Benchmark Report:

Lateral Chemical Boundary Conditions for CMAQ

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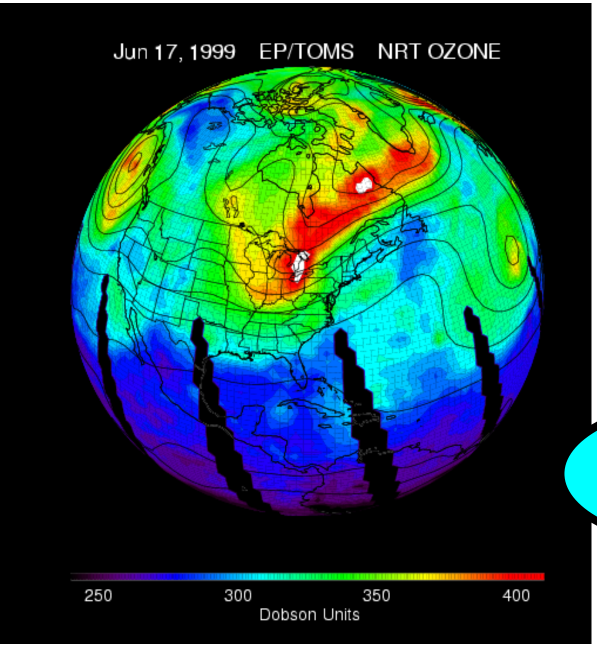
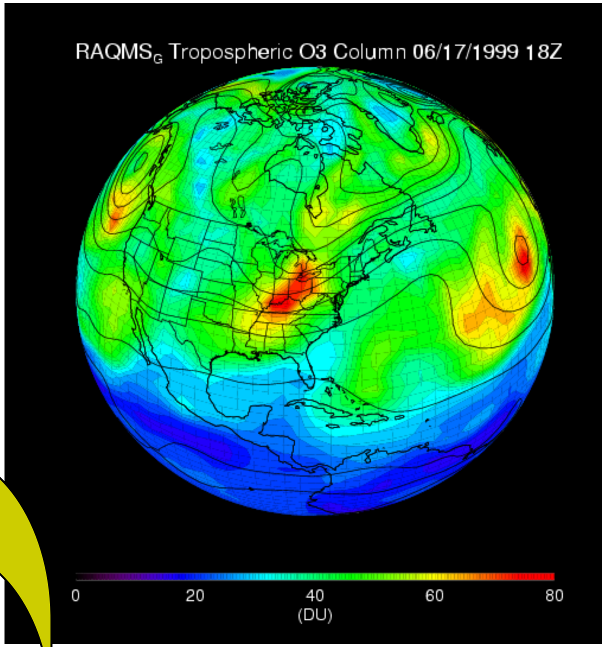
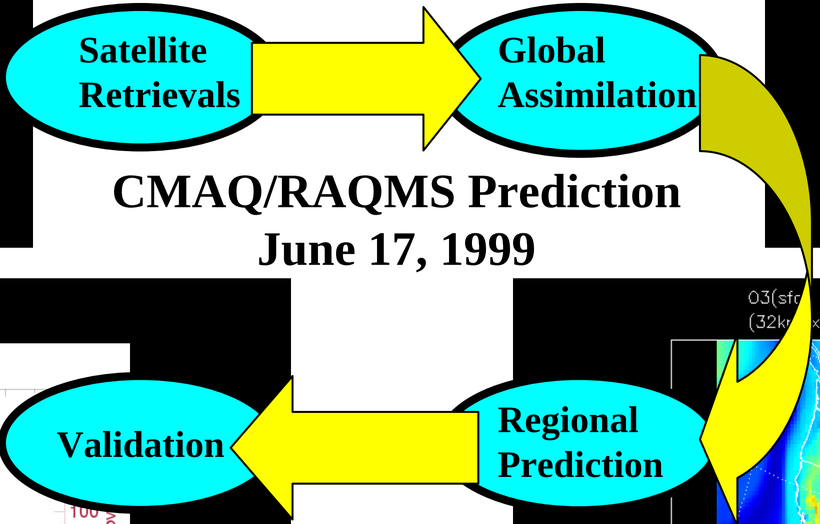
Presented by Daewon Byun (Univ. Houston),

Objective: prototype/evaluate potential for NASA global satellite measurements and data assimilation systems to improve EPA air quality assessment modeling

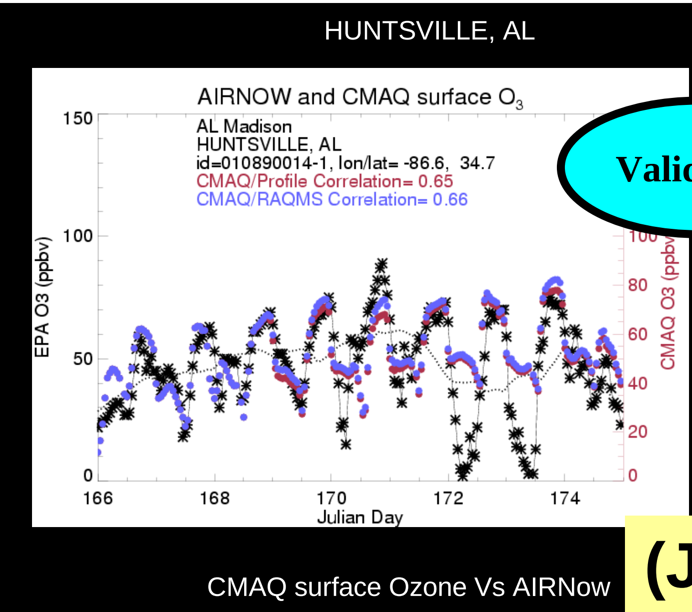


Benchmarking studies conducted in collaboration with EPA/ORD (Alice Gilliland, Ken Schere) and the University of Houston Institute for Multidimensional Air Quality Studies (Daewon Byun) using RAQMS global chemical analyses as lateral boundary conditions for the EPA CMAQ model.

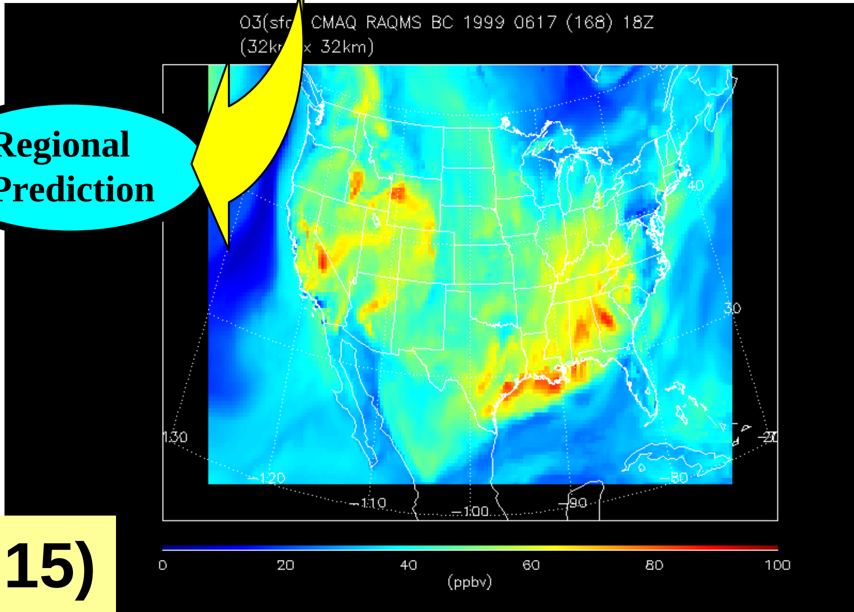




CMAQ/RAQMS Prediction
June 17, 1999



(June 15-July 15)



Overview: DSSs, User/Partners, Earth Science Products

Primary Partners: EPA ORD/NERL
NOAA NESDIS/ORA
University of Houston (UH) /SAIC
University of Wisconsin (UW)

Partner DSS: CMAQ assessment model

Earth Science measurements:
NASA: TOMS, HALOE, SAGE
Partners: POAM, GOES, AIRNow, WMO Sondes

Earth Science models:
NASA: RAQMS modeling system, SDF assimilation
Partners: CMAQ (assessment)

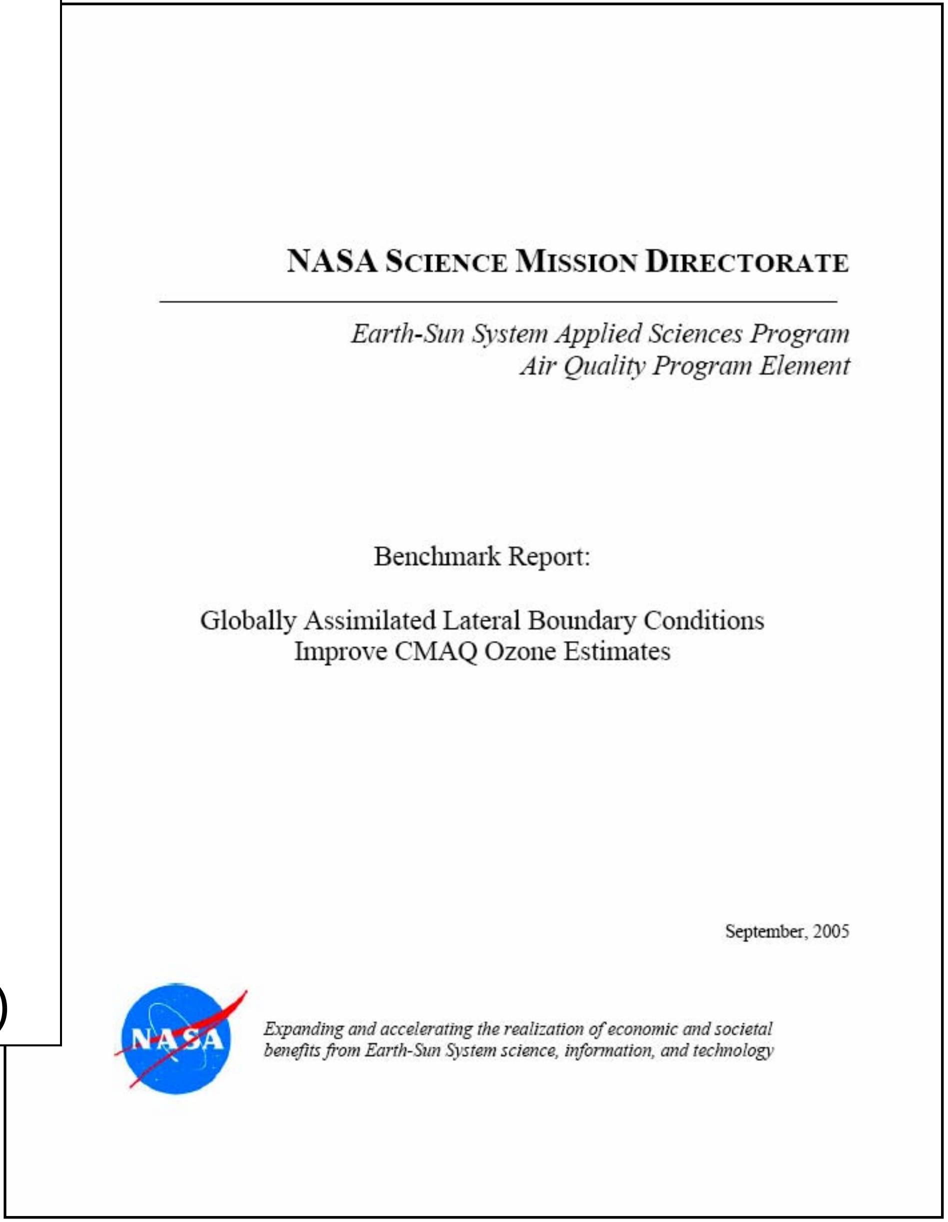
Work was closely linked to 2002-2005 NASA Earth Science Proposal (B. Pierce, PI)

Expected benefits

- **Benefit to partner(s):** Improved constraints on upper tropospheric ozone for EPA assessment modeling
- **Benefit to NASA Earth science:** Utilization of NASA satellite data/modeling tools for Improved understanding of the links between global chemical composition and regional air quality, boundary layer exchange processes, strat/trop exchange; development of modeling/data assimilation tools for linking global and regional satellite measurements
- **Benefit to NASA Applied science:** <u>Benchmark</u> impact of NASA global satellite measurements/data assimilation systems on EPA Air Quality assessment modeling DSS.

Timeline

- Funding started April 2004
- CMAQ assessment runs conducted during 2004 at University of Houston due to EPA resource commitments
- CMAQ/RAQMS task completed and benchmark report submitted September 2005
- Manuscript submitted to JGR, "Song, C.-K., et al., Downscale linkage of global model output for regional chemical transport modeling: Method and general performance" (March 2007)
- Transition to GFS Project (2005 Decisions CAN, FY'07 direct funding)


NASA SCIENCE MISSION DIRECTORATE

Earth-Sun System Applied Sciences Program
Air Quality Program Element

Benchmark Report:

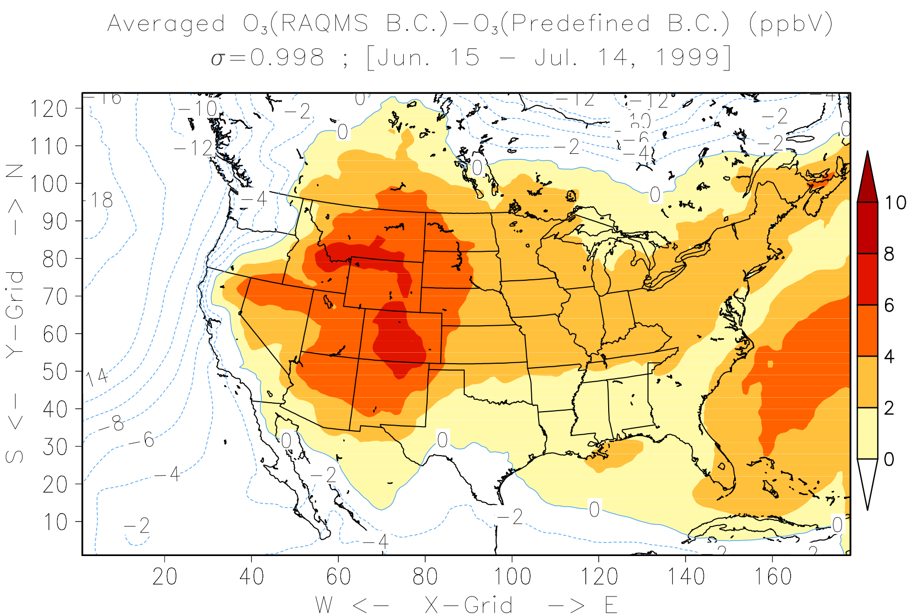
Globally Assimilated Lateral Boundary Conditions
Improve CMAQ Ozone Estimates

September, 2005

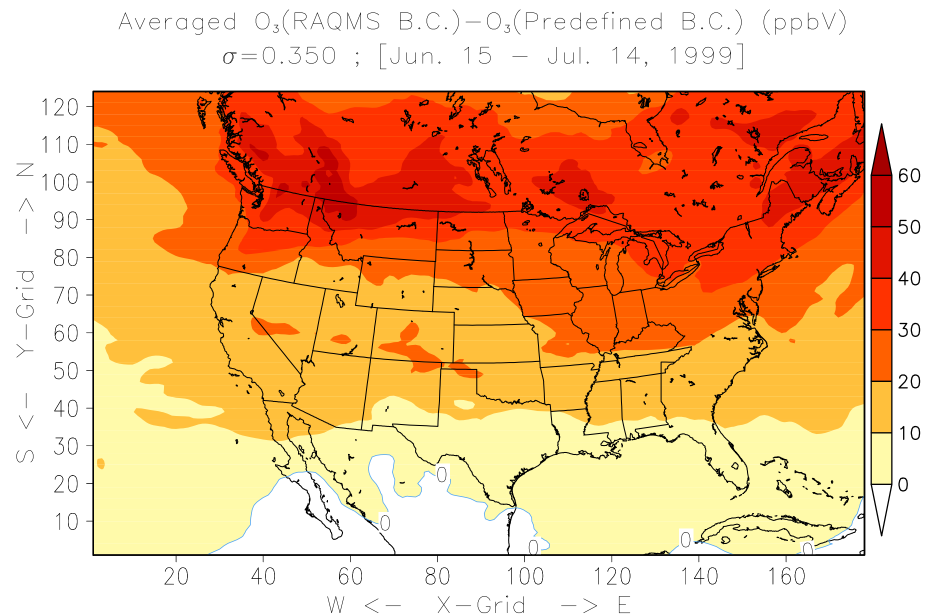
Expanding and accelerating the realization of economic and societal benefits from Earth-Sun System science, information, and technology

Mean Ozone differences (ppbv) between baseline and RAQMS CMAQ June 15-July 15, 1999 assessment

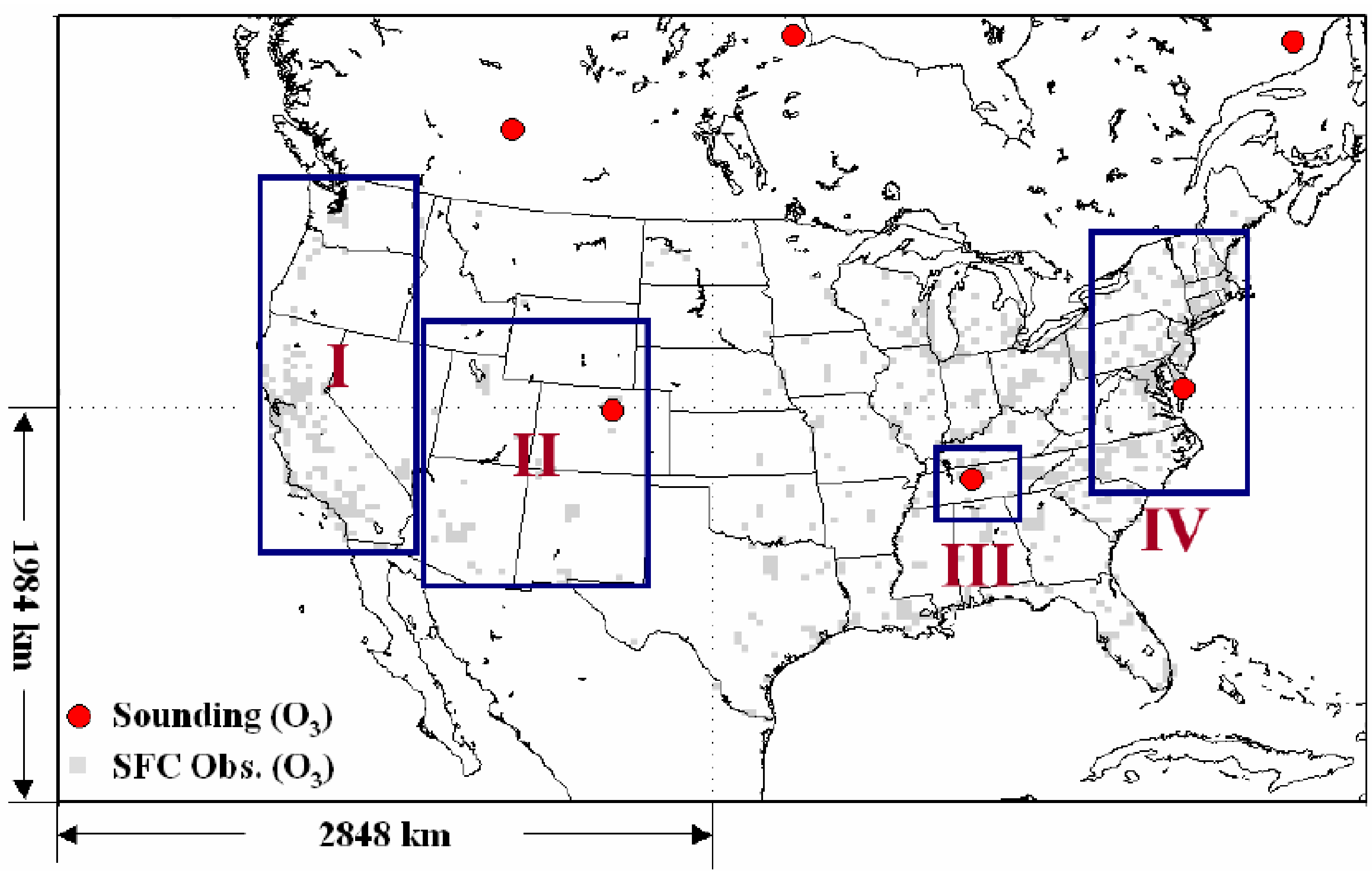
surface (sigma=0.998)



upper troposphere (sigma=0.350)

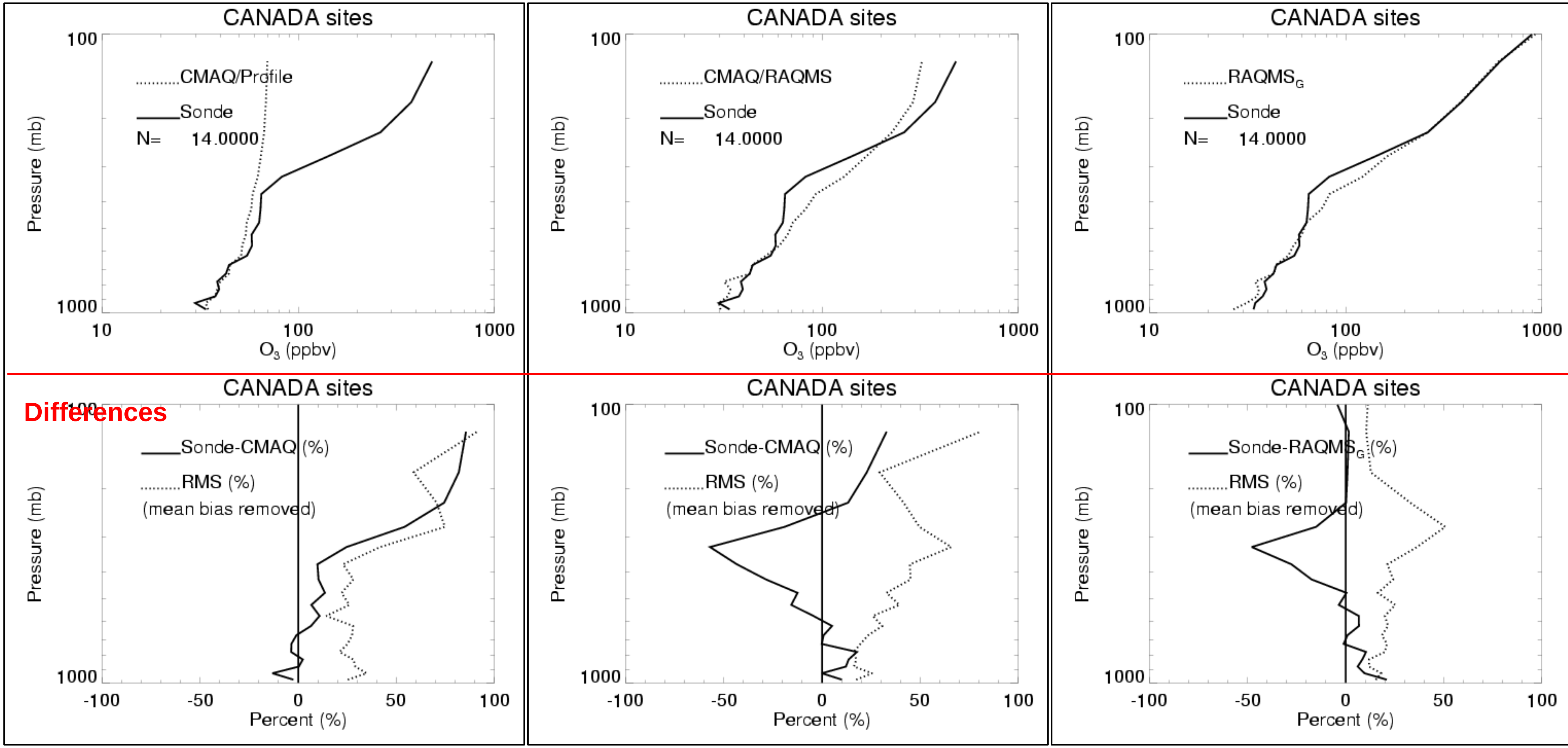


Significant increases in ozone mixing ratios in the upper troposphere and moderate increases in surface ozone mixing ratios over the mountainous regions of the western US when BC from RAQMS are included.


I
II
III
IV
Sounding (O_3)
SFC Obs. (O_3)
2848 km
1984 km

Comparison with Canadian Ozonesonde Data (14 Ozonesondes)

Direct Comparison

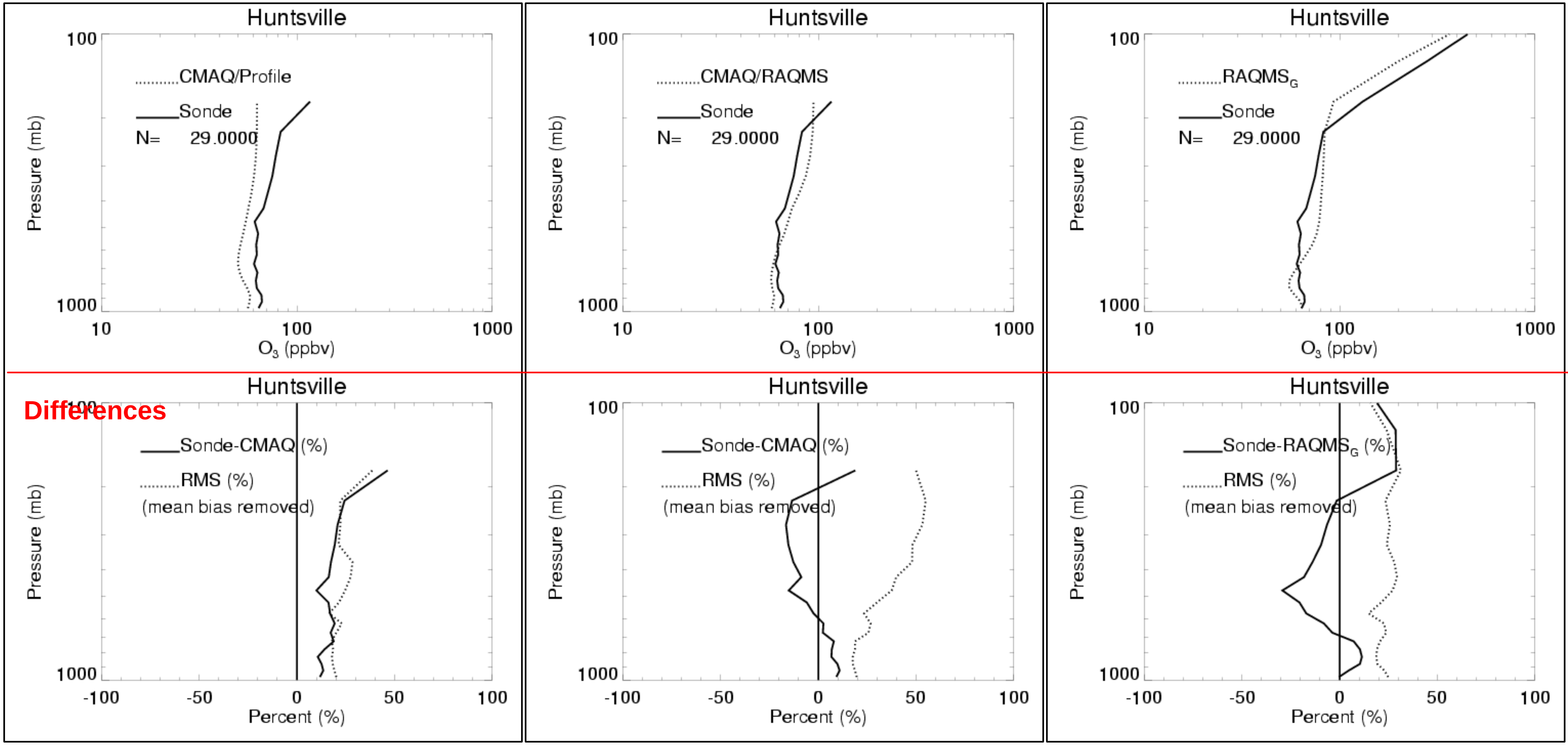


CMAQ/Profile — CMAQ/RAQMS — RAQMS

Comparisons with Canada (Edmonton, Goose Bay, Churchill) ozone sondes show that RAQMS boundary conditions improve CMAQ representation of tropopause ozone profile, increasing biases in the upper troposphere and decreasing biases in the lower stratosphere.

Comparison with Huntsville Ozonesonde Data (29 Ozonesondes)

Direct Comparison

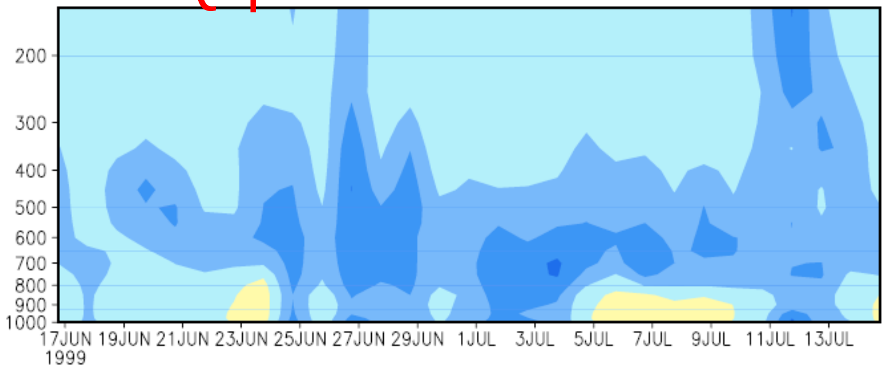


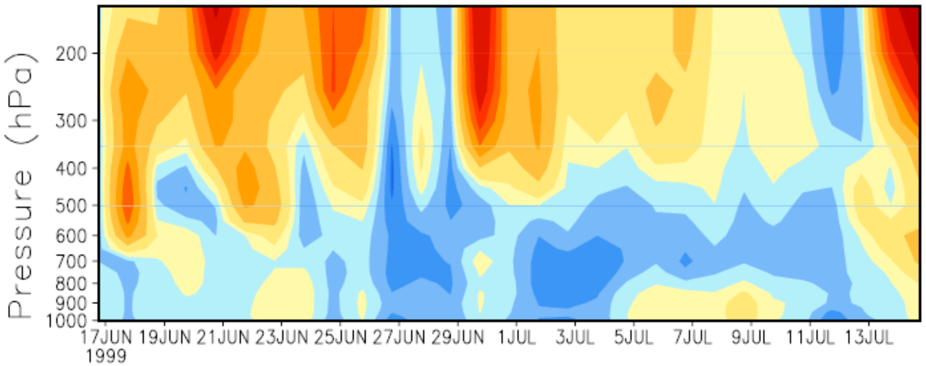
CMAQ/Profile CMAQ/RAQMS RAQMS

Comparison with the ozone soundings indicates that the BC from RAQMS improve the mean CMAQ/Sonde profile comparisons. However, increases in RMS errors in the free troposphere are likely associated with upper troposphere vertical resolution.

Comparison with Ozone Sonde Data for SOS99 (15 June-15 July)

CMAQ-profile





RAQMS-CMAQ

Old Hickory, TN

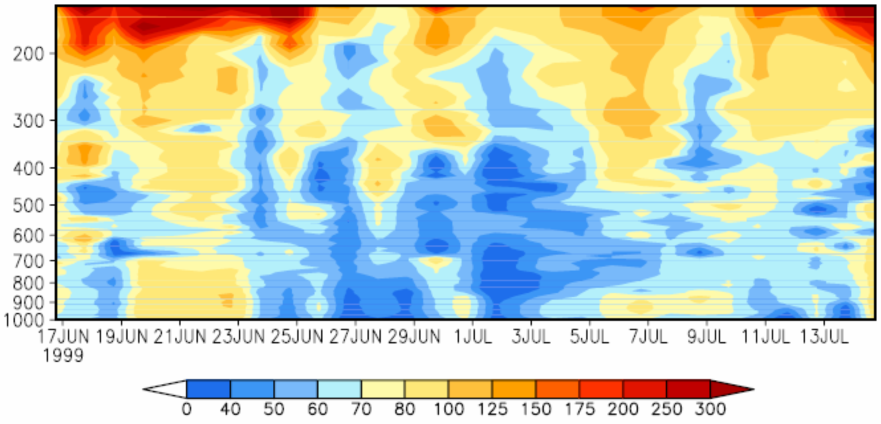


Figure 7f. Model results (CMAQ/Profile; Upper and CMAQ/RAQMS; middle) versus observation Lower) on Old Hickory, TN during SOS-99 period.

Comparison with AIRNow Surface Data

Whole Domain

Table 1. Averaged statistics for surface ozone concentrations at 09 UTC and 21 UTC

	B.C. file	OBS.		MODEL		Regression			Bias	IOA	RMSE	Sys. RMSE	Unsys. RMSE	Skill_e	Skill_v	Skill_r
		AVG	SD	AVG	SD	b	a	r^2								
09 UTC	Profile	34.66	12.59	39.24	10.64	0.85	9.93	0.13	4.58	0.60	14.00	12.03	4.97	0.96	0.85	1.11
	RAQMS	34.75	12.58	41.57	11.84	0.94	8.98	0.12	6.82	0.59	15.51	13.47	6.87	1.07	0.94	1.23
21 UTC	Profile	52.74	18.99	55.73	15.43	0.81	12.87	0.41	3.00	0.78	15.21	13.06	4.65	0.69	0.81	0.80
	RAQMS	52.80	18.97	58.11	16.69	0.88	11.73	0.42	5.31	0.78	16.04	14.02	5.79	0.74	0.88	0.85

Note: AVG=arithmetic average; SD=standard deviation; b=slope; a=intercept; IOA=index of agreement (close to 1 shows skill); Sys. RMSEs=systematic root mean square error; Unsys. RMSEu = unsystematic root mean square error; Skill_e = Unsys.RMSEu /observed SD (<1 shows skill); Skill_v = model SD/observed SD (close to 1 shows skill); Skill_r = RMSE/ observed SD (<1 shows skill).

Both CMAQ simulations overestimate average surface O3 concentrations by 3 – 7 ppb. The use of RAQMS BC increased surface O3 concentrations about +2 ppb over the baseline CMAQ run and increased the magnitude of diurnal variation of surface O3 up to 10 %

Comparison with AIRNow Surface Data

Area II & IV, monthly mean

sigma

Level		Rocky Mountain Area (Area II)						New England Area (Area IV)					
		O_3 (ppv)*			O_3 (ppv)**			O_3 (ppv)*			O_3 (ppv)**		
Index	Sigma	$CMAQ^R$	$CMAQ^P$	Diff.	$CMAQ^R$	$CMAQ^P$	Diff.	$CMAQ^R$	$CMAQ^P$	Diff.	$CMAQ^R$	$CMAQ^P$	Diff.
1	0.9980	49.5	44.8	4.7	48.5	43.7	4.8	46.0	43.6	2.4	38.3	37.3	1.0
2	0.9925	50.6	45.8	4.8	48.5	43.6	4.9	47.7	45.2	2.5	38.3	37.4	0.9
3	0.9875	51.4	46.5	4.8	48.5	43.6	4.9	48.8	46.3	2.5	38.4	37.4	1.0
10	0.9000	55.5	50.3	5.2	48.9	44.0	4.9	55.7	52.7	3.0	39.3	37.9	1.4
11	0.8800	55.8	50.5	5.2	49.0	44.2	4.8	56.2	53.1	3.1	39.2	38.1	1.1
12	0.8500	55.9	50.7	5.3	49.1	44.3	4.8	56.6	53.2	3.4	40.0	38.5	1.5
13	0.8100	56.1	50.8	5.4	49.7	44.6	5.1	57.5	53.4	4.1	41.5	39.0	2.5
14	0.7400	56.5	50.9	5.6	50.2	45.2	5.0	58.9	52.9	6.0	45.2	40.7	4.5
18	0.3500	74.1	58.9	15.2	69.3	56.9	12.4	82.9	56.7	26.2	75.3	51.4	23.9
19	0.2500	82.1	61.7	20.4	77.0	59.5	17.5	96.0	59.6	36.3	87.9	54.3	33.6
20	0.1500	90.9	63.3	27.6	88.0	63.5	24.5	110.7	61.6	49.2	108.0	58.3	49.7
21	0.0500	99.3	63.5	35.7	99.0	64.7	34.3	131.5	62.6	68.8	141.2	63.3	77.9

*CMAQ-O3 (full chem) **CMAQ-O3 trace only *CMAQ-O3 (full chem) **CMAQ-O3 trace only

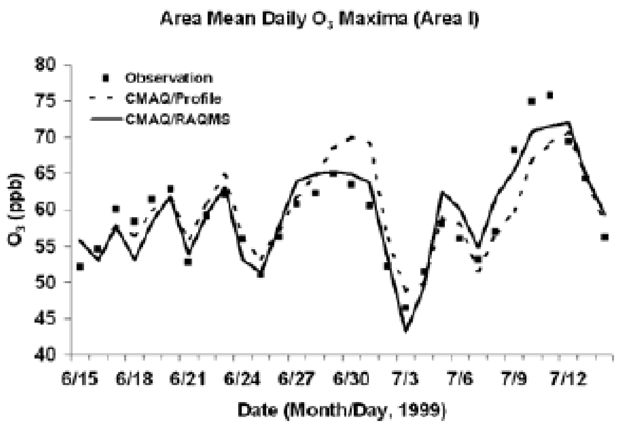
Richer gets richer, i.e., more O3 BC, more O3 production

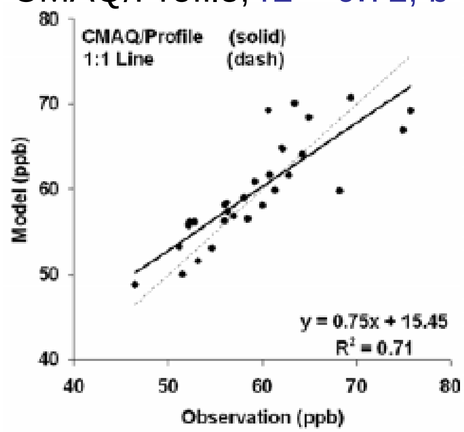
O3 Daily Max. time series & Scatter

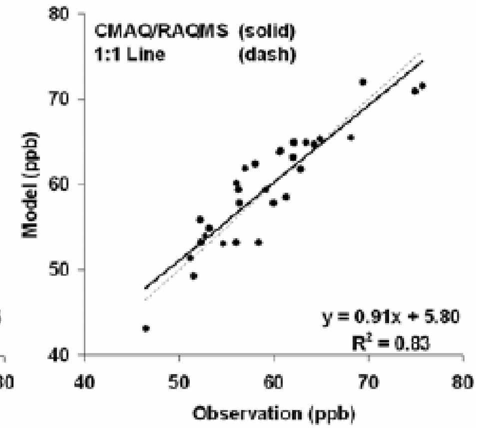
Area I: Western region of U.S. continent,

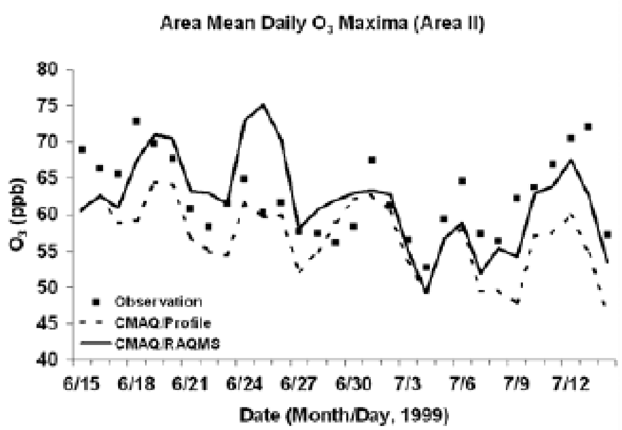
CMAQ/RAQMS, r2 = 0.83, b=0.91

CMAQ/Profile, r2 = 0.71, b=0.75

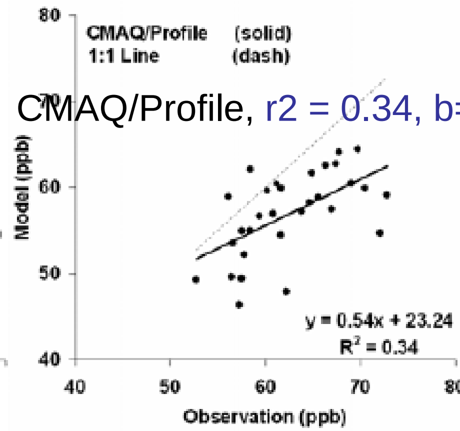


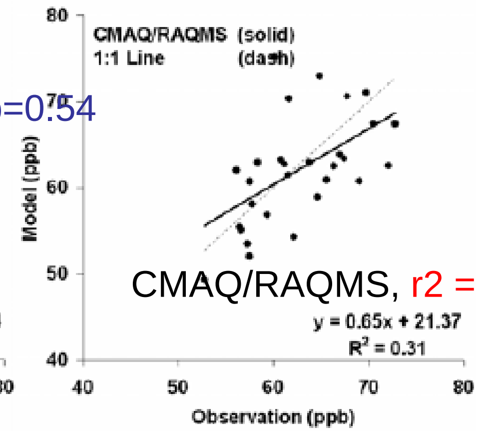






CMAQ/Profile, r2 = 0.34, b=0.54



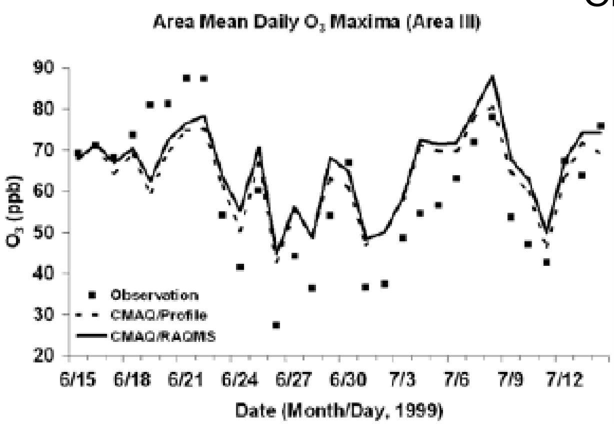


CMAQ/RAQMS, r2 = 0.31, b=0.65

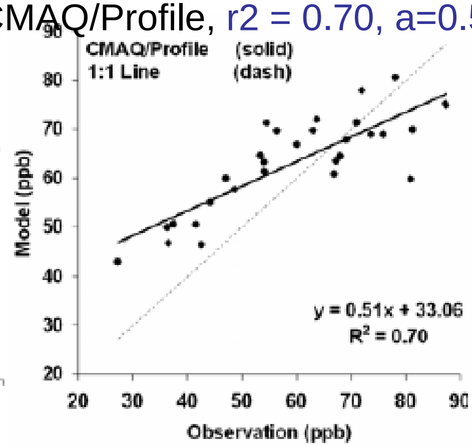
Area II: Rocky mountain region,

Improved Comparison

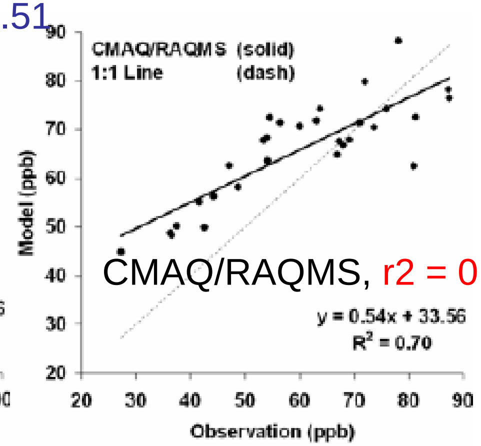
Area III: Tennessee (SOS-99 Nashville experiment)

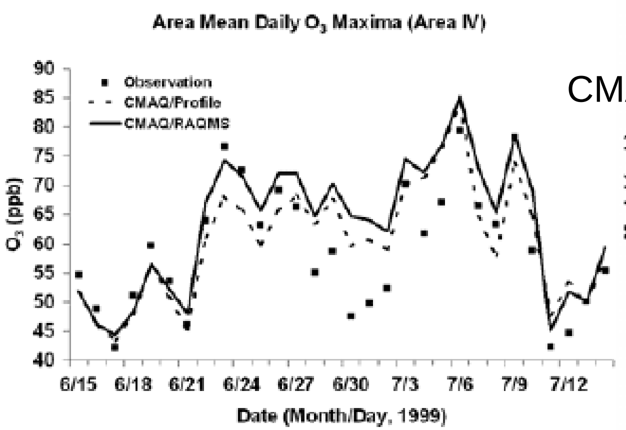


CMAQ/Profile, r2 = 0.70, a=0.51

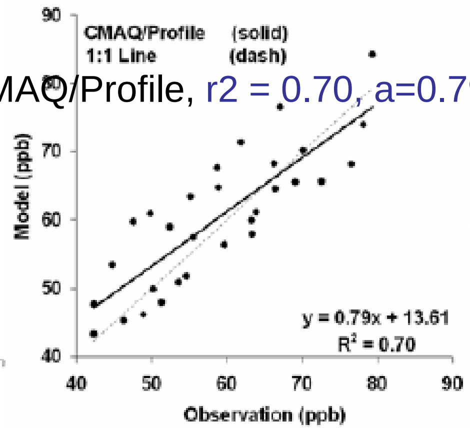


CMAQ/RAQMS, r2 = 0.70, b=0.54

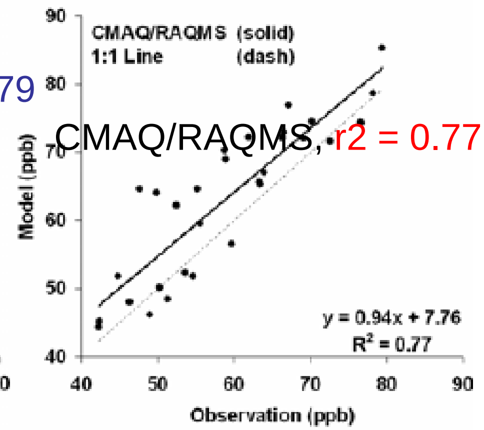




CMAQ/Profile, r2 = 0.70, a=0.79



CMAQ/RAQMS, r2 = 0.77, b=0.94



Area IV: NE US

SOS99 CMAQ/RAQMS Technical Summary

•Including RAQMS assimilated boundary conditions results in significant increases in CMAQ ozone mixing ratios in the upper troposphere and moderate increases in surface ozone mixing ratios over the mountainous regions of the western US.

•The CMAQ/RAQMS/SONDE statistics show that, in general, the BC information has been translated into the interior CMAQ domain, however, increased RMS errors compared to the RAQMS/SONDE statistics point to issues that need to be resolved in terms of CMAQ vertical resolution and/or convective exchange processes in the middle/upper troposphere.

•Comparisons with surface ozone from AIRNow showed that both CMAQ simulations overestimated average surface O_3 concentrations by 3 – 7 ppb and that CMAQ tends to underestimate peak O_3 concentration during daytime and overestimate lower O_3 concentrations at nighttime. The use of RAQMS BC **increased surface O_3 concentrations about +2 ppb** over the baseline CMAQ run and **increased the magnitude of diurnal variation of surface O_3 up to 10 %. (whole domain average)**

•**Nominal but appreciable improvement in CMAQ simulations at surface (compared with AIRNow) and substantial improvement for Area I, IV; Some improvement in Area II; Area III and southern US (June 15 – July 15, 1999)**

•**Future Study at UH: Duplicate simulations for the TexAQS-II period (June-Sept, 2006) and compare with surface, aircraft, lidar, and ozone sonde data to demonstrate impacts at higher temporal frequency for a whole summer season.**

Applications Air Quality Modeling Focus at Langley Research Center

Objective: Benchmark prototype chemical data assimilation procedures to provide NASA constituent observations to environmental decision support systems of NOAA, EPA, Regional Planning Organizations, and State and Local air quality management agencies

CMAQ Project (FY '04 - '05)

Prototype/evaluate techniques for improving boundary conditions of *National* air quality assessment model

GFS Project (FY '06 - '07)

Improve operational *National* AQ forecasts through incorporation of NASA models and satellite data

TexAQS Rapid Prototype (FY '07)

Improve capability of *State/Local* agencies to assess extra-regional influences on local air quality

Enabling Synergies: EPA AMI projects, ROSES 2007 proposals

Tools, capabilities and *inter-organizational partnerships* developed under previous and ongoing projects applied to emerging opportunities/needs