Appendix O: CMAQ Model Performance Evaluation for 2001

An operational model performance evaluation for $PM_{2.5}$ and its related speciated components was conducted using the 2001 data in order to estimate the ability of the CMAQ modeling system to replicate the base year concentrations for 36-km continental United States domain[1].[2] The PM2.5 components covered in this evaluation include sulfate (SO_4), nitrate (NO_3), total nitrate (TNO_3=NO_3+HNO_3), ammonium (NH_4), elemental carbon (EC), and organic carbon (OC). This evaluation principally comprises statistical assessments of model versus observed pairs that were paired in time and space on a daily or weekly basis, depending on the sampling frequency of each network (measured data). It should be noted when pairing model and observed data that each CMAQ concentration represents a grid-cell volume-averaged value, while the ambient network measurements are made at specific locations. Performance statistics were calculated for each month and season individually and for the entire year, as a whole. Seasons were defined as: winter (December-January-February), spring (March-April-May), summer (June-July-August), and fall (September-October-November). Ambient measurements for 2001 were obtained from the following networks for model evaluation: **S**peciation **T**rends **N**etwork (STN), **I**nteragency **M**onitoring of **PRO**tected **V**isual **E**nvironments (IMPROVE), and **C**lean **A**ir **S**tatus and **T**rends **Net**work (CASTNet). The pollutant species included in the evaluation for each network are listed in Table A-1. For PM2.5 species that are measured by more than one network, we calculated separate sets of statistics for each network. Statistics were generated for the following geographic groupings: 36-km domainwide, and Eastern vs. Western (divided along the 100th meridian).

Table A-1. Monitoring networks and pollutants species included in the CMAQ performance evaluation.

Ambient Monitoring Networks	Particulate Species						
	$PM_{2.5}$ Mass	SO_4	NO_3	TNO_3	NH_4	EC	OC
IMPROVE	X	X	X		X	X	X
CASTNet		X		X	X		
STN	X	X	X		X	X	X

Note that $TNO_3 = (NO_3 + HNO_3)$

There are various statistical metrics available for model performance evaluation. For this evaluation, the principal evaluation statistics used to evaluate CMAQ performance were two bias metrics, fractional bias and normalized mean bias; and two error metrics, fractional error and normalized mean error. Fractional bias is defined as:

[1] See Chapter 4, Section 4.1.2 of the PM NAAQS RIA for the map of the CMAQ modeling domain.
[2] This evaluation includes updates to the CMAQ Model Performance Evaluation Report for 2001 updated March 2005 (CAIR Docket OAR-2005-0053-2149).

$$FB = \frac{1}{n}\left(\frac{\sum_{1}^{n}(P-O)}{\sum_{1}^{n}\left(\frac{(P+O)}{2}\right)}\right) *100,$$ where P = predicted concentrations and O = observed concentrations. FB is a useful model performance indicator because it has the advantage of equally weighting positive and negative bias estimates. The single largest disadvantage in this estimate of model performance is that the estimated concentration (i.e., prediction, P) is found in both the numerator and denominator. Fractional error (FE) is similar to fractional bias except the absolute value of the difference is used so that the error is always positive. Fractional error is defined as:

$$FE = \frac{1}{n}\left(\frac{\sum_{1}^{n}|P-O|}{\sum_{1}^{n}\left(\frac{(P+O)}{2}\right)}\right) *100$$

Normalized mean bias (NMB) is used as a normalization to facilitate a range of concentration magnitudes. This statistic averages the difference (model - observed) over the sum of observed values. NMB is a useful model performance indicator because it avoids over inflating the observed range of values, especially at low concentrations. Normalized mean bias is defined as:

$$NMB = \frac{\sum_{1}^{n}(P-O)}{\sum_{1}^{n}(O)} *100$$

Normalized mean error (NME) is also similar to NMB, where the performance statistic is used as a normalization of the mean error. NME calculates the absolute value of the difference (model - observed) over the sum of observed values. Normalized mean error is defined as:

$$NME = \frac{\sum_{1}^{n}|P-O|}{\sum_{1}^{n}(O)} *100$$

The "acceptability" of model performance was judged by comparing our CMAQ 2001 performance results to the range of performance found in recent regional $PM_{2.5}$ model applications for other, non-EPA studies[3]. Overall, the FB, FE, NMB, and NME statistics shown in Tables A-2 – A-8 below for CMAQ in 2001 are within the range or close to that found by other groups in recent applications. The CMAQ model performance results give us confidence that our applications of CMAQ using this modeling platform provide a scientifically credible

[3] See Appendix C of the CMAQ Model Performance Evaluation Report for 2001 updated March 2005 (CAIR Docket OAR-2005-0053-2149). These other modeling studies represent a wide range of modeling analyses which cover various models, model configurations, domains, years and/or episodes, chemical mechanisms, and aerosol modules.

approach for assessing $PM_{2.5}$ concentrations for the purposes of the PM NAAQS assessment. We discuss in the following sections the bias and error results for the annual and seasonal $PM_{2.5}$ and its related speciated components.

Annual PM2.5 Species Evaluation

Table A-2 provides annual model performance statistics for PM2.5 and its component species for the 36-km national domain and the East and West domains. Nationally, annual total PM2.5 mass is under-predicted, with a NMB of -8%, FB of -10%, NME of 39%, and FE of 42% for STN sites and a NMB of -11%, FB of -11%, NME of 47%, and FE of 51% for IMPROVE sites. PM2.5 model performance compared at STN network sites is better in the East than in the West, whereas the comparison at East and West IMPROVE sites are similar. Although not shown here, the mean observed concentrations of PM2.5 are approximately twice as high at the STN sites (~6μg m^{-3}) as the IMPROVE sites (~13μg m^{-3}), thus illustrating the statistical differences between the urban STN and rural IMPROVE networks. Sulfate is consistently under-predicted at STN, IMPROVE, and CASTNet sites, with NMB values ranging from -51% to -9%. Overall, sulfate performance is best in the East at urban STN sites (NMB=-9%, FB= -8%, NME=34%, and FE=41%). Nitrate is under-predicted both nationally and in the West, while nitrate is over-predicted in the East at both STN and IMPROVE networks. Model performance of total nitrate at CASTNet sites shows an over-prediction domainwide (NMB= 9%; FB=4%) and in the East (NMB=14%; FB=13%). Total nitrate performance was slightly worse in the West, with a NMB of -27% and FB of -21%. Ammonium model performance varies across STN and CASTNet, with STN showing an over-prediction in the national and Eastern domains and CASTNet showing an under-prediction in the national, East and West domains. Elemental carbon is over-predicted at STN sites in the East with a NMB of 34%, FB of 26%, NME of 71% and FE=59%. Although, EC is under-predicted at IMPROVE sites in the East with a NMB of -18%, FB of -26%, NME of 46% and FE=53%. In the West, EC model performance is similar between the STN and IMPROVE networks when comparing FB statistics (STN: FB=-8%; IMPROVE: FB=-7), however NMB statistics are significantly different (STN: NMB=-13%; IMPROVE: NMB=19%). Organic carbon is moderately under-predicted for all domains in the STN network. For the IMPROVE network, OC is under-predicted in the East and over-predicted in the West. Differences in model predictions between IMPROVE and STN networks could be attributed to both the rural versus urban characteristics as well as differences in the measurement methodology between the two networks (e.g. blank correction factors, and filter technology used).

Table A-2. Annual model performance statistics for PM NAAQS CMAQ 2001

PM NAAQS CMAQ 2001 Annual			No. of Obs.	FB (%)	FE (%)	NMB (%)	NME (%)
$PM_{2.5}$ Total Mass	STN	National	6356	-10	42	-8	39
		East	5124	-5	39	-2	35
		West	1232	-29	53	-36	54
	IMPROVE	National	13218	-11	51	-11	47
		East	5606	-11	47	-11	41

		West	7612	-10	54	-12	55
Sulfate	STN	National	6723	-16	45	-13	36
		East	5478	-8	41	-9	34
		West	1245	-52	64	-51	58
	IMPROVE	National	13477	-21	50	-20	39
		East	5657	-15	41	-16	34
		West	7790	-26	57	-33	52
	CASTNet	National	3791	-29	37	-21	27
		East	2784	-22	29	-19	25
		West	1007	-47	59	-45	51
Nitrate	STN	National	5883	-39	89	-15	74
		East	4673	-23	81	14	70
		West	1210	-103	116	-76	82
	IMPROVE	National	13398	-72	116	-10	86
		East	5636	-53	109	16	90
		West	7762	-85	121	-42	82
Total Nitrate (NO3 + HNO3)	CASTNet	National	3788	4	38	9	35
		East	2781	13	34	14	33
		West	1007	-21	51	-27	47
Ammonium	STN	National	6723	20	63	6	54
		East	5478	27	59	16	51
		West	1245	13	78	-53	75
	CASTNet	National	3791	-17	38	-11	31
		East	2784	-8	32	-10	29
		West	1007	-39	57	-37	51
Elemental Carbon	STN	National	6842	19	60	22	69
		East	5551	26	59	34	71
		West	1291	-8	65	-13	63
	IMPROVE	National	13441	-15	60	-2	63
		East	5646	-26	53	-18	46
		West	7795	-7	66	19	85
Organic Carbon	STN	National	6685	-46	65	-43	54
		East	5401	-45	65	-41	51
		West	1284	-46	68	-47	61
	IMPROVE	National	13428	6	63	4	68
		East	5658	-28	60	-24	51
		West	7770	31	64	38	88

Seasonal PM2.5 Total Mass Performance

Seasonal model performance statistics for PM2.5 total mass are shown in Table A-3. Total PM2.5 mass is generally over-predicted in the cooler seasons (winter and fall) in the East for both STN and IMPROVE networks. In the winter season, in the West, PM2.5 is moderately

under-predicted for urban STN sites with a NMB of -47% and FB of -42%, and over-predicted for rural IMPROVE sites with a NMB of 24% and FB of 15%. Note that for comparison of West versus East STN sites, the total number of Western sites is usually less than a quarter of the Eastern sites. In the fall season, PM2.5 is slightly over-predicted for Eastern STN and IMPROVE networks with NMB values ranging from 6% to 8% and FB values ranging from 2% to 6%. In the west, PM2.5 performance shows an under-prediction for STN (NMB=-42%, FB=-37%, NME=57%, and FE=58%) and IMPROVE (NMB=-7%, FB=-5%, NME=50%, and FE=47%) in the fall. In the spring and summer seasons, CMAQ under-predicts PM2.5 in the East and West for STN and IMPROVE. Better PM2.5 performance is achieved during the spring season in the East, with STN showing a slight under-prediction (NMB=-3%, FB=-8%) and IMPROVE showing a moderate under-prediction (NMB=-15%, FB=-20%).

Table A-3. Seasonal model performance statistics for PM2.5 total mass

PM2.5 total mass - PM NAAQS 2001			No. of Obs.	FB (%)	FE (%)	NMB (%)	NME (%)
Winter	STN	National	1179	-4	46	19	54
		East	947	7	42	12	42
		West	232	-42	63	-47	59
	IMPROVE	National	2869	19	54	21	59
		East	1140	15	47	20	50
		West	1729	22	59	24	74
Spring	STN	National	1292	-10	42	-6	38
		East	1033	-8	41	-3	36
		West	259	-18	46	-17	46
	IMPROVE	National	3271	-26	52	-22	46
		East	1394	-15	46	-15	41
		West	1877	-33	57	-33	54
Summer	STN	National	1901	-20	40	-17	34
		East	1547	-20	38	-15	32
		West	354	-20	46	-27	48
	IMPROVE	National	3378	-30	52	-26	44
		East	1471	-42	51	-34	40
		West	1907	-21	52	-13	52
Fall	STN	National	1984	-4	41	-4	40
		East	1597	4	37	8	35
		West	387	-37	58	-42	57
	IMPROVE	National	3700	-2	45	1	44
		East	1601	2	43	6	39
		West	2099	-5	47	-7	50

Seasonal Sulfate Performance

As seen in Table A-4, CMAQ generally under-predicts sulfate nationally throughout the entire year. Sulfate predictions during the winter season show NMB values ranging from -15% to -27% and FB values ranging from -9% to -29% in the East and with NMB values ranging from -10% to -40% and FB values ranging from 0.1% to -32% in the West. Sulfate predictions during the fall seasons are nearly unbiased in the East, with NMB values ranging from 2% to -6% across STN, IMPROVE, and CASTNet networks. Sulfate is moderately under-predicted in the West during the fall season. In the spring, sulfate predictions are moderately under-predicted in the East and West, with NMB values ranging from -22% to -43% and FB values ranging from -29% to -53%. Sulfate predictions during the summer season are somewhat under-predicted in the East across the available monitoring data, while sulfate predictions in the West were moderately under-predicted.

Table A-4. Seasonal model performance statistics for sulfate

Sulfate - PM NAAQS 2001			No. of Obs.	FB (%)	FE (%)	NMB (%)	NME (%)
Winter	STN	National	1292	-14	48	-17	43
		East	1030	-9	47	-15	42
		West	262	-32	51	-40	52
	IMPROVE	National	2979	-5	49	-14	41
		East	1143	-12	43	-16	39
		West	1836	0.1	52	-10	48
	CASTNet	National	878	-23	35	-26	30
		East	656	-29	34	-27	30
		West	222	-6	37	-11	36
Spring	STN	National	1345	-26	55	-23	37
		East	1083	-22	42	-22	36
		West	262	-46	56	-42	49
	IMPROVE	National	3372	-26	48	-24	38
		East	1422	-22	40	-22	34
		West	1950	-29	54	-30	49
	CASTNet	National	963	-36	41	-29	32
		East	713	-30	34	-27	30
		West	250	-53	60	-43	49
Summer	STN	National	2005	-20	46	-11	35
		East	1672	-9	40	-8	33
		West	333	-72	78	-60	64
	IMPROVE	National	3385	-38	58	-26	40
		East	1483	-21	45	-20	35
		West	1902	-51	67	-46	57
	CASTNet	National	952	-37	42	-21	25
		East	689	-22	28	-19	23
		West	263	-77	79	-58	59
Fall	STN	National	2081	-8	42	-4	36
		East	1693	2	37	2	33

		West	388	-51	65	-52	60
	IMPROVE	National	3711	-14	47	-12	36
		East	1609	-4	37	-4	31
		West	2102	-22	55	-31	51
	CASTNet	National	990	-19	31	-9	21
		East	721	-9	21	-6	19
		West	269	-48	57	-44	49

Seasonal Nitrate Performance

Table A-5 provides the seasonal model performance statistics for nitrate and total nitrate for the national domain and the East and West domains. Typically, nitrate and total nitrate performance for all of the seasonal assessments tend to be better in the East (NMB range of 51% to -11%) as compared to the West (NMB range of 37% to -80%). Nitrate is generally under-predicted domainwide during the winter season when nitrate is most abundant. In the East, during the winter, nitrate (NMB ~-5%) and total nitrate (NMB ~2%) performance is slightly under-predicted. Nitrate and total nitrate performance is mixed for the fall, spring and summer seasons, with moderate under-predictions occurring in the West and moderate over-predictions occurring in the East.

Table A-5. Seasonal model performance statistics for nitrate

Nitrate - PM NAAQS 2001			No. of Obs.	FB (%)	FE (%)	NMB (%)	NME (%)
Nitrate (Winter)	STN	National	1196	-39	79	-27	62
		East	939	-25	73	-6	55
		West	257	-91	103	-74	78
	IMPROVE	National	2957	-64	108	-25	74
		East	1137	-39	92	-5	70
		West	1820	79	118	-50	79
Total Nitrate (Winter)	CASTNet	National	877	6	37	1	31
		East	655	7	33	2	30
		West	222	4	48	-9	46
Nitrate (Spring)	STN	National	1344	-32	85	4	69
		East	1082	-21	83	15	68
		West	262	-77	95	-54	70
	IMPROVE	National	3356	-55	104	3	81
		East	1415	-39	102	25	87
		West	1941	-66	105	-28	73
Total Nitrate (Spring)	CASTNet	National	962	-1	33	1	29
		East	712	5	30	4	27
		West	250	-18	43	-21	43
Nitrate (Summer)	STN	National	1561	-62	103	-26	87
		East	1243	-45	93	6	86
		West	318	-129	139	-82	89

	IMPROVE	National	3379	-111	138	-35	97
		East	1475	-94	129	-11	105
		West	1904	-125	145	-55	90
Total Nitrate (Summer)	CASTNet	National	952	-2	42	13	40
		East	689	17	34	26	37
		West	263	-51	65	-41	52
Nitrate (Fall)	STN	National	1782	-25	85	-11	83
		East	1409	-4	76	41	81
		West	373	107	121	-80	85
	IMPROVE	National	3706	-58	115	13	105
		East	1609	-39	110	51	116
		West	2097	-74	119	37	90
Total Nitrate (Fall)	CASTNet	National	989	13	42	23	43
		East	720	25	39	31	43
		West	269	-18	49	-25	46

Seasonal Ammonium Performance

Table A-5 lists the performance statistics for ammonium PM at the STN and CASTNet sites. In the winter, ammonium performance varies across the STN and CASTNet networks, with STN showing an over-prediction in the East (NMB=10%) and the West (NMB=58%) and CASTNet showing an under-prediction in the East (NMB=-13) and West (NMB=-15%). Likewise, ammonium performance for the spring season in the East is similar to that of the winter season, with NMB of 11% for STN and NMB of -7% for CASTNet. However, in the West, model predictions in the spring are generally under-predicted for the West. Ammonium predictions in the summer are moderately under-predicted for the East and West in both the rural and urban sites. In the fall, ammonium predictions are over-predicted in the East (STN: NMB=54%, CASTNet: NMB=8%), whereas in the ammonium predictions are under-predicted in the West (STN: NMB=-58%, CASTNet: NMB=-38%).

Table A-6. Seasonal model performance statistics for ammonium

Ammonium - PM NAAQS 2001			No. of Obs.	FB (%)	FE (%)	NMB (%)	NME (%)
Winter	STN	National	1292	13	64	-4	53
		East	1030	20	58	10	48
		West	262	-13	87	58	75
	CASTNet	National	878	-12	37	-13	31
		East	656	-12	34	-13	30
		West	222	-13	48	-15	48
Spring	STN	National	1345	15	51	8	47
		East	1083	19	51	11	45
		West	262	-3	55	-19	59
	CASTNet	National	963	-11	34	-8	28
		East	713	-4	29	-7	27

		West	250	-32	51	-28	48
Summer	STN	National	2005	-1	53	-6	43
		East	1672	6	49	-0.4	39
		West	333	-40	73	-59	73
	CASTNet	National	952	-37	44	-23	29
		East	689	-25	33	-20	27
		West	263	-70	72	-52	55
Fall	STN	National	2081	47	79	30	78
		East	1693	57	77	54	77
		West	388	2	91	-58	81
	CASTNet	National	990	-6	39	3	35
		East	721	7	33	8	34
		West	269	-40	55	-38	50

Seasonal Elemental Carbon Performance

Table A-7 presents the seasonal performance statistics of elemental carbon for the urban and rural 2001 monitoring data. In the winter, elemental carbon performance is mixed across the STN and IMPROVE networks, with a slight under-prediction in the East (NMB=-3%) and slight over-prediction (NMB=10%) in the West for IMPROVE and a moderate over-prediction in the East (NMB=44%) and a moderate under-prediction in the West (NMB=-31%). Nationally, elemental carbon predictions are moderately over-predicted for the spring and summer seasons for STN, however, elemental carbon is generally under-predicted for the East and West at IMPROVE. Fall elemental carbon predictions are similar to that of the winter predictions, with an under-prediction in the East and slight over-prediction in the West for IMPROVE and an over-prediction in the East and a moderate under-prediction in the West. These biases and errors are not unexpected since there are known uncertainties among the scientific community in carbonaceous emissions/measurements, transport, and deposition processes.

Table A-7. Seasonal model performance statistics for elemental carbon

Elemental Carbon - PM NAAQS 2001			**No. of Obs.**	**FB (%)**	**FE (%)**	**NMB (%)**	**NME (%)**
Winter	STN	National	1292	19	67	16	75
		East	1025	31	66	44	83
		West	267	-28	69	-31	61
	IMPROVE	National	2953	-18	68	3	71
		East	1144	-16	52	-3	52
		West	1809	-19	78	10	96
Spring	STN	National	1390	31	63	47	82
		East	1117	37	64	55	86
		West	273	11	62	20	67
	IMPROVE	National	3363	-25	55	-13	53
		East	1416	-26	51	-20	45
		West	1947	-23	58	-3	65

Summer	STN	National	2042	31	60	46	76
		East	1694	34	60	51	77
		West	348	19	61	27	72
	IMPROVE	National	3385	-2	62	9	73
		East	1471	-37	56	-32	44
		West	1914	26	67	61	110
Fall	STN	National	2118	-0.2	55	0.2	56
		East	1715	7	52	10	55
		West	403	-30	68	-27	59
	IMPROVE	National	3740	-17	58	-7	56
		East	1615	-24	52	-15	45
		West	2125	-12	63	2	70

Seasonal Organic Carbon Performance

Seasonal organic carbon performance statistics are provided in Table A-8. The model predictions show moderate under-predictions for all Eastern sites located in the urban STN sites (NMB values range from -28% to -51%) and rural IMPROVE sites (NMB values range from -2% to -45%). For STN, organic carbon performance in the West shows under-predictions, with the largest underestimations during the colder months, winter and fall. For IMPROVE, organic carbon performance in the West shows a positive bias and error with moderate over-predictions. These biases and errors reflect sampling artifacts among each monitoring network. In addition, uncertainties exist for primary organic mass emissions and secondary organic aerosol formation. Research efforts are ongoing to improve fire emission estimates and understand the formation of semi-volatile compounds, and the partitioning of SOA between the gas and particulate phases.

Table A-8. Seasonal model performance statistics for organic carbon

Organic Carbon - PM NAAQS 2001			No. of Obs.	FB (%)	FE (%)	NMB (%)	NME (%)
Winter	STN	National	1251	-36	66	-41	58
		East	986	-27	59	-28	50
		West	265	-72	90	-61	70
	IMPROVE	National	2945	18	65	20	76
		East	1144	-6	53	-2	53
		West	1801	33	72	52	109
Spring	STN	National	1363	-42	61	-38	50
		East	1092	-43	62	-39	49
		West	271	-37	59	-35	51
	IMPROVE	National	3360	0.4	55	-5	56
		East	1417	-23	56	-22	50
		West	1943	17	54	18	63
Summer	STN	National	2013	-57	69	-47	54
		East	1665	-63	73	-51	54
		West	348	-26	52	-31	51

	IMPROVE	National	3396	-5	68	2	74
		East	1483	-62	74	-45	54
		West	1913	39	64	54	97
Fall	STN	National	2058	-43	64	-43	53
		East	1658	-40	62	-41	50
		West	400	-53	73	-47	62
	IMPROVE	National	3727	11	63	4	66
		East	1614	-19	56	-18	49
		West	2113	34	68	28	85