TSD-1b

Processing of Biogenic Emissions for OTC / MANE-VU Modeling

Bureau of Air Quality Analysis and Research

Division of Air Resources

New York State Department of Environmental Conservation

Albany, NY 12233

September 19, 2006

Biogenic emissions for the time period from January 1, 2002 – December 31, 2002 were calculated by NYSDEC using the Biogenic Emissions Inventory System (BEIS) version 3.12 integrated within SMOKE2.1. General information about BEIS is available at http://www.epa.gov/AMD/biogen.html while documentation about biogenic emissions processing within SMOKE2.1 is available at http://cf.unc.edu/cep/empd/products/smoke/version2.1/html/ch06s10.html and http://cf.unc.edu/cep/empd/products/smoke/version2.1/html/ch06s17.html . Note that the SMOKE documentation refers to BEIS3.09 and has not yet been updated for BEIS3.12. This affects the number of species modeled as well as the use of different speciation profiles. However, the general processing approach has not changed from BEIS3.09 to BEIS3.12. In short, this processing approach is as follows and was utilized by NYSDEC for its biogenic emission processing for 8-hr ozone and $PM_{2.5}$ modeling:

1. **Normbeis3** reads gridded land use data and emissions factors and produces gridded normalized biogenic emissions for 34 species/compounds. The gridded land use includes 230 different land use types. Both summer and winter emissions factors for each species/compound are provided for each of the 230 land use types. On output, **Normbeis3** generates a file `B3GRD` which contains gridded summer and winter emission fluxes for the modeling domain that are normalized to 30 °C and a photosynthetic active radiation (PAR) of 1000 µmol/m^2s. In addition, gridded summer and winter leaf area indices (LAI) are also written to `B3GRD`.

2. **Tmpbeis3** reads the gridded, normalized emissions file `B3GRD` and meteorological data from the MCIP-processed MM5 meteorological fields generated by the University of Maryland for MANE-VU/OTC modeling. Specifically, the following MM5/MCIP meteorological variables are used by **Tmpbeis3** to compute hour-specific, gridded biogenic emissions from the normalized emission fluxed contained in `B3GRD`: layer-1 air temperature (“TA”), layer-1 pressure (“PRES”), total incoming solar radiation at the surface (“RGRND”), and convective (“RC”) and non-convective (“RN”) rainfall. Additionally, the emissions for the 34 species/compounds modeled by BEIS3.12 are converted to CO, NO, and the CB-IV

VOC species utilized in CMAQ via the use of the BEIS3.12-CB-IV speciation profile. In adition, an optional seasonal switch file, `BIOSEASON`, was utilized to decide whether to use summer or winter emissions factors for any given grid cell on any given day. This file was generated by the SMOKE2.1 utility **Metscan** based on MM5 layer-1 air temperatures to determine the date of the last spring frost and first fall frost at each grid cell. Summer emission factors are used by **Tmpbeis3** for the time period between the last spring frost and first fall frost at any given grid cell, and winter emission factors are used for the remaining time period. Documentation for the **Metscan** utility is available at http://cf.unc.edu/cep/empd/products/smoke/version2.1/html/ch05s07.html . An animated GIF file showing the `BIOSEASON` file used by NYSDEC can be found at ftp://ftp.dec.state.ny.us/dar/air_research/chogrefe/biog_reports/b3season_movie.gif

3. For reporting purposes, the hourly, speciated, gridded emissions were aggregated to the county level for each day. For any given grid cell, emissions are distributed among the counties intersecting this grid cell in proportion to the area of each of these counties within the grid cell. The area gridding surrogates needed for this aggregration are based on a file obtained from EPA via http://www.epa.gov/ttn/chief/emch/spatial/new/bgpro.12km_041604.us.gz followed by windowing for the MANE-VU/OTC modeling domain.

Table 1 County and State totals of estimated biogenic emissions (tpy)

State	FIPS	County	NO [TPY]	CO [TPY]	VOC [TPY]
Connecticut	009001	Fairfield	52	894	7150
	009003	Hartford	88	915	8537
	009005	Litchfield	98	1261	12221
	009007	Middlesex	54	615	5587
	009009	New Haven	80	876	7544
	009011	New London	74	906	8960
	009013	Tolland	55	651	5999
	009015	Windham	60	772	8019
Connecticut		**TOTAL**	560	6889	64017
Deleware	010001	Kent	308	1354	15912
	010003	New Castle	143	875	8834
	010005	Sussex	539	2045	21595
Deleware		**TOTAL**	990	4274	46342
DC	011001	Washington	30	150	1726
DC		**TOTAL**	30	150	1726
Maine	023001	Androscoggin	35	885	8204
	023003	Aroostook	741	15531	140877
	023005	Cumberland	49	1298	11528
	023007	Franklin	72	3269	32111
	023009	Hancock	66	2950	27090
	023011	Kennebec	73	1425	12849
	023013	Knox	30	689	6680
	023015	Lincoln	32	849	8072
	023017	Oxford	79	3224	34189
	023019	Penobscot	211	7249	63128
	023021	Piscataquis	146	8638	80748
	023023	Sagadahoc	37	526	4504
	023025	Somerset	173	8413	77850
	023027	Waldo	57	1833	18125
	023029	Washington	144	6459	58678
	023031	York	73	1698	15571
Maine		**TOTAL**	2018	64936	600203
Maryland	024001	Allegany	63	661	8664
	024003	Anne Arundel	79	945	12786
	024005	Baltimore	166	847	8102
	024009	Calvert	59	798	10048
	024011	Caroline	202	648	7907

	024013	Carroll	189	822	7853
	024015	Cecil	86	654	10093
	024017	Charles	78	1079	15042
	024019	Dorchester	134	829	10337
	024021	Frederick	204	1123	10964
	024023	Garrett	102	930	11391
	024025	Harford	141	911	9053
	024027	Howard	75	562	4460
	024029	Kent	177	498	4761
	024031	Montgomery	134	813	6786
	024033	Prince Georges	87	732	10214
	024035	Queen Annes	222	684	7146
	024037	St Marys	99	886	10793
	024039	Somerset	58	498	5796
	024041	Talbot	131	495	5225
	024043	Washington	112	781	7538
	024045	Wicomico	124	796	10304
	024047	Worcester	158	1121	13079
	024510	Baltimore	54	235	1762
Maryland		**TOTAL**	2934	18350	210104
Massachusetts	025001	Barnstable	261	668	5905
	025003	Berkshire	73	1182	11029
	025005	Bristol	107	753	7142
	025007	Dukes	115	252	1728
	025009	Essex	55	794	7128
	025011	Franklin	61	1031	9424
	025013	Hampden	51	904	9201
	025015	Hampshire	61	820	7056
	025017	Middlesex	68	1085	11630
	025019	Nantucket	56	159	1362
	025021	Norfolk	49	615	5513
	025023	Plymouth	170	1197	11876
	025025	Suffolk	26	177	1351
	025027	Worcester	103	1955	23612
Massachusetts		**TOTAL**	1257	11594	113957
New Hampshire	033001	Belknap	25	693	6915
	033003	Carroll	40	1512	14981
	033005	Cheshire	49	1019	10099
	033007	Coos	72	3239	33668
	033009	Grafton	91	2442	23151
	033011	Hillsborough	48	1337	14503
	033013	Merrimack	48	1314	13566
	033015	Rockingham	39	1120	10080
	033017	Strafford	25	686	6617
	033019	Sullivan	45	943	8314
New Hampshire		**TOTAL**	482	14306	141894

New Jersey	034001	Atlantic	135	1225	18890
	034003	Bergen	37	239	2455
	034005	Burlington	151	1827	25255
	034007	Camden	68	491	7751
	034009	Cape May	90	566	7763
	034011	Cumberland	122	773	10699
	034013	Essex	57	199	1831
	034015	Gloucester	119	556	8444
	034017	Hudson	26	125	701
	034019	Hunterdon	81	706	5743
	034021	Mercer	85	475	4889
	034023	Middlesex	98	456	5267
	034025	Monmouth	125	1152	15423
	034027	Morris	63	604	7288
	034029	Ocean	128	1871	27063
	034031	Passaic	41	339	3841
	034033	Salem	123	535	8304
	034035	Somerset	49	518	5548
	034037	Sussex	67	718	7768
	034039	Union	21	168	2191
	034041	Warren	125	517	4505
New Jersey		**TOTAL**	1813	14058	181618
New York	036001	Albany	59	730	6253
	036003	Allegany	129	1218	9526
	036005	Bronx	25	100	657
	036007	Broome	107	879	7861
	036009	Cattaraugus	148	1654	13540
	036011	Cayuga	227	986	7928
	036013	Chautauqua	202	1260	8144
	036015	Chemung	88	521	3911
	036017	Chenango	149	1120	7833
	036019	Clinton	138	1631	13341
	036021	Columbia	96	896	8484
	036023	Cortland	101	616	4280
	036025	Delaware	133	1672	13435
	036027	Dutchess	90	1096	10288
	036029	Erie	165	1127	6898
	036031	Essex	94	2547	20888
	036033	Franklin	228	2337	17197
	036035	Fulton	90	764	5275
	036037	Genesee	201	645	3993
	036039	Greene	47	886	8182
	036041	Hamilton	78	2092	16056
	036043	Herkimer	175	1783	12846
	036045	Jefferson	251	1754	12503
	036047	Kings	15	60	309

	036049	Lewis	154	1693	12116
	036051	Livingston	222	888	6048
	036053	Madison	149	1049	7528
	036055	Monroe	223	990	6237
	036057	Montgomery	106	579	4715
	036059	Nassau	81	408	2859
	036061	New York	16	76	473
	036063	Niagara	335	940	5182
	036065	Oneida	214	1515	10021
	036067	Onondaga	171	929	6259
	036069	Ontario	178	767	6024
	036071	Orange	110	1065	13024
	036073	Orleans	195	635	3314
	036075	Oswego	119	1277	7911
	036077	Otsego	157	1190	7958
	036079	Putnam	32	473	5243
	036081	Queens	20	105	543
	036083	Rensselaer	96	894	7316
	036085	Richmond	47	173	1292
	036087	Rockland	26	300	4006
	036089	St. Lawrence	376	3876	28960
	036091	Saratoga	76	1125	9010
	036093	Schenectady	39	377	3032
	036095	Schoharie	95	737	5496
	036097	Schuyler	87	438	3193
	036099	Seneca	127	438	3305
	036101	Steuben	267	1475	12085
	036103	Suffolk	368	1328	12886
	036105	Sullivan	76	1325	12538
	036107	Tioga	102	730	5400
	036109	Tompkins	96	576	4128
	036111	Ulster	82	1493	15714
	036113	Warren	46	1396	11568
	036115	Washington	183	1109	8355
	036117	Wayne	270	920	5940
	036119	Westchester	35	549	5347
	036121	Wyoming	194	720	3813
	036123	Yates	107	507	4017
New York		**TOTAL**	8313	63436	492483
Pennsylvania	042001	Adams	186	892	8926
	042003	Allegheny	182	948	6727
	042005	Armstrong	108	940	9955
	042007	Beaver	69	600	4895
	042009	Bedford	128	1249	14127
	042011	Berks	280	1377	14146
	042013	Blair	91	729	7579
	042015	Bradford	224	1265	9423

042017	Bucks	144	954	8399
042019	Butler	149	1032	8602
042021	Cambria	128	805	6545
042023	Cameron	25	627	7563
042025	Carbon	53	585	8121
042027	Centre	158	1344	16886
042029	Chester	264	1176	10474
042031	Clarion	85	848	10743
042033	Clearfield	149	1368	13267
042035	Clinton	71	1230	18191
042037	Columbia	106	802	9080
042039	Crawford	204	1297	10839
042041	Cumberland	193	816	9505
042043	Dauphin	116	799	8502
042045	Delaware	35	410	3250
042047	Elk	49	949	8921
042049	Erie	199	1107	8273
042051	Fayette	156	1087	9277
042053	Forest	26	577	7122
042055	Franklin	271	1057	10296
042057	Fulton	93	744	9341
042059	Greene	91	830	6966
042061	Huntingdon	135	1093	12606
042063	Indiana	144	1078	9156
042065	Jefferson	101	865	7362
042067	Juniata	79	588	8263
042069	Lackawanna	58	586	5569
042071	Lancaster	464	1299	9565
042073	Lawrence	114	503	3755
042075	Lebanon	155	623	5827
042077	Lehigh	149	594	6040
042079	Luzerne	75	1013	13215
042081	Lycoming	152	1457	16633
042083	Mc Kean	57	1044	7113
042085	Mercer	175	865	7114
042087	Mifflin	107	620	7508
042089	Monroe	75	773	8856
042091	Montgomery	106	812	6736
042093	Montour	85	321	3306
042095	Northampton	144	506	4416
042097	Northumberland	92	570	6340
042099	Perry	113	804	10216
042101	Philadelphia	29	194	1420
042103	Pike	37	757	9946
042105	Potter	89	1129	9027
042107	Schuylkill	123	1050	15001
042109	Snyder	88	538	6373
042111	Somerset	221	1251	11228

	042113	Sullivan	45	684	5112
	042115	Susquehanna	126	978	6448
	042117	Tioga	176	1313	10942
	042119	Union	71	541	6435
	042121	Venango	72	855	9086
	042123	Warren	76	1031	7352
	042125	Washington	166	1068	7429
	042127	Wayne	89	862	5954
	042129	Westmoreland	199	1297	10589
	042131	Wyoming	60	551	4634
	042133	York	366	1393	12758
Pennsylvania		**TOTAL**	8645	59945	585271
Rhode Island	044001	Bristol	40	90	441
	044003	Kent	41	328	3471
	044005	Newport	37	183	1646
	044007	Providence	39	591	6901
	044009	Washington	54	572	6775
Rhode Island		**TOTAL**	211	1764	19233
Vermont	050001	Addison	186	922	6274
	050003	Bennington	43	896	7349
	050005	Caledonia	58	1149	10239
	050007	Chittenden	74	606	3633
	050009	Essex	61	1315	11795
	050011	Franklin	208	971	5927
	050013	Grand Isle	50	490	3506
	050015	Lamoille	36	727	5627
	050017	Orange	57	1182	10120
	050019	Orleans	120	1570	12842
	050021	Rutland	102	1257	9867
	050023	Washington	47	1099	9502
	050025	Windham	42	1232	10898
	050027	Windsor	57	1330	10796
Vermont		**TOTAL**	1142	14745	118376
Virginia	051001	Accomack	187	959	9472
	051003	Albemarle	140	1246	12533
	051005	Alleghany	35	522	7369
	051007	Amelia	70	915	10717
	051009	Amherst	80	905	10823
	051011	Appomattox	76	830	10447
	051013	Arlington	17	64	531
	051015	Augusta	135	1049	13291
	051017	Bath	46	771	11636
	051019	Bedford	189	1279	13052
	051021	Bland	41	515	7097
	051023	Botetourt	74	780	10211

051025	Brunswick	98	1458	18254
051027	Buchanan	32	722	9557
051029	Buckingham	76	1287	18830
051031	Campbell	112	1078	12933
051033	Caroline	73	1173	16020
051035	Carroll	132	634	6885
051036	Charles City	93	415	4711
051037	Charlotte	84	1219	14277
051041	Chesterfield	69	802	10686
051043	Clarke	56	369	4009
051045	Craig	39	538	7314
051047	Culpeper	105	894	10720
051049	Cumberland	56	814	10677
051051	Dickenson	20	550	6910
051053	Dinwiddie	82	1207	16511
051057	Essex	58	671	7403
051059	Fairfax	111	533	5538
051061	Fauquier	150	1166	14084
051063	Floyd	47	593	6493
051065	Fluvanna	54	775	10756
051067	Franklin	119	1297	15933
051069	Frederick	64	588	8798
051071	Giles	38	508	4918
051073	Gloucester	32	510	5945
051075	Goochland	47	670	10392
051077	Grayson	60	627	8260
051079	Greene	57	434	5727
051081	Greensville	63	735	9009
051083	Halifax	201	1852	22730
051085	Hanover	91	950	12493
051087	Henri	81	427	5468
051089	Henry	59	805	9772
051091	Highland	44	608	8579
051093	Isle Of Wight	178	813	8049
051095	James City	41	314	3989
051097	King And Queen	77	673	7615
051099	King George	62	540	6111
051101	King William	102	712	7846
051103	Lancaster	33	311	3669
051105	Lee	97	680	7221
051107	Loudoun	137	942	8999
051109	Louisa	78	1142	16780
051111	Lunenberg	88	1108	13611
051113	Madison	70	598	7305
051115	Mathews	27	367	4025
051117	Mecklenburg	145	1478	18507
051119	Middlesex	42	480	5561
051121	Montgomery	70	501	5366

051125	Nelson	67	979	12465
051127	New Kent	35	600	8240
051131	Northampton	90	263	2019
051133	Northumberland	88	778	9298
051135	Nottoway	74	894	10670
051137	Orange	98	759	8265
051139	Page	77	540	6705
051141	Patrick	75	884	10255
051143	Pittsylvania	203	1806	22102
051145	Powhatan	47	675	10194
051147	Prince Edward	69	942	12042
051149	Prince George	73	572	6484
051153	Prince William	38	718	10979
051155	Pulaski	61	450	6510
051157	Rappahannock	61	521	7141
051159	Richmond	63	383	4548
051161	Roanoke	63	427	5278
051163	Rockbridge	101	813	9710
051165	Rockingham	189	1020	12959
051167	Russell	56	703	7975
051169	Scott	95	753	9943
051171	Shenandoah	117	757	10570
051173	Smyth	78	603	7159
051175	Southampton	177	1306	15588
051177	Spotsylvania	46	911	12575
051179	Stafford	27	637	8344
051181	Surry	85	784	10024
051183	Sussex	102	1267	16362
051185	Tazewell	77	639	7477
051187	Warren	44	438	6310
051191	Washington	142	632	6822
051193	Westmoreland	101	777	9357
051195	Wise	35	462	5685
051197	Wythe	109	596	7803
051199	York	35	271	3423
051510	Alexandria	38	145	1065
051515	Bedford	22	101	604
051520	Bristol	37	135	1220
051530	Buena Vista	6	43	381
051540	Charlottesville	18	98	528
051550	Chesapeake	71	666	8477
051560	Clifton Forge	27	61	436
051570	Colonial Heights	35	88	662
051580	Covington	24	114	1605
051590	Danville	55	343	3405
051595	Emporia	19	234	3300
051600	Fairfax	18	96	1518
051610	Falls Church	16	98	1120

	051620	Franklin	66	142	1041
	051630	Fredericksburg	14	250	3012
	051640	Galax	45	94	519
	051650	Hampton	24	127	1112
	051660	Harrisonburg	73	143	746
	051670	Hopewell	26	79	711
	051678	Lexington	8	62	620
	051680	Lynchburg	45	250	2135
	051683	Manassas	17	86	743
	051685	Manassas Park	17	50	268
	051690	Martinsville	19	190	1625
	051700	Newport News	63	231	2187
	051710	Norfolk	42	197	2692
	051720	Norton	13	120	1305
	051730	Petersburg	58	171	1419
	051735	Poquoson	17	122	1351
	051740	Portsmouth	34	285	3215
	051750	Radford	27	76	609
	051760	Richmond	29	239	3517
	051770	Roanoke	33	91	770
	051775	Salem	14	61	568
	051790	Staunton	69	205	1550
	051800	Suffolk	118	964	11269
	051810	Virginia Beach	186	924	8724
	051820	Waynesboro	43	120	895
	051830	Williamsburg	3	38	446
	051840	Winchester	42	117	772
Virginia		**TOTAL**	9267	80615	981848

TSD-1c

Emissions Processing for 2002 OTC Regional and Urban 12km Base Year Simulation

Bureau of Air Quality Analysis and Research
Division of Air Resources
New York State Department of Environmental Conservation
Albany, NY 12233

March 19, 2007

Overview

All emissions processing for the revised 2002 OTC regional and urban 12 km base case simulations was performed with SMOKE2.1 compiled on a Red Hat 9.0 Linux operating system with the Portland group fortran compiler version 5.1. The emissions processing was performed on a month-by-month and RPO-by-RPO basis, i.e. SMOKE processing was performed for each month for each of the RPOs (MANE-VU, VISTAS, CENRAP, MRPO) individually as well as for Canada. For each month/RPO combination, a separate SMOKE ASSIGNS file was created, and the length of the episode in each of these ASSIGNS files was set to the entire month. Also, as discussed in Section 3, there was no difference between "episode-average" temperatures and "monthly-average" temperatures for the Mobile6 simulations that used the option of temperature averaging.

This document is structured as follows: A listing of all emission inventories is given in Section 2, organized by RPO and source category. Section 3 discusses the Mobile6 processing approach employed for the different RPOs, while Section 4 describes the processing of biogenic emissions with BEIS3.12. Finally, Sections 5 through7 describe the temporal allocation, speciation, and spatial allocation of the emissions inventories, respectively.

1. Emission Inventories

1.1 MANE-VU

Version 3 of the MANE_VU inventory was utilized to generate CMAQ-ready emissions. This emissions inventory data were obtained from the MANEVU archive in April 2006.

1.1.1 Area Sources

- Files: MANEVU_AREA_SMOKE_INPUT_ANNUAL_SUMMERDAY_040606.txt and MANEVU_AREA_SMOKE_INPUT_ANNUAL_WINTERDAY_040606.txt prepared by PECHAN, downloaded from **ftp.marama.org** (username mane-vu, password exchange)
- Fugitive dust correction: This was applied as county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing

1.1.2 Nonroad Sources

- File: MANEVU_NRD2002_SMOKE_030306 prepared by PECHAN; downloaded from **ftp.marama.org** (username mane-vu, password exchange)

1.1.3 Mobile Sources

- VMT/Speed: MANEVU_2002_mbinv_02022006_addCT.txt prepared by PECHAN and NESCAUM; downloaded from http://bronze.nescaum.org/Private/junghun/MANE-VU/onroad_ver3_update/MANEVU_V3_update.tar

1.1.4 Point Sources

- Files: MANEVU_Point_SMOKE_INPUT_ANNUAL_SUMMERDAY_041006.txt and MANEVU_Point_SMOKE_INPUT_ANNUAL_WINTERDAY_041006.txt prepared by PECHAN were downloaded from **ftp.marama.org** (username mane-vu, password exchange)
- Fugitive dust correction: This was applied as county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing
- Corrected the omission of 2,100 tons/year VOC emissions from several point sources in NJ. NJDEP provided updated IDA files on June 30 that were used for modeling.

1.2 CENRAP

The inventory data were obtained from the CENRAP ftp site in March 2006 and reflect version BaseB of the CENRAP inventory.

1.2.1 Area Sources

- Files:
  - CENRAP_AREA_SMOKE_INPUT_ANN_STATES_081705.txt
  - CENRAP_AREA_MISC_SMOKE_INPUT_ANN_STATE_071905.txt
  - CENRAP_AREA_BURNING_SMOKE_INPUT_ANN_TX_ NELI_071905.txt
  - CENRAP_AREA_MISC_SMOKE_INPUT_NH3_MONTH_{MMM} _072805.txt where {MMM} is JAN, FEB, … DEC
  - CENRAP_AREA_SMOKE_INPUT_NH3_MONTH_{MMM} _071905.txt where {MMM} is JAN, FEB, … DEC
- Fugitive dust correction: This was applied as county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing
- Note about area and nonroad source SMOKE processing for the CENRAP region: All area source inventories (both annual and month-specific) were processed in

one step through SMOKE. SMK_AVEDAY_YN was set to N, so seasonal profiles were used to apportion the annual inventories numbers by month. This setting was also used for the nonroad processing performed in a separate step. This was necessary since the month-specific files had zero in their 'average-day' column and the annual total column reflects the "monthly emissions as annual totals" as per header line. Therefore, seasonal profiles are used to apportion both the annual and month-specific files. As described below, we utilized the temporal profiles and cross-reference files generated by CENRAP. However, we did not verify that this approach indeed leads to the intended monthly allocation of ammonia and nonroad emissions.

1.2.2 Nonroad Sources

- Files:
  - CENRAP_NONROAD_SMOKE_INPUT_ANN_071305.txt
  - CENRAP_NONROAD_SMOKE_INPUT_MONTH_{MMM}_071305.txt where {MMM} is JAN, FEB, … DEC

1.2.3 Mobile Sources

- VMT/Speed files:
  - mbinv02_vmt_cenrap_ce.ida
  - mbinv02_vmt_cenrap_no.ida
  - mbinv02_vmt_cenrap_so.ida
  - mbinv02_vmt_cenrap_we.ida

1.2.4 Point Sources

- File: CENRAP_POINT_SMOKE_INPUT_ANNUAL_DAILY_072505.txt
- Fugitive dust correction: This was applied as county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing.

1.3 VISTAS

All VISTAS emission files were obtained from the Alpine Geophysics ftp site. They reflect version BaseG of the VISTAS inventory with the exception of fire emissions which reflect BaseF and BaseD. These files were downloaded between February and August, 2006.

1.3.1 Area Sources

- Files:

    - arinv_vistas_2002g_2453922_w_pmfac.txt
    - ida_ar_fire_2002_vistaonly_basef.ida
- Note: the header lines of these files indicate that the fugitive dust correction was already applied, so no further correction was performed.

1.3.2 Nonroad Sources

- Files:
    - nrinv_vistas_2002g_2453908.txt
    - marinv_vistas_2002g_2453972.txt

1.3.3 Mobile Sources

- VMT/Speed file: mbinv_vistas_02g_vmt_12jun06.txt

1.3.4 Point Sources

- Files:
    - Annual:
        - egu_ptinv_vistas_2002typ_baseg_2453909.txt
        - negu_ptinv_vistas_2002typ_baseg_2453909.txt
        - ptinv_fires_{MM}_typ.vistas.ida where {MM} is 01, 02, 03, etc. depending on the month; these annual point fire files were generated as part of the VISTAS BaseD inventory and were obtained in January 2005
    - Hour-specific:
        - pthour_2002typ_baseg_{MMM}_28jun2006.ems where {MMM} is jan, feb, mar, etc.
        - pthour_fires_{MM}_typ.vistas.ida where {MM} is 01, 02, 03, etc. depending on the month; these hourly point fire files were generated as part of the VISTAS BaseD inventory and were obtained in January 2005
- Note: No fugitive dust correction was performed for these files.

1.4 MRPO

MRPO emissions for SMOKE modeling were generated by Alpine Geophysics through a contract from MARAMA to convert the MRPO BaseK inventory from NIF to IDA format. The files were downloaded from the MARAMA ftp site **ftp.marama.org** (username mane-vu, password exchange) between April and June 2006.

1.4.1 Area Sources

- Files:
    - Annual:
        - arinv_mar_mrpok_2002_27apr2006.txt
        - arinv_other_mrpok_2002_20jun2006.txt
    - Month-specific:

        - arinv_nh3_2002_mrpok_{mmm}_3may2006.txt where {mmm} is jan, feb, etc.
        - dustinv_2002_mrpok_{mmm}_23may2006.txt where {mmm} is jan, feb, etc.
- Fugitive dust correction: This correction was performed only to the arinv_other_mrpok_2002_20jun2006.txt file using county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing.
- Note about area source SMOKE processing: SMOKE processing was performed separately for the annual and month-specific files. For the annual inventory processing, SMK_AVEDAY_YN was set to N, so seasonal profiles were used to apportion the annual inventories numbers by month. For the month-specific inventory processing, this variable was set to Y so that no seasonal profiles would be applied and the inventory numbers in the 'average day' column would be used. To save a SMOKE processing step, the annual "marine" inventory "arinv_mar_mrpok_2002_27apr2006.txt" was processed together with the annual "other area source" inventory "arinv_other_mrpok_2002_20jun2006.txt" even though it technically is part of the nonroad inventory.

1.4.2 Nonroad Sources

- Files: nrinv_2002_mrpok_{mmm}_3may2006.txt where {mmm} is jan, feb, etc.

1.4.3 Mobile Sources

- VMT/Speed file: mbinv_mrpo_02f_vmt_02may06.txt

1.4.4 Point Sources

- Files: ptinv_egu_negu_2002_mrpok_1may2006.txt
- Fugitive dust correction: This correction was performed only to the arinv_other_mrpok_2002_20jun2006.txt file using county-specific correction factors for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from EPA's CAIR NODA ftp site http://www.airmodelingftp.com (password protected).; this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing.

1.5 Canada

1.5.1 Area Sources

- File: AS2000_SMOKEready.txt obtained from ftp://ftp.epa.gov/EmisInventory/canada_2000inventory
- Fugitive dust correction: We applied "divide-by-four" correction for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; this adjustment was performed outside SMOKE with in-house Fortran programs. No county/province-specific correction factors were available for Canada

1.5.2 Nonroad Sources

- File: NONROAD2000_SMOKEready.txt obtained from ftp://ftp.epa.gov/EmisInventory/canada_2000inventory

1.5.3 Mobile Sources

- File: MOBILE2000_SMOKEready.txt obtained from ftp://ftp.epa.gov/EmisInventory/canada_2000inventory
- Fugitive dust correction: applied "divide-by-four" correction for SCC's listed at http://www.epa.gov/ttn/chief/emch/invent/index.html#dust; this adjustment was performed outside of SMOKE with in-house Fortran programs. No county/province-specific correction factors were available for Canada.

1.5.4 Point Sources

There has long been difficulty in obtaining an up-to-date Canadian criteria emissions inventory for point sources. This is due largely to confidentiality rights afforded to Canadian facilities. Thus far, the most recent inventory of Canadian point sources is rooted in the 1985 NAPAP data and is close to two decades old. Because there are a number of high emitting industrial facilities in southern Canada it is of particular importance to have a reasonably accurate inventory of these sources especially when modeling air quality over the Northeast and Midwest United States. Toward this end, an effort was made to obtain more recent Canadian point source data and incorporate it into an inventory database, which could then be used for the 2002 OTC air quality modeling.

Perhaps the most accurate and publicly accessible source of Canadian pollutant data is now available from the National Pollutant Release Inventory (NPRI) database. This database contains 268 substances. Facilities that manufacture, process or otherwise use one of these substances and that meet reporting thresholds are required to report these emissions to Environment Canada on an annual basis. The NPRI data are available at Environment Canada's website and can be found at the link http://www.ec.gc.ca/pdb/npri/npri_home_e.cfm. The page hosts an on-line search engine where one can locate emissions by pollutant or location. In addition, the entire database is available for download as an MS Access or Excel file. The NPRI database contains

numerous pages with a rather comprehensive list of information. Detailed information is available about each facility, including location, activity and annual emissions. In addition, facilities having stacks with a height of 50 meters or more are required to report stack parameters.

Unfortunately, one of the limitations of the NPRI database for modeling purposes is that the data are only available at the facility level. Emissions models require process level information, so in order to use this data, a few generalizations had to be made. Each facility has a Standard Industrial Classification (SIC) code associated with it; however, emissions models require Source Classification Codes (SCC's). SCC's are of critical importance as the emissions models use these codes for assignment of temporal and speciation profiles. SIC codes describe the general activity of a facility while SCC codes describe specific processes taking place at each facility. While no direct relationship exists between these two codes, a general albeit subjective association can be made.

For the purposes of creating a model-ready inventory file it was necessary to obtain the whole NPRI database. After merging all the necessary components from the NPRI database required in the SMOKE inventory file, the SIC code from each facility was examined and assigned an SCC code. In most cases, only a SCC3 level code was assigned with confidence. While this is admittedly a less than desirable process, it does allow for the use of the most recent emissions from the NPRI database to be used in modeling. Furthermore, having some level of SCC associated with these emissions will ensure that they will be assigned a temporal and speciation profile by the model, other than the default. Once the model-ready inventory file was developed, it was processed through SMOKE.

2. Mobile6 Processing

2.1 MANE-VU

2.1.1 Mobile6 input files

- Month-specific input files were prepared by PECHAN and NESCAUM and were downloaded from http://bronze.nescaum.org/Private/junghun/MANE-VU/onroad_ver3_update/MANEVU_V3_update.tar
- Added the line "REBUILD EFFECTS :0.10" to each file before the SCENARIO record to override the Mobile6 default setting of 0.9 (90%) for the "chip reflash" effectiveness

2.1.2 SMOKE/Mobile6 auxiliary files

- SMOKE/Mobile6 auxiliary files were prepared by PECHAN and NESCAUM and were downloaded from http://bronze.nescaum.org/Private/junghun/MANE-VU/onroad_ver3_update/MANEVU_V3_update.tar

2.1.3 Temperature averaging

- Following the setting in the MANEVU_2002_mvref.txt files, the following procedures were used by SMOKE for temporal and spatial temperature averaging in the calculation of emission factors:
    - Spatial averaging: temperatures were averaged over all counties that share a common reference county (i.e. Mobile6 input file)
    - Temporal averaging for May – September emissions processing: no temporal averaging was used, i.e. day-specific temperatures were used to calculate emission factors for each day.
    - Temporal averaging for non-summer-months emissions processing: Temporal averaging over the duration of the episode (i.e. the entire month, see introduction) was used, i.e. monthly average temperatures were used to calculate the emission factors.

2.2 CENRAP

2.2.1 Mobile6 input files

- Mobile6 input files for the CENRAP region for January and July were contained in the files central_M6_{MMM}.zip, north_M6_{MMM}.zip, south_M6_{MMM}.zip, west_M6_{MMM}.zip where {MMM} is either jan or jul. July input files were used for April – September processing, while January input files were used for the remaining months
- All files were downloaded from the CENRAP ftp site in March 2006.

2.2.2 SMOKE/Mobile6 auxiliary files

- SMOKE/Mobile6 auxiliary files were contained in the files central_M6_RD.zip, north_M6_RD.zip, south_M6_RD.zip, and west_M6_RD.zip. The SMOKE MCREF, MVREF, and MCODES files were contained in the file MOBILESMOKE_Inputs.zip. The MCREF and MVREF files were combined for the different regions (“central”, “east”, “west”, “north”)
- All files were downloaded from the CENRAP ftp site in March 2006.

2.2.3 Temperature averaging

- The following procedures were used by SMOKE for temporal and spatial temperature averaging in the calculation of emission factors according to the setting in the mvref files:
    - Spatial averaging: no spatial averaging of temperatures, i.e. the temperatures for the reference county is used to calculate emission factors for all counties that share this reference county (i.e. Mobile6 input file)
    - Temporal averaging: Temporal averaging over the duration of the episode (i.e. the entire month, see introduction) was used, i.e. monthly average temperatures were used to calculate the emission factors.

2.3 VISTAS

2.3.1 Mobile6 input files

- Month-specific Mobile6 input files were obtained from the Alpine Geophysics ftp site in July 2006. They reflect version BaseG of the VISTAS inventory.

2.3.2 SMOKE/Mobile6 auxiliary files

- SMOKE/Mobile6 auxiliary files utilized were obtained from the Alpine Geophysics ftp site in July 2006. They reflect version BaseG of the VISTAS inventory.

2.3.3 Temperature averaging

- The following procedures were used by SMOKE for the temporal and spatial temperature averaging in the calculation of emission factors according to the setting in the mvref_baseg.36k.ag.txt file:
    - Spatial averaging: temperatures averaged over all counties that share a common reference county (i.e. Mobile6 input file)
    - Temporal averaging: Temporal averaging over the duration of the episode (i.e. the entire month, see introduction) was used, i.e. monthly average temperatures were used to calculate the emission factors.

2.4 MRPO

2.4.1 Mobile6 input files

- Month-specific Mobile6 input files for SMOKE modeling were generated by Alpine Geophysics through a contract from MARAMA. They are based on version BaseK of the MRPO inventory. The files were downloaded from the MARAMA ftp site **ftp.marama.org** (username mane-vu, password exchange) in May 2006.

2.4.2 SMOKE/Mobile6 auxiliary files

- SMOKE/Mobile6 auxiliary files for SMOKE modeling were generated by Alpine Geophysics through a contract from MARAMA. They are based on version BaseK of the MRPO inventory. The files were downloaded from the MARAMA ftp site **ftp.marama.org** (username mane-vu, password exchange) in May 2006.

2.4.3 Temperature averaging

- The following procedures were used by SMOKE for the temporal and spatial temperature averaging in the calculation of emission factors according to the setting in the mvreg_mrpo_basek.txt file:
    - Spatial averaging: temperatures averaged over all counties that share a common reference county (i.e. Mobile6 input file)

- Temporal averaging: Temporal averaging over the duration of the episode (i.e. the entire month, see introduction) was used, i.e. monthly average temperatures were used to calculate the emission factors.

3. Biogenic Emission Processing

Hourly gridded biogenic emissions for the 12 km and 36 km modeling domains were calculated by BEIS3.12 through SMOKE, using MCIP-processed MM5 fields for temperature ("TA", layer-1 temperature), solar radiation ("RGRND"), surface pressure ("PRES"), and precipitation ("RN" and "RC"). A 'seasonal switch' file was generated by the SMOKE utility metscan to determine whether winter or summer emission factors should be used for any given grid cell on any given day. Winter emission factors are used from January 1st through the date of the last frost and again from the data of the first frost in fall through December 31st. Summer emission factors are used for the time period in between. This calculation is performed separately for each grid cell.

4. Temporal Allocation

4.1 MANE-VU

4.1.1 Area and nonroad sources

- Generated as part of the MANE-VU version 1 inventory
- amptpro.m3.us+can.manevu.030205.txt
- amptref.m3.manevu.012405.txt
- downloaded from **ftp.marama.org** (username mane-vu, password exchange) in January 2005

4.1.2 Mobile sources

- MANEVU_2002_mtpro_02022006_addCT.txt
- MANEVU_2002_mtref_02022006_addCT.txt
- prepared by PECHAN and NESCAUM and downloaded from http://bronze.nescaum.org/Private/junghun/MANE-VU/onroad_ver3_update/MANEVU_V3_update.tar

4.1.3 Point Sources

- Based on the same files as for the MANE-VU area and nonroad temporal files listed above, but added the CEM-based 2002 state-specific temporal profiles and cross-references for EGU sources for the MANE-VU states that were generated by VISTAS for their BaseD modeling and obtained in February 2005.
- No CEM-based hour-specific EGU emissions were utilized

4.2 CENRAP

The following temporal profiles and cross-reference files were used:

- Area and nonroad sources:
    - amptpro.m3.us+can.cenrap.010605_incl_nrd.txt
    - amptref.m3.cenrap.010605_add_nh3_and_nrd.txt
- Mobile sources:
    - mtpro.cenrap.v3.txt
    - mtref.cenrap.v3.txt
- Point sources:
    - ptpro.{QQ}.cenrap_egus_cem.00-03avg.121205.txt where {QQ} is Q1 for January/February/March, Q2 for April/May/June, etc.
    - ptref.{QQ}.cenrap_egus_cem.00-03avg.121205.txt where {QQ} is Q1 for January/February/March, Q2 for April/May/June, etc.
- All files were downloaded from the CENRAP ftp site in March 2006.

4.3 VISTAS

The following month-specific temporal profiles and cross-reference files were used:

- Area and nonroad sources:
    - atpro_vistas_basef_15jul05.txt
    - atref_vistas_basef_15jul05.txt
- Mobile sources:
    - mtpro_vistas_basef_04jul05.txt
    - mtref_us_can_vistas_basef_04jul05.txt
- Point sources:
    - ptpro_typ_{MMM}_vistasg_28jun2006.txt where {MMM} is jan, feb, mar, etc.
    - ptref_typ_vistas_baseg_28jun2006.txt
- These files were obtained from the Alpine Geophysics ftp site. They reflect version BaseG of the VISTAS inventory for the point source allocation files and version BaseF for the area, nonroad, and mobile source allocation files. These files were downloaded between February and July, 2006.

4.4 MRPO

The following month-specific temporal profiles and cross-reference files were used for all source categories:

- amptpro_typ_us_can_{MMM}_vistas_27nov04.txt where {MMM} is jan, feb, mar, etc.
- amptref_2002_us_can_vistas_17dec04.txt
- These files were obtained from VISTAS in January 2005 and reflect their BaseD modeling. No updated temporal profiles or cross-reference files were developed for use with the MRPO BaseK inventory.

4.5 Canada

For Canada, the SMOKE2.1 default temporal profiles and cross-reference files (amptpro.m3.us+can.txt and amptref.m3.us+can.txt) were utilized.

5. Speciation

The same speciation profiles (gspro.cmaq.cb4p25.txt) and cross-references (gsref.cmaq.cb4p25.txt) were utilized for all regions and all source categories. Different versions of these files were obtained (SMOKE2.1 default, EPA-CAIR modeling, VISTAS, CENRAP and MANE-VU) and compared. After comparing the creation dates and header lines of these files, it was determined that the EPA-CAIR and MANE-VU files had the most recent updates, and consequently the final speciation profile and cross-reference files used for all regions and source categories was based on the EPA-CAIR files with the addition of MANE-VU specific updates.

6. Spatial Allocation

6.1 U.S.

The spatial surrogates for the 12km domain were extracted from the national grid 12km U.S. gridding surrogates posted at EPA's website at
http://www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html
The gridding cross-references were also obtained from this website, but for the processing of MANE-VU area source emissions, MANE-VU specific cross-reference entries posted on the MARAMA ftp site were added.

6.2 Canada

The spatial surrogates for Canadian emissions for the 12km domain were extracted from the national grid 12km Canadian gridding surrogates posted at EPA's website at
http://www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html
The gridding cross-references were also obtained from this website.

Reference:

Pechan: (2006) Technical Support document for 2002 MANE-VU SIP Modeling inventories, version 3. Prepared by E. H. Pechan & Associates, Inc. 3622 Lyckan Parkway, Suite 2005, Durham, NC 27707.

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TSD-1d

8-h Ozone modeling using the SMOKE/CMAQ system

Bureau of Air Quality Analysis and Research

Division of Air Resources

New York State Department of Environmental Conservation

Albany, NY 12233

February 1, 2006

Air Quality Modeling Domain

The modeling domain utilized in this application represented a sub-set of the inter-RPO's continental modeling domain that covered the entire 48-state region with emphasis on the Ozone Transport Region. The OTC modeling domain at 12km horizontal mesh is displayed in Figure 1 is part of the 36km continental domain that is designed to provide boundary conditions (BCs). The particulars of the two modeling domains are:

The 36km domain covered the continental US by a 149 by 129 mesh in the east-west and north-south directions, respectively. The domain is based on Lambert Conformal Projection with the center at (97ºW 40ºN) and parallels at 33ºN and 45ºN. As evident from Figure 1, the 12km domain utilized in this analysis covers most areas of the eastern US and has 172 by 172 mesh in the horizontal. Both domains utilize 22 layers in the vertical extending to about 16km with 16 layers placed within the lower 3km.

Photochemical Modeling -- CMAQ

The CMAQ (version 4.5.1) with CB4 chemistry, aerosol module for $PM_{2.5}$ and RADM cloud scheme was utilized in this study. Photochemical modeling was performed with the CCTM software that is part of the CMAQ modeling package. Version 4.5.1 of this modeling software was obtained from the CMAS modeling center at http://www.cmascenter.org. The following module options were used in compiling the CCTM executable:

- Horizontal advection: yamo
- Vertical advection: yamo
- Horizontal diffusion: multiscale
- Vertical diffusion: eddy
- Plume-in-Grid: non operational
- Gas phase chemical mechanism: CB-4
- Chemical solver: EBI
- Aerosol module: aero3
- Process analysis: non operational

The following computational choices were made during compilation:

- Compiler version: PGI 6.0
- Fortran compiler flags:-Mfixed -Mextend -Bstatic -O2 -module ${MODLOC} -I.
- C compiler flags: -v -O2 -I${MPICH}/include
- IOAPI library: version 3.0
- NETCDF library: version 3.6.0
- Parallel processing library version: mpich 1.2.6
- Static compilation on 32-bit system

The following choices were made for running the executable:

- Number of processors: 8
- Domain decomposition for parallel processing: 4 columns, 2 rows
- Number of species written to the layer-1 hourly-average concentration output (ACONC) file: 39 (O3, NO, CO, NO2, HNO3, N2O5, HONO, PNA, PAN, NTR, NH3, SO2, FORM, ALD2, PAR, OLE, ETH, TOL, XYL, ISOP, ASO4I, ASO4J, ANO3I, ANO3J, ANH4I, ANH4J, AORGAI, AORGAJ, AORGPAI, AORGPAJ, AORGBI, AORGBJ, AECI, AECJ, A25I, A25J, ACORS, ASEAS, ASOIL)
- Each daily simulation was performed for 24 hours starting at 05:00 GMT (00:00 EST)

The following postprocessing steps were performed using utility tools from the "ioapi" software package obtained from http://www.baronams.com/products/ioapi/AA.html#tools:

- Extract and combine the following species for each hour for the first 16 model layers from the full 3-D instantaneous concentration output file: O3, CO, NO, NO2, NOY_1 (=*NO + NO2 + PAN + HNO3*), NOY_2 (=*NO + NO2 + PAN + HNO3 + HONO + N2O5 + NO3 + PNA + NTR*), HOX (=*OH + HO2*), VOC (=*2*ALD2 + 2*ETH + FORM + 5*ISOP + 2*OLE + PAR + 7*TOL + 8*XYL*), ISOP, PM2.5 (=*ASO4I + ASO4J + ANO3I + ANO3J + ANH4I + ANH4J + AORGAI + AORGAJ + 1.167*AORGPAI + 1.167*AORGPAJ + AORGBI + AORGBJ + AECI + AECJ + A25I + A25J*), PM_SULF (=*ASO4I + ASO4J*), PM_NITR (=*ANO3I + ANO3J*), PM_AMM (=*ANH4I + ANH4J*), PM_ORG_SA (=*AORGAI + AORGAJ*), PM_ORG_PA (=*1.167*AORGPAI + 1.167*AORGPAJ*), PM_ORG_SB(=*AORGBI + AORGBJ*), PM_ORG_TOT (=*AORGAI + AORGAJ + 1.167*AORGPAI + 1.167*AORGPAJ + AORGBI + AORGBJ*), PM_EC (=*AECI + AECJ*), PM_OTH (=*A25I + A25J*), PM_COARS (=*ACORS + ASEAS + ASOIL*), SO2, HNO3, NH3, H2O2
- Extract all species for all model layers for the last hour of each daily instantaneous concentration output file to enable "hot" restarts of modeling simulations
- Create daily files of hourly running-average 8-hr ozone concentrations with time stamps assigned to the first hour of the averaging interval

The following files are archived on LTO2 computer tapes (each tape holds approximately 200 Gb of data) for each day:

- Aerosol/visibility file
- Layer-1 hourly-average concentration output file (contains 39 species)
- Dry deposition file
- Wet deposition file
- Extracted 16-layer species file
- Restart file (last hour of full 3-D instantaneous concentration file)
- Hourly 8-hr concentration file

Photolysis Rates

One of the inputs to CMAQ is the photolysis rates. In this study, photolysis rate lookup tables were generated for each day of 2002 with the JPROC software that is part of the CMAQ modeling package. This software was obtained from the CMAS modeling center at http://www.cmascenter.org. Rather than using climatological ozone column data, daily ozone column measurements from the NASA Earthprobe TOMS instrument were downloaded from ftp://toms.gsfc.nasa.gov/pub/eptoms/data/ozone/Y2002/ and used as input to the JPROC processor. It should be noted that TOMS data were missing for the time period from August 3 – 11, 2002. The missing period was filled as follows-- TOMS data file for August 2 was used as JPROC input for August 3rd through August 7th, and the TOMS data file for August 12th was used as JPROC input for August 8th through August 11th.

Boundary Conditions (BCs)

The boundary conditions for the 12km grid were extracted from the 36km CMAQ simulation. The 36km simulation utilized boundary conditions that were based on a one-way nest approach to GEOS-CHEM global model outputs (Moon and Byun 2004, Baker 2005). As stated above, the intent of the 36km CMAQ simulation was to provide the BCs for the 12km model that would be more reflective of the emissions and meteorology rather than to use either clean or arbitrary pollutant fields. Also, in this study the CMAQ simulations utilized a 15-day ramp-up period, thereby minimizing the propagation of the boundary fields into the areas of concern. A report on the setup and application of the 36km CMAQ and the extraction of the BCs is available from NYSDEC.

Meteorological data

The meteorological data for this study was based on MM5 modeling (see Meteorological Modeling, 2007). The MM5 fields are then processed by MCIP version 3.0, a utility available as part of the CCTM software from CMAS Modeling Center (see http://www.cmascenter.org) to provide CMAQ model-ready inputs.

Emissions

The emissions data for 2002 were generated by individual states within the OTR and were assembled and processed through the Mid Atlantic Northeast Visibility Union (MANE-VU), a Regional Planning Organization (RPO). These emissions were then processed by NYSDEC using SMOKE processor to provide CMAQ compatible inputs (Anthro-Emissions 2006). The 2002 emissions for the non-OTR areas within the modeling domain were obtained from the corresponding RPOs and were processed using SMOKE, in a manner similar to that of the OTR.emissions. Details of this processing are outlined in the report (Pechan 2007), and the hourly biogenic emissions (Bio-Emissions, 2006)

CMAQ simulations

CMAQ simulations were performed using the one-way nesting approach in which we perform the continental CMAQ simulation at 36km grid spacing. For this simulation we utilized clean initial conditions with boundary conditions extracted from the simulation of GEOS-CHEM global chemical model. The interface program used in this application was developed by University of Huston (Moon and Byun 2004), which was applied to obtain hourly 36km boundary concentrations from GEOS-CHEM outputs. The CMAQ 36km simulation was initiated from December 15, 2001 with the first 15 days as spin up period and terminated on December 31, 2002. The simulation utilized the 2002 emissions data available from the RPOs and 2002 MM5 meteorological fields developed by the University of Maryland (TSD-1a). The hourly boundary fields for the 12km CMAQ domain were obtained by application of BCON program to the 3-D concentration fields generated by the 36km CMAQ simulation.

The 12km simulations for both base and future year were assigned the boundary conditions based on the 36km CMAQ simulation and clean initial conditions. The simulation period covered was from April 15 through September 30, with the first 15 days of April set as ramp-up or spin-up period and that only data from May 1 through September 30 were used in the analysis. Details on CMAQ setup and run scripts are available from NYSDEC.

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Anthro-Emissions: (2006) Emission Processing for the Revised 2002 OTC Regional and Urban 12 km Base Case Simulations. TSD-1c

Figure 1 Display of 36- and 12km air quality modeling domains.

TSD-1e

CMAQ Model Performance and Assessment

8-h OTC Ozone Modeling

Bureau of Air Quality Analysis and Research

Division of Air Resources

New York State Department of Environmental Conservation

Albany, NY 12233

March 19, 2006

Air quality model evaluation and assessment

One of the tasks that is required as part of demonstrating attainment for the 8-hr ozone NAAQS is the evaluation and assessment of the air quality modeling system that has been utilized to predict future air quality over the region of interest. As part of the attainment demonstration, the SMOKE/CMAQ modeling system was applied to simulate the pollutant concentration fields for the base year 2002 emissions with the corresponding meteorological information. The modeling databases for meteorology using MM5 (TSD-1a), the emissions using SMOKE (TSD-1b and TSD-1c), and application of CMAQ (TSD-1d) provides simulated pollutant fields that are compared to measurements, in order to establish the credibility of the simulation. In the following sections a comparison between the measured and predicted concentrations is performed and results are presented, demonstrating on an overall basis the utility of the modeling system in this application.

The results presented here should serve as an illustration of some of the evaluation and assessment performed on the base 2002 CMAQ simulation. Additional information can be made available by request from the New York State Department of Environmental Conservation.

Summary of measured data

The ambient air quality data, both gaseous and aerosol species, for the simulation period of May through September 2002 were obtained from the following sources:

- EPA Air Quality System (AQS)
- EPA fine particulate Speciation Trends Network (STN)
- EPA Clean Air Status & Trends Network (CASTNet)
- Interagency Monitoring of PROtected Visual Environments (IMPROVE)
- Pinnacle State Park, NY operated by Atmospheric Science Research Center, University at Albany, Albany, NY
- Harvard Forest, Petersham, MA operated by Harvard University, Boston, MA
- Atmospheric Investigation, Regional Modeling, Analysis and Prediction (AIRMAP) operated by University of New Hampshire, Durham, NH
- NorthEast Ozone & Fine Particle Study (NE-OPS), led by Penn State University and other research groups in Philadelphia, PA
- Aircraft data obtained by the University of Maryland, College Park MD
- Wet deposition data from the National Atmospheric Deposition Program/National Trends Network (NADP/NTN), Atmospheric Integrated Research Monitoring Network (AIRMoN), and the New York State Department of Environmental Conservation (NYSDEC)

Measured data from sites within the Ozone Transport Region (OTR) plus the rest of Virginia were included here. The model-based data were obtained at the grid-cell corresponding to the monitor location; no interpolation was performed.

Ozone (O_3)

Hourly O_3 is measured at a large number of State, Local, and National Air Monitoring Stations (SLAMS/NAMS) across the US on a routine basis, and the data from 208 sites were extracted from the AQS database (http://www.epa.gov/ttn/airs/airsaqs/aqsweb/aqswebhome.html). Hourly O_3 concentrations from the Harvard Forest Environmental Management Site in Petersham, MA (http://www.as.harvard.edu/data/nigec-data.html); Pinnacle State Park in Addison, NY (http://www.asrc.cestm.albany.edu); and the four University of New Hampshire AIRMAP sites (http://airmap.unh.edu) were also included in this database. The EPA CASTNet program collects hourly O_3 at generally rural locations across the US (http://www.epa.gov/castnet); data from 22 sites, including two from West Virginia, were used in the model evaluation.

Fine particulate matter ($PM_{2.5}$)

The 24-hour average Federal Reference Method (FRM) $PM_{2.5}$ mass data collected routinely at SLAMS/NAMS sites across the US were extracted from AQS (257 sites). Hourly $PM_{2.5}$ mass was also included in this database, primarily extracted from AQS (54 sites). Hourly $PM_{2.5}$ mass were also taken from the Thompson Farm, NH AIRMAP site, Pinnacle State Park, and the NE-OPS site in Philadelphia, PA (http://lidar1.ee.psu.edu).

Fine particulate speciation

The 24-hour average $PM_{2.5}$ and fine particulate speciation (sulfate (SO_4), nitrate (NO_3), elemental carbon (EC), organic carbon/organic mass (OC/OM), and soil/crustal matter) from Class I areas across the US, collected every 3rd day, were obtained from the IMPROVE web site (http://vista.cira.colostate.edu/IMPROVE/Default.htm). In addition to these parameters, the EPA STN (http://www.epa.gov/ttn/amtic/speciepg.html) also reports ammonium (NH_4) to AQS; data from this network are collected every 3rd or 6th day. Data from 49 STN sites, generally in urban areas and often collocated with FRM monitors, and 21 IMPROVE sites (including Dolly Sods, WV) were used in this analysis. Organic mass is assumed to equal 1.8×OC, and soil/crustal matter is assumed to consist of oxides of Al, Ca, Fe, Si, and Ti. The STN OC data are blank-corrected by removing a monitor-specific, constant blank, and these values are available from http://www.epa.gov/airtrends/aqtrnd03/pdfs/2_chemspec0fpm25.pdf; the IMPROVE OC blanks are assumed to equal zero.

Criteria gaseous pollutants

Hourly carbon monoxide (CO; 97 sites), nitric oxide (NO; 75 sites), nitrogen dioxide (NO_2; 97 sites) and sulfur dioxide (SO_2; 134 sites) are also included in this model evaluation database. A large majority of these sites are SLAMS/NAMS monitors located primarily in urban in suburban areas, but data from the Harvard Forest, Pinnacle State Park, and AIRMAP sites are also included here.

Non-methane hydrocarbons

While there are several dozen hydrocarbon species measured routinely, for this model evaluation database the focus was on Carbon Bond IV species groups that consist of a single primary species. For this reason only ethene (C_2H_4), isoprene (C_5H_8), and formaldehyde (HCHO) concentrations were extracted from AQS. Hourly C_2H_4 and C_5H_8 data from 19 Photochemical Assessment Monitoring Stations (PAMS) sites and 24-hour average HCHO from 18 air toxics sites are included in this database.

University of Maryland aircraft data

The University of Maryland performed 144 aircraft spirals at 41 regional airport locations over 26 days from May-August 2002 (http://www.atmos.umd.edu/~RAMMPP). Spirals are approximately 20-45 minutes in duration, over which time the atmosphere from about 0-3 km is sampled. The concentrations of O_3, CO, and SO_2 from these spirals were included in this database, and help provide a semi-quantitative evaluation of CMAQ performance above the ground surface. Minute average aircraft data were compared to the nearest instantaneous 3-dimensional CMAQ output.

Wet deposition

The NADP (http://nadp.sws.uiuc.edu) collects wet deposition samples across the US, through the NTN and the AIRMoN. Weekly wet deposition samples are collected by the NTN, while daily or event-based samples were collected by the AIRMoN. The NYSDEC (http://www.dec.state.ny.us) also collects weekly wet deposition samples independently from the NADP. The wet deposition of SO_4^{2-}, NO_3^-, and NH_4^+ from 43 NADP/NTN sites, 7 NADP/AIRMoN sites, and 19 NYSDEC sites are included in this model evaluation database.

Evaluation of CMAQ predictions

The following sections provide model evaluation information for the above referenced pollutants over the OTR portion of the 12-km modeling domain. The statistical formulations that have been computed for each species are as follows: P_i and O_i are the individual (daily maximum 8-hour O_3 or daily average for the other species) predicted and observed concentrations, respectively; $\overline{P}$ and $\overline{O}$ are the average concentrations, respectively, and N is the sample size.

Observed average, in ppb:

$$\overline{O} = \frac{1}{N}\sum O_i$$

Predicted average, in ppb (only use P_i when O_i is valid):

$$\overline{P} = \frac{1}{N}\sum P_i$$

Correlation coefficient, R^2:

$$R^2 = \frac{\left[\sum (P_i - \overline{P})(O_i - \overline{O})\right]^2}{\sum (P_i - \overline{P})^2 \sum (O_i - \overline{O})^2}$$

Normalized mean error (NME), in %:

$$NME = \frac{\sum |P_i - O_i|}{\sum O_i} \times 100\%$$

Root mean square error (RMSE), in ppb:

$$RMSE = \left[\frac{1}{N}\sum (P_i - O_i)^2\right]^{1/2}$$

Fractional error (FE), in %:

$$FE = \frac{2}{N}\sum \left|\frac{P_i - O_i}{P_i + O_i}\right| \times 100\%$$

Mean absolute gross error (MAGE), in ppb:

$$MAGE = \frac{1}{N}\sum \left|P_i - O_i\right|$$

Mean normalized gross error (MNGE), in %:

$$MNGE = \frac{1}{N}\sum \frac{\left|P_i - O_i\right|}{O_i} \times 100\%$$

Mean bias (MB), in ppb:

$$MB = \frac{1}{N}\sum (P_i - O_i)$$

Mean normalized bias (MNB), in %:

$$MNB = \frac{1}{N}\sum \frac{(P_i - O_i)}{O_i} \times 100\%$$

Mean fractionalized bias (MFB), in %:

$$MFB = \frac{2}{N}\sum \left[\frac{P_i - O_i}{P_i + O_i}\right] \times 100\%$$

Normalized mean bias (NMB), in %:

$$NMB = \frac{\sum (P_i - O_i)}{\sum O_i} \times 100\%$$

Daily maximum 8-hour O_3 concentrations

Model evaluation statistics, based on daily maximum 8-hour average O_3 levels on those days having (1) at least 18 valid observations, or (2) fewer than 18 valid observations but the observed daily maximum O_3 concentration was at least 85 ppb, are presented here for all sites across the OTR and all of VA. The data covered the period May 15 through September 29, excluding July 6-9, when many sites across the eastern US were affected by large forest fires in Quebec. There are 208 SLAMS/NAMS sites and 28 special sites.

These model evaluation statistics were computed using two different threshold values for observed daily maximum 8-hour O_3. First, the statistics were computed using only those days when the observed daily maximum 8-hour O_3 concentration exceeded 40 ppb. Second, the statistics were computed using only those days when the observed daily maximum 8-hour O_3 exceeded 60 ppb. This latter method focuses on the highest O_3 days.

Figures 1-4 display time series of observed and predicted daily maximum 8-hour O_3 concentrations averaged over all sites across the OTR, at SLAMS/NAMS and special sites and for the daily maximum two thresholds. These averages were computed for each day considering all sites that met the corresponding threshold criteria. In general the observed and predicted composite average O_3 concentrations track each other rather well, although there was fairly substantial underprediction during the mid-August period. Also, the model performance tends to be better when the lower cutoff (40 ppb) was considered.

Figures 5-8 display spatial maps of fractional error and mean fractionalized bias for the two threshold levels. At each site the statistics were computed over the entire modeling season. Both the SLAMS/NAMS and special monitors are displayed here. In general, the model performance was better in the vicinity of urban areas and along the northeastern corridor, compared to the performance in rural areas where the model tended to underpredict daily maximum concentrations. The other statistical metrics yielded similar results to FE and MFB.

Table 1 lists the median and range in fractional error, and the mean fractionalized bias of daily maximum 8-hour O_3 calculated at each site over the season, for both observed thresholds (40 and 60 ppb), as well as all sites versus just the SLAMS/NAMS sites. Considering just SLAMS/NAMS sites, FE was always less than 32% for the 40 ppb threshold, and less than 40% for the 60 ppb threshold. Similarly, the MFB at SLAMS/NAMS sites ranged from -29 to +23% for the 40 ppb threshold, and ranged from -40 to +22% for the 60 ppb threshold. Adding the special sites did not affect the statistics substantially.

Diurnal variations of gases

Figures 9-17 display the composite diurnal variations of the species reported hourly – O_3 (SLAMS/NAMS and other/special sites, displayed separately), continuous $PM_{2.5}$, CO, NO, NO_2, SO_2, ethene, and isoprene. The average diurnal variations are for the period of May 15-September 30 – again excluding July 6-9 – considering all sites in the OTR. Note that the O_3 diurnal variations were computed from running 8-hour averages, with hours denoting the start of the 8-hour block. The number of monitors used to compute each composite diurnal variation is shown in each figure.

For O_3, the composite diurnal pattern predicted by CMAQ is fairly similar to that observed, especially at the more urban SLAMS/NAMS monitors. However, on average CMAQ predicts the daily maximum about an hour earlier than observed. For most of the other species presented here, CMAQ tends to predict two daily peaks, one morning and one late afternoon. For some species, such as $PM_{2.5}$ mass the observed concentration on a composite basis has very little diurnal variation. On the other hand, primary pollutants like CO, NO, and ethane, CMAQ exhibits qualitative agreement with the observations.

Daily average concentrations of co-pollutant trace gases

Composite daily average predicted and observed concentrations of CO, NO, NO_2, SO_2, C_2H_4, HCHO, and C_5H_8 across the OTR are displayed in Figures 18-24. Daily average concentrations of the criteria gases, C_2H_4 and C_5H_8 were computed from hourly averages, and only those days having at least 12 hours of valid observed data were considered here. The HCHO data shown here are based on 24-hour average values every 6th day. The criteria gas data cover the period May 15 – September 30, whereas the NMHC data only cover the June 1 – August 31 period, since these data are predominantly PAMS data; however, excluded from this analysis is the July 6-9 period when many sites across the eastern US were affected by large forest fires in Quebec.

Table 2 lists the median and range in mean fractionalized bias calculated at each site over the season used in this analysis. The values listed in Table 2 were computed at each site over the entire season. While the range in MFB is rather large for each species across all sites, the median MFB was below 50% for all species except C_2H_4, which is substantially overpredicted by CMAQ. It should be noted that these species can vary substantially from day to day, and days with very low modeled or observed values can contribute to high MFB.

$PM_{2.5}$ mass and speciation

Composite daily average predicted and observed concentrations of $PM_{2.5}$ mass (both daily average FRM data and continuous data), as well as major speciation –SO_4, NO_3, NH_4, EC, OM (defined here operationally as 1.8×blank-corrected organic carbon), and crustal mass (sum of oxides of Al, Ca, Fe, Si, and Ti) – across the OTR were compared in this analysis. The data cover the period May 15 – September 30, and again the July 6-9 period was excluded, when numerous sites in the eastern US were affected

by large forest fires in Quebec. The continuous and FRM $PM_{2.5}$ data are shown every day, since there are ample daily FRM sites across the OTR. The speciation data included here are daily averages every third day, and consist of the largely urban EPA STN and the largely rural IMPROVE network. The two speciation networks collect $PM_{2.5}$, SO_4, NO_3, EC, OM, and crustal mass, while only the STN reports NH_4 at a sufficient number of locations.

Table 3 lists the median and range in mean fractionalized bias calculated at each site over the season used in this analysis. The values listed in Table 3 were computed at each site over the entire season. Figures 25-39 display time series of composite average observed and predicted daily concentrations; in these figures, for each day the statistics were computed using all monitors with valid data. The best qualitative agreement between observed and modeled concentrations is exhibited for $PM_{2.5}$ and SO_4. Note that in the case of crustal mass, the data from July 4 are also not included since this day is greatly affected by fireworks. On July 4, the composite average observed and predicted crustal concentrations were 4.59 $\mu g\ m^{-3}$ and 1.74 $\mu g\ m^{-3}$, respectively at the STN monitors, and 4.46 $\mu g\ m^{-3}$ and 0.99 $\mu g\ m^{-3}$, respectively at the IMPROVE monitors.

As with the gaseous co-pollutant data, there is a substantial spread in MFB across the sites. However, the median MFB for $PM_{2.5}$ mass and SO_4 was generally small (<12%) for both urban and rural sites. CMAQ tends to overpredict NO_3, more so at the IMPROVE sites. CMAQ also tends to underpredict OM at both urban and rural sites, although some of this discrepancy may be attributed to the fact that OM is operationally defined and is highly dependent on the blank correction and multiplier to account for other components of OM not directly measured. CMAQ tends to overpredict both EC and crustal mass, especially at urban sites; similar to OM, the crustal mass overprediction is related to the fact that this parameter is operationally defined.

Wet deposition of sulfate, nitrate, and ammonium

Observed and predicted wet deposition of SO_4, NO_3, and NH_4 were compared over the period May 14 – September 30. For this analysis, weekly or event-based wet deposition amounts from the NADP/NTN (43 sites), NADP/AIRMoN (7 sites), and New York State DEC (19 sites) covering the entire OTR plus all of VA and WV were integrated over the four-and-a-half months. Because the observed weekly wet deposition samples did include July 6-9, the corresponding CMAQ predictions also include this period. Table 4 lists the model evaluation statistics for integrated wet deposition of SO_4, NO_3, and NH_4 at each site over the season, while Figures 40-42 compare the observed and predicted weekly values relative to the 1:1 line.

Overall CMAQ tended to overpredict wet deposition of these ions. On a percentage basis, the overprediction was least for SO_4 and highest for NO_3. The NME, MNGE, MNB, and NMB were less than 50% for the three ions. Given that precipitation is very difficult to predict, especially during the summer months when rainfall can vary tremendously over a 12 km by 12 km area represented by this model grid, CMAQ did a rather good job reproducing seasonal wet deposition over the OTR.

Upper-air O_3, CO, and SO_2 data

The University of Maryland operated an instrumented light aircraft during the summer of 2002. On 26 days from May-August meteorological, trace gas, and particle scattering/absorption data were collected during ascent or descent spirals over 41 regional airports. In all, 144 spirals were performed from near the surface to about 3 km above ground level. For this analysis, composite average profiles of O_3, CO, and SO_2 were created over three time periods: "morning" (08-11 EST), "afternoon" (12-16 EST), and "evening" (17-19 EST). The minute average observed concentrations were aggregated into layer averages, which correspond to the lowest 15 model layers. Model layers are increasingly thick away from the surface; the surface layer is about 20 m thick while the 15th layer is about 500 m thick (and centered about 2.8 km above the ground). Figures 43-51 display the observed and predicted composite vertical profiles of O_3, CO, and SO_2 for the three time periods. In terms of profile shape, CMAQ was in good qualitative agreement for all three species above the surface during the afternoon hours. For CO, the model tends to greatly underpredict observed levels near the surface, whereas the predicted O_3 and SO_2 concentrations are closer to the respective observed values.

Summary

Various model evaluation statistics are presented here for a variety of gaseous and aerosol species in addition to O_3. In general, the CMAQ results were best for daily maximum O_3 and daily average $PM_{2.5}$ and SO_4 mass. Many other species vary tremendously over the course of a day, or from day to day, and small model over- or underprediction at low concentrations can lead to large biases on a composite basis. It is important to demonstrate that the model performs reasonably over the diurnal cycle, not just in terms of daily maximum or average values. Also, it is important to demonstrate that the model can reproduce concentrations above the ground level.

Table 1. Median and range in fractional error (FE, %) and mean fractionalized bias (MFB, %) for daily maximum 8-hour O_3 using the 40 ppb and 60 ppb observed thresholds. The values using only SLAMS/NAMS sites are boldfaced, the values using all sites are in regular font.

Metric, threshold	Range (%)	Median (%)
FE, 40 ppb	+10 to +34% **+10 to +32%**	+15% **+15%**
MFB, 40 ppb	-34 to +23% **-29 to +23%**	-6% **-6%**
FE, 60 ppb	+9 to +40% **+9 to +40%**	+15% **+15%**
MFB, 60 ppb	-40 to +22% **-40 to +22%**	-12% **-11%**

Table 2. Median and range in mean fractionalized bias (%) for daily average CO, NO, NO_2, SO_2, C_2H_4, HCHO, and C_5H8.

Pollutant	Range in MFB (%)	Median MFB (%)
CO (97 sites)	-128 to +144%	-10%
NO (75 sites)	-182 to +116%	-46%
NO_2 (97 sites)	-125 to +107%	+13%
SO_2 (134 sites)	-139 to 140%	+3%
C_2H_4 (19 sites)	+28 to +168%	+86%
HCHO (18 sites)	-66 to +96%	-13%
C_5H_8 (19 sites)	-54 to +165%	+43%

Table 3. Median and range in mean fractionalized bias (%) for daily average $PM_{2.5}$, SO_4, NO_3, NH_4, EC, and OM.

Pollutant	Range in MFB (%)	Median MFB (%)
$PM_{2.5}$ (FRM; 257 sites)	-59 to +119%	-4%
$PM_{2.5}$ (continuous; 57 sites)	-39 to +85%	+5%
STN $PM_{2.5}$ (49 sites)	-45 to +102%	-9%
IMPROVE $PM_{2.5}$ (21 sites)	-36 to +19%	-10%
STN SO_4 (49 sites)	-21 to +60%	+12%
IMPROVE SO_4 (21 sites)	-26 to +16%	-7%
STN NO_3 (49 sites)	-73 to +406%	+25%
IMPROVE NO_3 (21 sites)	-57 to +358%	+64%
STN NH_4 (49 sites)	-36 to +112%	+16%
STN EC (49 sites)	-42 to +269%	+34%
IMPROVE EC (21 sites)	-60 to +146%	-27%
STN OM (49 sites)	-82 to -25%	-58%
IMPROVE OM (21 sites)	-60 to +7%	-40%
STN crustal (49 sites)	+2 to +546%	+182%
IMPROVE crustal (21 sites)	-18 to +163%	+38%

Table 4. Model evaluation statistics for integrated wet deposition of SO_4, NO_3, and NH_4

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Parameter	SO_4	NO_3	NH_4
Observed average, mg m^{-2}	1063	704	185
Predicted average, mg m^{-2}	946	367	117
Correlation coefficient, R^2	0.17	0.22	0.12
NME, %	34	49	48
RMSE, mg m^{-2}	490	417	109
FE, %	36	62	57
MAGE, mg m^{-2}	365	344	89
MNGE, %	36	45	46
MB, mg m^{-2}	-118	-337	-68
MNB, %	-3	-44	-28
MFB, %	-13	-61	-44
NMB, %	-11	-48	-37

Figure 1.

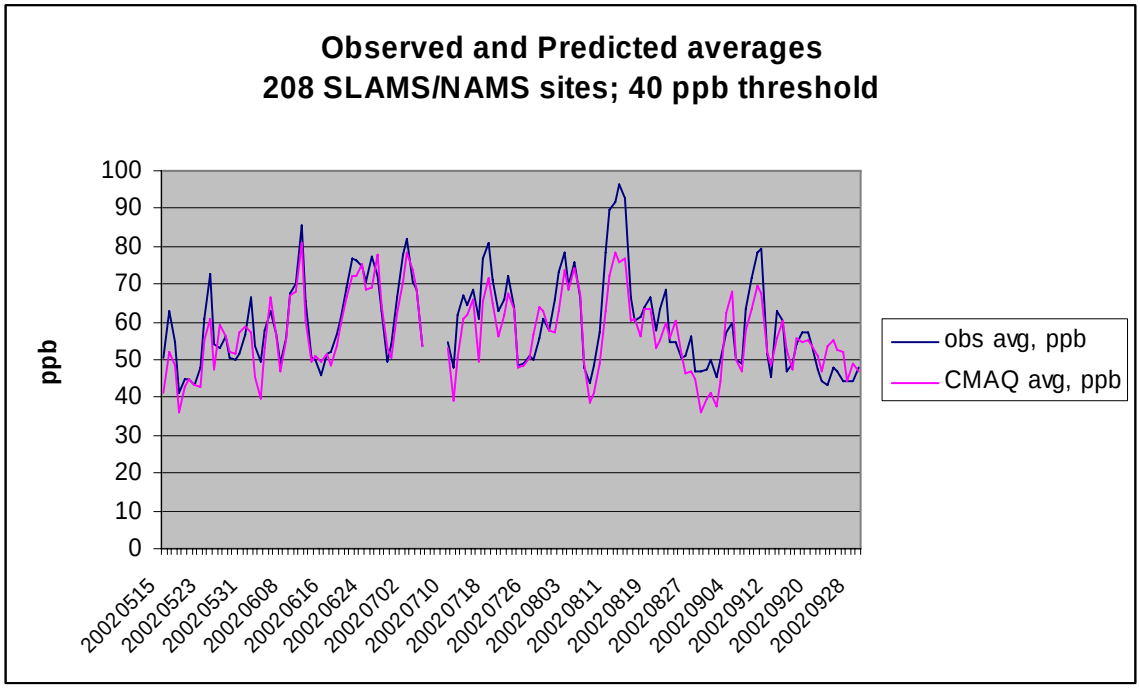


Figure 2.

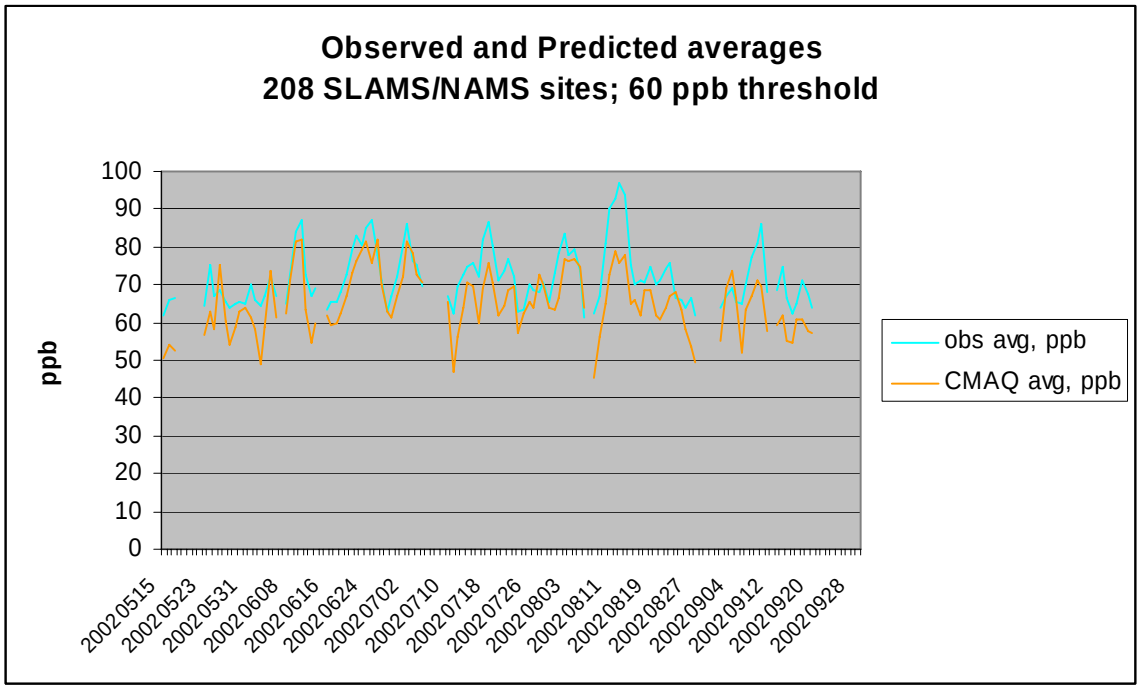


Figure 3.

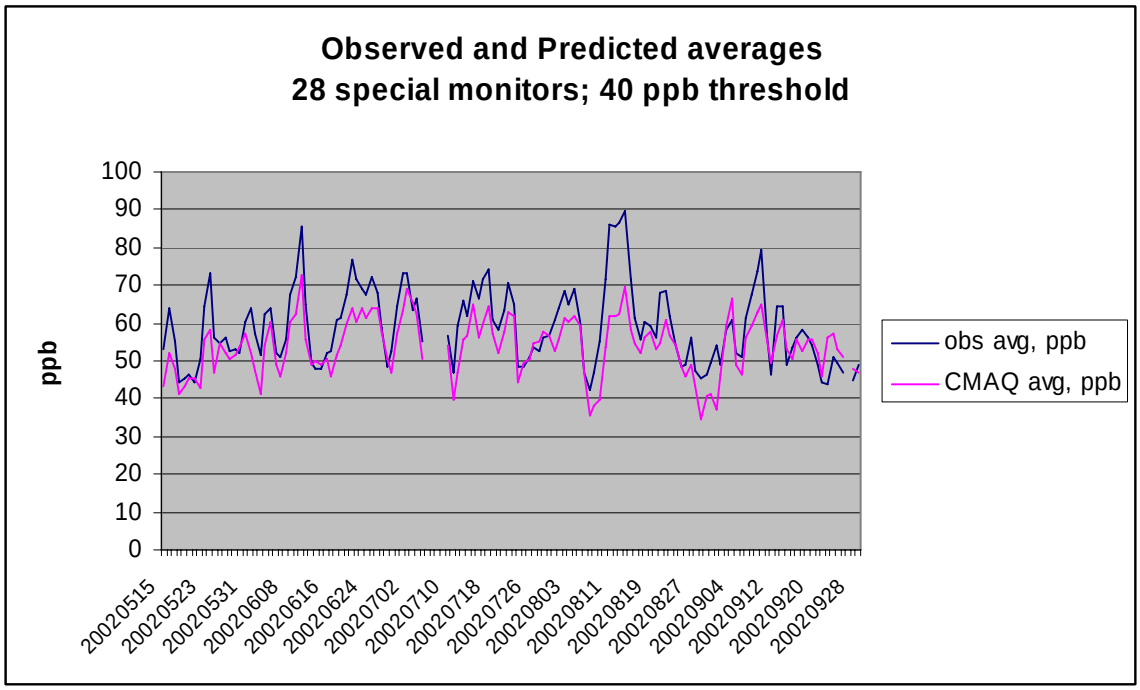


Figure 4.

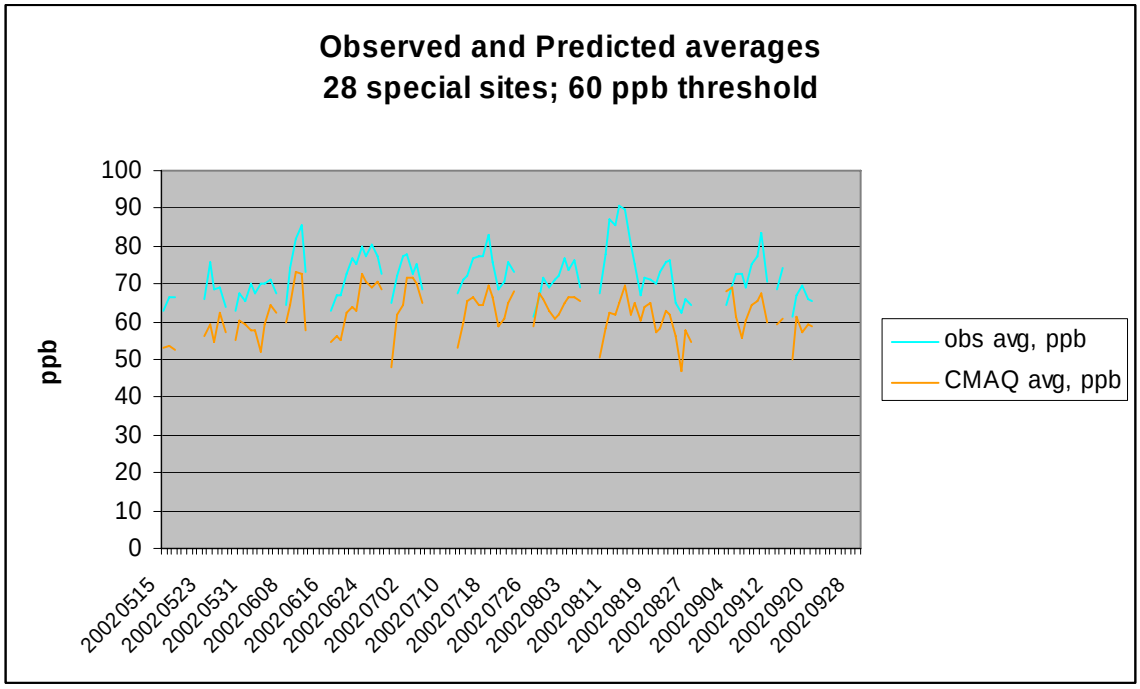


Figure 5.

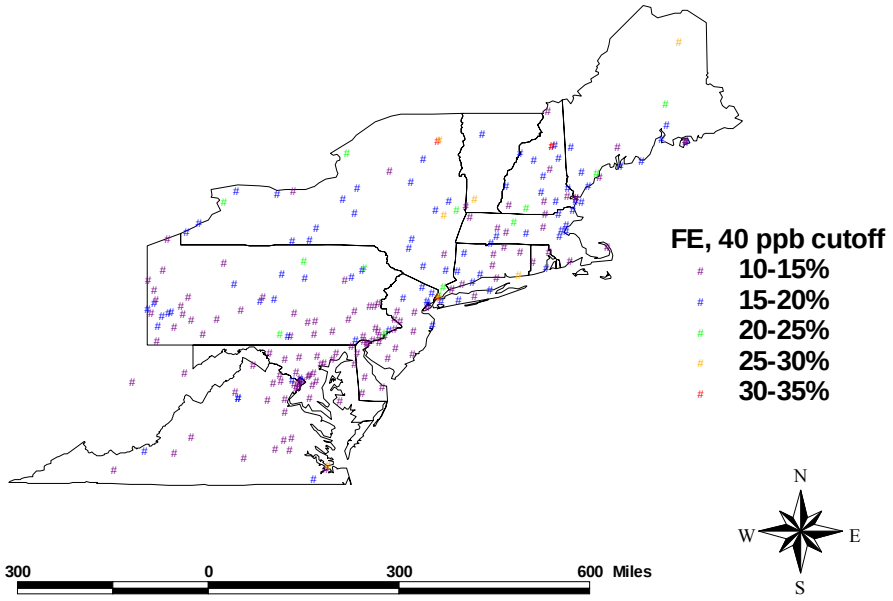


Figure 6.

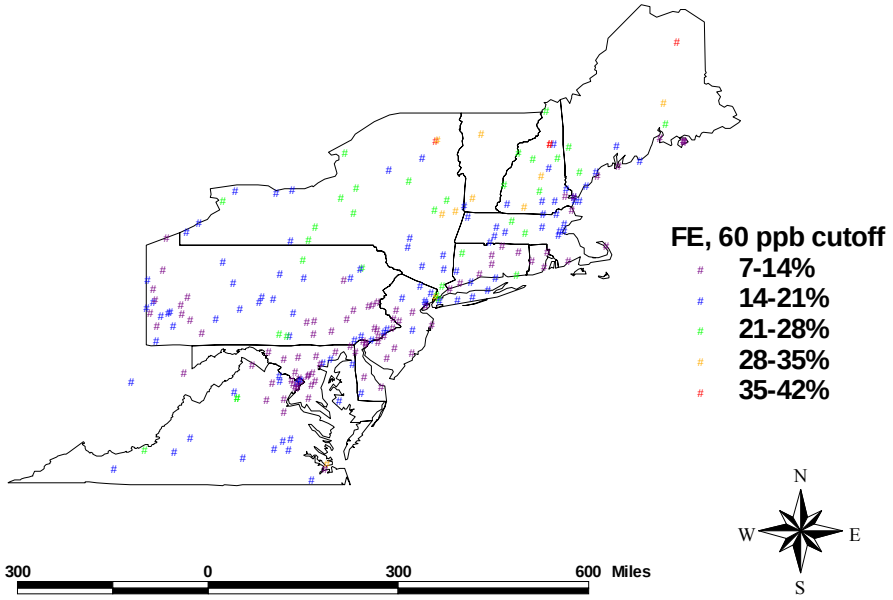
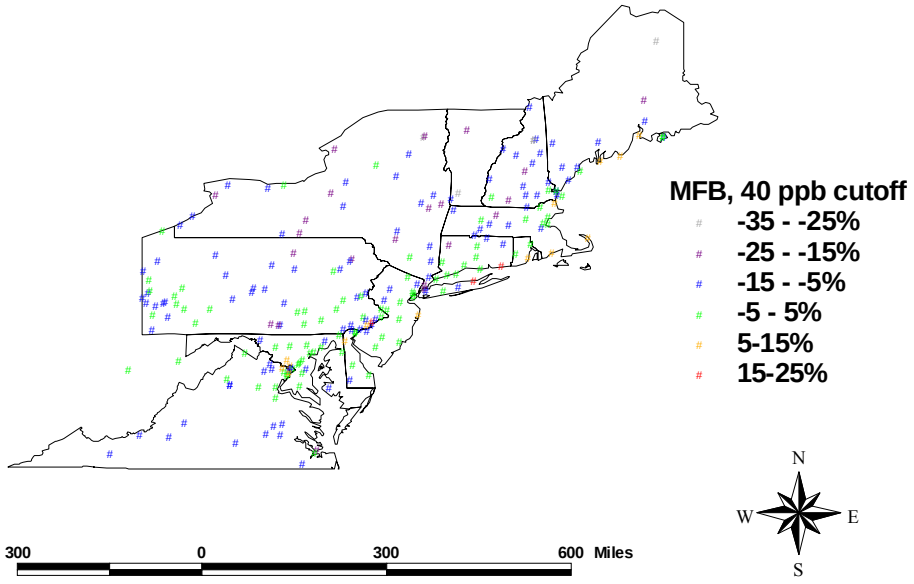


Figure 7.



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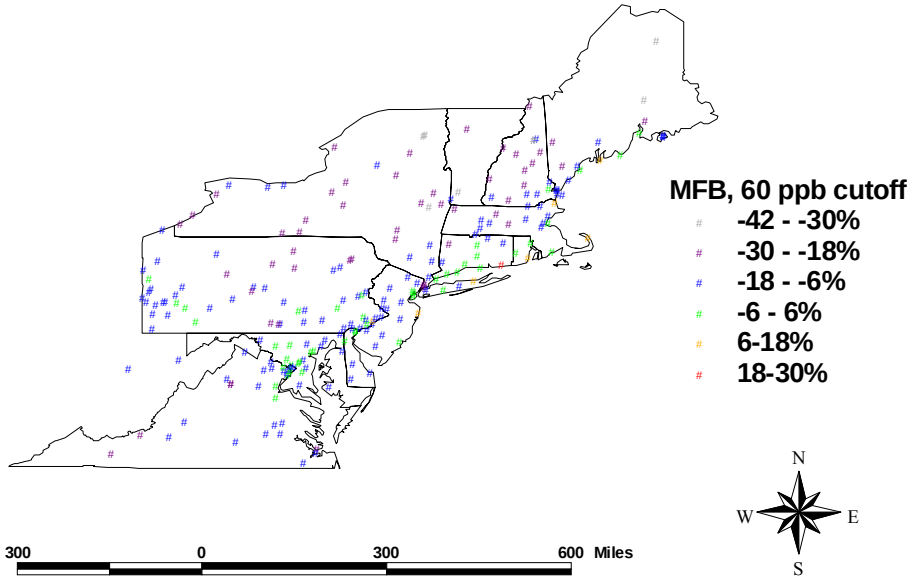

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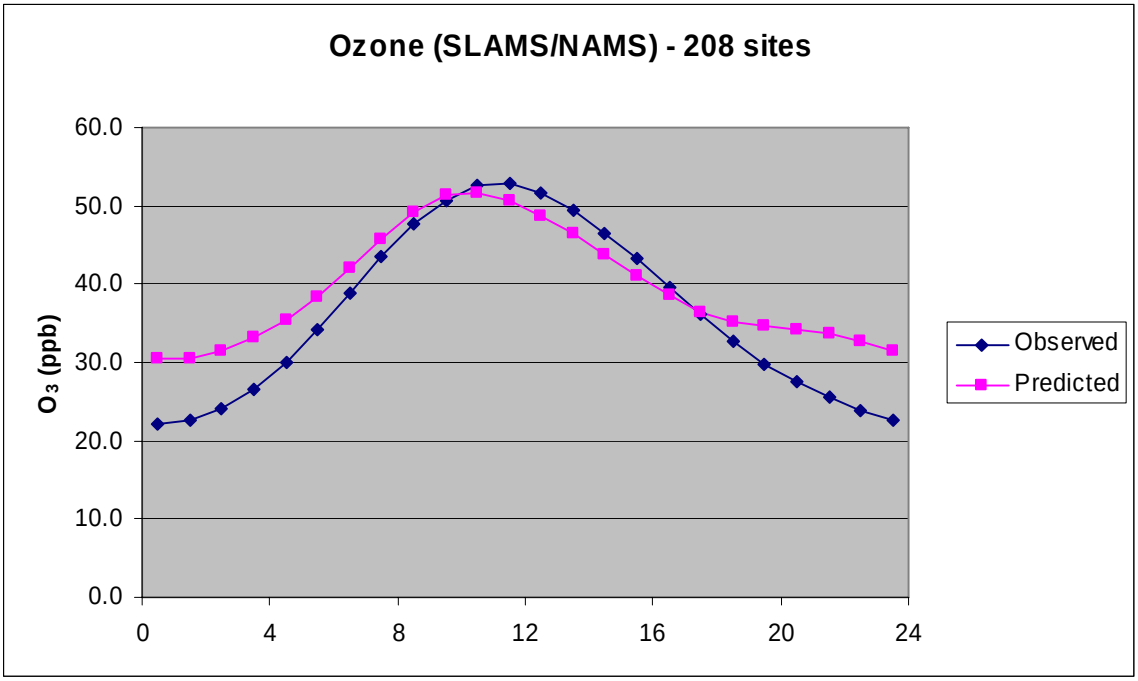

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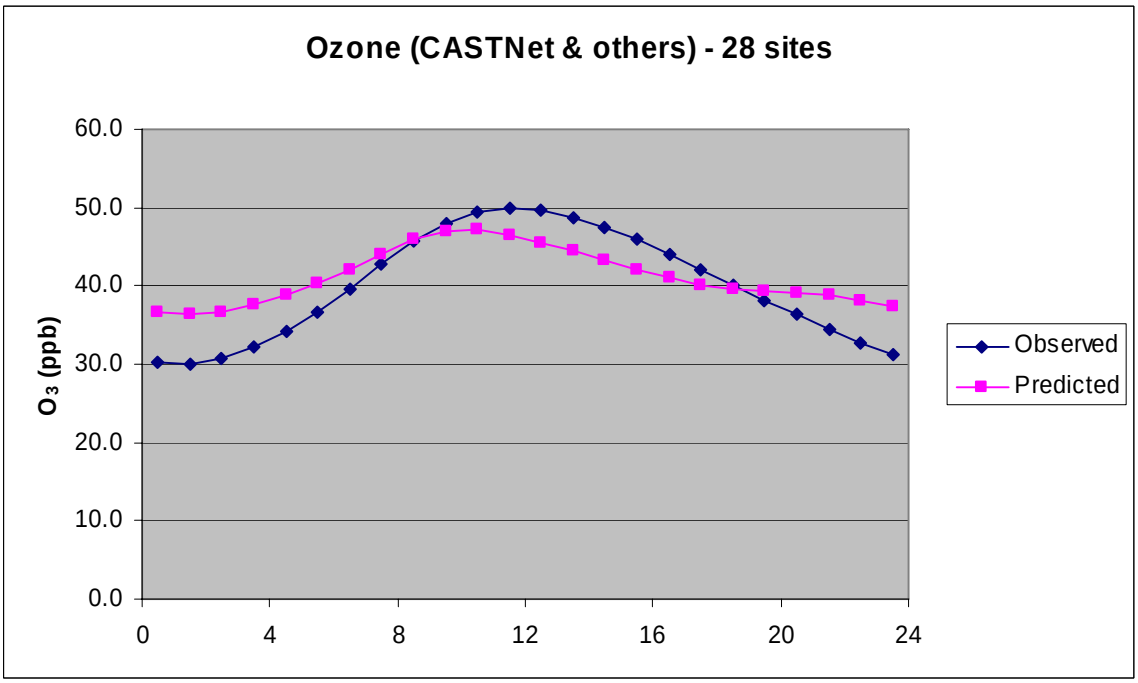

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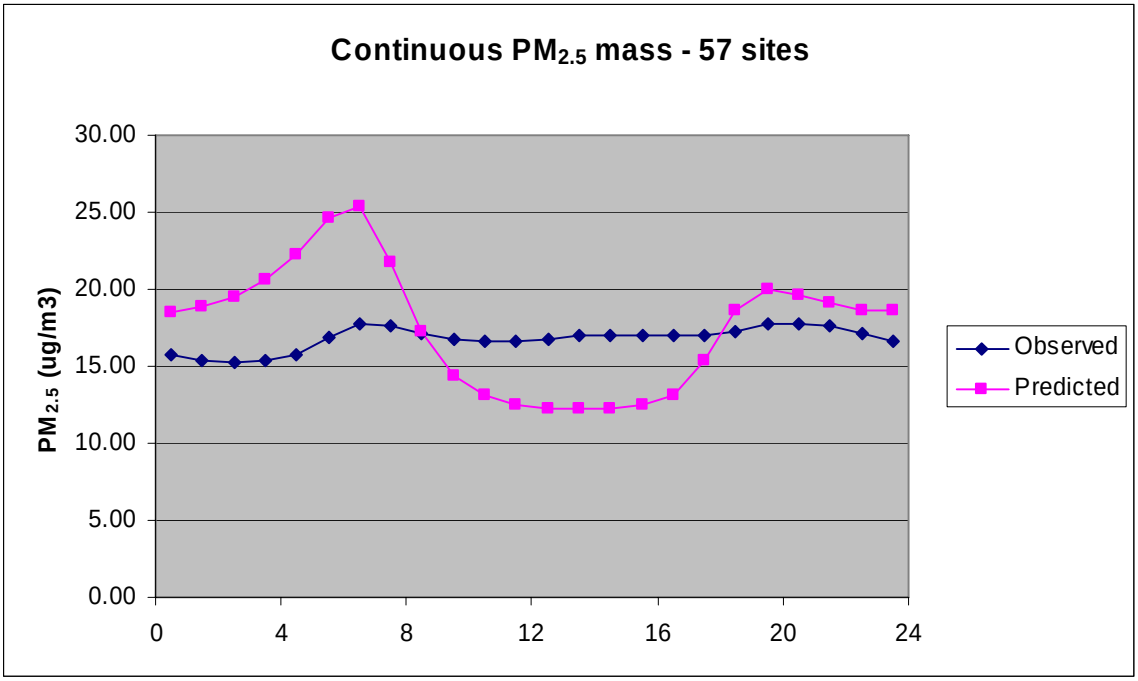

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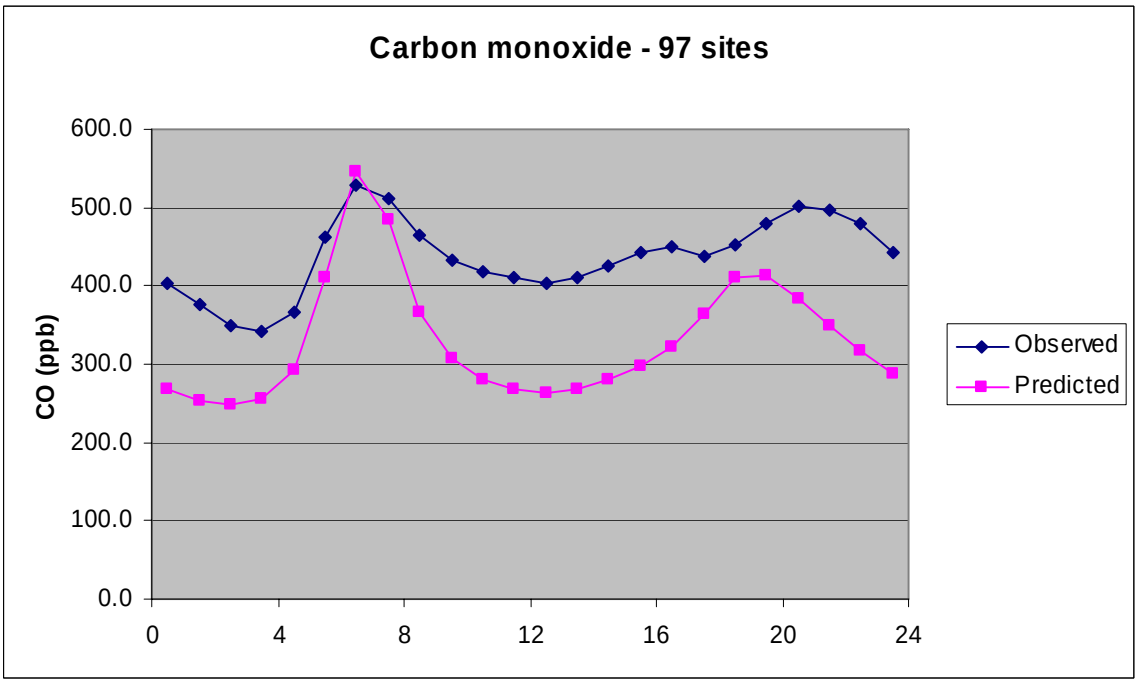

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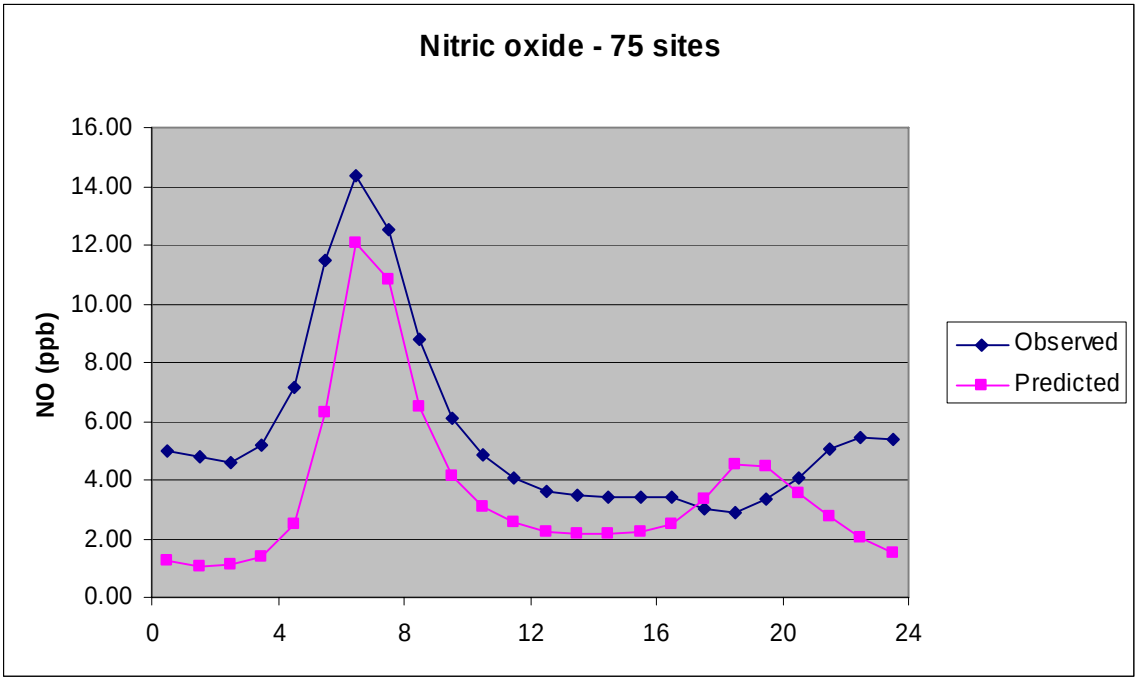

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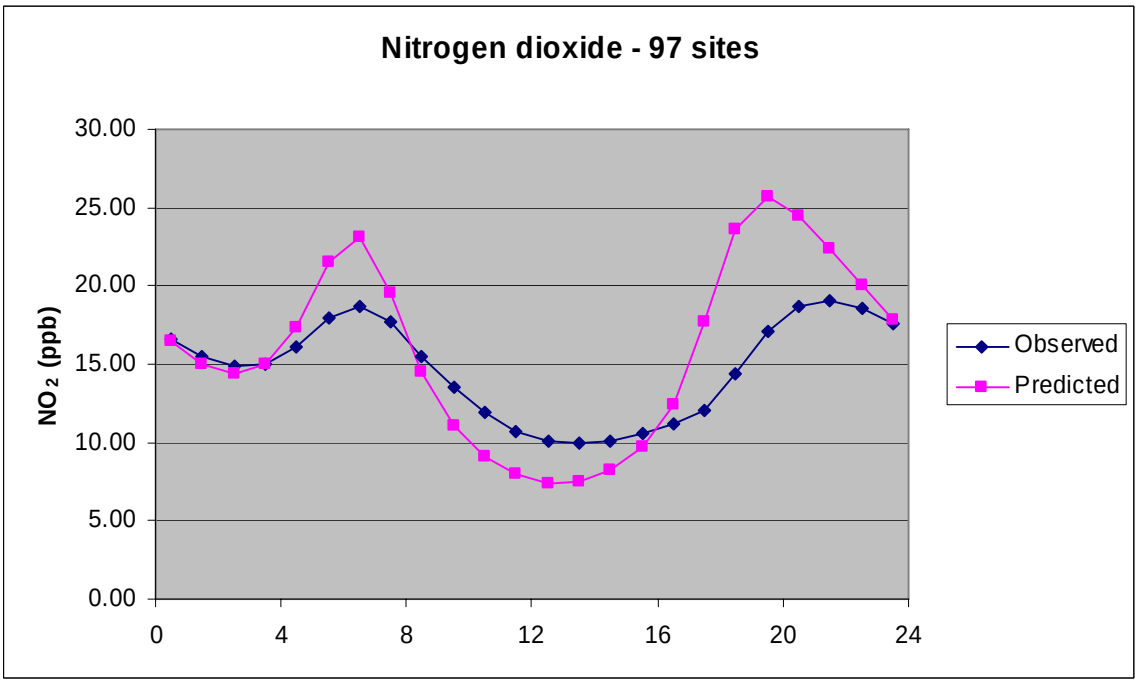

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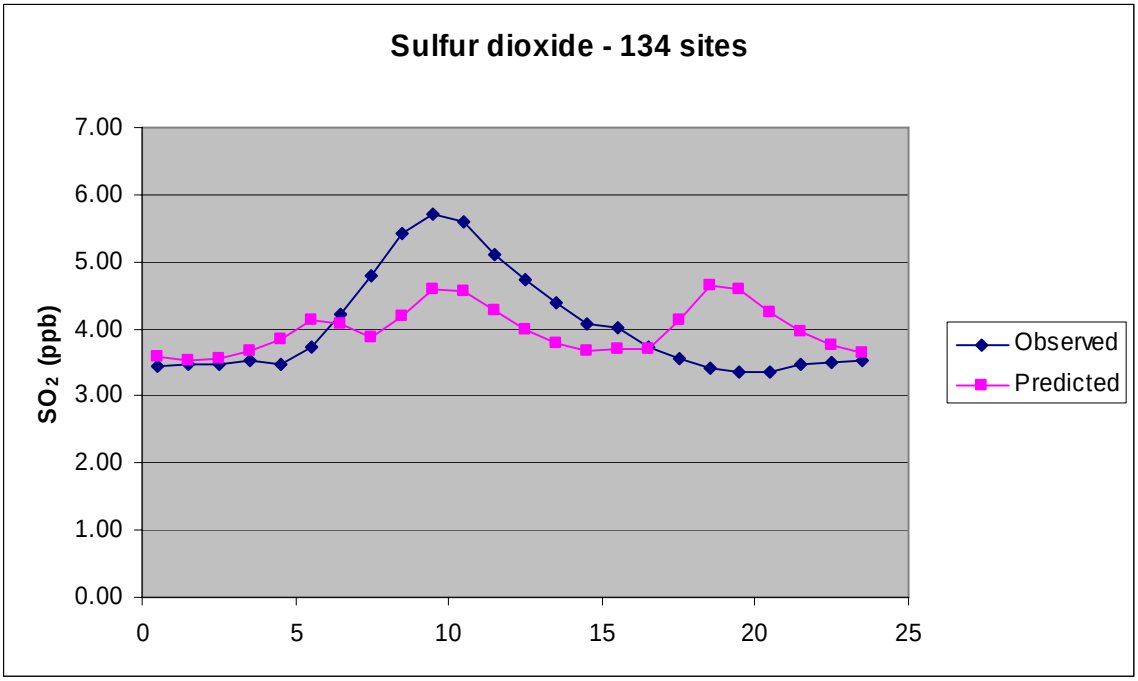

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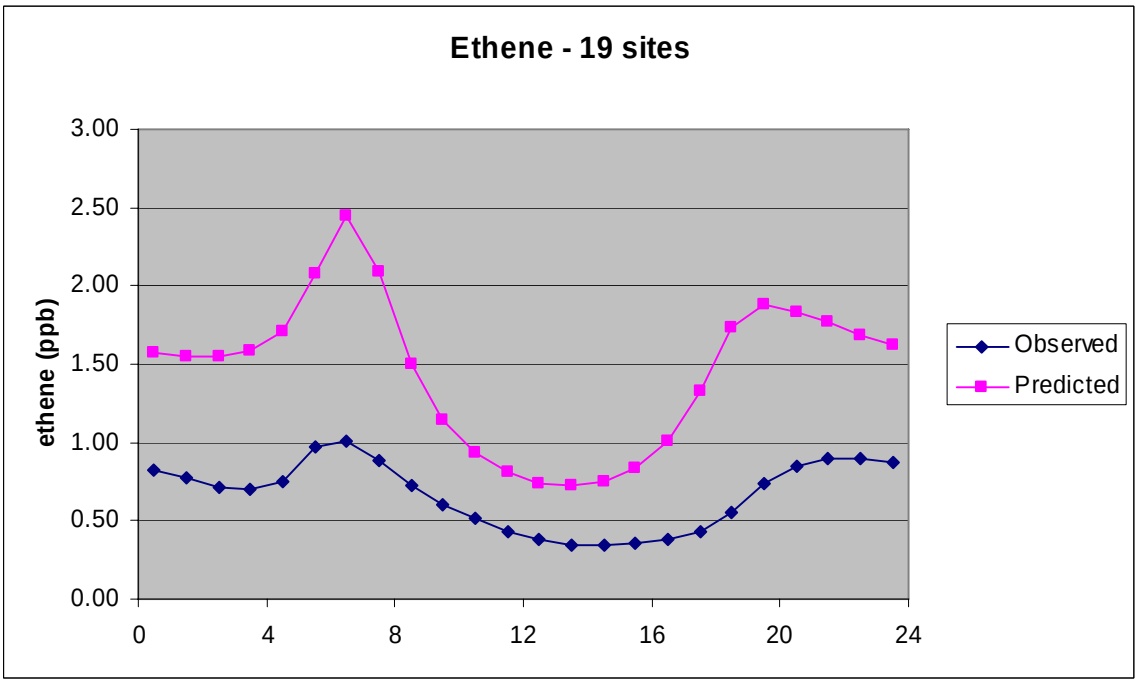

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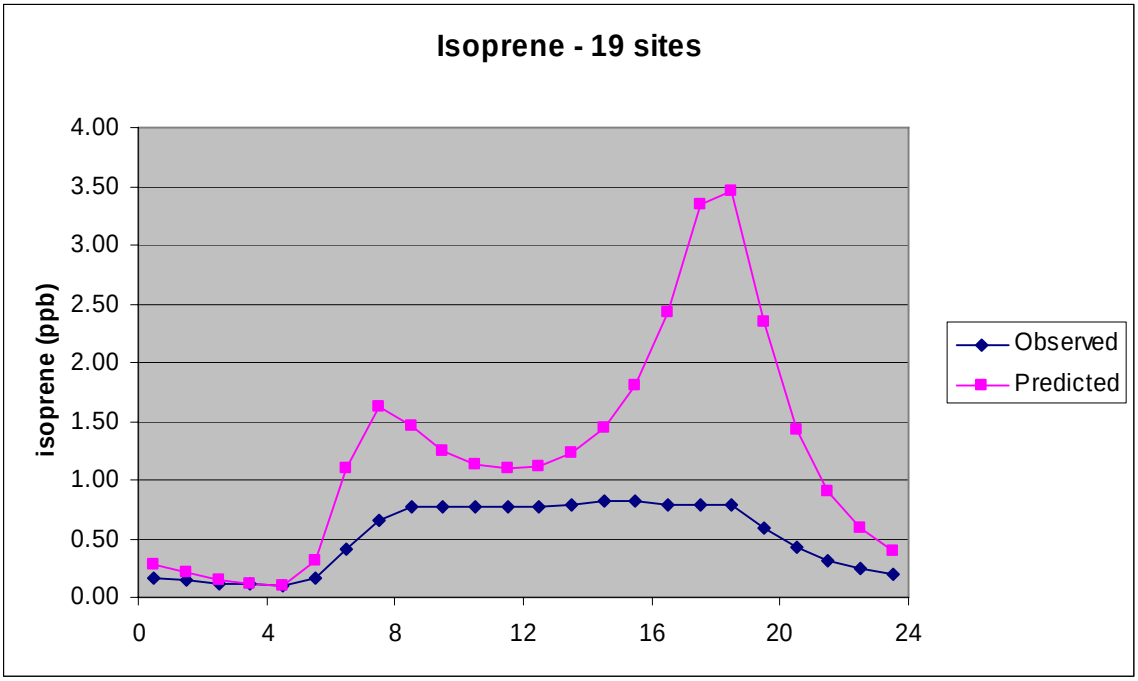

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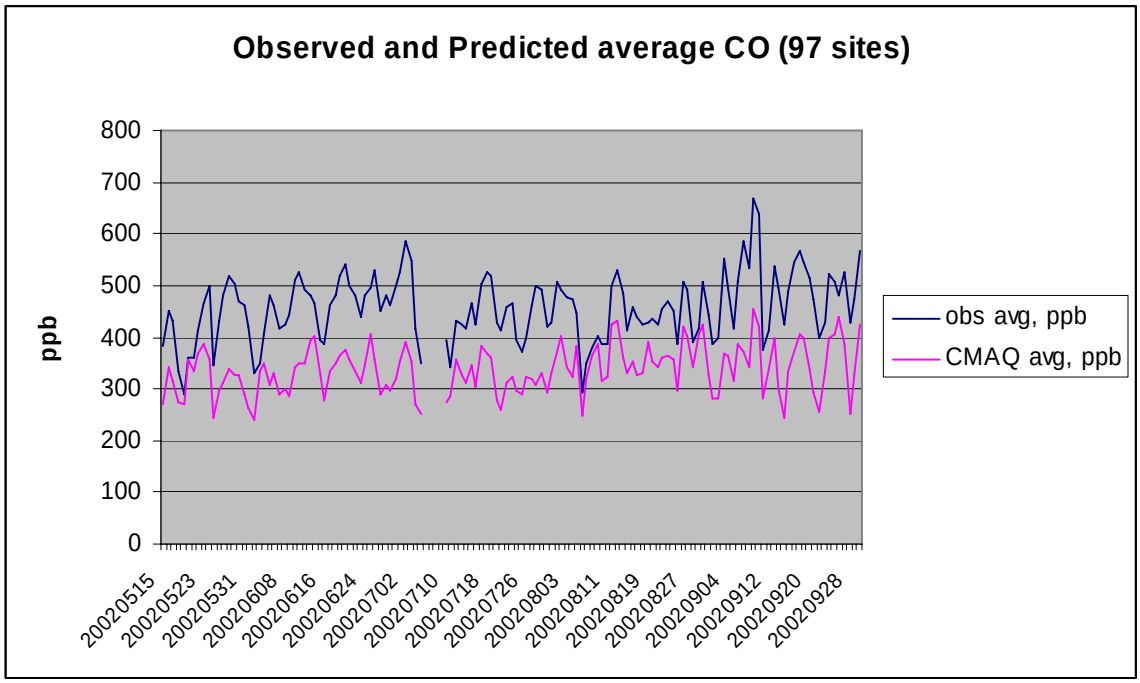

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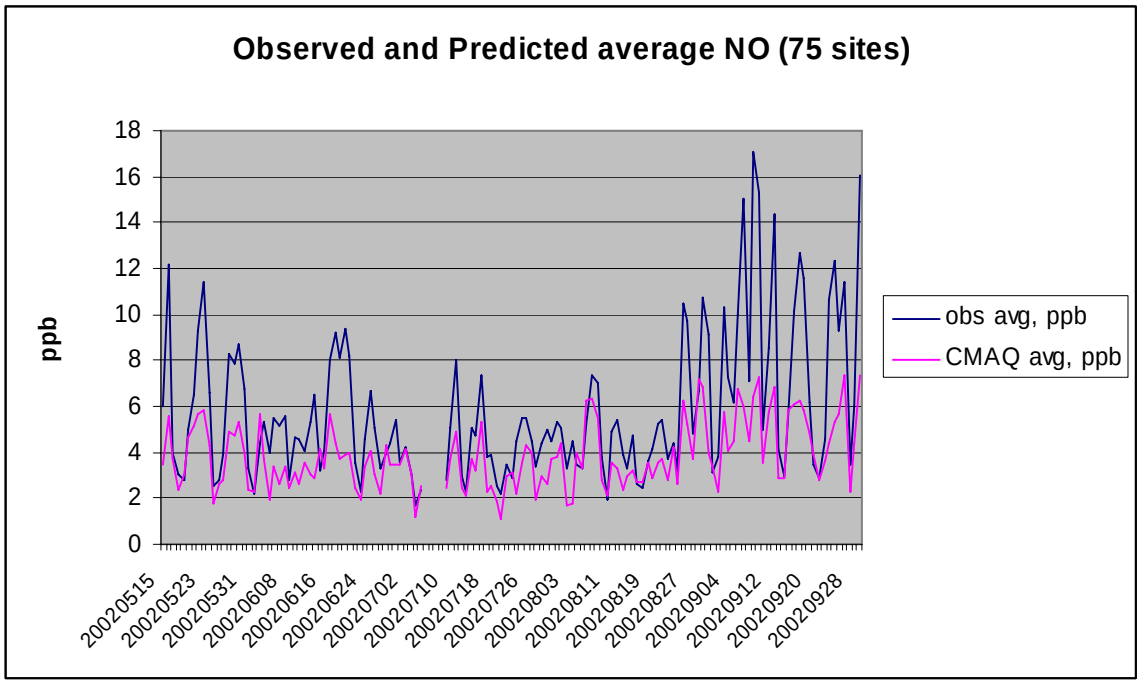

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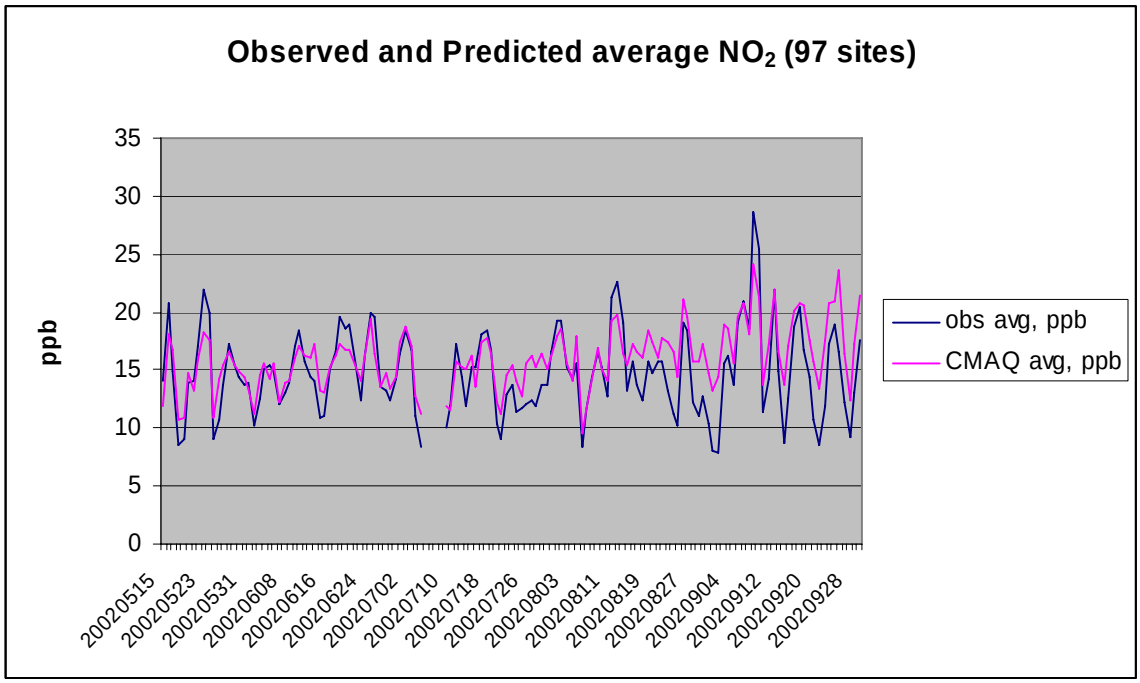

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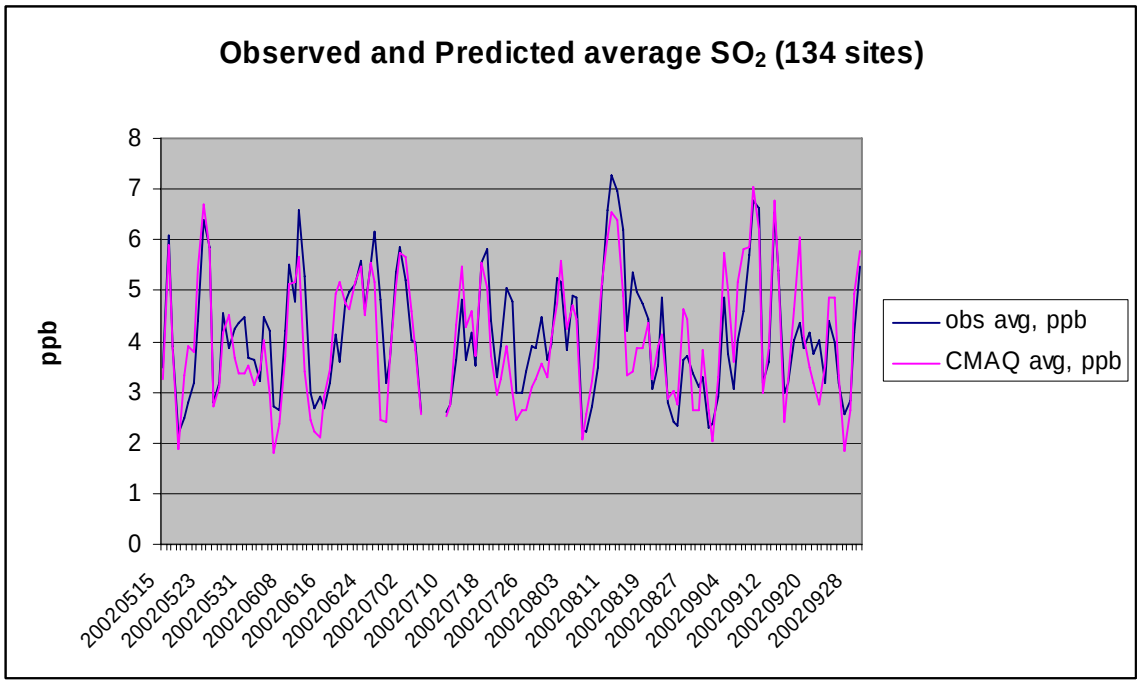

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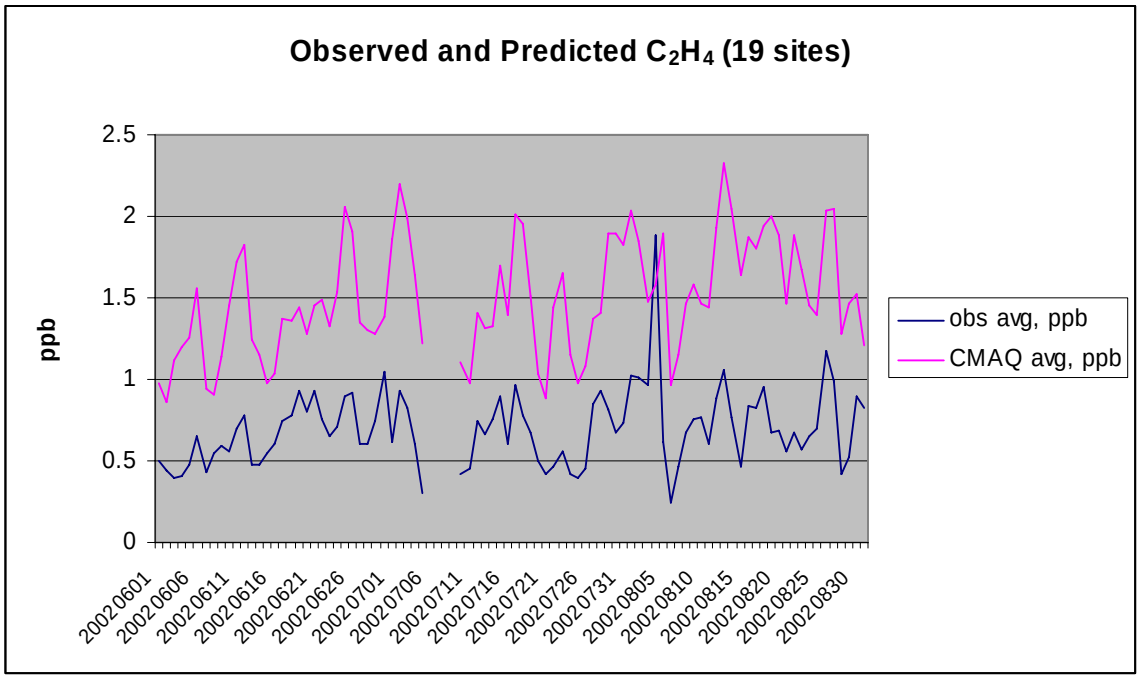

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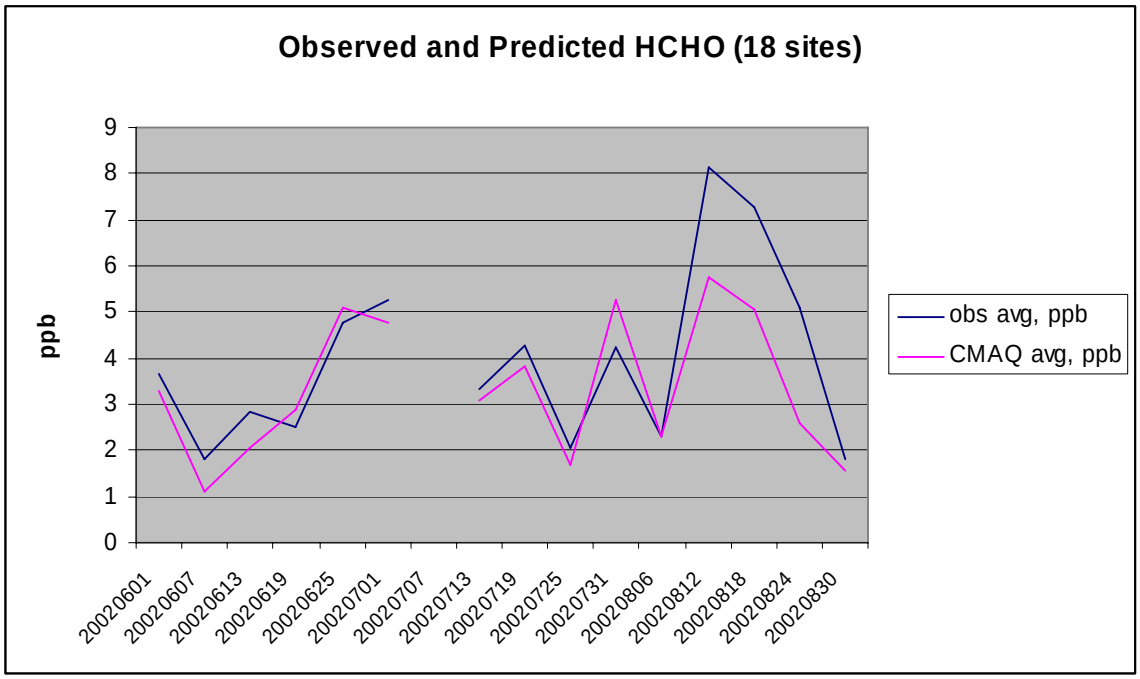

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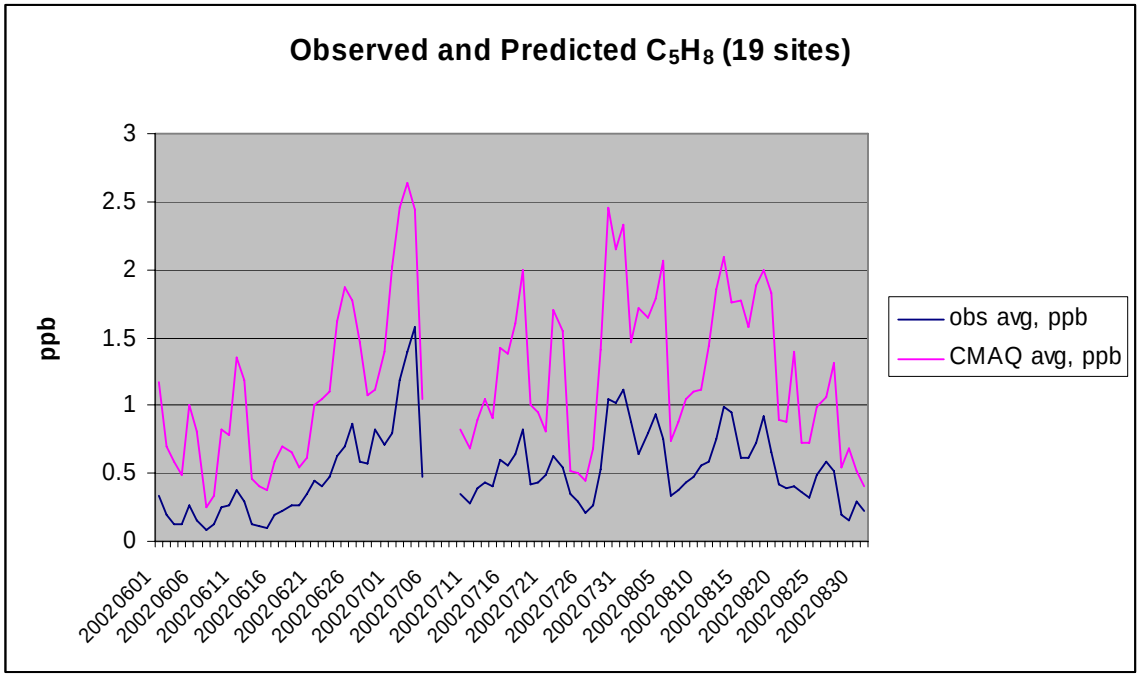

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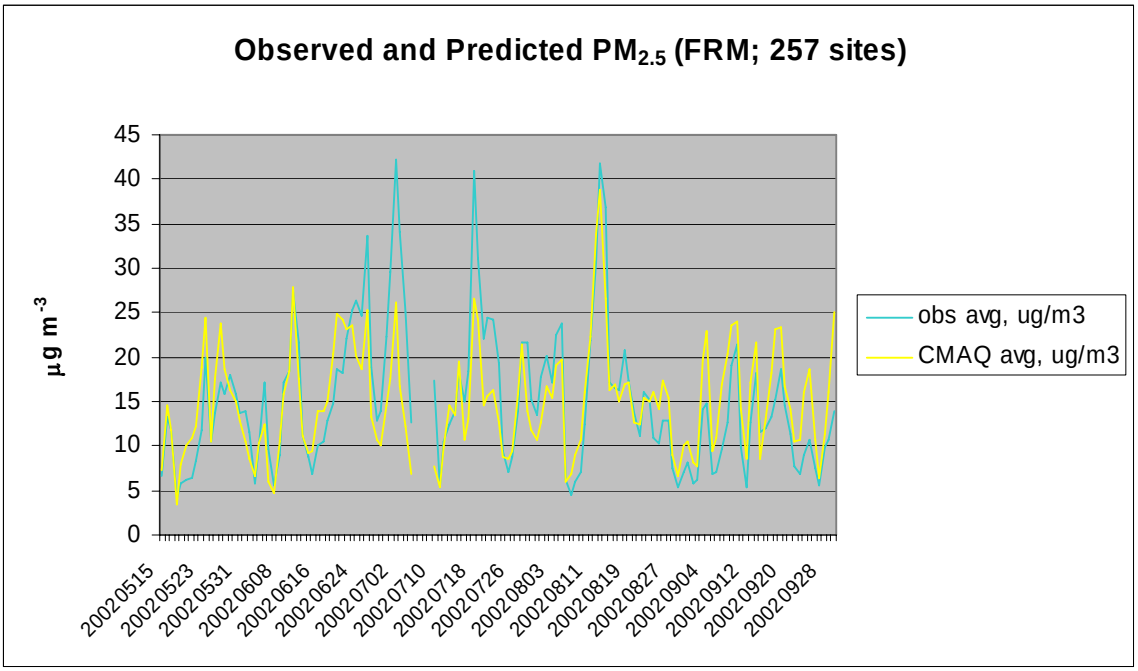

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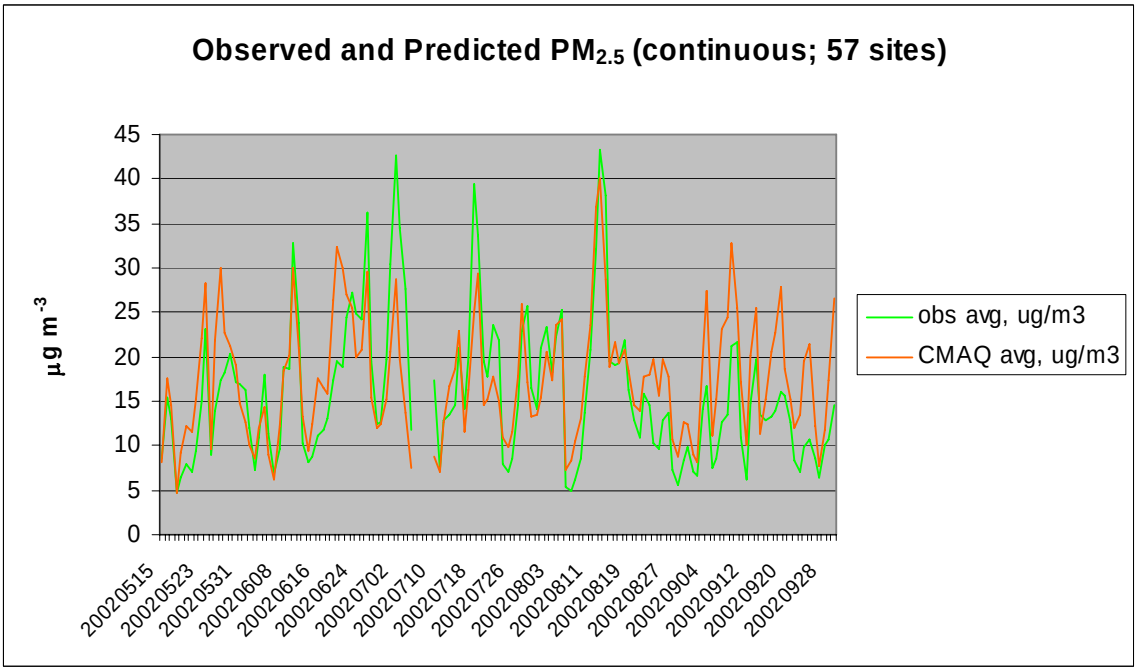

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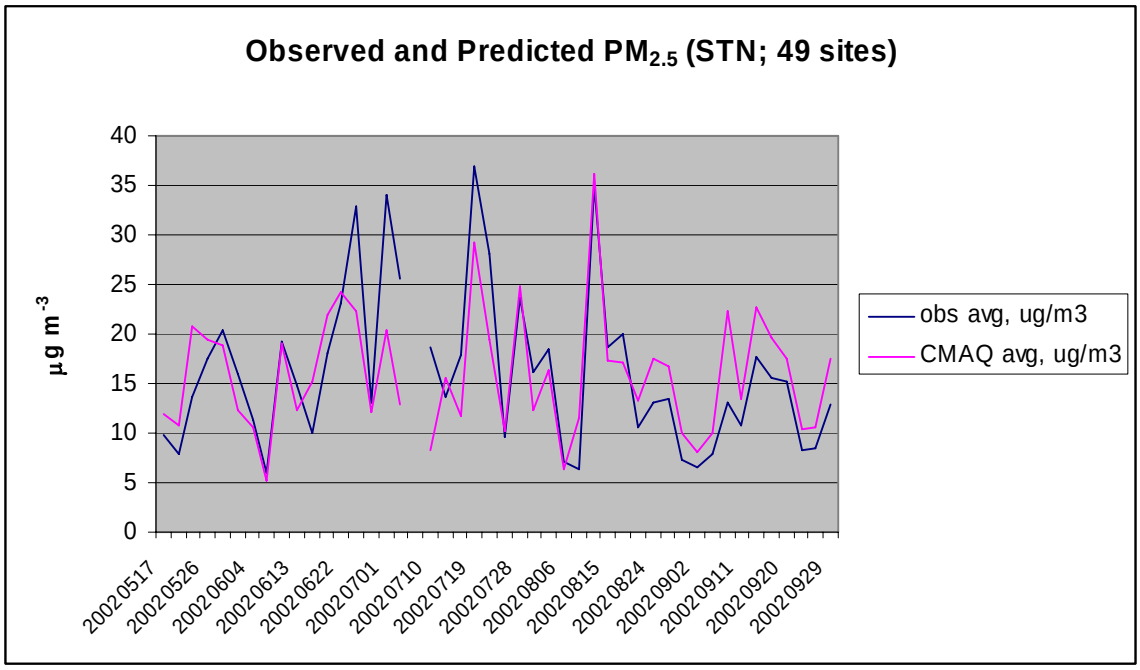

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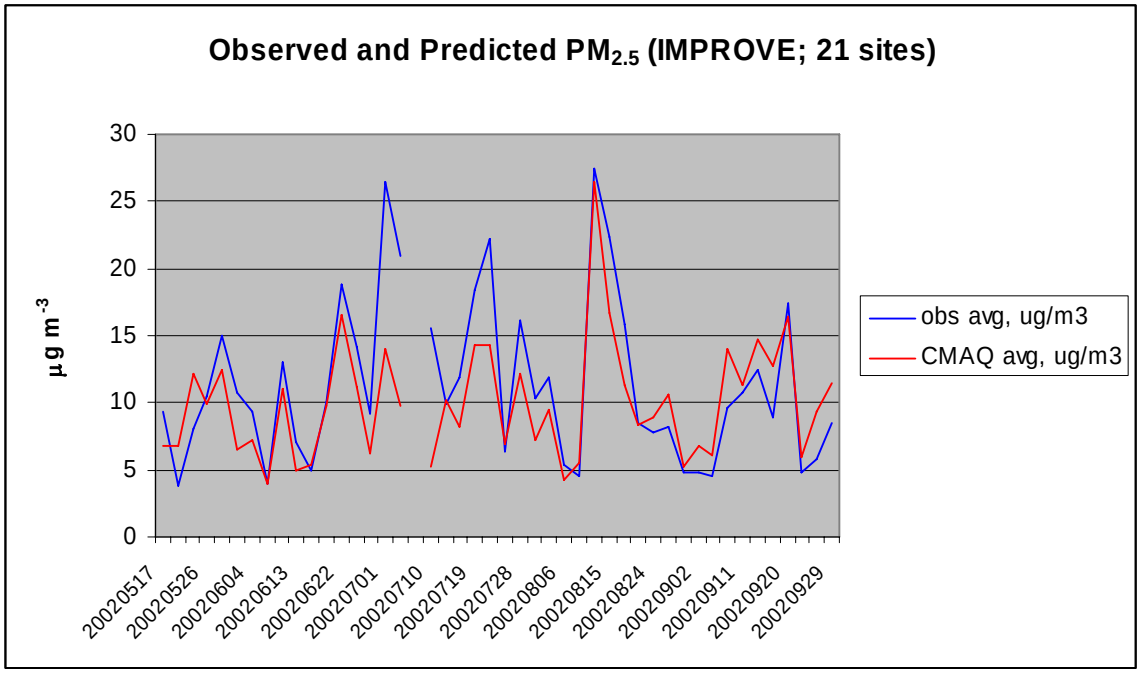

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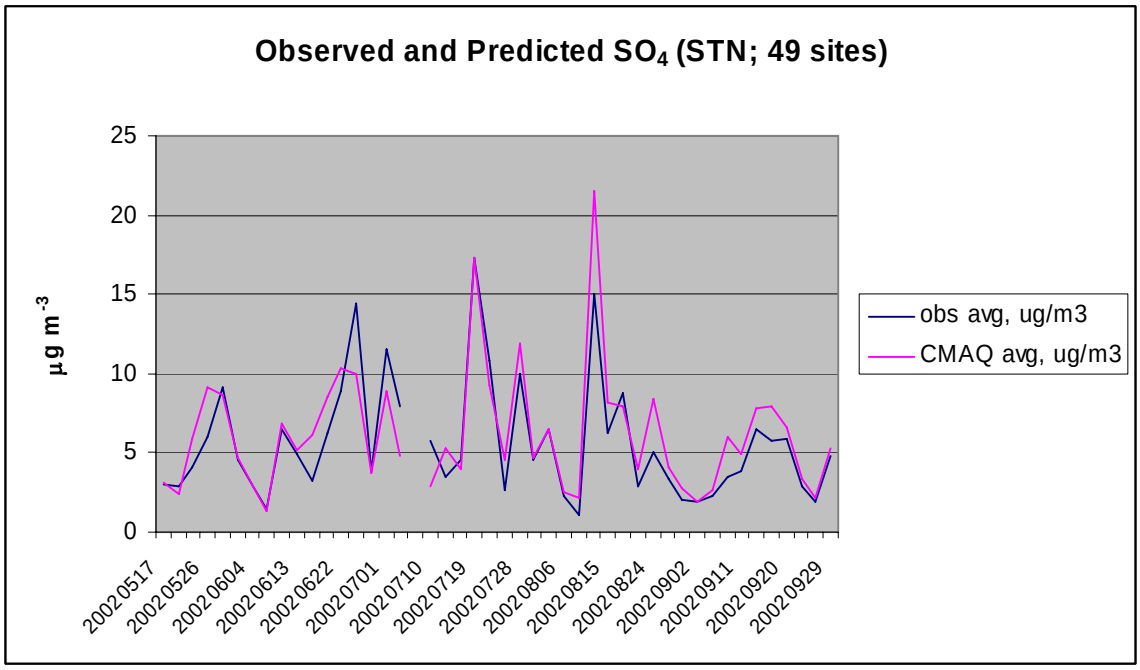

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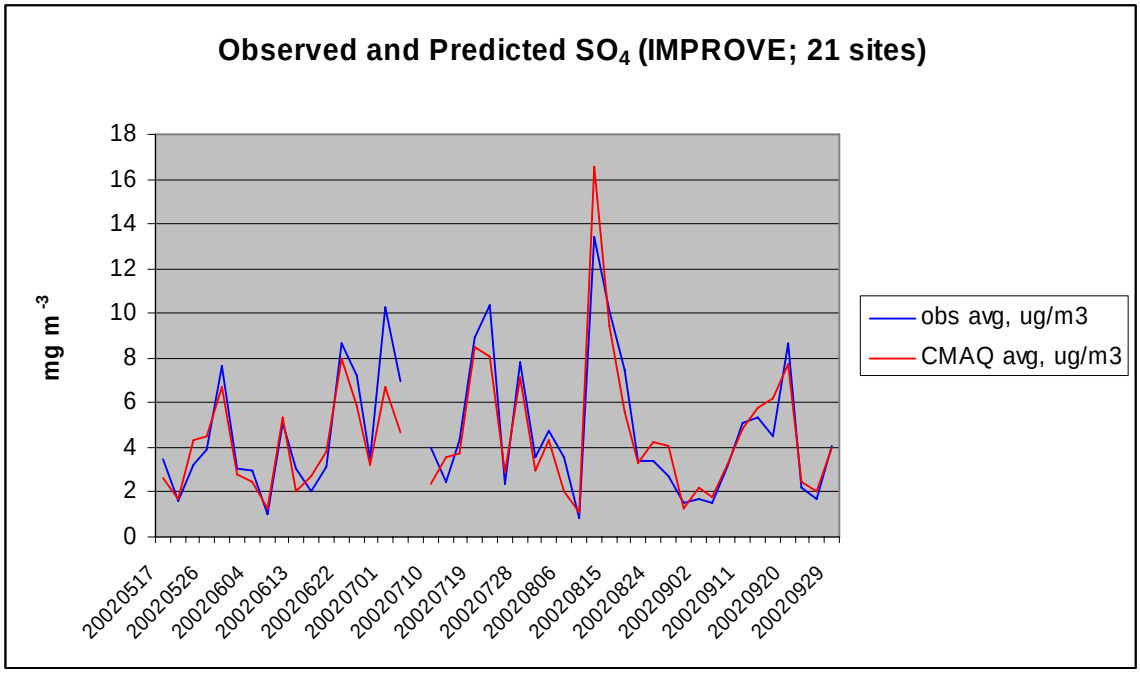

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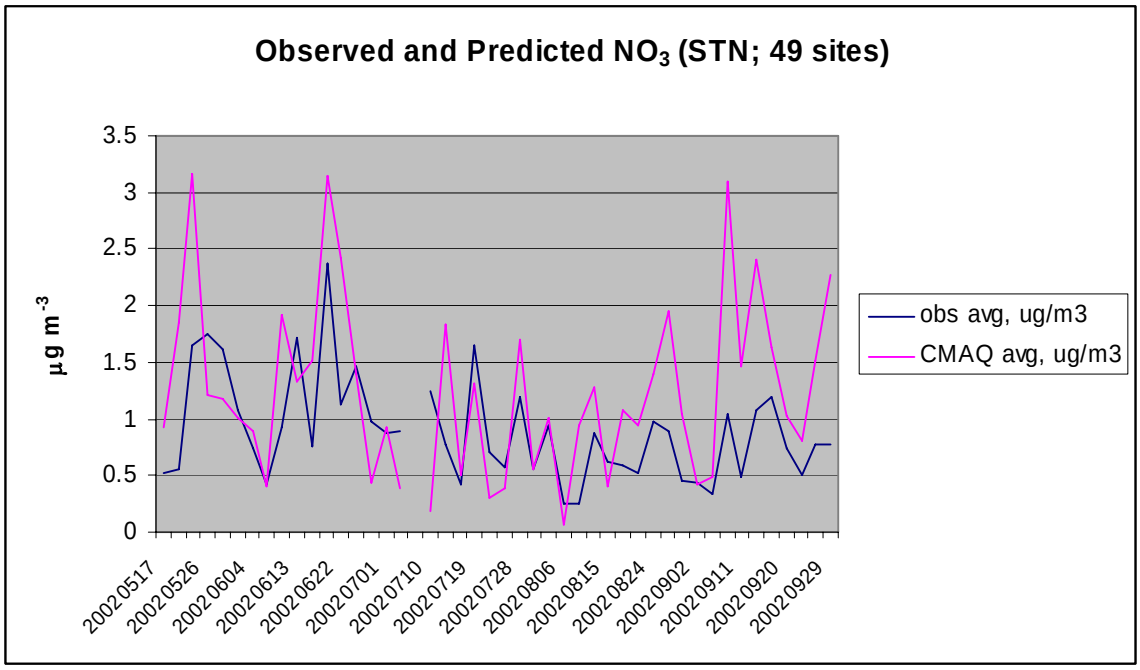

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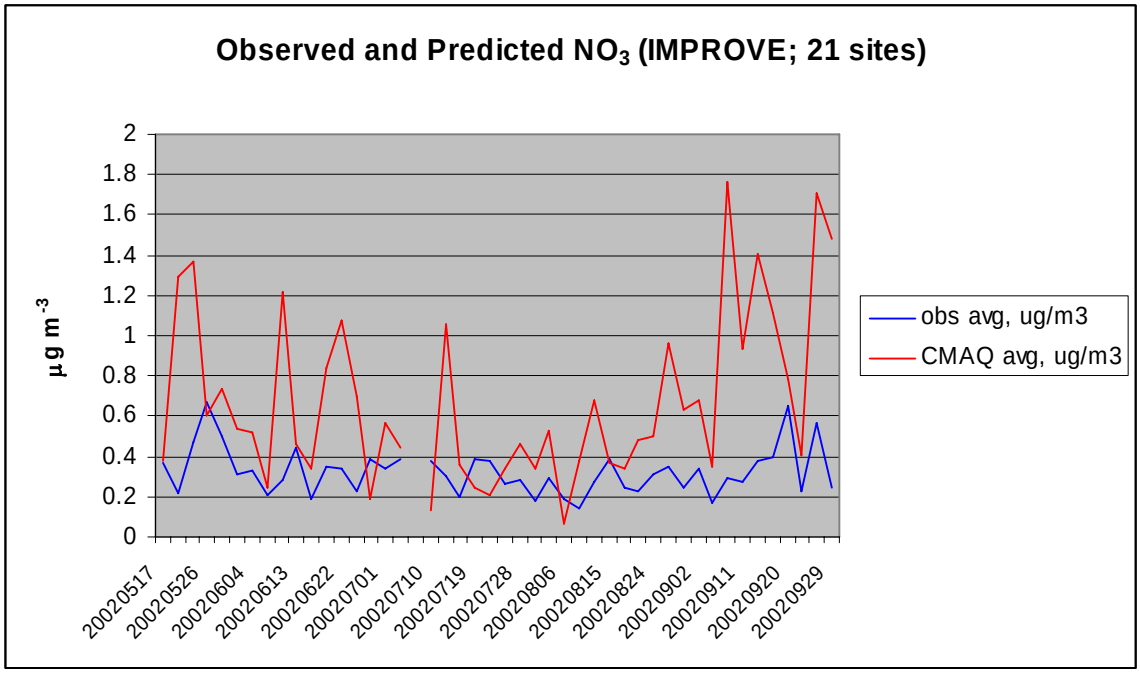

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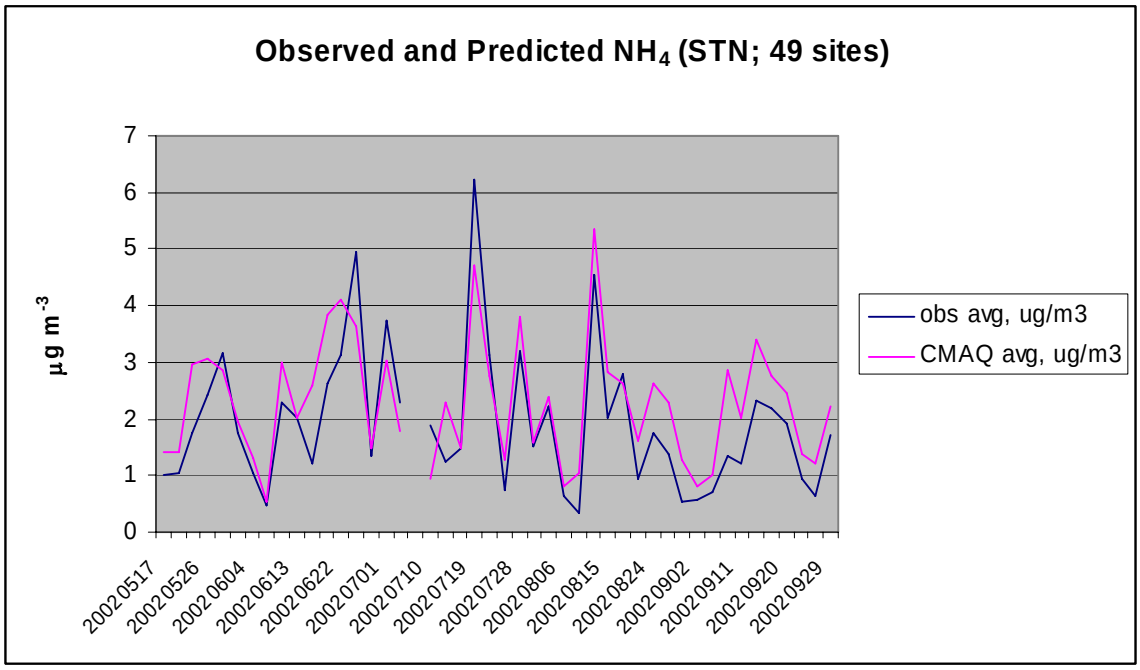

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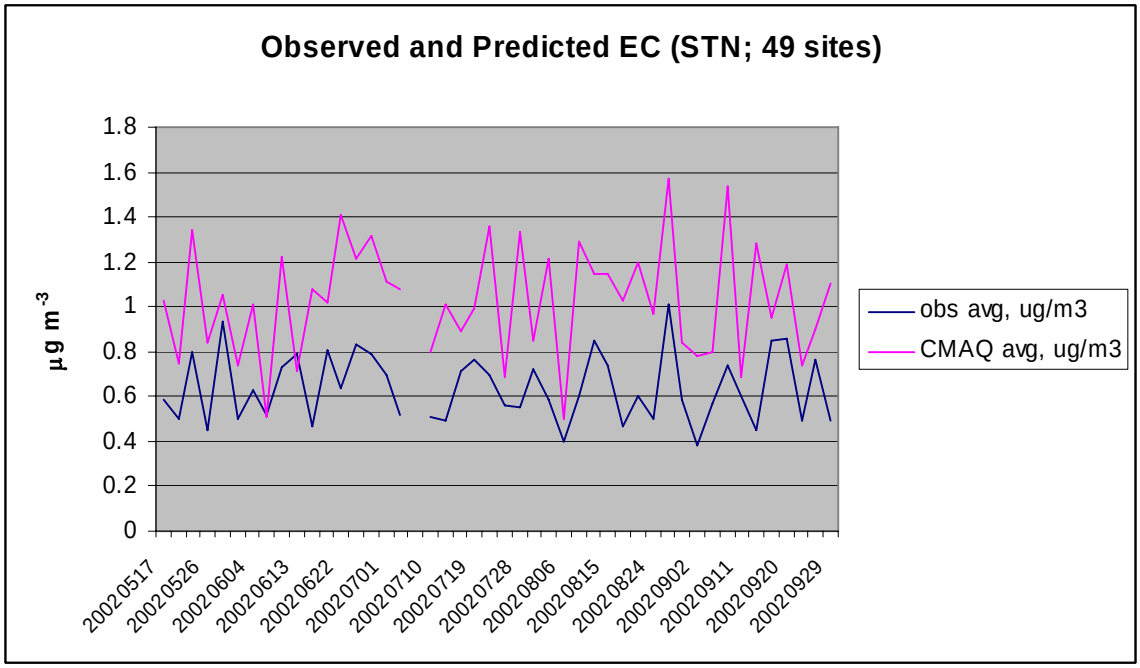

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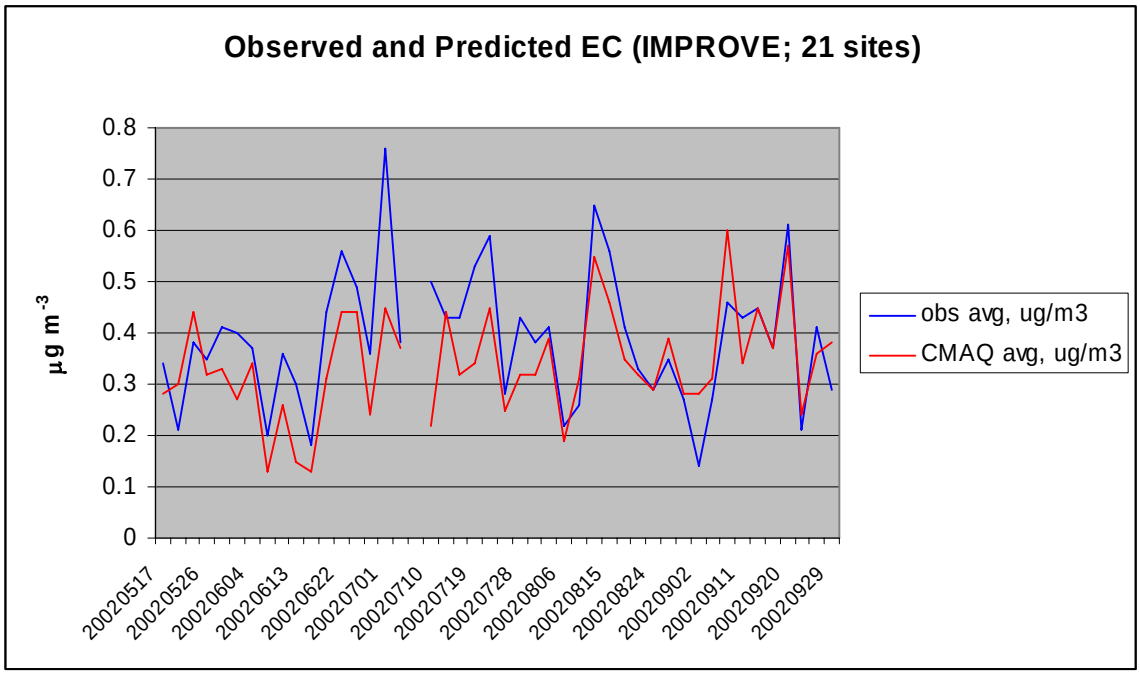

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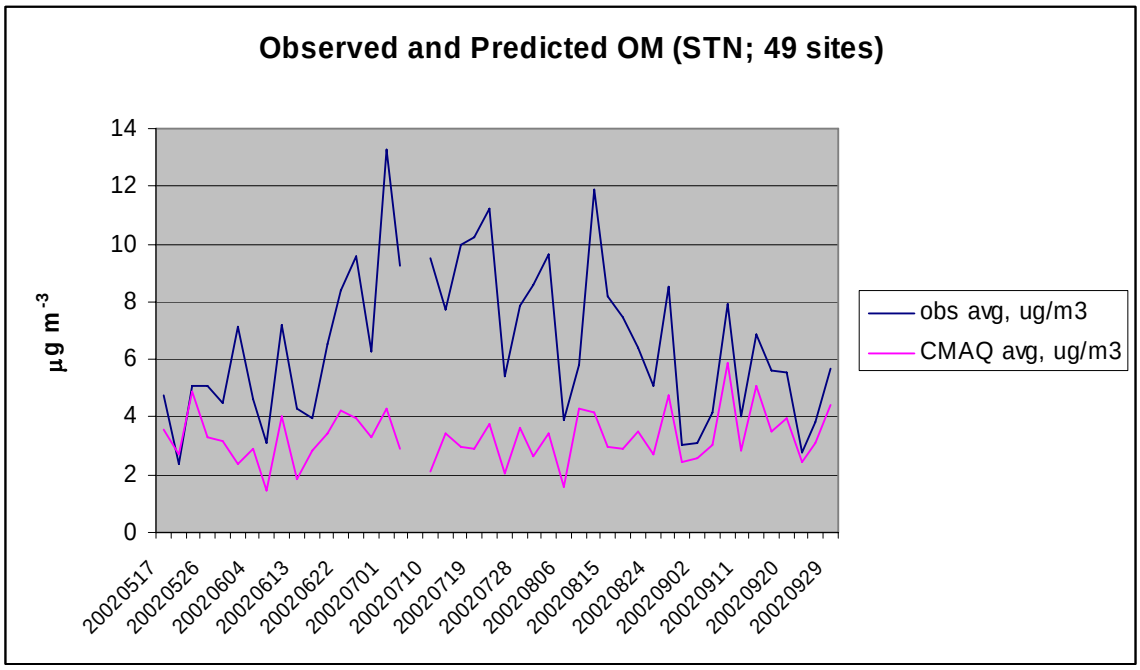

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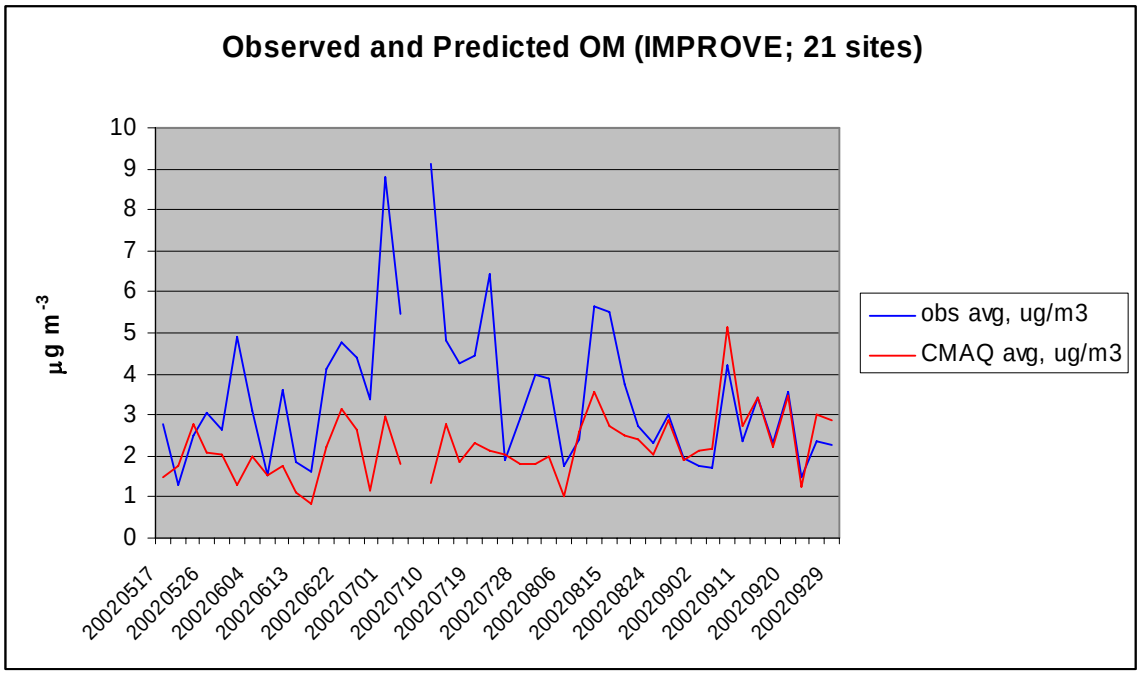

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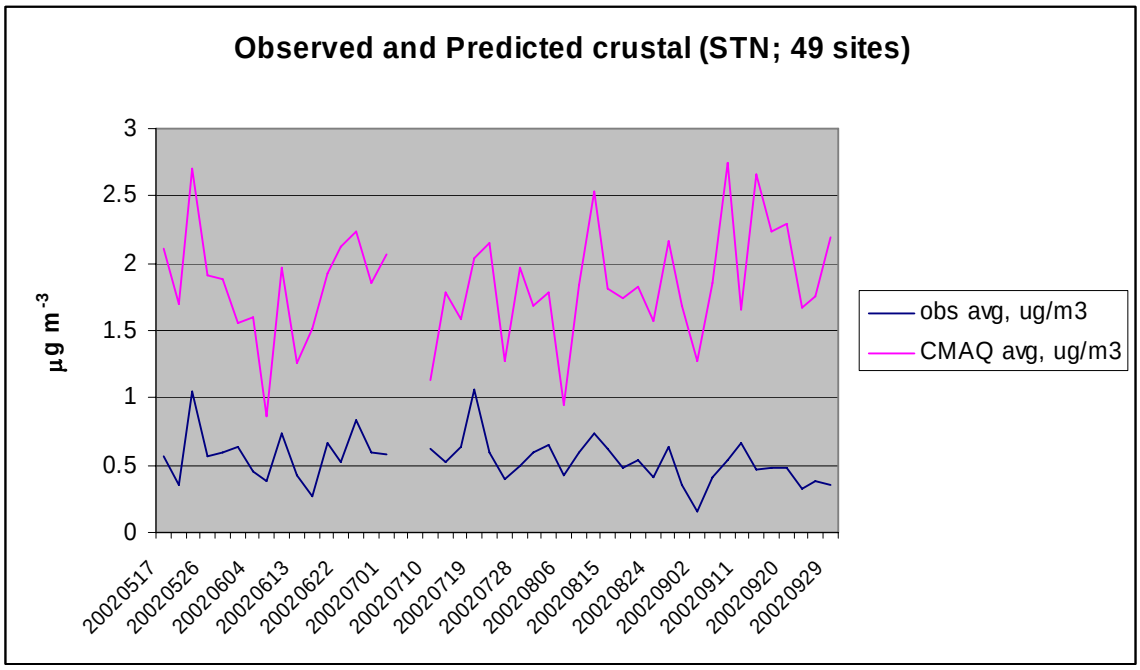

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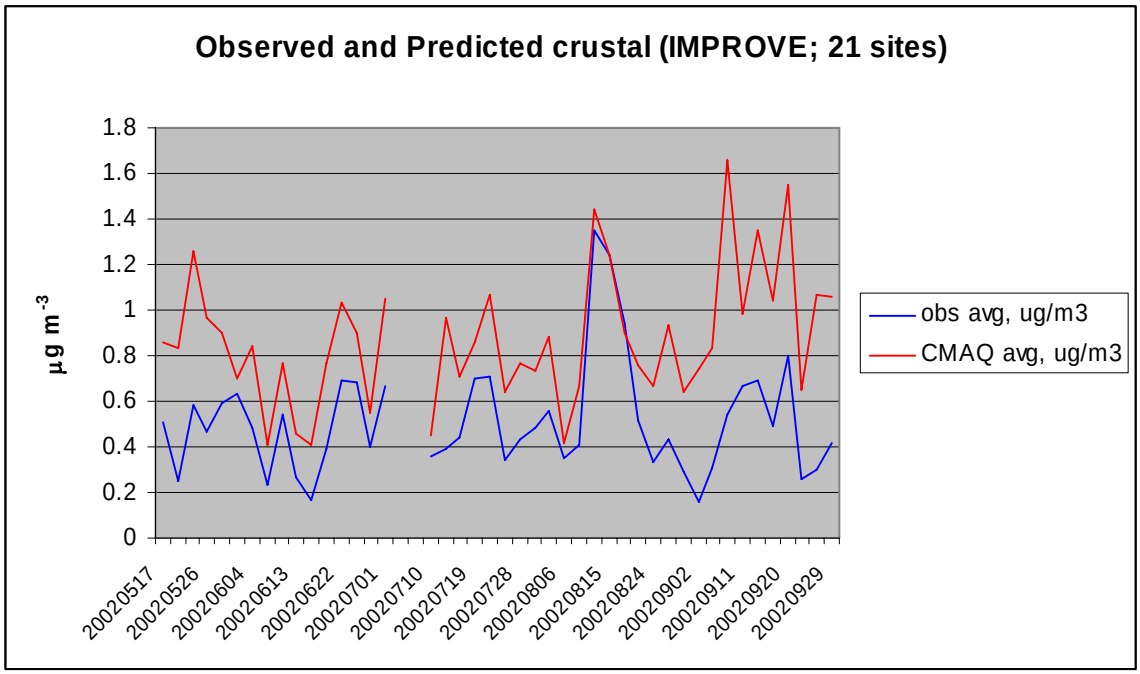

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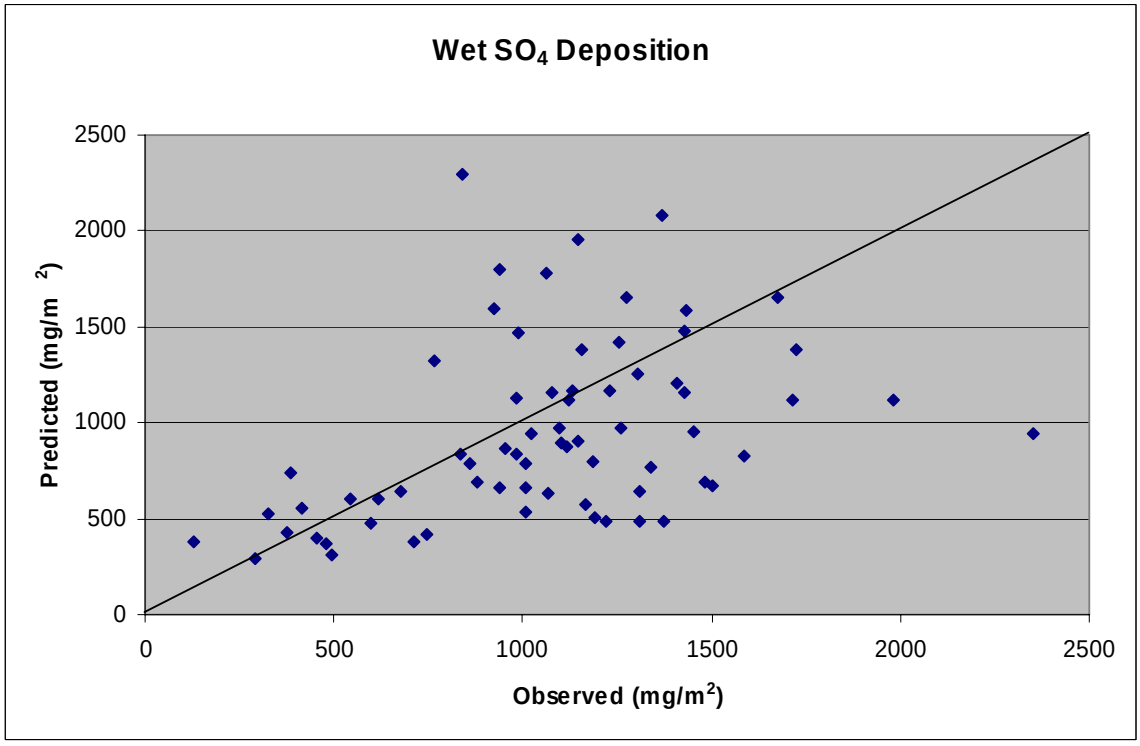

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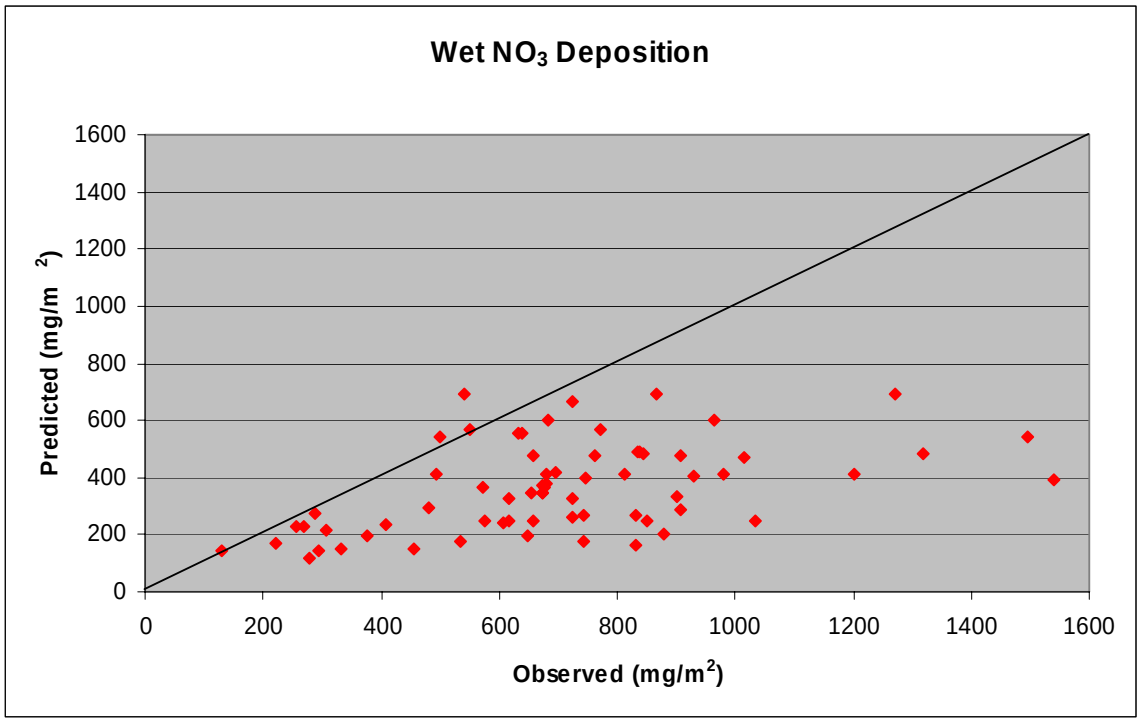

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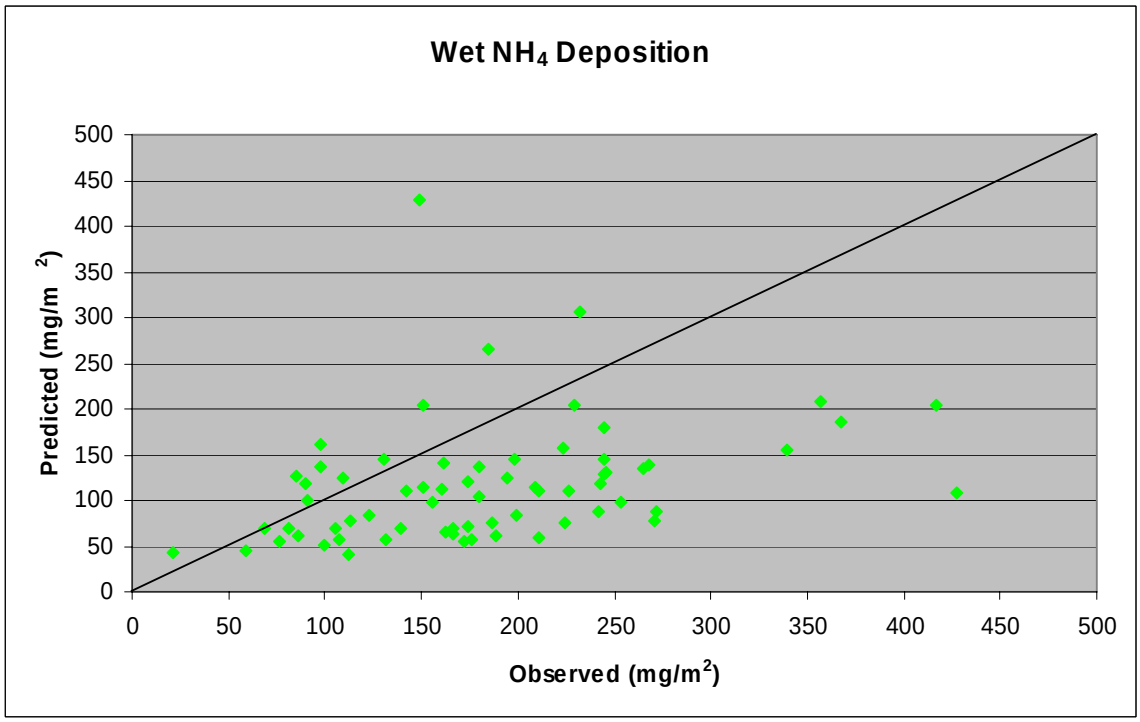

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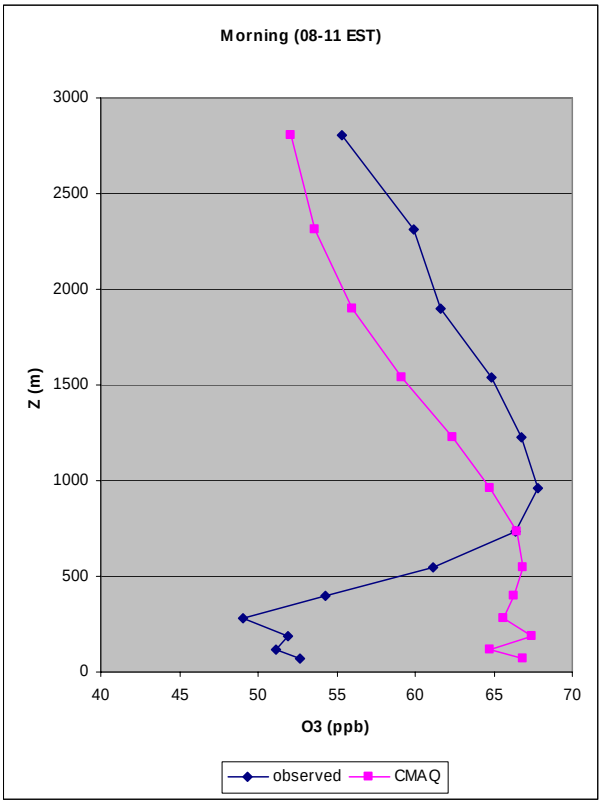

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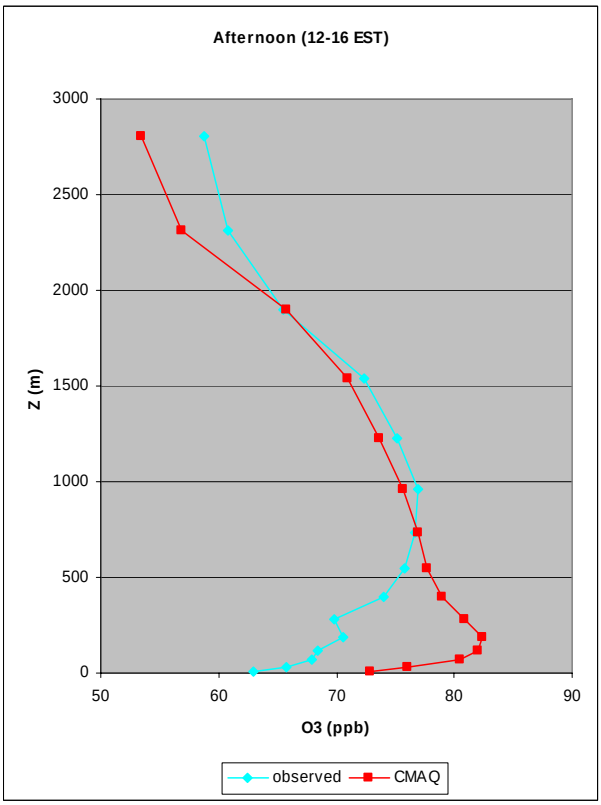

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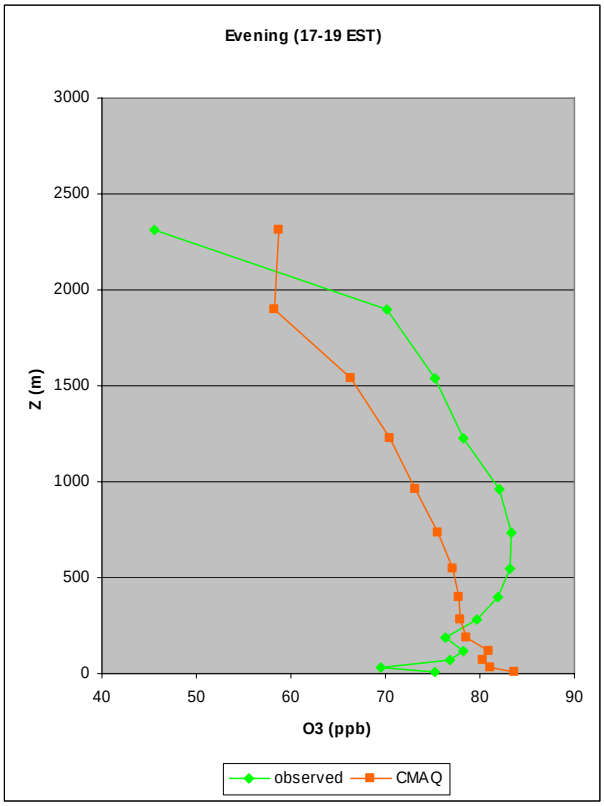

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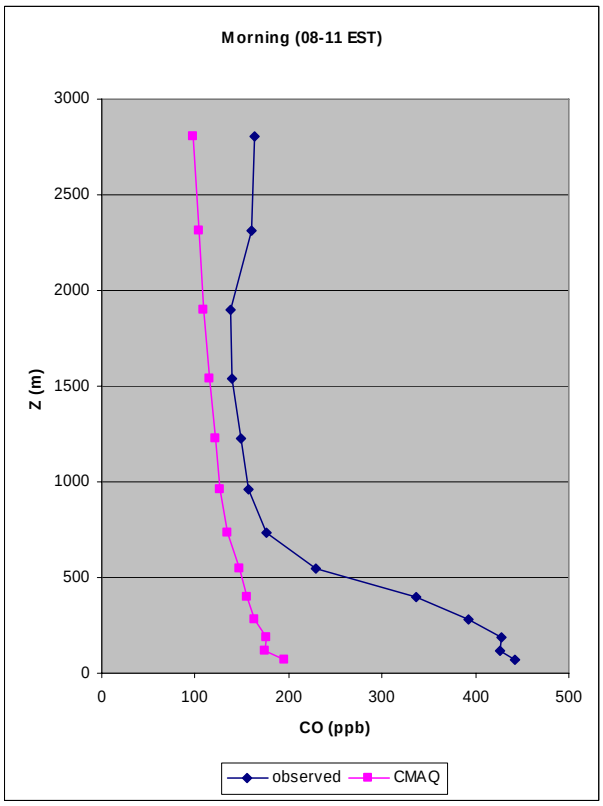

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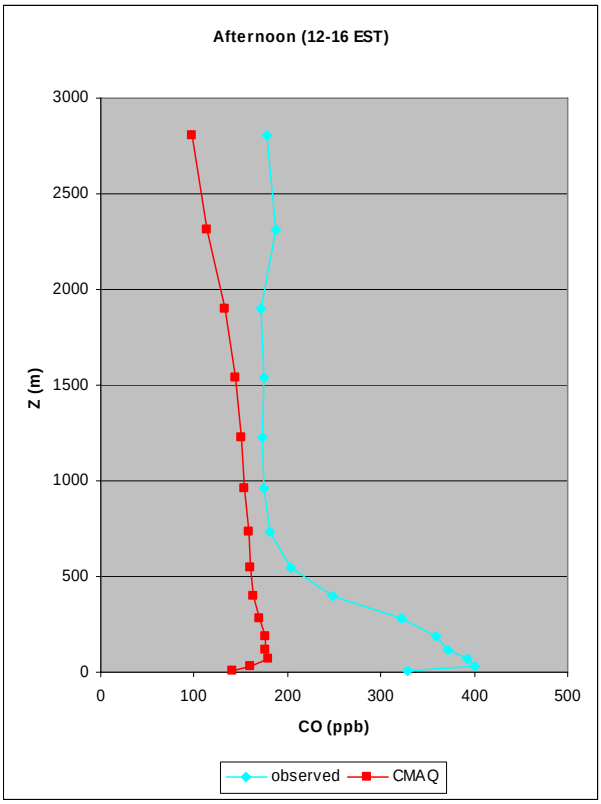

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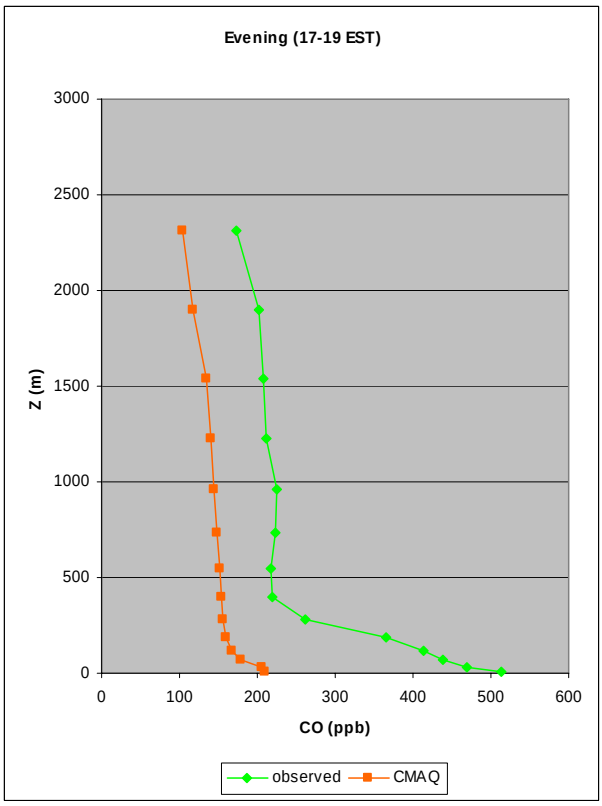

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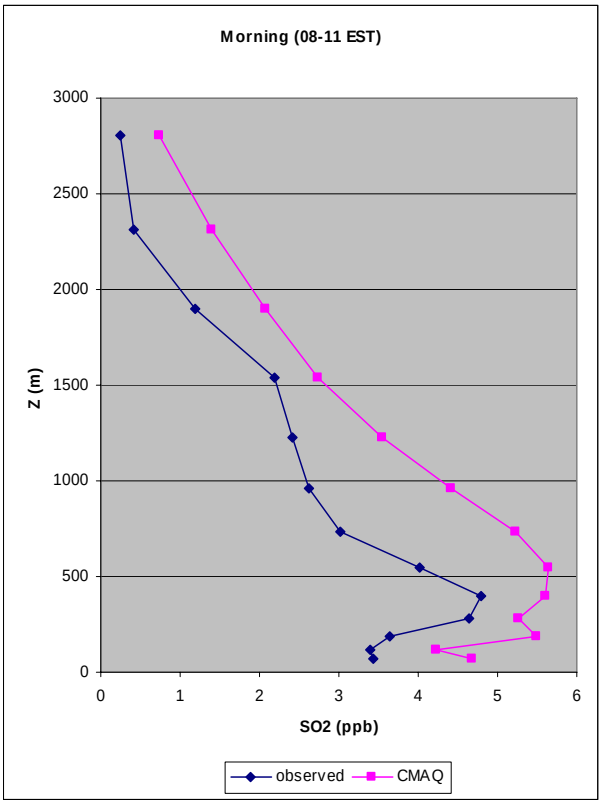

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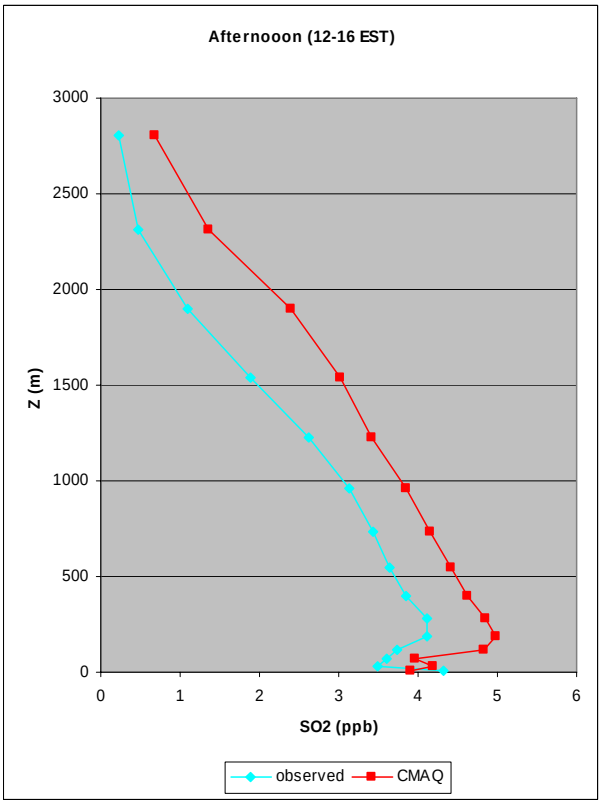

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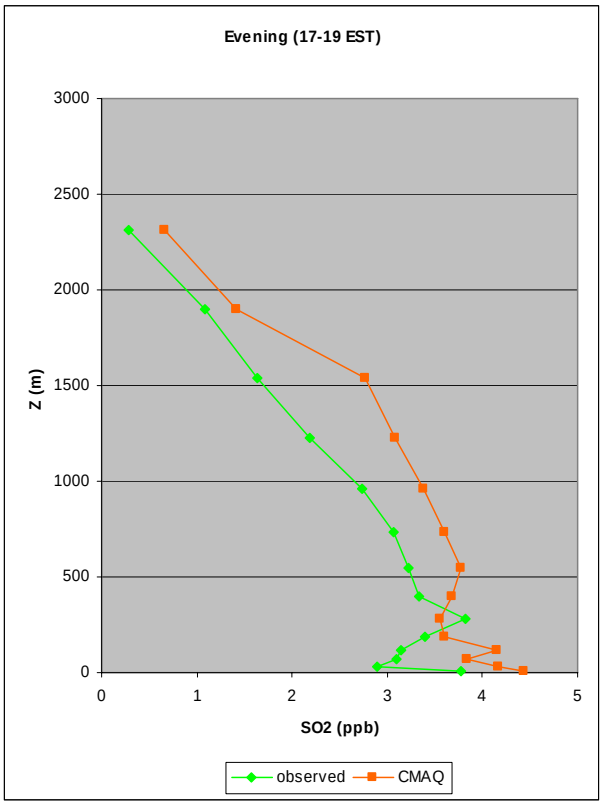
Evening (17-19 EST)
3000
2500
2000
1500
1000
500
0
Z (m)
0
1
2
3
4
5
SO2 (ppb)
observed
CMAQ

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TSD-1f

Future Year Emissions Inventory for 8-h OTC Ozone Modeling

Bureau of Air Quality Analysis and Research
Division of Air Resources
New York State Department of Environmental Conservation
Albany, NY 12233

February 22, 2007

Following the designation of an area as non-attainment for the criteria pollutant Ozone, the Clean Air Act requires submission of an implementation plan, commonly referred to as State Implementation Plan (SIP), demonstrating as to how that area will be meeting the NAAQS in the time period established by the Act. Several areas of the OTR were designated as being in nonattainment for 8-hr ozone (see http://www.epa.gov/ozonedesignations/) with a maximum attainment date of June 2009 and June 2010. However, given that ozone precursors also contribute to $PM_{2.5}$ and other logistics, it was recommended and agreed by the member states that the future year for demonstrating attainment would be 2009. Therefore the OTR states initiated the development of emissions inventories reflecting growth and control from 2002 to 2009 as well as for 2012 and 2018. The 2018 inventory was in response to the need for submission of regional haze SIP, and the 2012 as a next step in the event that attainment for ozone was not feasible in 2009.

Future year emissions inventories within the OTR

The OTR states through MANE-VU contracted MACTEC Federal Programs (called Contractor) develop the 2009, 2012 and 2018 inventories based upon 2002 inventories that the states had previously developed for use in the base year model work. The Contractor in consultation with the states developed the necessary growth and control factors and applied to the 2002 inventory. It should be noted that emissions for mobile sources and the electric energy generating units (EGUs) was not part of the Contractor's effort. The states provided VADEQ and NESCAUM appropriate MOBILE 6 input files along with the projected VMTs, which coupled with the hourly gridded temperature information was used to generate mobile source emissions. As for the emissions from the EGU sector, the inter-RPO work group utilized the Integrated Planning Model (IPM) to develop the state and unit-level emissions. Details on these topics can be found in MACTEC (2007) for non-EGU sectors and in ICF (2005a, 2005b) for the EGU sector. These inventories are identified as 2009 on the way (2009OTW), since they reflect all emission control measures that were promulgated or would become effective on or before 2009.

In addition to these OTW inventories, states have also requested the development of what is termed as beyond on the way (BOTW) inventories for 2009, 2012, and 2018. These inventories are to be based on additional OTC model rules, which would result in reduction in emissions from specific source categories. Details on the development of these controls and the corresponding inventories can be found in MACTEC (2007).

Future year emission inventories outside the OTR

MANE-VU obtained inventories for 2009OTW and 2018OTW as part of the inter-RPO workgroup. However, only MRPO provided emissions for 2012OTW. For the VISTAS region, 2012 emissions were obtained by interpolating area, nonroad, and non-EGU emissions between 2009 and 2018. For mobile sources, VMT were interpolated between

2009 and 2018 and the 2012 emissions were calculated with MOBILE6 using these interpolated VMT and 2012 emission factors. For the CENRAP region, no 2012 emissions were generated, and therefore the 2009 emissions were used in the 2012 CMAQ simulation.

Canadian Emissions

In the case of Canadian emissions, 2010 and 2020 area, non-road, and mobile source emissions were obtained from USEPA (ftp://ftp.epa.gov/EmisInventory/canada_2000inventory/). Primary $PM_{2.5}$ and PM_{10} emissions for the SCCs listed in http://www.epa.gov/ttn/chief/emch/invent/tf_scc_list2002nei_v2.xls were divided by a factor of 4 to account for the fugitive dust transport fraction correction. EGU point source emissions for 2010 and 2020 were obtained from Environment Canada (Bloomer, 2006), while non-EGU point source emissions were assumed to be the same as those developed for 2002 and described elsewhere (see TSD-1c). The 2010 inventories were used in preparing CMAQ input files for the 2009OTW, 2009BOTW, and 2012BOTW scenarios.

Emissions processing – Application of SMOKE

The 2009OTW, 2009BOTW, and 2012 BOTW inventories were processed by VADEQ and NYSDEC using a template similar to that was used for processing 2002 base year emissions (see TSD-1d, TSD-1j) for the 12 km domain. In particular, all gridding and speciation profiles and cross-reference files as well as all temporal allocation profiles and cross-reference files used in the 2002 processing were also used for future year processing. For each day, the following files were prepared:

2009OTW:

- MANE-VU
  - 2009 OTW V3 area source (VADEQ)
  - 2009 V3 nonroad source (VADEQ)
  - 2009 mobile source (NYSDEC)
  - 2009 OTW V3 non-EGU point source (VADEQ)
  - 2009 IPM2.1.9. EGU point source (VADEQ)
  - 2009 EGU point source, IPM2.1.9. non-fossil fuel units (VADEQ)
- VISTAS
  - 2009 BaseG area source (VADEQ)
  - 2009 BaseG nonroad source (VADEQ)
  - 2009 BaseG non-EGU point source (VADEQ)
  - 2009 IPM2.1.9. EGU point source (incl. post-IPM adjustments) (VADEQ)
  - 2009 BaseG low-level fires (VADEQ)
  - 2009 BaseG elevated source fires (VADEQ)
- MRPO
  - 2009 BaseK area source (NYSDEC)
  - 2009 BaseK area source NH3/dust (NYSDEC)

    - 2009 BaseK nonroad source (NYSDEC)
    - 2009 non-EGU point source (VADEQ)
    - 2009 IPM2.1.9. EGU point source (incl. post-IPM adjustments) (VADEQ)
- CENRAP
    - 2009 BaseB area source (VADEQ)
    - 2009 BaseB nonroad source (VADEQ)
    - 2009 non-EGU point source (VADEQ)
    - 2009 IPM2.1.9. EGU point source (VADEQ)
- VISTAS/MRPO/CENRAP ("non-MANE-VU RPOs")
    - 2009 mobile sources for all non-MANE-VU RPOs as implemented in VISTAS 2009 BaseG processing (VADEQ)
- Canada
    - 2010 area sources (NYSDEC)
    - 2010 nonroad sources (NYSDEC)
    - 2010 mobile sources (NYSDEC)
    - point sources (2002 non-EGU point sources; 2010 EGU point sources from IPM) (NYSDEC)
- Biogenics
    - Same as for 2002 base case, calculated with hourly MM5 meteorological fields for 2002 (NYSDEC)

2009 BOTW:

As above for 2009 OTW, with the following two exceptions:

- MANE-VU
    - 2009 BOTW V3 area source (NYSDEC)
    - 2009 BOTW V3 non-EGU point source (NYSDEC)

2012 BOTW:

- MANE-VU
    - 2012 OTW V3 area source (NYSDEC)
    - 2012 V3 nonroad source (NYSDEC)
    - 2012 mobile source (NYSDEC)
    - 2012 OTW V3 non-EGU point source (NYSDEC)
    - 2012 IPM2.1.9. EGU point source (NYSDEC)
    - 2009 EGU point source, IPM2.1.9. non-fossil fuel units (VADEQ)
- VISTAS
    - 2012 BaseG area source (interpolated between 2009 BaseG and 2018 BaseG) (NYSDEC)
    - 2012 BaseG nonroad source (interpolated between 2009 BaseG and 2018 BaseG) (NYSDEC)
    - 2012 BaseG mobile source (interpolated VMT between 2009 BaseG and 2018 BaseG) (NYSDEC)

    - 2012 BaseG non-EGU point source (interpolated between 2009 BaseG and 2018 BaseG) (NYSDEC)
    - 2012 IPM2.1.9. EGU point source (incl. post-IPM adjustments) (NYSDEC)
    - 2009 BaseG low-level fires (VADEQ)
    - 2009 BaseG elevated source fires (VADEQ)
- MRPO
    - 2012 BaseK area source (NYSDEC)
    - 2012 BaseK area source NH3/dust (NYSDEC)
    - 2012 BaseK nonroad source (NYSDEC)
    - 2012 BaseK nonroad source (NYSDEC)
    - 2012 non-EGU point source (NYSDEC)
    - 2012 IPM2.1.9. EGU point source (incl. post-IPM adjustments) (NYSDEC)
- CENRAP
    - 2009 BaseB area source (VADEQ)
    - 2009 BaseB nonroad source (VADEQ)
    - 2009 mobile source (based on VISTAS 2009 BaseG processing) (NYSDEC)
    - 2009 non-EGU point source (VADEQ)
    - 2009 IPM2.1.9. EGU point source (VADEQ)
- Canada
    - 2010 area sources (NYSDEC)
    - 2010 nonroad sources (NYSDEC)
    - 2010 mobile sources (NYSDEC)
    - point sources (2002 non-EGU point sources; 2010 EGU point sources from IPM) (NYSDEC)
- Biogenics
    - Same as for 2002 base case, calculated with hourly MM5 meteorological fields for 2002

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