A Preliminary Evaluation of A Regional Air Quality Model with Measurements from MODIS and Surface Monitoring Networks

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Introduction

The objective of this project is to study the effects of urban and regional pollution on the global atmosphere. The project involves three major tasks:

(1) gathering and gridding appropriate satellite and in-situ data for comparison with models,

(2) comparing model simulation results with the satellite retrievals and the in-situ data, and

(3) using the models to address the following science questions:

a. What are the effects of future emission changes on regional/global air quality?

b. To what extent does the export of O_3, aerosols, and their precursors, such as NO_x and VOCs, from urban/regional scale affect their formation and distribution on the global scale?

c. What are the effects of individual organic gas emissions (e.g., isoprene), subgrid treatment (e.g., cloud chemistry and plume-in-grid treatment) and grid resolution on the fate of pollutants leaving the urban/regional scale?

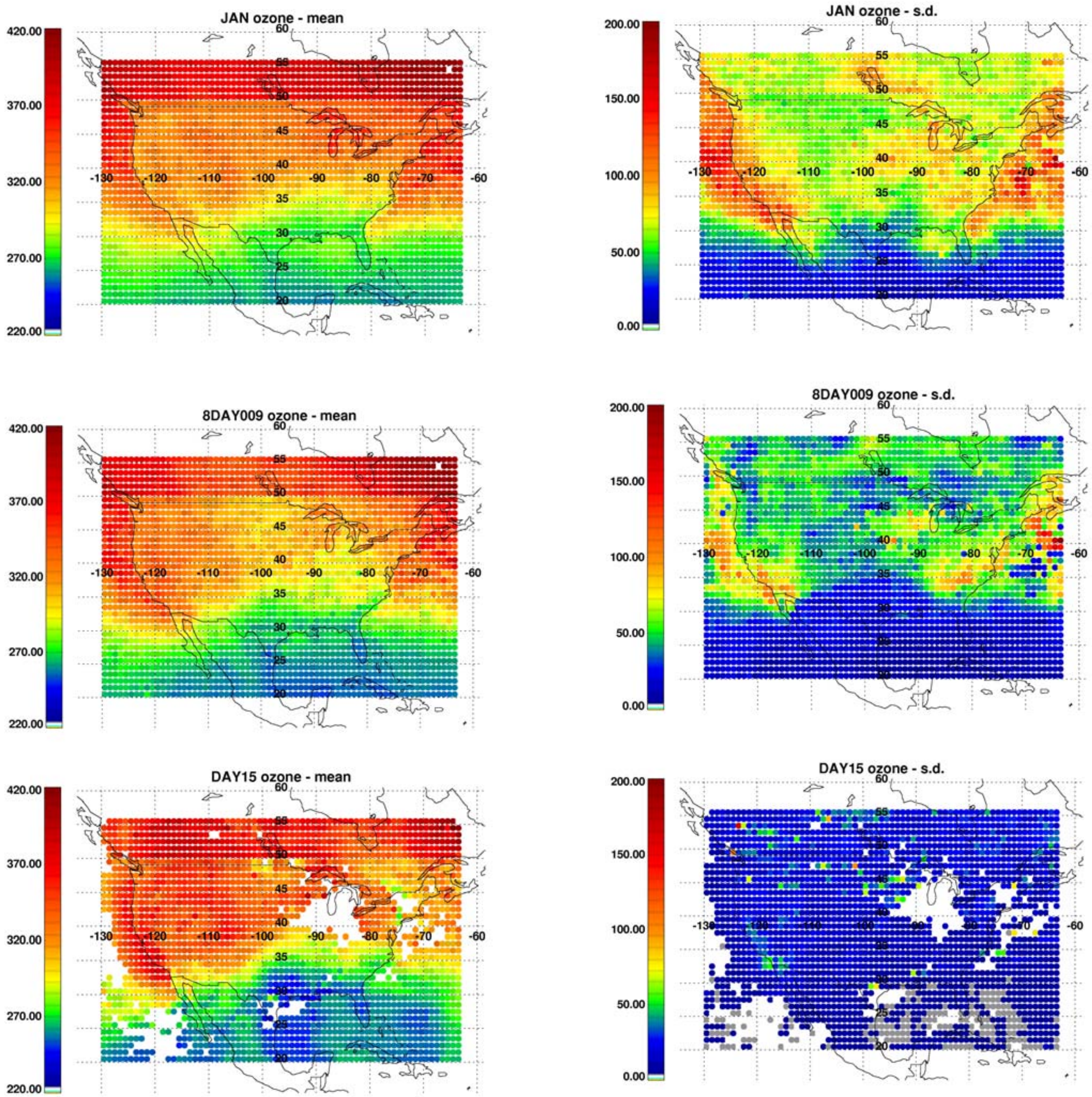

Figure 1. The differences in MODIS Level 3 products with different time-averaging for the total column ozone abundance in Dobson units (DU) in January, 2001. The figures on the left show the mean ozone amount, while the figures on the right show its standard deviation. Compared to daily data, the 8-day and monthly mean data smooth most of the spatial variations.

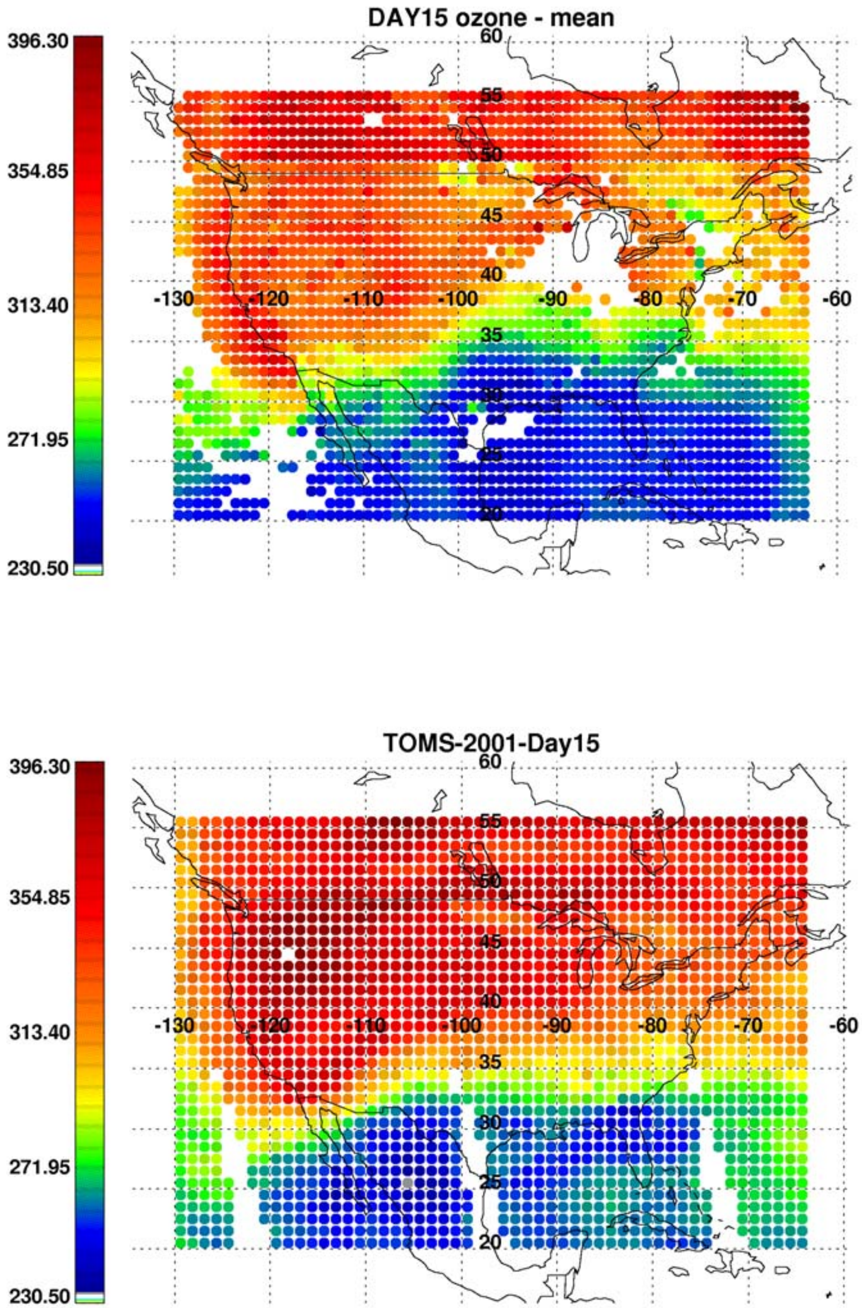

Figure 2. The daily-mean total column ozone abundance in DU from MODIS (top) and TOMS (bottom) on 15 Jan., 2001. The figures show a general agreement with some notable discrepancies. Namely, the transition between low ozone and high ozone (blue to red) is somewhat different. Also, the intrusion of low ozone air into upper New England is not as evident in the TOMS data.

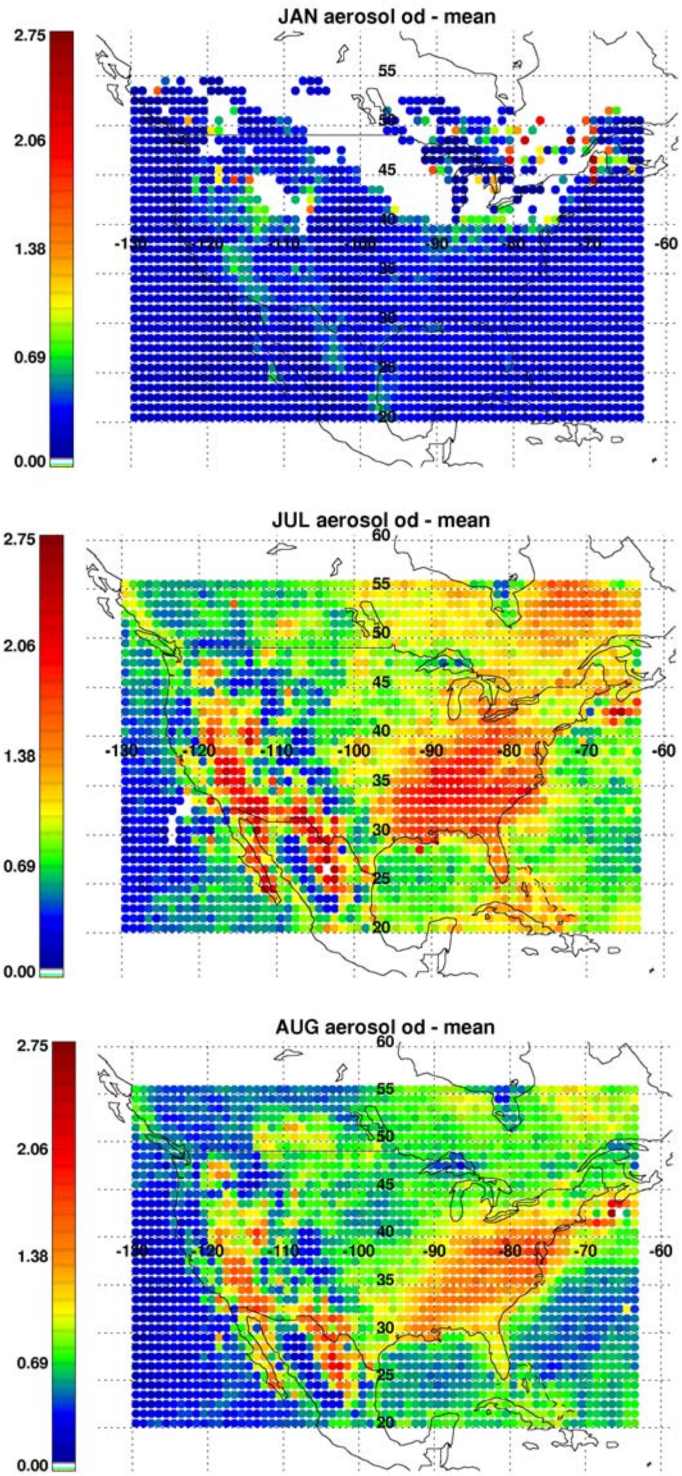

Figure 3. The monthly-mean aerosol optical depth (AOD) in January, July and August 2001 from MODIS.

Regional Model Simulations

Domain

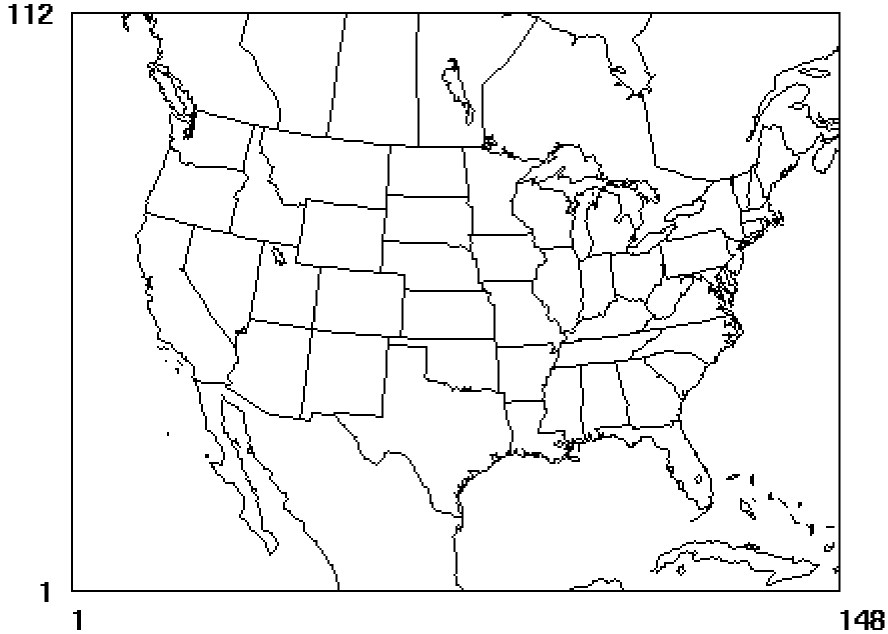

Figure 4. The modeling domain of CMAQ

Simulation Period	**22 December 2000-31 December 2001**
Grid Resolution	**36×36 km, 148×112 grid cells, 14 layers (0-15 km)**
Meteorology	**MM5/FDDA from U.S. EPA**
Emissions	**EPA's NEI 2001 Inventory**
	MOBILES6/BEIS 3.12/SMOKE1.4
ICONs/BCONs	**A global model (GEOS-CHEM)**
3-D Model	**EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System v4.4 released Oct. 2001**
Model Initialization	**10-day spin-up (22-31 December, 2000)**
Current Status	**Simulation of Jan.-Mar. 2001 completed**

Table 1. The overall statistical performance of CMAQ for the max 1-hr and the max 8-hr average O_3 mixing ratios at the CASTNet[1] sites for each month and the JFM period.

Variables[2]	Jan.		Feb.		Mar.		JFM	
	Max 1-hr	Max 8-hr	Max 1-hr	Max 8-hr	Max 1-hr	Max 8-hr	Max 1-hr	Max 8-hr
MeanObs	35.35	31.08	40.27	35.41	46.58	41.79	40.79	36.15
MeanMod	31.50	28.61	36.86	33.82	43.68	40.56	37.50	34.33
Number	1936	2652	1749	2399	2034	2818	5697	7980
Corr	0.49	0.66	0.38	0.65	0.36	0.55	0.52	0.69
MB	-3.85	-2.47	-3.42	-1.59	-2.90	-1.23	-3.29	-1.81
MAGE	7.87	7.46	7.43	6.50	7.33	6.62	7.43	6.90
RMSE	12.79	9.20	14.86	8.27	13.47	8.47	13.12	8.73
MNB	-0.07	-0.02	-0.03	0.02	-0.03	0.00	-0.04	0.00
MNGE	0.24	0.30	0.19	0.23	0.15	0.17	0.20	0.24
NMB	-0.11	-0.08	-0.08	-0.04	-0.06	-0.03	-0.08	-0.05
NME	0.22	0.24	0.18	0.18	0.16	0.16	0.18	0.19
FB	-0.12	-0.10	-0.07	-0.04	-0.06	-0.03	-0.08	-0.06
FGE	0.25	0.29	0.19	0.21	0.16	0.17	0.20	0.22
NMFB	-0.12	-0.08	-0.09	-0.05	-0.06	-0.03	-0.08	-0.05
NMFGE	0.24	0.25	0.19	0.19	0.16	0.16	0.19	0.20
MNFB	-0.17	-0.12	-0.10	-0.02	-0.07	-0.03	-0.11	-0.06
MNGFE	0.34	0.40	0.26	0.28	0.19	0.20	0.26	0.30
NMBF	-0.12	-0.09	-0.09	-0.05	-0.07	-0.03	-0.09	-0.05
NMEF	0.25	0.26	0.20	0.19	0.17	0.16	0.20	0.20

1. **CASTNet - the Clean Air Status and Trends Network.**
2. **MB - the mean bias; MAGE - the mean absolute gross error; RMSE - the root mean squared error, (MAGE), MNB - the mean normalized bias; MNGE - the mean normalized gross error; NMB - the normalized mean bias; NME - the normalized mean error; FB - the fractional bias; FGE - the fractional gross error; NMFB - the normalized mean fractional bias; NMFGE - the normalized mean fractional gross error; MNFB - the mean normalized factor bias, MNGFE - the mean normalized gross factor error; NMBF - the normalized mean bias factor; and NMEF - the normalized mean error factor.**

Table 2. The overall statistical performance of CMAQ for the max 1-hr and the max 8-hr average O_3 mixing ratios at AQS[1] sites for each month and the JFM period.

Variables[2]	Jan.		Feb.		Mar.		JFM	
	Max 1-hr	Max 8-hr	Max 1-hr	Max 8-hr	Max 1-hr	Max 8-hr	Max 1-hr	Max 8-hr
MeanObs	33.00	27.58	37.02	32.12	46.01	40.64	39.28	33.68
MeanMod	34.58	30.69	37.67	33.77	45.60	41.49	39.86	35.59
Number	15632	15550	13562	13505	18255	18201	48299	48086
Corr	0.56	0.54	0.61	0.61	0.60	0.59	0.66	0.64
MB	1.59	3.10	0.65	1.65	-0.41	0.85	0.58	1.91
MAGE	7.93	8.34	6.90	7.08	7.52	7.51	7.48	7.74
RMSE	10.58	11.03	9.08	9.14	10.15	9.95	10.00	10.28
MNB	0.19	0.29	0.11	0.17	0.05	0.10	0.11	0.18
MNGE	0.38	0.48	0.27	0.32	0.20	0.24	0.27	0.36
NMB	0.05	0.11	0.02	0.05	-0.01	0.02	0.01	0.06
NME	0.24	0.30	0.19	0.22	0.16	0.18	0.19	0.23
FB	0.04	0.09	0.03	0.06	0.00	0.03	0.02	0.07
FGE	0.27	0.33	0.21	0.25	0.18	0.20	0.22	0.26
NMFB	0.05	0.11	0.02	0.05	-0.01	0.02	0.01	0.06
NMFGE	0.23	0.29	0.18	0.21	0.16	0.18	0.19	0.22
MNFB	0.10	0.19	0.07	0.11	0.02	0.06	0.06	0.12
MNGFE	0.47	0.58	0.31	0.38	0.23	0.28	0.33	0.42
NMBF	0.05	0.11	0.02	0.05	-0.01	0.02	0.01	0.06
NMEF	0.24	0.30	0.19	0.22	0.16	0.18	0.19	0.23

1. AIRS-AQS - the Aerometric Information Retrieval System-Air Quality System.
2. MB - the mean bias; MAGE - the mean absolute gross error; RMSE - the root mean squared error, (MAGE), MNB - the mean normalized bias; MNGE - the mean normalized gross error; NMB - the normalized mean bias; NME - the normalized mean error; FB - the fractional bias; FGE - the fractional gross error; NMFB - the normalized mean fractional bias; NMFGE - the normalized mean fractional gross error; MNFB - the mean normalized factor bias, MNGFE - the mean normalized gross factor error; NMBF - the normalized mean bias factor; and NMEF - the normalized mean error factor.

Table 3. The overall statistical performance of CMAQ for PM and its compositions at CASTNet, IMPROVE, and STN sites[1] for the JFM, 2001.

Variables[2]	CASTNet			IMPROVE						STN					
	SO_4	NO_3	NH_4	$PM_{2.5}$	SO_4	NO_3	NH_4	BC	OC	$PM_{2.5}$	SO_4	NO_3	NH_4	BC	OC
Mean Obs.	2.33	1.80	1.18	4.10	1.18	0.82	1.01	0.20	0.79	11.56	3.59	3.57	2.38	1.53	4.73
Mean Sim.	1.72	2.34	1.25	5.27	1.03	0.98	1.45	0.20	1.01	14.14	2.18	2.66	1.54	0.99	2.63
Total #	868	867	868	2826	2919	2908	90	2894	2888	834	990	990	990	1006	986
Corr. Coeff.	0.87	0.75	0.87	0.71	0.76	0.61	0.61	0.58	0.50	0.39	0.28	0.41	0.27	-0.11	0.07
MB	-0.61	0.54	0.07	1.17	-0.16	0.16	0.44	0.00	0.22	2.58	-1.41	-0.91	-0.84	-0.54	-2.10
MAGE	0.69	1.13	0.33	2.32	0.45	0.69	0.59	0.12	0.57	7.91	2.01	2.51	1.61	1.55	3.36
RMSE	0.94	1.55	0.47	3.76	0.87	1.34	0.83	0.22	1.01	11.29	3.88	4.49	3.76	3.99	6.31
MNB	-0.17	1.51	0.23	0.66	0.57	1.20	0.70	0.28	1.31	15082	937	2233	457	218	1408
MNGE	0.30	1.80	0.41	0.86	0.95	1.82	0.84	0.83	1.54	15082	937	2233	457	219	1409
NMB	-0.26	0.30	0.06	0.28	-0.13	0.20	0.44	-0.02	0.29	0.22	-0.39	-0.25	-0.35	-0.35	-0.44
NME	0.29	0.63	0.28	0.57	0.38	0.85	0.58	0.60	0.72	0.68	0.56	0.70	0.68	1.01	0.71
FB	-0.24	0.31	0.10	0.26	-0.09	-0.13	0.31	-0.19	0.30	0.30	-0.33	-0.19	0.00	0.27	-0.37
FGE	0.33	0.73	0.33	0.52	0.43	0.91	0.50	0.60	0.62	0.74	0.62	0.86	0.71	0.85	0.76
NMFB	-0.30	0.26	0.06	0.25	-0.14	0.18	0.36	-0.02	0.25	0.20	-0.49	-0.29	-0.43	-0.43	-0.57
NMFGE	0.34	0.55	0.27	0.50	0.40	0.77	0.48	0.61	0.63	0.62	0.70	0.81	0.82	1.23	0.91
MNFB	-0.34	0.72	0.15	0.49	0.19	-431.25	0.49	-0.45	1.07	15081	935	2225	455	214	1406
MNGFE	0.46	2.59	0.49	1.04	1.33	434.27	1.06	1.56	1.78	15082	938	2241	459	223	1411
NMBF	-0.35	0.30	0.06	0.28	-0.16	0.20	0.44	-0.02	0.29	0.22	-0.65	-0.34	-0.54	-0.55	-0.80
NMEF	0.40	0.63	0.28	0.57	0.44	0.85	0.58	0.61	0.72	0.68	0.92	0.94	1.05	1.57	1.28

1. IMPROVE - Interagency Monitoring of Protected Visual Environments; CASTNet - the Clean Air Status and Trends Network; and STN - the Speciation Trends Network.
2. MB - the mean bias; MAGE - the mean absolute gross error; RMSE - the root mean squared error, (MAGE), MNB - the mean normalized bias; MNGE - the mean normalized gross error; NMB - the normalized mean bias; NME - the normalized mean error; FB - the fractional bias; FGE - the fractional gross error; NMFB - the normalized mean fractional bias; NMFGE - the normalized mean fractional gross error; MNFB - the mean normalized factor bias, MNGFE - the mean normalized gross factor error; NMBF - the normalized mean bias factor; and NMEF - the normalized mean error factor.

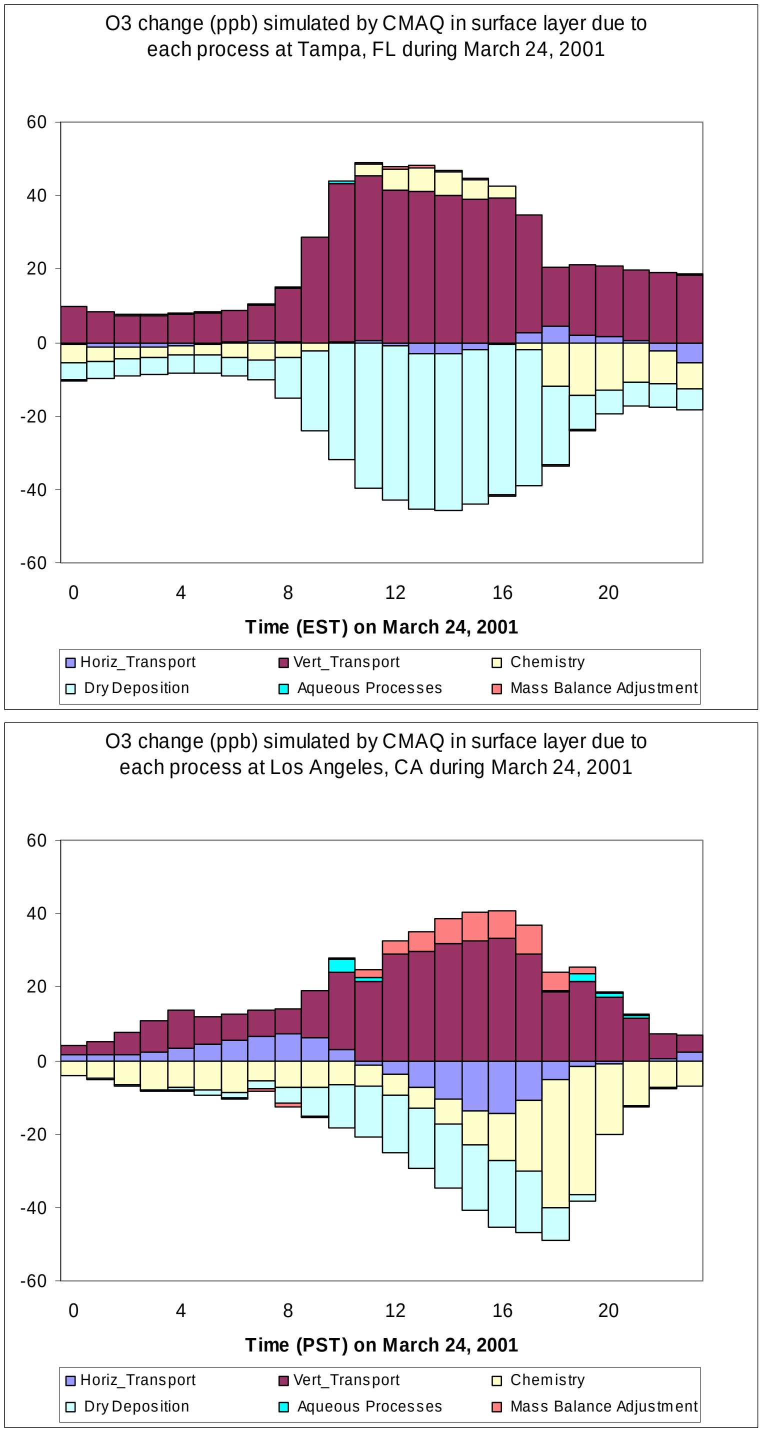

Figure 5. The hourly O_3 change in ppb at TAM and LAX on March 24 during which the peak O_3 mixing ratio was the highest among all days in March and in JFM.

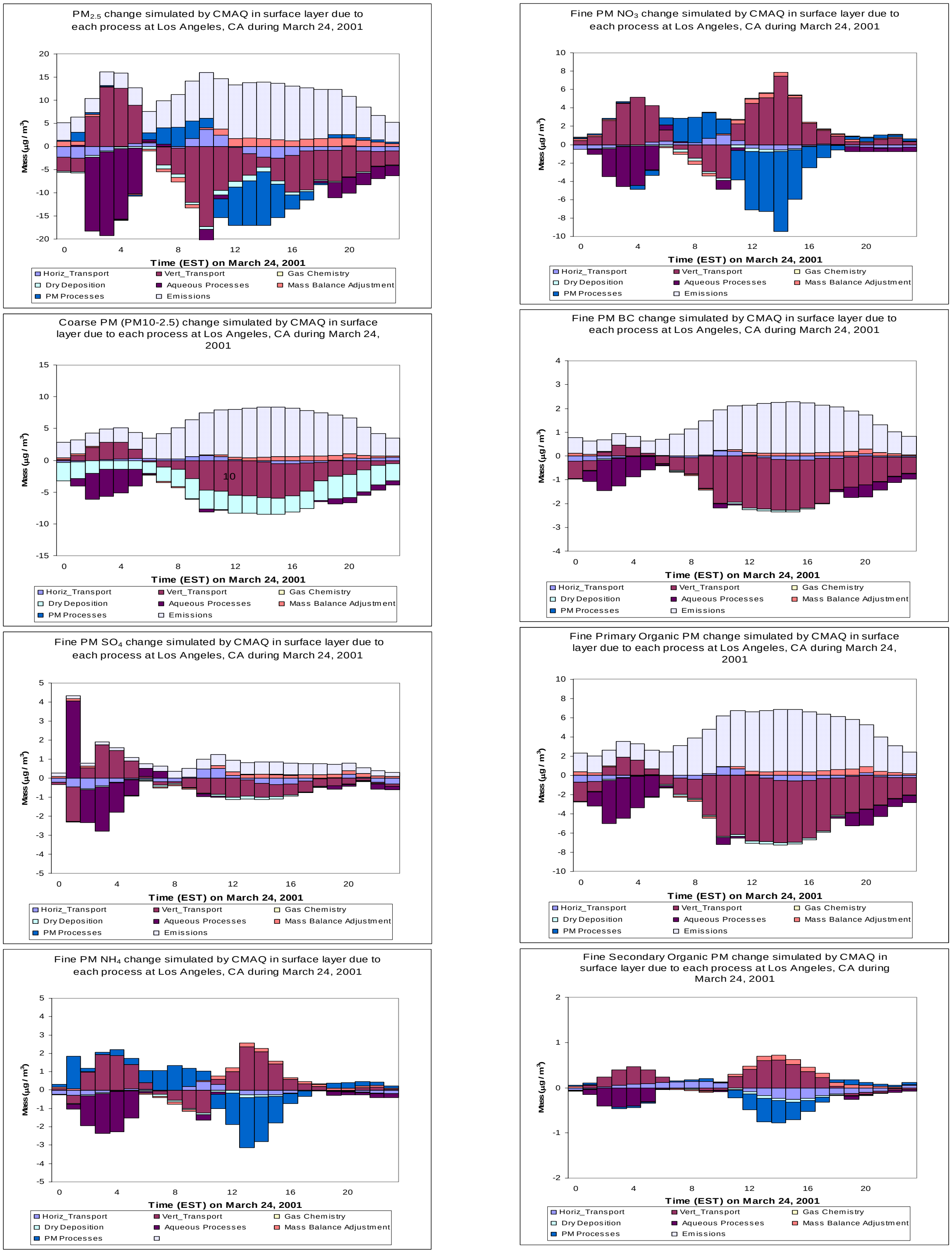

Figure 6. The daily contributions of individual processes to the mass concentrations of $PM_{2.5}$, $PM_{10\text{-}2.5}$ and $PM_{2.5}$ compositions including sulfate, ammonium, nitrate, BC, primary OC (POC), and second organic aerosols (SOA) on March 24 at LAX.

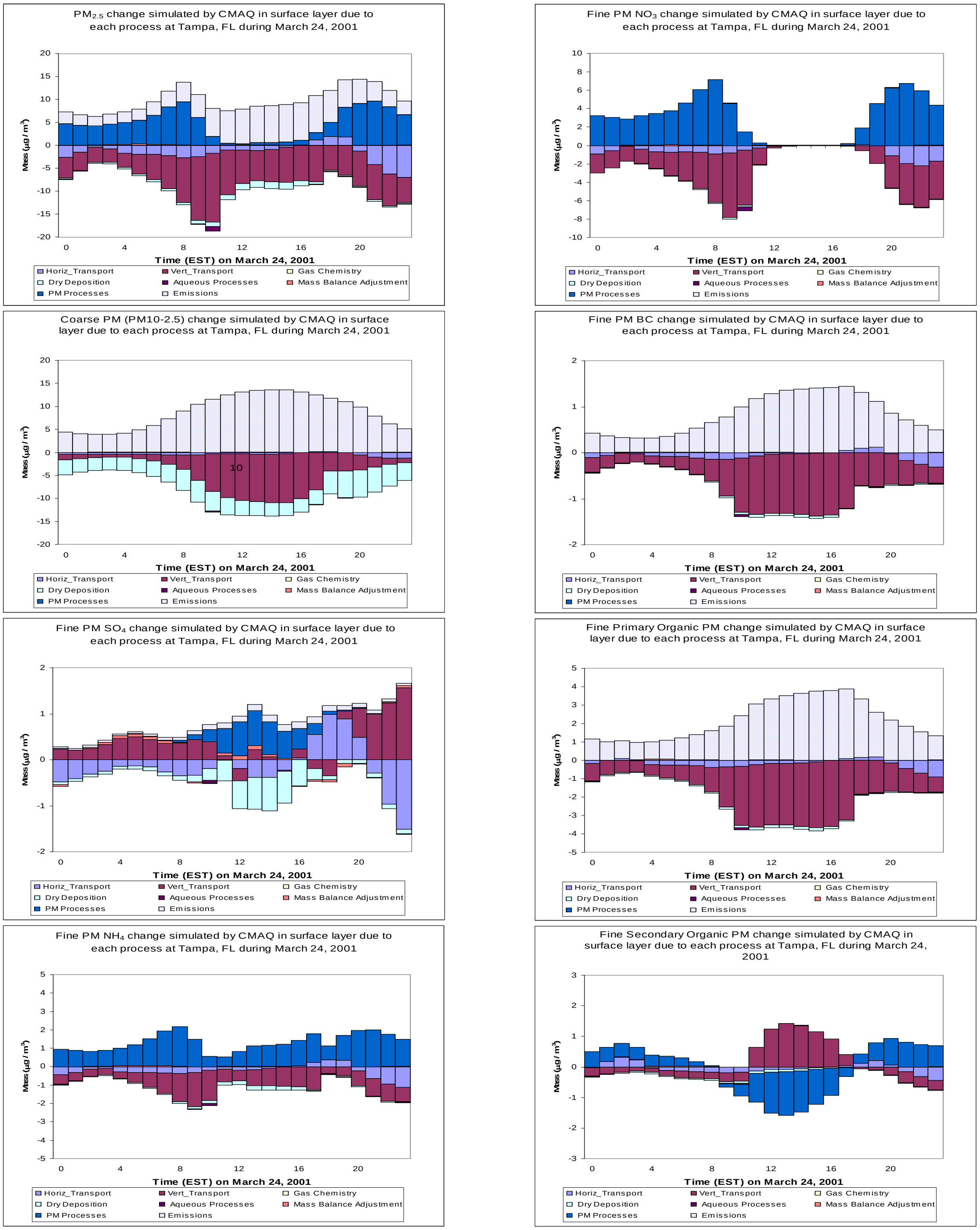

Figure 7. The daily contributions of individual processes to the mass concentrations of $PM_{2.5}$, $PM_{10\text{-}2.5}$ and $PM_{2.5}$ compositions including sulfate, ammonium, nitrate, BC, primary OC (POC), and second organic aerosols (SOA) on March 24 at TAM.

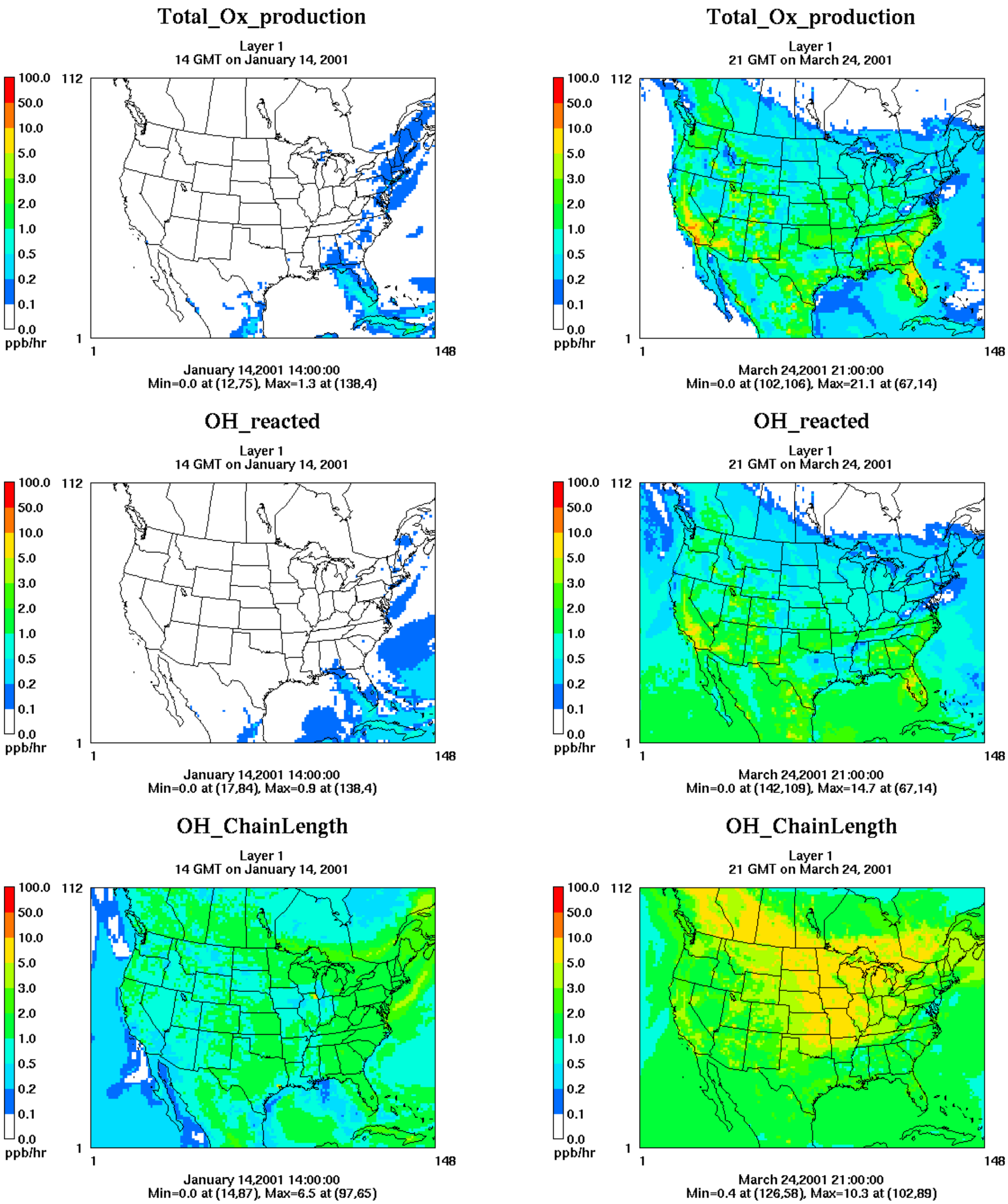

Figure 8. The spatial distribution of total O_x production, total HO_2 production, and total OH production in the surface layer at 14 GMT on 14 Jan., 2001 and 21 GMT on 24 Mar. at which the peak O_3 occurred.

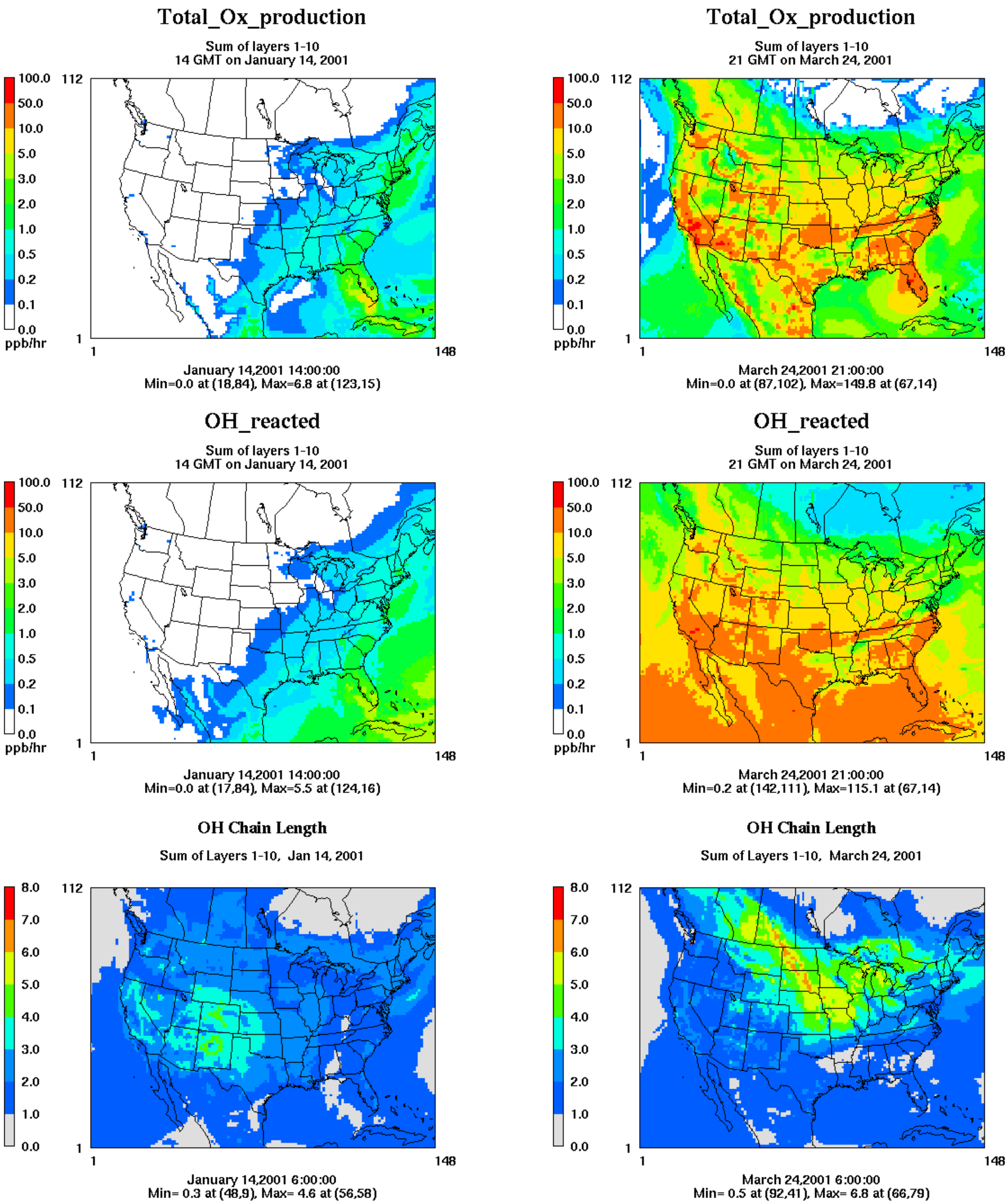

Figure 9. The spatial distribution of total O_x production, total HO_2 production, and total OH production in the PBL (0-2.9 km) at 14 GMT on 14 Jan., 2001 and 21 GMT on 24 Mar. at which the peak O_3 occurred.

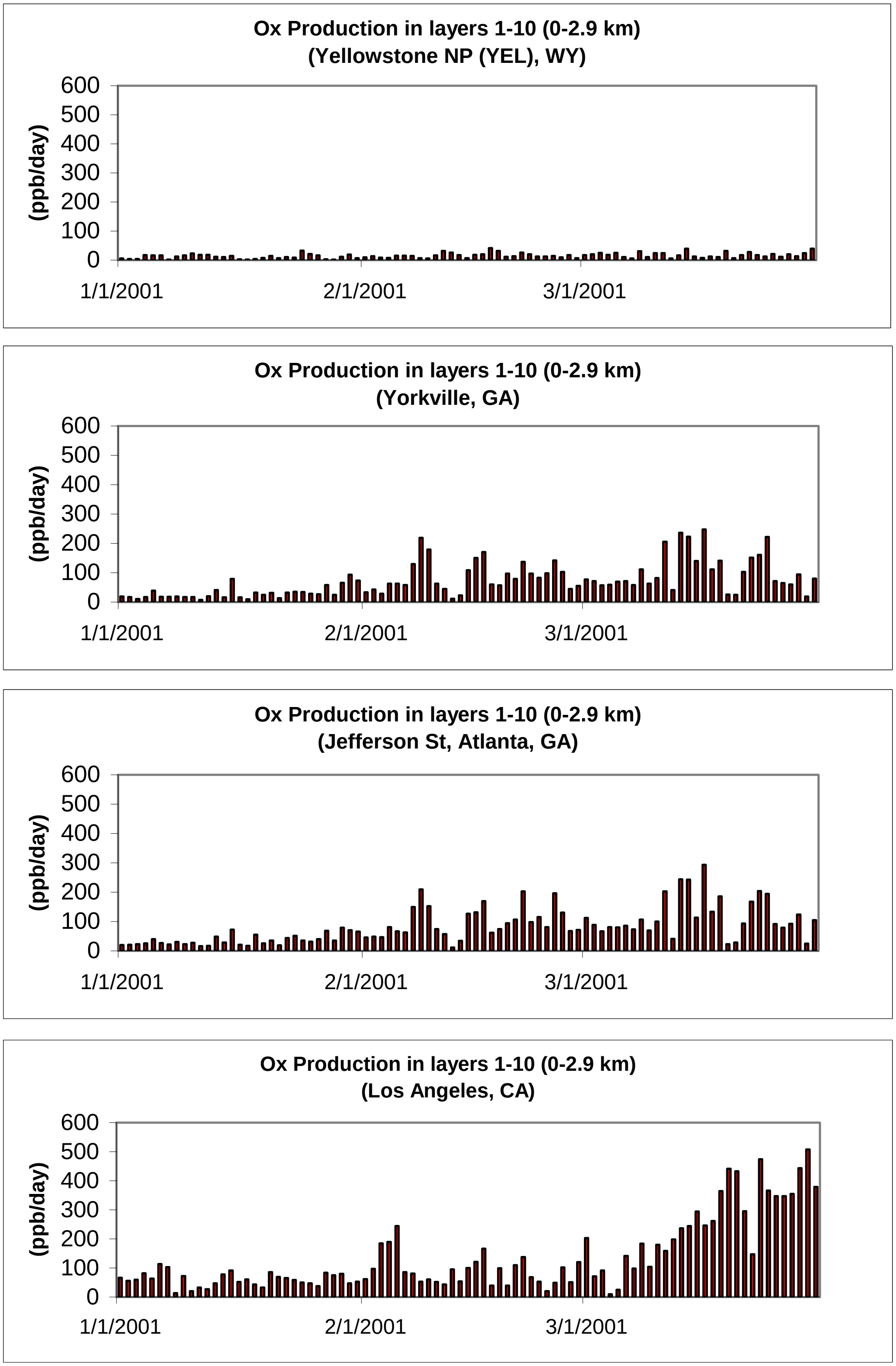

Figure 10. The sum of the total O_x production in the PBL (i.e., layers 1-10, correspond to 0-2.9 km) at Yorkville (YRK), GA; Yorkville, GA; Jefferson St., Atlanta, GA; and Los Angeles, CA.

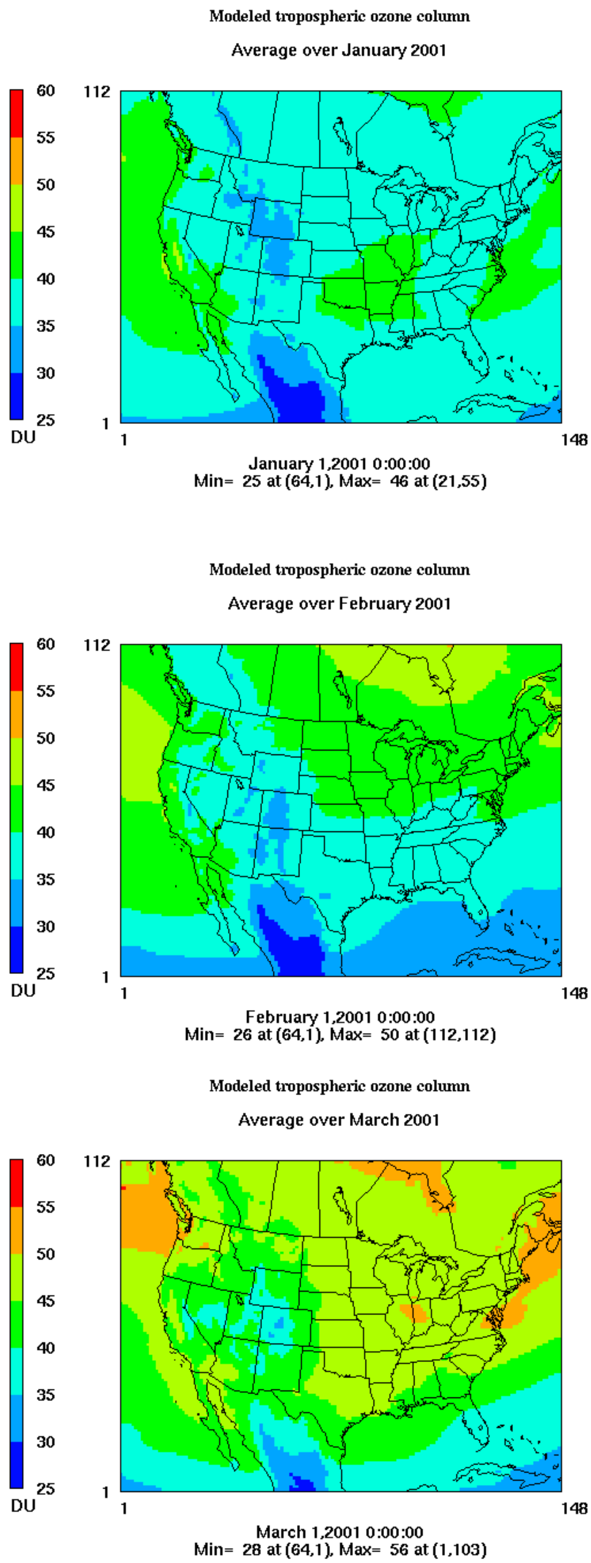

Figure 11. The simulated monthly-mean total tropospheric O_3 abundance in DU for Jan., Feb., and Mar., 2001.

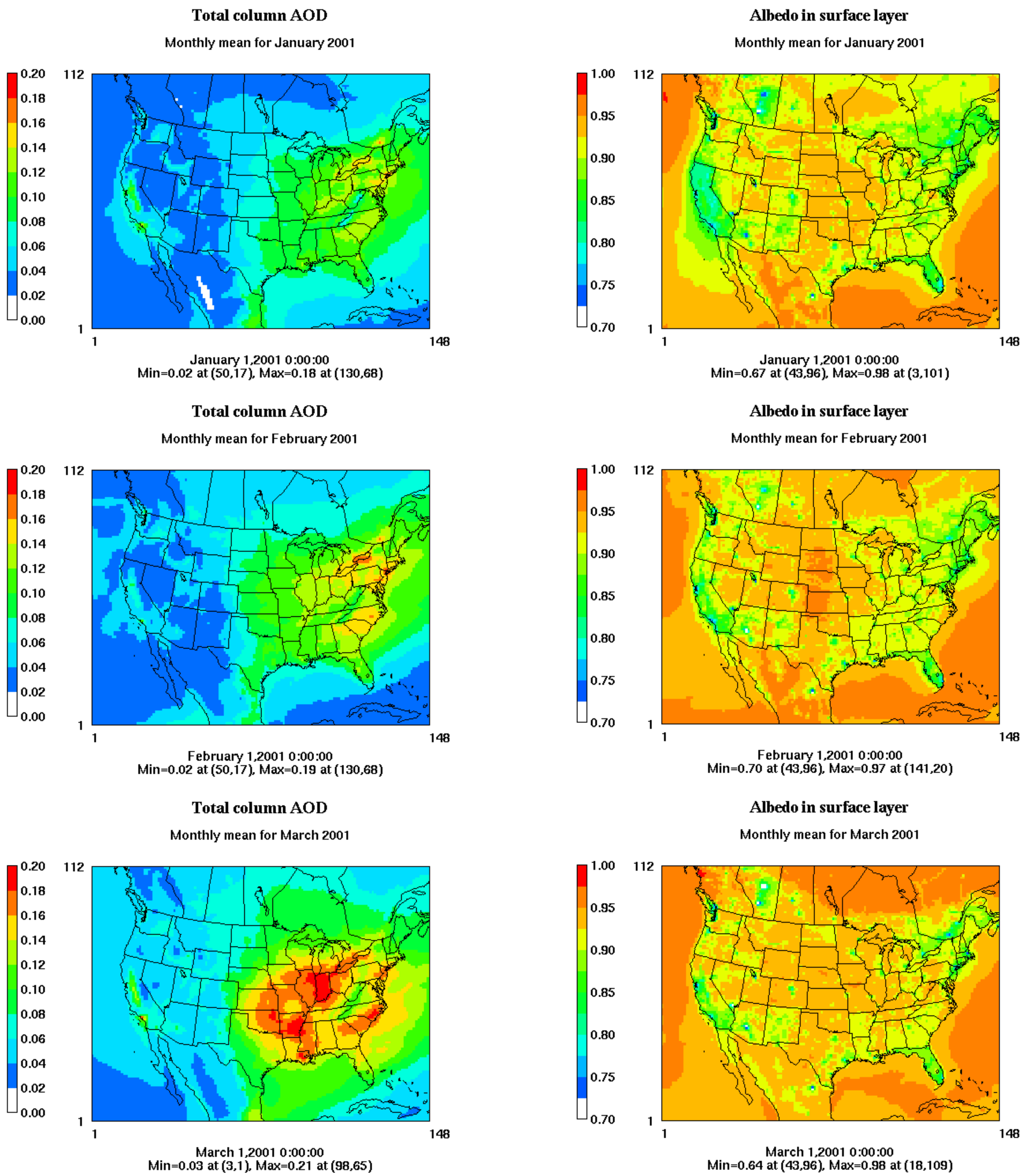

Figure 12. The model-estimated monthly-mean total column AOD and the monthly-mean SSA in the surface layer in Jan., Feb., and Mar., 2001.

Budget for O_x and $PM_{2.5}$ on Urban/Regional Scale during JFM 2001

Process	O_x	O_3	NO_x	NO_y	HNO_3	SO_2	AVOC[1]	BVOC[1]	$PM_{2.5}$
X - Advection	-14.942	-13.991	-0.241	-0.969	-0.443	-0.312	-4.513	-0.005	-57.02
Y - Advection	6.622	6.567	0.003	0.056	0.059	0.098	-0.412	-0.03	-7.14
Z - Advection	9.298	9.645	-0.091	-0.363	-0.138	-0.123	-1.807	0.004	-27.14
Mass balance adjustment	1.141	1.099	0.007	0.033	0.012	0.01	0.268	0.014	1.49
Horizontal diffusion	0	0	0	0	0	0	0	0	-0.001
Vertical diffusion	-4.057	-4.451	1.467	0.956	-0.382	-0.068	7.349	1.738	44.25
Dry deposition	-2.806	-2.283	-0.06	-0.516	-0.346	-0.268	-0.382	0	-3.03
Gas-phase chemistry	4.132	1.057	-3.148	0	1.008	-0.121	-4.595	-3.277	0.0
Aerosol process	-0.768	0	0	-0.288	0.667	0	0	0	58.50
Aqueous process	1.936	3.105	0.03	-0.916	-0.427	-0.93	-1.057	0.074	-48.58
Emissions	0.197	0	2.022	2.022	0	1.719	5.187	1.494	41.21
Net export	0.752	0.747	-0.013	0.015	0.011	0.005	0.040	0.013	1.54

1. $O_x = O_3 + NO_2 + 2 \times NO_3 + O + O^1D + PAN + 3 \times N_2O_5 + HNO_3 + HNO_4 +$ unknown organic nitrate. AVOC = Anthropogenic Volatile Organic Compounds. BVOC = Biogenic Volatile Organic Compounds.
2. All quantities are 3-month averages in Gigamoles/day for gas-phase species and Gigagrams/day for $PM_{2.5}$ for the boundary layer (0-2.9 km) over the modeling domain.

Summary

We have conducted a preliminary evaluation of the CMAQ simulation results for Jan.-Mar., 2001 for a modeling domain that covers the contiguous U.S., southern Canada, and northern Mexico using MODIS data and ground-based measurements. We have explored the use of process analysis tool embedded in CMAQ to gain in-depth understanding of the controlling processes for the fate of air pollutants on urban/regional scales.

Our preliminary model evaluation results for Jan.-Mar. 2001 using four ground-based databases have shown that CMAQ's performance for O_3 is generally satisfactory or marginally satisfactory at most sites but its performance slightly deteriorates for urban sites and for the max 8-hr average O_3 mixing ratios. Its PM performance is generally consistent with current PM model performance, with worst performance at STN sites and relatively high biases in nitrate, ammonium, and OC based on NMBF. Our preliminary model evaluation results using MODIS measurements have shown that CMAQ generally reproduces the magnitudes and spatial variations of the monthly-mean AOD from MODIS. The SSA predicted by CMAQ is within the typical range of satellite measurements. The process analysis has shown that the net export is 0.75 Gigamoles/day for O_x and 1.54 Gigagrams/day for $PM_{2.5}$ for the planetary boundary layer (0-2.9 km) during January, February and March 2001 over the modeling domain.

We are continuing the CMAQ simulation and model evaluation. The likely causes for the discrepancies between model simulation results and observations are being identified. We will process additional satellite products (e.g., the total mass column for NO_x and CO, total Angstrom exponent and aerosol mass concentrations) for model evaluation. We plan to conduct a set of sensitivity experiments to study the effect of urban/regional emissions on the large-scale environment and quantify the export of O_3, aerosols and their precursors such as NO_x and VOCs, from the urban/regional scale into the global atmosphere.