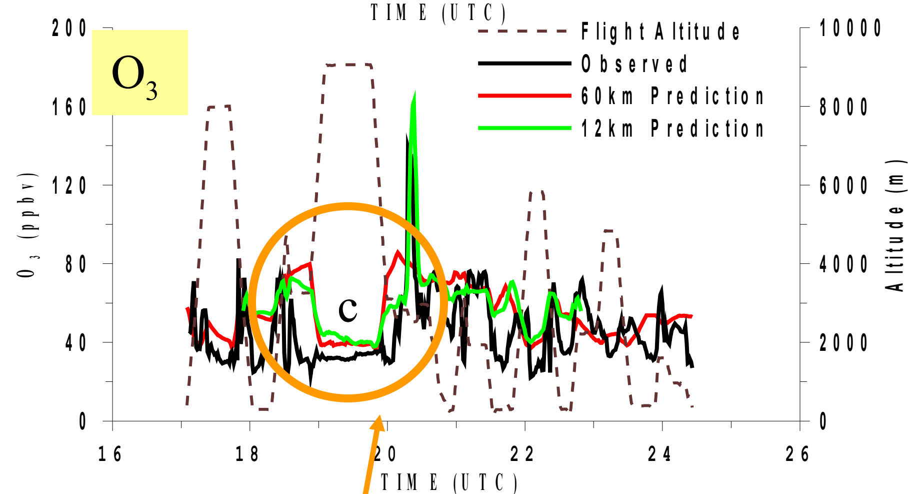
The high-resolution simulation yield different results not only due to the improved resolution of emissions, but also due to the terrain/land use meteorology differences.

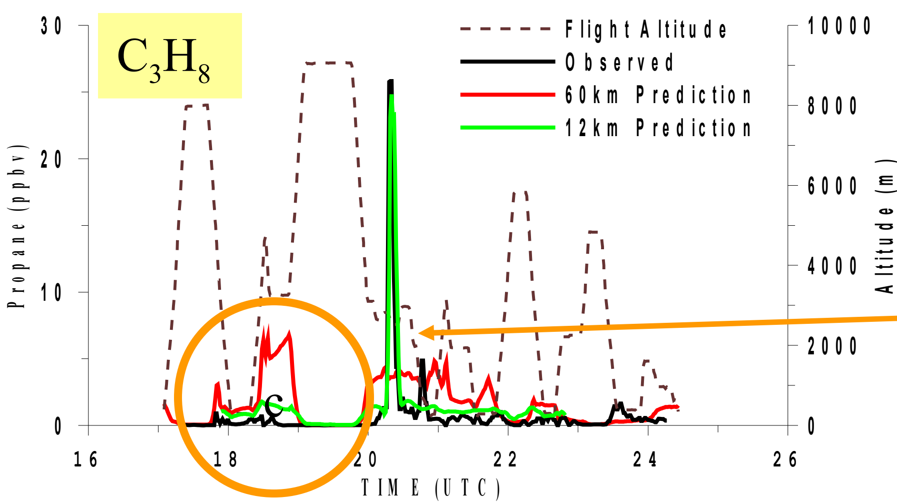
Effect of model resolution II

DC-8 flight #5 on 03/11









Lower resolution causes broader, dilute plumes

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Effect of model resolution on nighttime ozone.

Minimum nighttime for city ~5-10 ppbv (12km) and ~15-20 ppbv (60km)

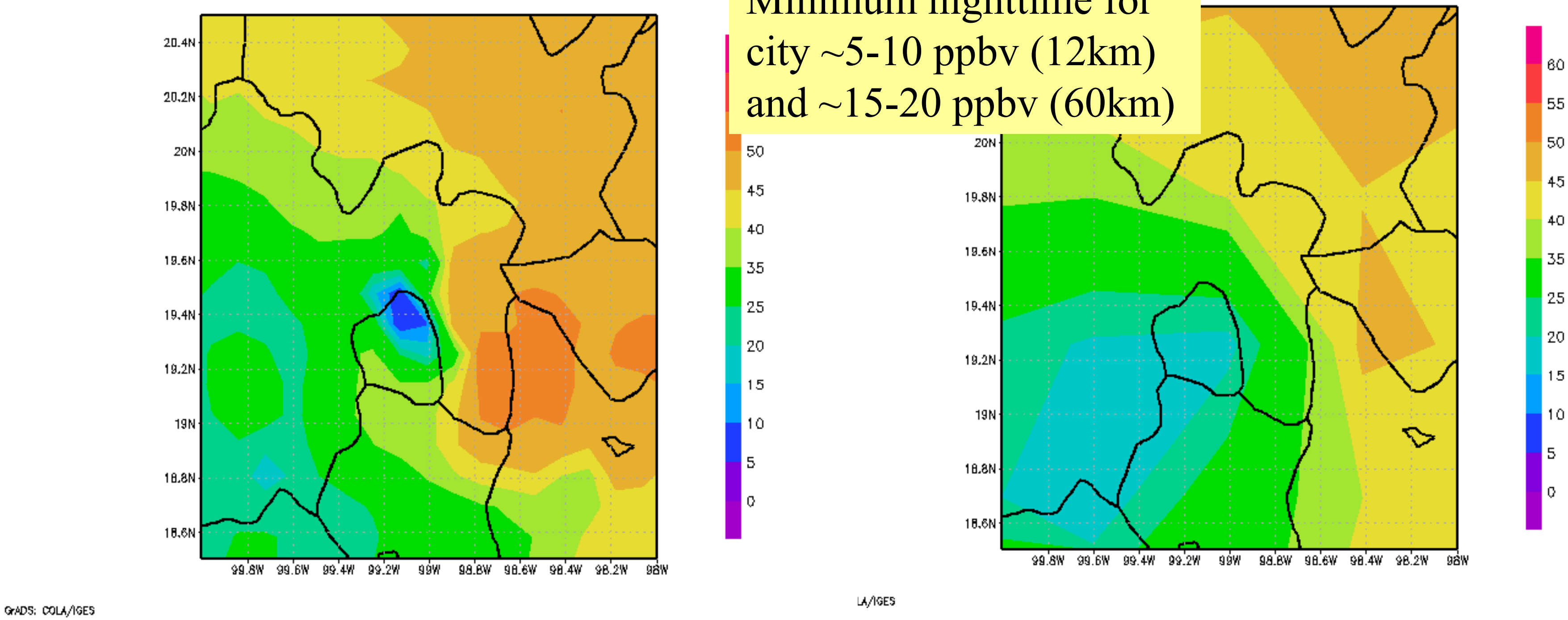

Figure 35 Comparison of mean modeled surface nighttime ozone from March 1-30, 2006 for 60km (left) and 12km (right) model resolutions, I run

Data Assimilation (4DVar)

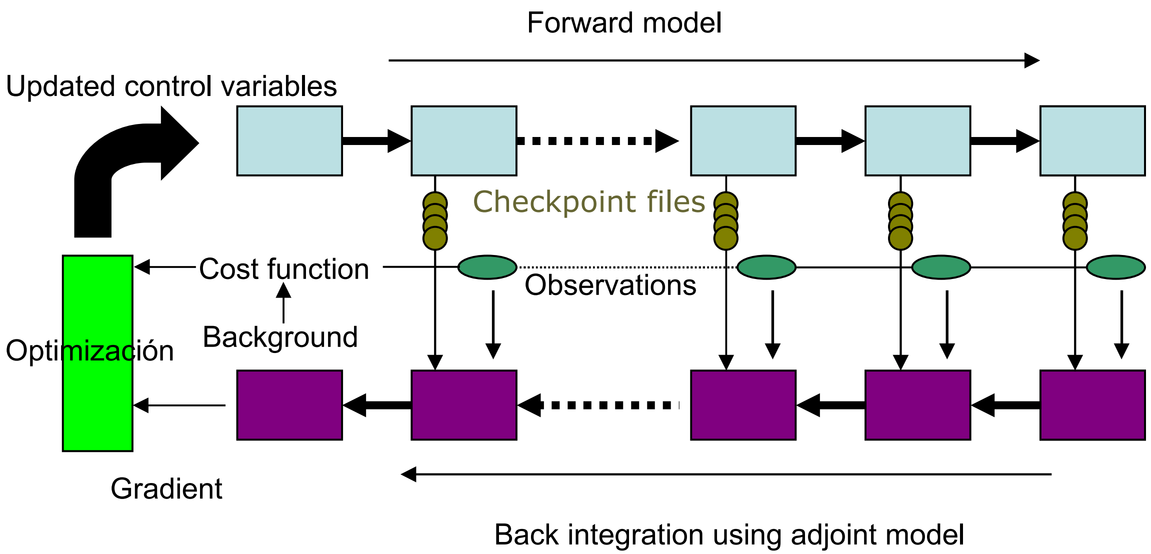

Figure 21 Conceptual model for four dimensional variational data assimilation (Pan et al., 2006)

$$J = \frac{1}{2\mu}[E_f - 1]^T B^{-1}[E_f - 1] + \frac{1}{2}[y - h(c)]^T O^{-1}[y - h(c)]$$

Cost function to recover emission scaling factors.

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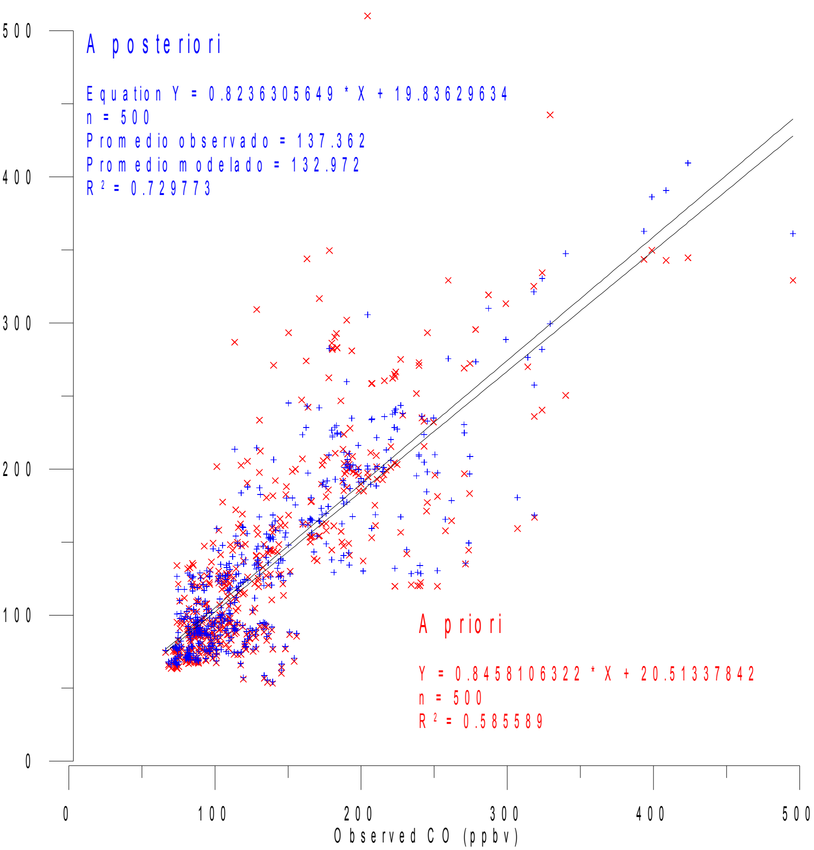
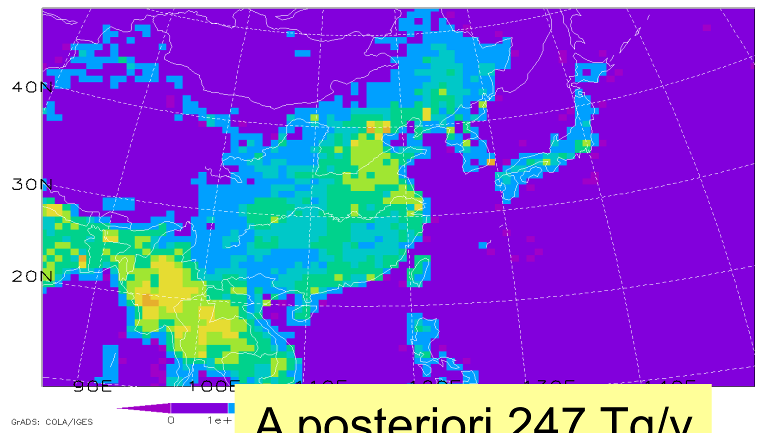
Recovery of emission scaling factors for Trace-P (Marzo 2001) (Mena Carrasco et al., 2008), NASA ACMAP Report

Modeling improvement

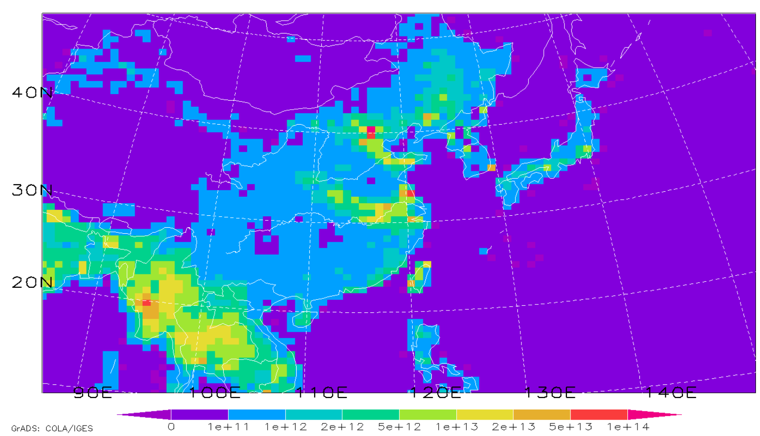


Emissions

A priori 299 Tg/y



A posteriori 247 Tg/y



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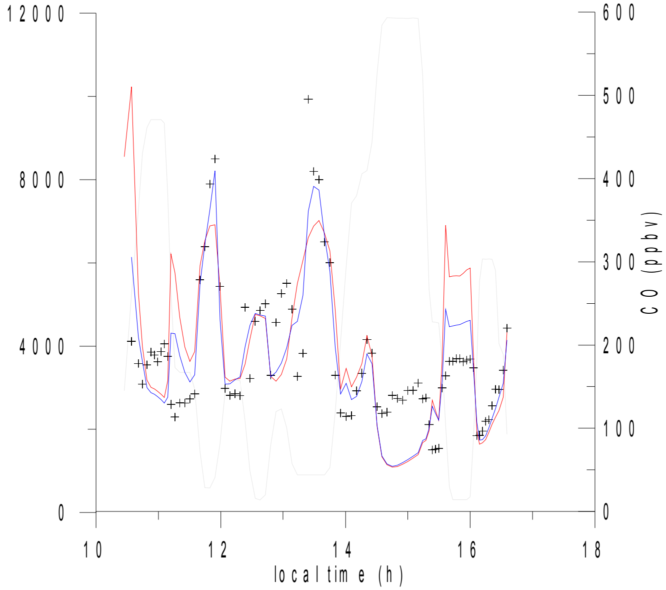
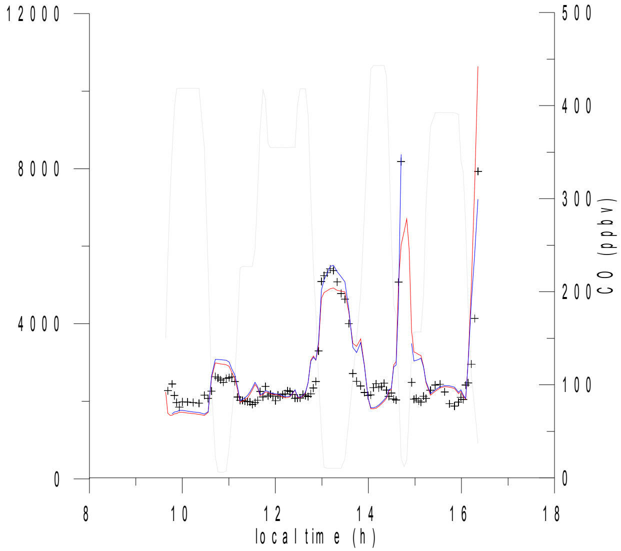
Day to day improvements

- Flight 1
  - A priori : R=0.85
  - Posteriori: 0.92
- Flight 2
  - A priori : R=0.70
  - Posteriori: 0.78
- Flight 3
  - A priori : R=0.93
  - Posteriori: 0.93
- Flight 4
  - A priori : R=0.63
  - Posteriori: 0.83
- Flight 5
  - A priori : R=0.80
  - Posteriori: 0.84





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Comparison of model performance between ICARTT and MILAGRO

	O_3			CO			NO_y		
Parameter	Forecast	Post-1	Post-2	Forecast	Post-1	Post-2	Forecast	Post-1	Post-2
R 0-1km (ICARTT)	0.71	0.70	0.72	0.61	0.68	0.68	0.59	0.59	0.56
R 1-4km (ICARTT)	0.40	0.48	0.50	0.49	0.65	0.65	0.49	0.52	0.51
R (MILAGRO)	0.54	0.60	0.58	0.60	0.66	0.67	0.59	0.66	0.63
Normalized Bias (ICARTT 0-1km)	22.91	5.92	2.6	7.05	-1.79	-1.33	184	76	60
Normalized Bias (ICARTT 1-4km)	2.84	-4.6	7.02	9.50	4.27	4.88	196	151	132
Normalized Bias (MILAGRO)	26	17	10	22	28	25	72	69	19

Model performance during MILAGRO was almost as good, and for some species much better than ICARTT, faster.

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Conclusions

- A method was presented to improve modeling of ozone by systematic analysis of model error using conventional statistics, vertical profiles and horizontal interpolation
- Model improvements were documented for the ICARTT and MILAGRO campaigns. In general ozone bias was highly correlated to bias of its precursors VOC and NO_x.
- Model performance during MILAGRO (hires urban, low res regional) was equal or sometimes better than during ICARTT.

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- Sensitivity studies for ICARTT showed that ozone formation in the United States is most sensitive to increased emission in NO_x. Sensitivities studies for MILAGRO showed that Mexico City is mostly VOC limited, and surrounding areas are NO_x limited.
- Effect of resolution shows that plumes are represented as broader and more dilute using low resolution
- Minimum ozone concentrations at night are dependent on emissions inventory resolution

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