

5) Forward Model Simulation of BRAVO Tracer Concentrations

The Regional Modeling System for Aerosols and Deposition (REMSAD) model is a prognostic, Eulerian-grid air quality model designed to simulate the formation and long-range transport of aerosols and their precursors (see section 2.2.1 for a full description). In this study, REMSAD was used to simulate the transport of sulfur from sources to Big Bend and other receptors and assess the source contributions of sulfate to these receptors. The CAPITA Monte Carlo (CMC) model is a particle dispersion model capable of simulating air mass advection and diffusion both forward and backward in time (see section 2.2.4 for a full description). The CMC model was used in both forward and backward air mass history analyses to analyze sulfur transport and estimate sulfur source apportionment.

In order to evaluate the ability of these two models to properly simulate the transport and diffusion processes, the models were used to simulate four conservative tracers that were released during the BRAVO study period. The models were then evaluated for their skill at reproducing the observed tracer time series in the Big Bend region. The REMSAD model was driven by the MM5 meteorological data while the CMC model was driven by both the MM5 and EDAS/FNL fields, and all simulations were run over the entire four month BRAVO period. The MM5 and EDAS/FNL field wind fields each have their advantages, the MM5 data having a higher resolution (36 km vs. 80 km), and the EDAS/FNL data incorporating more measured data in its data assimilation process.

This chapter reports on the comparison of the simulated to observed tracer concentrations to evaluate the ability of these models and wind fields to simulate medium- to long-range transport. The evaluation was conducted over the entire four month period, generating an aggregated model performance over a range of meteorological conditions. Identifying particular meteorological conditions and events that the models performed well and not well was not conducted. The performance of the two models using the MM5 meteorological data are also compared, as well as the difference between the CMC performance using the MM5 and EDAS meteorological drivers.

5.1 Perfluorocarbon Tracer Data and Model Simulation Requirements

The BRAVO tracer network consisted of four unique perfluorocarbon tracers released from or representing urban/electric utilities and measured at 24 monitors throughout West Texas. The tracer data are fully described in section 2.1.1.2 and this section summarizes these tracer release and monitoring networks. Figure 5-1 presents both the tracer release sites and the monitoring network. The perfluorocarbon tracer experiment was conducted in two phases. In the first phase (July 5–September 13, 1999), two “timing” tracers were released at Eagle Pass to help characterize transport times from Eagle Pass to Big Bend NP. During the second phase of the study (September 17–November 1), the two timing tracers were moved to sites in eastern Texas in San Antonio and the Parish power plant in Houston where they were continually released. The tracer release sites were 230–750 km from the Big Bend National Park, which allowed for evaluating both near and distant mesoscale transport (100–1000 km). However, Big Bend is impacted from sources throughout North America, and this evaluation was unable to assess the regional scale (1000–5000) transport abilities of these models.

The tracer network included six 6-hour receptor sites, located along an arc extending from Big Bend to about 300 km north-northeast (Figure 5-1). These sites collected data throughout the four month period with high collection efficiencies. The other sites collected data

in July and only part of August and October and generally had lower collection efficiency. Only the 6-hour sites were used in this evaluation study due to their extended sampling period and their good collection efficiency.

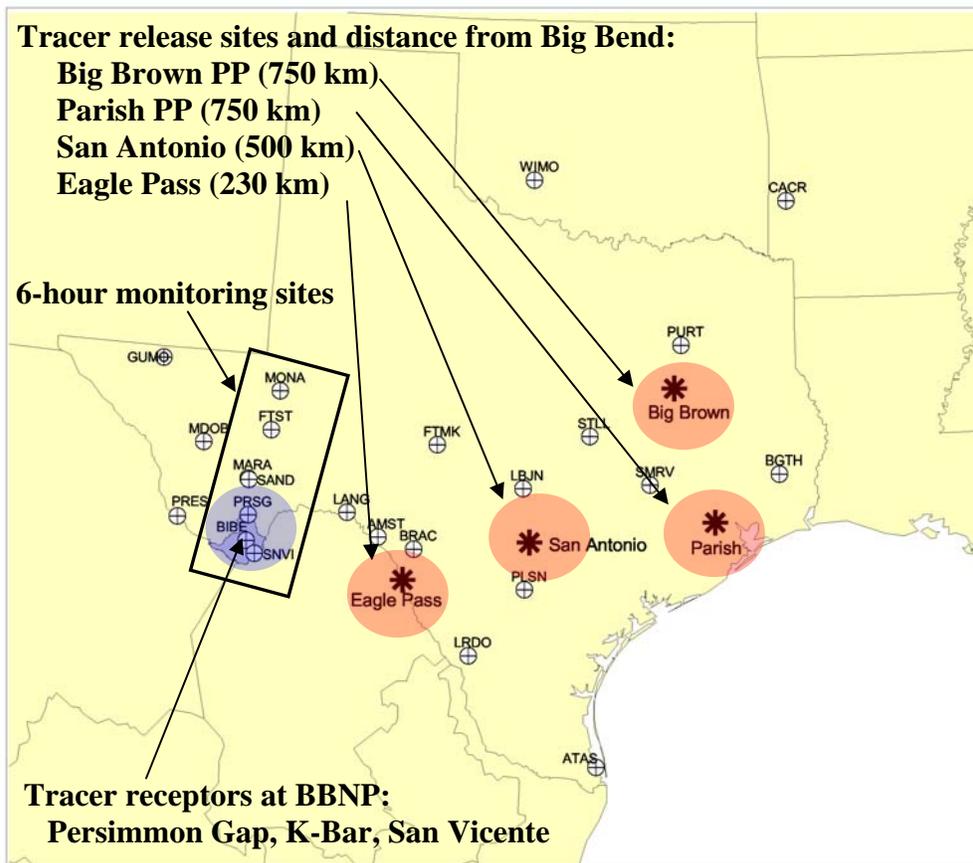


Figure 5-1. The location of the tracer release sites and tracer monitoring network. The distance from the tracer release sites to Big Bend is also noted.

5.1.1 Spatial Variability in the Tracer Concentration Field

The simulation of the BRAVO tracer data requires properly simulating the transport direction and speed from the tracer release sites to the receptor sites as well as the vertical and horizontal spreading of the tracer plume. This requires simulating the microscale processes of molecular and turbulent diffusion and the mesoscale process of advection, both of which are influenced by the topography and meteorology. The tracer concentration fields are sensitive to transport directions, since small errors can be the difference between a tracer impacting or missing a receptor site. In addition, the horizontal and vertical dilution of a plume is critical to properly simulating the concentration for a plume hit.

These processes result in a spatially and temporally heterogeneous concentration field. This is shown in Table 5-1, the correlation of the ocPDCH tracer released from Eagle Pass between the six 6-hour tracer monitoring sites. As shown, the correlation coefficients fall off rapidly with distance. For example, Marathon is about 100 km north of K-Bar Ranch in Big Bend National Park and the $r=0.36$ between these two sites. Consequently, the K-Bar tracer concentrations can explain only about 13% of the variance in Marathon's concentrations. Table

5-1 also presents the correlation between the sites for the 6-hour concentrations aggregated up to 24-hour concentrations. As shown, the correlations between the monitoring sites do improve somewhat for the nearby sites, e.g., r increased from 0.42 to 0.62 between K-Bar and Persimmon Gap.

Table 5-1. A) The correlation between the measured ocPDCH tracer concentrations at the six 6-hour monitoring sites. B) The same correlation matrix as in A) but the data were aggregated up to 24 hours. The distance between the receptor sites in km are in parentheses.

A) Eagle Pass (ocPDCH) Observed Tracer 6 hr Average Correlation Matrix

	San Vicente	K-Bar	Persimmon	Marathon	Ft Stocton	Monahans
San Vicente	1 (0)	0.76 (25)	0.32 (62)	0.32 (122)	0.34 (200)	0.12 (265)
K-Bar	0.76 (25)	1 (0)	0.42 (41)	0.36 (100)	0.28 (182)	-0.05 (245)
Persimmon	0.32 (62)	0.42 (41)	1 (0)	0.41 (60)	0.44 (140)	0.09 (205)
Marathon	0.32 (122)	0.36 (100)	0.41 (60)	1 (0)	0.53 (85)	0.06 (148)
Ft Stocton	0.34 (200)	0.28 (182)	0.44 (140)	0.53 (85)	1 (0)	0.22 (63)
Monahans	0.12 (265)	-0.05 (245)	0.09 (205)	0.06 (148)	0.22 (63)	1 (0)

B) Eagle Pass (ocPDCH) Observed Tracer 24 hr Average Correlation Matrix

	San Vicente	K-Bar	Persimmon	Marathon	Ft Stocton	Monahans
San Vicente	1 (0)	0.77 (25)	0.53 (62)	0.31 (122)	0.27 (200)	0.13 (265)
K-Bar	0.77 (25)	1 (0)	0.62 (41)	0.42 (100)	0.23 (182)	-0.07 (245)
Persimmon	0.53 (62)	0.62 (41)	1 (0)	0.69 (60)	0.3 (140)	-0.07 (205)
Marathon	0.31 (122)	0.42 (100)	0.69 (60)	1 (0)	0.64 (85)	0.12 (148)
Ft Stocton	0.27 (200)	0.23 (182)	0.3 (140)	0.64 (85)	1 (0)	0.41 (63)
Monahans	0.13 (265)	-0.07 (245)	-0.0 (205)	0.12 (148)	0.41 (63)	1 (0)

The correlation between the fine particulate sulfur and sulfur dioxide for the same six sites are presented in Table 5-2. The correlation between sites for particulate sulfur is greater than 0.8 for all site pairs indicating a spatially uniform concentration field compared to the tracer data. On the other hand, the sulfur dioxide correlations decrease more rapidly with distance than the tracer data. The spatially homogeneous particulate sulfur concentrations are due to it being a long-lived secondary species with characteristic lifetimes often in excess of 5 days, and the concentrations are impacted by emission from sources over a broad region. Sulfur dioxide is a shorter-lived species, with lifetimes on the order of 1–3 days, and the receptors are impacted by more nearby sources resulting in a more heterogeneous concentration field. The large variability in the tracer and sulfur dioxide concentrations make it a challenge to properly simulate their concentrations with regional scale models. However, the scale of variability in particulate sulfur is better matched to these regional models.

Table 5-2. The correlation of the A) 24-hour particulate sulfur concentrations and B) 24-hour sulfur dioxide between the same six monitoring sites as in Table 5-1.

A) Particle Sulfur observed 24 hr Average Correlation Matrix

	San Vicente	K-Bar	Persimmon	Marathon	Ft Stocton	Monahans
San Vicente	1 (0)	0.94 (25)	0.93 (62)	0.88 (122)	0.86 (200)	0.84 (265)
K-Bar	0.94 (25)	1 (0)	0.9 (41)	0.86 (100)	0.83 (182)	0.82 (245)
Persimmon	0.93 (62)	0.9 (41)	1 (0)	0.94 (60)	0.89 (140)	0.87 (205)
Marathon	0.88 (122)	0.86 (100)	0.94 (60)	1 (0)	0.92 (85)	0.89 (148)
Ft Stocton	0.86 (200)	0.83 (182)	0.89 (140)	0.92 (85)	1 (0)	0.89 (63)
Monahans	0.84 (265)	0.82 (245)	0.87 (205)	0.89 (148)	0.89 (63)	1 (0)

B) SO₂ 24 hr Observed Average Correlation Matrix

	San Vicente	K-Bar	Persimmon	Marathon	Ft Stocton	Monahans
San Vicente	1 (0)	0.8 (25)	0.2 (62)	0.29 (122)	0.07 (200)	0.06 (265)
K-Bar	0.8 (25)	1 (0)	0.34 (41)	0.17 (100)	0.06 (182)	0 (245)
Persimmon	0.2 (62)	0.34 (41)	1 (0)	0.58 (60)	0.27 (140)	0.11 (205)
Marathon	0.29 (122)	0.17 (100)	0.58 (60)	1 (0)	0.45 (85)	0.1 (148)
Ft Stocton	0.07 (200)	0.06 (182)	0.27 (140)	0.45 (85)	1 (0)	0.11 (63)
Monahans	0.06 (265)	0 (245)	0.11 (205)	0.1 (148)	0.11 (63)	1 (0)

5.1.2 Inherent Uncertainty in the Tracer Simulation

The above section illustrated the high degree of variability in the tracer concentrations at distances as little as 25 and 40 km. The grid size of the REMSAD model is 36 km and in the CMC model it varied between 36 and 180 km depending on the wind field used. These models cannot capture the sub-grid variability in the tracer concentration. In addition, the true model resolution is four times the grid spacing [Pielke, 1984; Grasso, 2000], and the models cannot reproduce a high degree of spatial variability below this resolution. In the case of REMSAD the true spatial resolution of the 36 km grid is 144 x 144 km².

The REMSAD and CMC model resolutions place an upper limit on the skill that the models can achieve when simulating the tracer data. For example, even if the REMSAD simulation of tracer perfectly matched the measured tracer concentrations at K-Bar, there would be errors when compared to San Vicente which is in the same grid cell as K-Bar. In addition to errors due to model resolution, uncertainties in the measured data exist due to errors in the measurements and in the background concentrations subtracted from the measured concentration. The models cannot account for these measurement uncertainties. The total error due to the spatial resolution of the model and errors in the measured data can be viewed as the inherent uncertainty in the model simulation.

In order to assess this inherent uncertainty in the simulated tracer, the tracer time series from K-Bar, San Vicente, and Persimmon Gap were compared to each other. These sites are between 25 and 62 km of each other, which is less than twice the 36 km MM5 grid spacing. Differences between these tracer data measured at these monitoring sites can be viewed as a measure of the sub-grid scale variability and tracer measurement error. The tracer time series were compared by examining ratios in the pair-wise average concentrations, the root mean square (RMS) difference between pairs of data, and the correlation coefficient (Tables 5-3 to 5-5). These metrics are similar to the standard model performance statistics of bias, RMS error, and correlation coefficient which are used to compare the simulated results to the observed values. The Big Brown tracer concentrations were usually below detection limit and negative, leading to poor data quality. The comparisons of the Big Brown data are included Tables 5-3 to 5-5 for completeness, but are not discussed.

As shown in Tables 5-3 to 5-5, the K-Bar and San Vicente monitoring sites had mean tracer concentrations within 15% of each other for all three tracers. However, the average concentration at Persimmon Gap was about a factor of 3 larger than at K-Bar or San Vicente for the Eagle Pass tracer and within a factor of two for the tracers released from the more distant San Antonio and Parish tracers. The RMS difference varies between 100–400% for the Eagle Pass tracer, while for the San Antonio and Parish tracers it varies between 50–200%. The largest differences for all tracers were for Persimmon Gap data compared to the other sites.

These results illustrate the difficulty in simulating the tracer data. Since San Vicente and K-Bar are in the same REMSAD grid cell, even if the model perfectly matched the Eagle Pass tracer at K-Bar it would have a 100% RMS error compared to San Vicente. In order to reduce this inherent uncertainty in the tracer simulation, the observed and modeled tracer data were compared by aggregating the results for the three Big Bend sites, San Vicente, K-Bar and Persimmon Gap, and for the six 6-hour tracer sites extending from San Vicente north 265 km to Monahans Sandhills. The Big Bend sites were aggregated together since the MM5 and EDAS/FNL wind fields could not resolve transport to individual sites 30 km apart. Aggregating the six sites over the 300 km range allowed for the examination of the capabilities of the models to properly simulate the timing of the tracer reaching the receptors, while allowing for small spatial displacements in the tracer plume. This is a less stringent and more appropriate test for the models and their intended use. To obtain as complete a time series as possible, data from only one monitoring site was needed to have a valid average observed tracer concentration. Also, due to the background tracer concentration being subtracted from the measured concentrations, negative concentration values do occur. These negative values represent the error in the data and zeroing them out would lead to biased measured values. Therefore all negative values were left in the comparison.

Table 5-3. Comparison of K-Bar and San Vicente's tracer data.

K-Bar Vs San Vicente's Tracer Data								
Tracer and Dates	#	Avg (ppq)		Ratio	RMS Difference			r
		K-Bar	San Vicente	SV/KB	Abs (ppq)	Relative to KB	Relative to SV	
Eagle Pass (7/1–10/31)	88	0.14	0.12	0.86	0.14	0.97	1.17	0.81
San Antonio (9/17–10/31)	32	0.41	0.37	0.89	0.25	0.44	0.67	0.90
Parish (9/17–10/31)	32	0.060	0.063	1.0	0.05	0.78	0.72	0.77
Big Brown (7/1–10/31)	88	-0.012	-0.001	0.07	0.03	-2.5	-33.3	0.66

Table 5-4. Comparison of K-Bar's and Persimmon Gap's tracer data.

K-Bar Vs Persimmons Gap's Tracer Data								
Tracer and Dates	#	Avg (ppq)		Ratio	RMS Difference			r
		K-Bar	Pers. Gap	PG/KB	Abs (ppq)	Relative to KB	Relative to PG	
Eagle Pass (7/1–10/31)	95	0.15	0.39	2.7	0.47	3.2	1.20	0.47
San Antonio (9/17–10/31)	38	0.59	0.35	0.59	0.45	0.80	1.28	0.88
Parish (9/17–10/31)	95	0.060	0.046	0.77	0.07	1.2	1.50	0.72
Big Brown (7/1–10/31)	38	-0.012	0.006	-0.48	0.05	-3.9	8.0	0.47

Table 5-5. Comparison of San Vicente and Persimmon Gap's tracer data.

San Vicente Vs Persimmon Gap's Tracer Data								
Tracer and Dates	#	Avg (ppq)		Ratio	RMS Difference			r
		San Vicente	Pers. Gap	PG/SV	Abs (ppq)	Relative to SV	Relative to PG	
Eagle Pass (7/1–10/31)	81	0.12	0.37	3.2	0.49	4.2	1.31	0.37
San Antonio (9/17–10/31)	31	0.33	0.18	0.54	0.40	1.2	2.29	0.58
Parish (9/17–10/31)	31	0.059	0.048	0.81	0.05	0.93	1.14	0.74
Big Brown (7/1–10/31)	81	-0.003	0.009	-2.8	0.05	-14.4	5.1	0.40

5.2 CAPITA Monte Carlo Model Simulation of Tracer Data

The CAPITA Monte Carlo model was used to simulate the tracer released from all four locations driven by either the BRAVO 36 km MM5 winds or a combination of the EDAS and FNL meteorological fields. The FNL data were used in October 1999 since the EDAS fields were not available. Section 2.1.3 provides detailed descriptions of the wind fields and data processing needed for input into the CMC model. The model was operated by releasing 100 particles every hour from each tracer release location at a fixed effective release height (Table 5-6). The Eagle Pass and San Antonio tracers were released from towers, so the effective stack height is the actual release point. The Big Brown and Parish tracers were injected into power plant stacks, and their effective release heights were the stack height plus a plume rise calculated from average stack and meteorological parameters. The particles were tracked for five days or until they left the meteorological grid. Each particle was weighted by the actual tracer emission rates divided by the number of particles release each hour. Simulated tracer concentration fields were generated every hour by summing the weights of all particles that fell in a given 36 km grid and below the mixed layer. This mass was normalized by the receptor cell's volume, the grid area times the mixing height, creating concentration fields.

Table 5-6. The tracer effective release heights and design tracer emission rates used in the CMC for each simulated tracer release location.

Release Site	Tracer	Release Rate (kg/day)	Release Schedule	Eff. Release Hgt. (m)	Distance from Big Bend (km)
Eagle Pass	ocPDCH	3.7	Continuous 7/1 – 11/1/99	100	230
San Antonio	PDCB	9.7	Continuous 9/17 – 11/1/99	20	500
Parish (Houston TX)	1PTCH	2.6	Continuous 9/17 – 11/1/99	400	750
Big Brown (Northeast TX)	iPPCH	2	Continuous 7/1 – 11/1/99	400	750

The actual tracer release rates used in the simulation are presented in Figures 2-3 to 2-6. These release rates were similar to the designed release rates reported in Table 5-6, but show some diurnal cycling and periods where no tracer was released. For example, PPCH was not released from the Big Brown power plant from October 8–16. This was unfortunate since this was one of the intensive modeling periods and a period when transport simulations showed transport from northern Texas.

5.2.1 Results of the Monte Carlo Model Tracer Simulation

The results of the simulation are presented in Figures 5-2 and 5-3 and Tables 5-7 and 5-8. As shown in Figure 5-2, the model simulations using the MM5 or the EDAS/FNL meteorological fields were able to reproduce the timing of the major Eagle Pass (ocPDCH) tracer impacts to Big Bend. The duration of the simulated tracer impacts tended to be about the same as measured or shorter. The MM5 simulation was better able to predict the Eagle Pass tracer pattern particularly from August 10 to September 12. Neither simulation was able to reproduce the day to day variability of the observed data with great skill, having correlation coefficients of 0.44 for MM5 and 0.53 for the EDAS/FNL meteorological fields. However, the correlation coefficient in both cases is significant at the 1% level. The EDAS simulation underestimated the Eagle Pass tracer by about a factor of 2 at Big Bend while the MM5 simulation underestimated the average

concentration by only 10%. Both simulations reproduce the measured data's standard deviation. Therefore, the MM5 simulation had a similar distribution as the observed values, while the EDAS simulation is biased low. Both simulations also had similar RMS errors of about 120% or an error greater than a factor of 2 in simulating transport from Eagle Pass to Big Bend.

The Eagle Pass tracer simulation averaged over all six monitoring sites is presented in Figure 5-3 and Table 5-8. Again, both model simulations reproduce the observed tracer pattern. The MM5 simulation properly identifies the time and duration of the Eagle Pass tracer impacts to this region and the correlation coefficient increased from 0.44 to 0.54 compared to the Big Bend simulation. However, the MM5 simulation does not fully capture the observed tracer peaks. This is reflected in the performance statistics (Table 5-8) where the predicted tracer concentrations are underestimated by 30% on average, and the standard deviation of the predicted values is 0.2 ppq compared to 0.29 ppq for the observed data. The RMS error decreased by almost half to 73%, indicating that the model is able to simulate the transport to within ± 150 km of the receptor with concentrations within less than a factor of 2 of the observed values.

The performance statistics for the EDAS/FNL winds averaged over all six sites did not show as large an improvement over those for just the Big Bend region. The EDAS/FNL simulation still underestimated the observed values by a factor of two and the correlation coefficient decreased from 0.53 to 0.46. The RMS error did improve from 120% to 95%. Examination of the vertical profiles of the EDAS/FNL simulations showed that, on average, ~50% of the mass was above the mixing layer. Therefore, the underestimation could be due to the particles being mixed too high prior to reaching Big Bend or the vertical velocities are inappropriately carrying mass above the mixed layer.

Tracer was released from San Antonio, Texas, and the Parish power plant in Houston, Texas, from September 17 through October. These tracer release sites are further from Big Bend than Eagle Pass, at ~500 km and 750 km, respectively. Therefore these tracers were a better test of the model's ability to simulate more regional scale transport. The tracer released from San Antonio was measured at Big Bend above the background a number of times in the first half of October. Impacts of the simulated tracer at Big Bend also occurred during this time period (Figure 5-2). The model run using EDAS/FNL had the most skill at reproducing the day to day variability with a correlation coefficient of 0.69 compared to 0.36 using the MM5 winds (Table 5-7). In addition, the EDAS/FNL simulation underestimated the San Antonio tracer at Big Bend by about 13% while the MM5 simulation overestimated the tracer by about 25%. The San Antonio RMS error was 140% using the EDAS/FNL winds, but 240% using the MM5 winds. The large RMS error for the MM5 simulation was due to the overestimation of the concentrations by about a factor of 5 on September 30 and October 24.

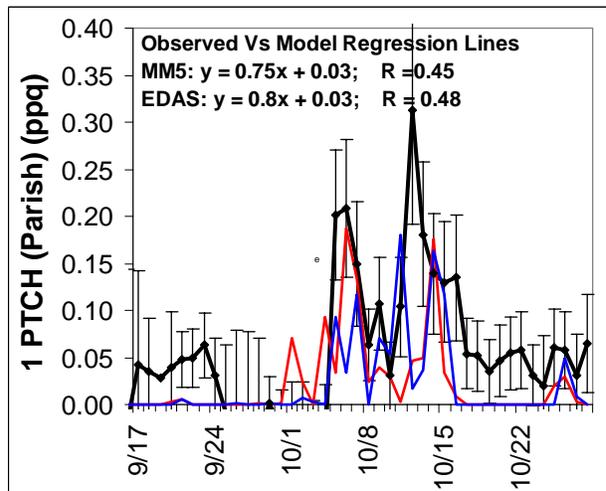
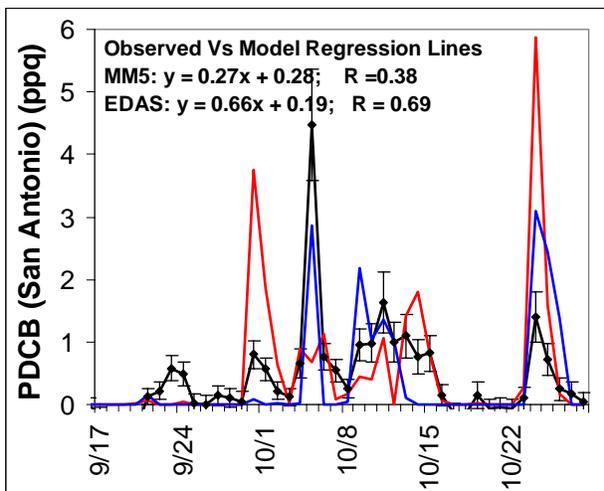
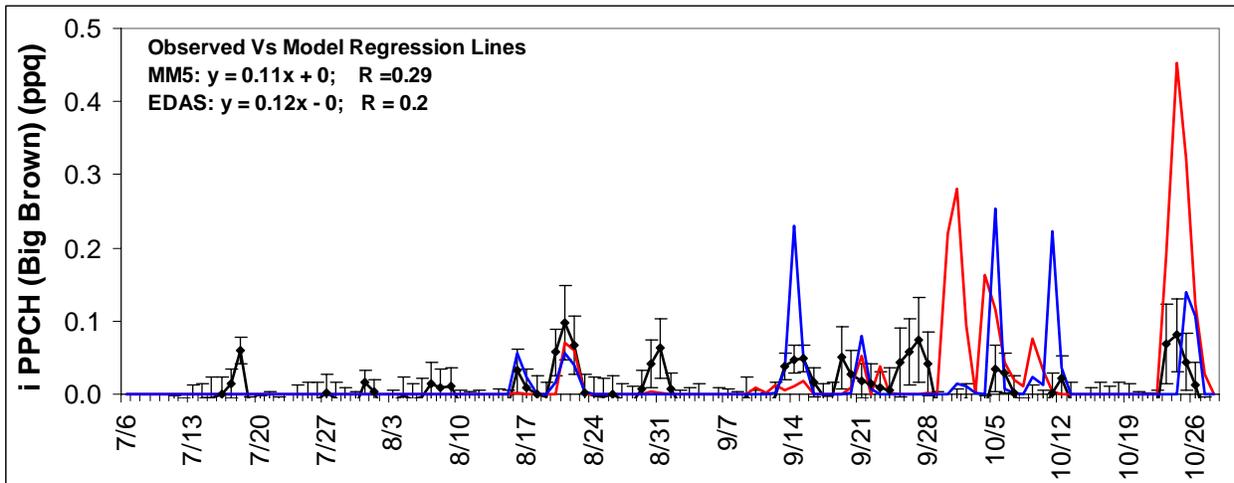
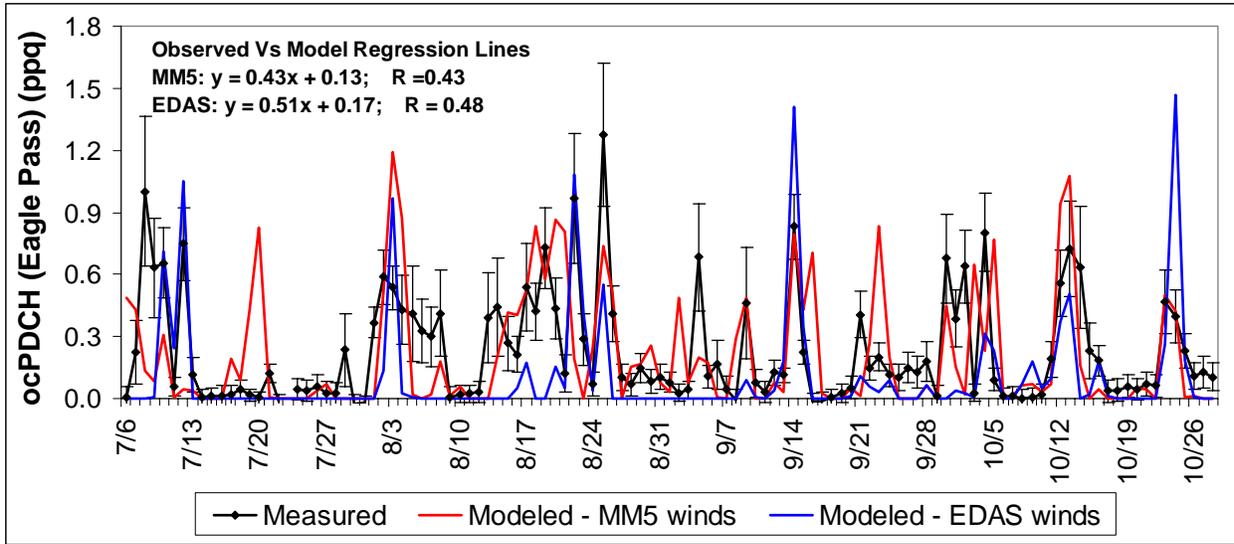


Figure 5-2. Comparison of observed and CMC modeled tracer data at Big Bend, Texas. The observed and modeled tracer data were averaged over the K-Bar, Persimmon Gap, and San Vicente monitoring sites which are in or at the boundary of the park. The measured data include error bars.

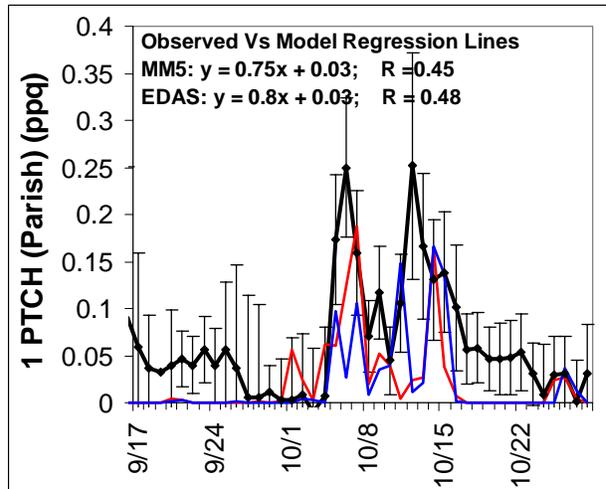
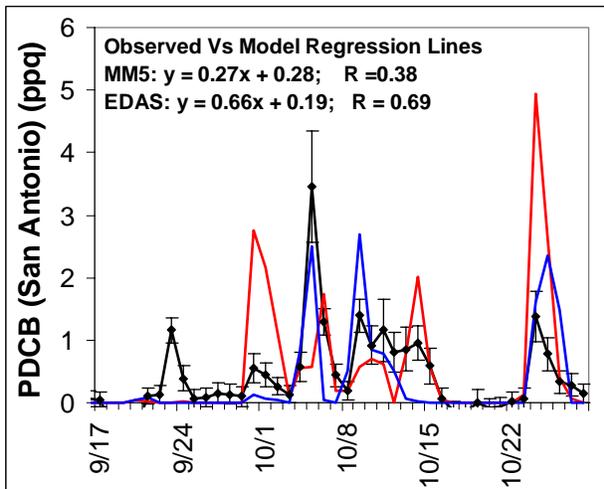
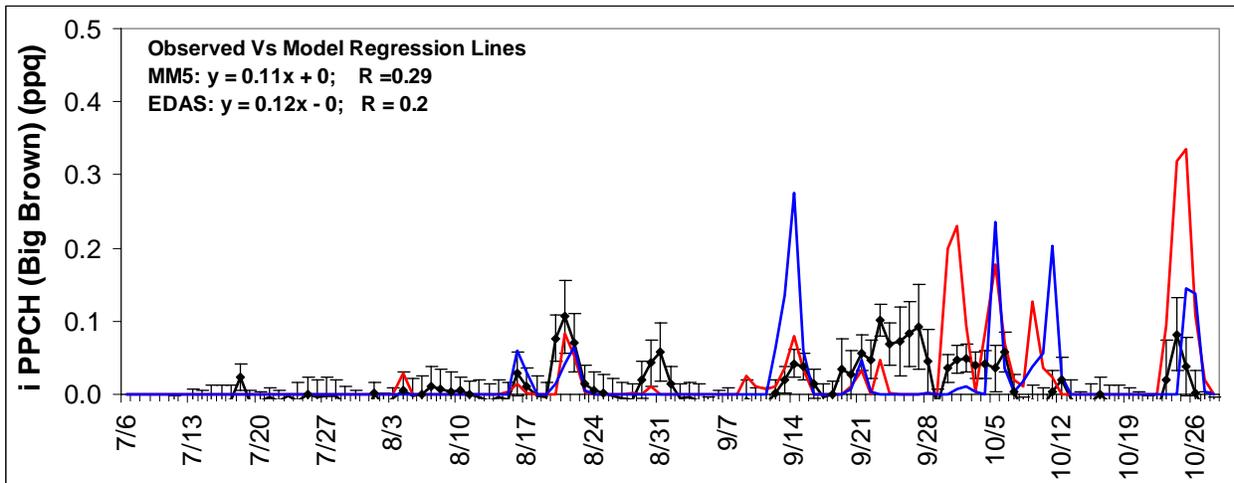
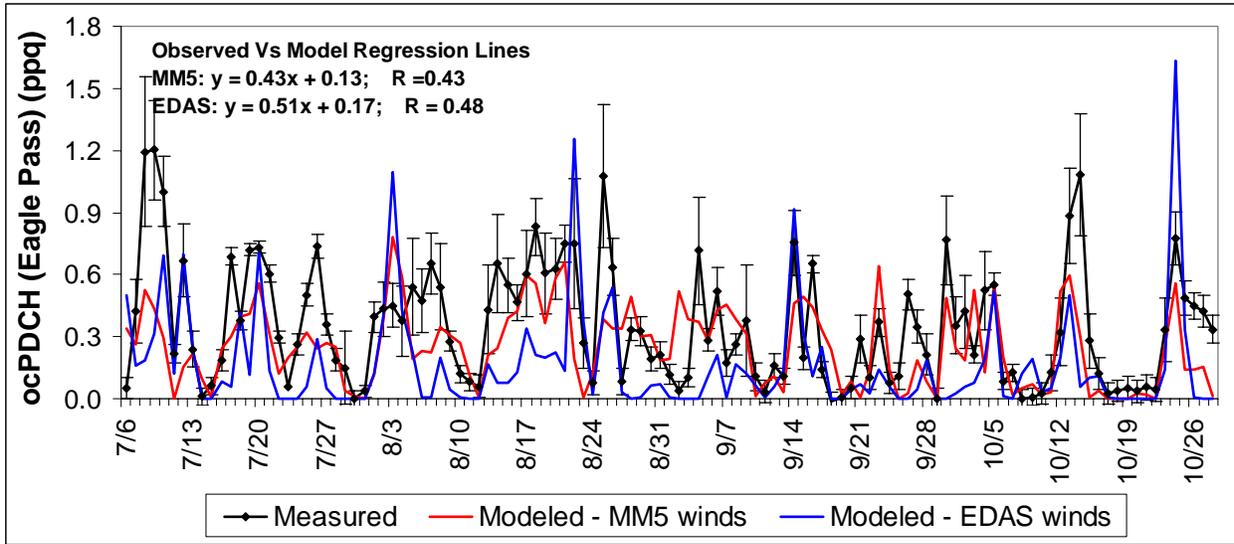


Figure 5-3. Comparison of observed and CMC modeled tracer data in southwest Texas. The observed and modeled tracer data were averaged over the six 6-hour monitoring sites: San Vicente, K-Bar, Persimmon Gap, Marathon, Fort Stockton, and Monahans Sandhills. The measured data include error bars.

Table 5-7. The CMC model performance statistics for the simulation of tracer average over the three Big Bend sites (San Vicente, K-Bar and Persimmon Gap). The modeled and observed statistics used the same days.

	MM5 Wind Fields Average Over Big Bend Sites (K-Bar, Persimmon Gap, San Vicente)												
	#	Average (ppq)		Bias Model/Obs	Std Dev (ppq)		Coef. of Variation		RMS Error		Correlation Line (ppq)		
		Obs	Model		Obs	Model	Obs	Model	Abs.(ppq)	Relative	r	Intercept	slope
Eagle Pass (ocPDCH)	109	0.24	0.21	0.89	0.28	0.29	1.12	1.4	0.29	1.23	0.44*	0.13	0.43
San Antonio (PDCB)	40	0.46	0.58	1.26	0.79	1.12	1.8	2.0	1.1	2.4	0.36	0.28	0.27
Parish (IPTCH)	40	0.057	0.025	0.44	0.08	0.05	1.4	1.8	0.072	1.26	0.51*	0.03	0.75
Big Brown (iPPCH)	109	0.001	0.021	16.90	0.03	0.07	30.0	3.3	0.07	54.76	0.29*	0.00	0.11

	EDAS Wind Fields Average Over Big Bend Sites (K-Bar, Persimmon Gap, San Vicente)												
	#	Average(ppq)		Bias Model/Obs	Std Dev (ppq)		Coef. of Variation		RMS Error		Correlation Line (ppq)		
		Obs	Model		Obs	Model	Obs	Model	Abs.(ppq)	Relative	r	Intercept	slope
Eagle Pass (ocPDCH)	109	0.24	0.11	0.47	0.28	0.26	1.12	2.5	0.30	1.22	0.53*	0.17	0.51
San Antonio (PDCB)	40	0.46	0.4	0.87	0.79	0.82	1.8	2.1	0.63	1.4	0.69*	0.19	0.66
Parish (IPTCH)	40	0.057	0.024	0.42	0.08	0.05	1.4	2.0	0.074	1.3	0.49*	0.03	0.80
Big Brown (iPPCH)	109	0.001	0.012	9.77	0.03	0.04	30.0	3.3	0.05	37.20	0.20	0.00	0.12

*Significant at the 1% level.

Table 5-8. The CMC model performance statistics for the simulation of tracer average over the six 6-hour tracer sites: San Vicente, K-Bar, Persimmon Gap, Marathon, Fort Stockton and Monahans Sandhills. The modeled and observed statistics used the same days.

	MM5 Wind Fields Average Over All 6-hour Tracer Sites												
	#	Average (ppq)		Bias Model/Obs	Std Dev (ppq)		Coef. of Variation		RMS Error		Correlation Line (ppq)		
		Obs	Model		Obs	Model	Obs	Model	Abs.(ppq)	Relative	r	Intercept	slope
Eagle Pass (ocPDCH)	111	0.37	0.26	0.7	0.29	0.19	0.78	0.74	0.27	0.73	0.54*	0.13	0.85
San Antonio (PDCB)	41	0.43	0.56	1.28	0.67	1.01	1.6	1.8	0.94	2.2	0.41*	0.27	0.28
Parish (IPTCH)	41	0.063	0.023	0.37	0.06	0.04	1.0	1.9	0.064	1.05	0.55*	0.04	0.81
Big Brown (iPPCH)	111	0.004	0.021	4.86	0.03	0.06	7.5	2.9	0.06	12.88	0.38*	0.00	0.21

	EDAS Wind Fields Average Over All 6-hour Tracer Sites												
	#	Average(ppq)		Bias Model/Obs	Std Dev (ppq)		Coef. of Variation		RMS Error		Correlation Line (ppq)		
		Obs	Model		Obs	Model	Obs	Model	Abs.(ppq)	Relative	r	Intercept	slope
Eagle Pass (ocPDCH)	111	0.37	0.17	0.46	0.29	0.26	0.78	1.6	0.34	0.95	0.46*	0.26	0.51
San Antonio (PDCB)	41	0.43	0.36	0.84	0.67	0.71	1.6	2.0	0.55	1.28	0.69*	0.20	0.63
Parish (IPTCH)	41	0.063	0.021	0.33	0.06	0.04	1.0	2.1	0.07	1.1	0.51*	0.04	0.74
Big Brown	111	0.004	0.015	3.45	0.03	0.04	7.5	2.7	0.05	11.88	0.17	0.00	0.12

*Significant at the 1% level.

The tracer released from the Parish site also had the largest impacts at Big Bend in the first half of October. Both EDAS/FNL and MM5 simulations reproduced these impacts and simulated the tracer with about equal skill, underestimating the average concentration by about a factor of 2 and correlation coefficients of ~ 0.5 . The large underestimation was primarily due to the simulations missing the tracer impacts in September and late October when the measured tracer was low. Also, the largest measured tracer concentration on October 12, 1999, was not reproduced in either simulation (Figure 5-2). The RMS error for the Parish tracer simulation was about 130% for both wind fields (Table 5-7).

The simulations compared to the measured tracer concentrations averaged over all 6 sites did not appreciably improve the model comparison statistics for the San Antonio tracer, with the RMS error decreasing by only $\sim 10\%$. However, the RMS error for the Parish tracer simulations decreased by more than 20% (Tables 5-8 and 5-9) from $\sim 130\%$ to $\sim 110\%$ for both simulations.

The Big Brown power plant is about 750 km from Big Bend located in northeastern Texas. The tracer released from this plant was only occasionally measured above the background concentrations at Big Bend, leading to poor quality tracer data. Both model runs were able to closely reproduce the timing and magnitudes of the August 15–24 Big Brown tracer episode; however, overall, the model simulation did not compare well with the observed concentration. It is not known whether this poor correspondence is due to errors in the measurements or the model simulations.

These modeling performance statistics were also calculated for each monitoring site. In nearly all cases, the simulation compared better to the spatially aggregated tracer concentrations than to the individual sites. This was expected, due to the large spatial heterogeneity in the measured tracer data.

5.3 REMSAD Simulation of Tracer Data

The REMSAD regional air quality model was used to simulate the transport and dispersion of the four inert tracers. The configuration of REMSAD for the tracer simulation was similar to the base emissions simulation, except that 1) the chemistry mechanism was not invoked, since the tracer did not undergo chemical transformation, 2) loss via depositional settling was not considered, since it was assumed that the tracers have very low deposition velocities, and 3) background concentrations were set to zero. Horizontal winds, temperature, and other meteorological fields were simulated by MM5.

Each of the four tracer releases was treated as a point source emission within REMSAD. REMSAD simulates the initial plume rise of an elevated point source. Two of the tracers – PPCH at the Big Brown power plant and 1PTCH at the Parish power plant – were released inside a plant stack and hence were lofted higher into the boundary layer due to buoyant and momentum plume rise. Plume rise can affect the subsequent transport of the tracer, as the transport can depend on the initial elevation of its release.

5.3.1 Results of the REMSAD Tracer Simulation

The performance of the REMSAD tracer simulation was evaluated by comparing the predicted tracer time series at the three Big Bend NP monitors with the observed tracer time series. Results for the Eagle Pass and northeast Texas tracers are shown for the entire four month BRAVO period, while results for the San Antonio and Parish tracers are shown for the last six weeks of the BRAVO period when the tracers were released from these sites. Observed and

predicted tracer time series plots are shown in Figure 5-4, and model performance statistics are shown in Table 5.9.

The Eagle Pass tracer (Figure 5-4) was designed to be a surrogate for the Carbón I/II power plants. Measured concentrations generally range between 0 and 1 ppq during the four month BRAVO period, except for a peak concentration of 1.6 ppq measured on August 25. Episodes of elevated concentration of the Eagle Pass tracer observed at Big Bend NP are generally well replicated by REMSAD, although the average predicted value of 0.5 ppq was about twice the observed value of 0.24 ppq, and from mid-August through September there is a clear tendency for REMSAD to over-predict tracer concentrations. The RMS error is 200% and the correlation coefficient is 0.46. One notable aspect of the Eagle Pass tracer is that the region between the tracer release and Big Bend NP is dominated by complex terrain, and is likely to be more difficult to simulate than the other three tracers.

The northeast Texas tracer (Figure 5-4), released from the Big Brown power plant, was measured in very low concentrations at the Big Bend NP monitors. The average observed tracer concentration during the four month study was only 0.003 ppq; this is nominally above the lower detection limit of the analytical method. The time series and performance statistics for the northeast Texas tracer are presented for completeness, but should be regarded with caution given the difficulties in quantifying the tracer concentration. Both the observed and predicted time series show concentrations ranging between 0 and 0.2 ppq, with REMSAD typically overestimating the peak concentration.

The time series of the predicted and observed San Antonio tracer (Figure 5-4) indicate that REMSAD is generally able to reproduce the timing of the observed tracer peaks; however, the simulated tracer is too low during the two episodes that occur during the first two weeks of October. This is especially true on October 5, when a peak value of 4.5 ppq was observed as compared to a predicted concentration of only about 1.5 ppq. Average observed and predicted concentrations of the San Antonio tracer are 0.46 ppq and 0.51 ppq, respectively. The normalized RMSE is 1.56 and the correlation coefficient is 0.53.

Similar to the San Antonio tracer, the Parish tracer (Figure 5-4) shows elevated concentrations during the first two weeks of October. The simulated tracer concentration is also highest during this period, but peak concentrations are under-predicted. Average observed and predicted concentrations of the Parish tracer are 0.057 ppq and 0.034 ppq, respectively. The normalized RMSE is 1.27 and the correlation coefficient is 0.41.

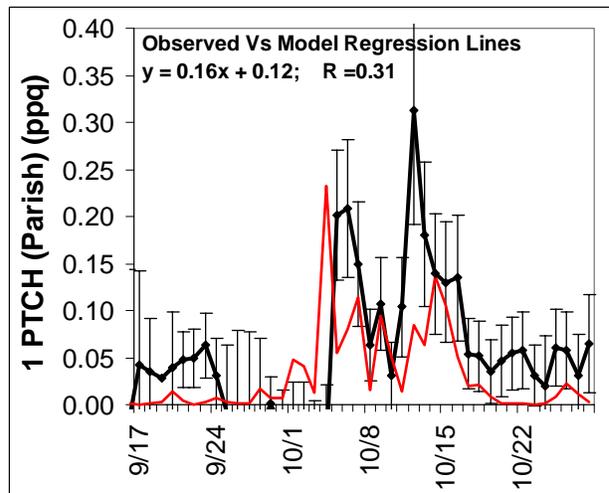
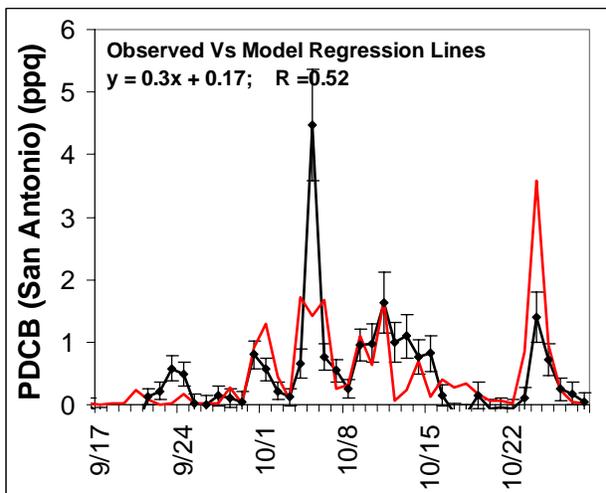
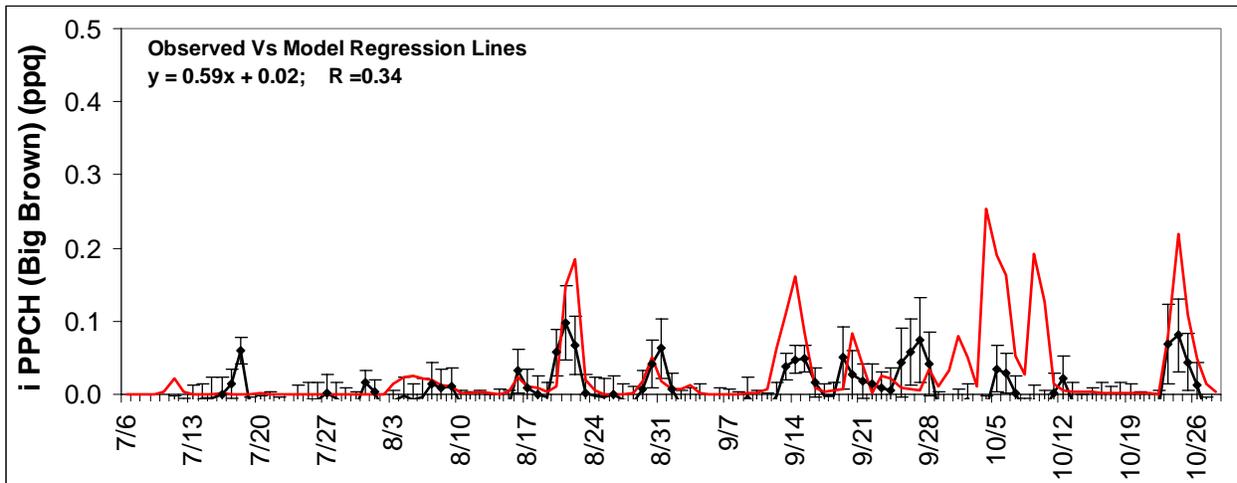
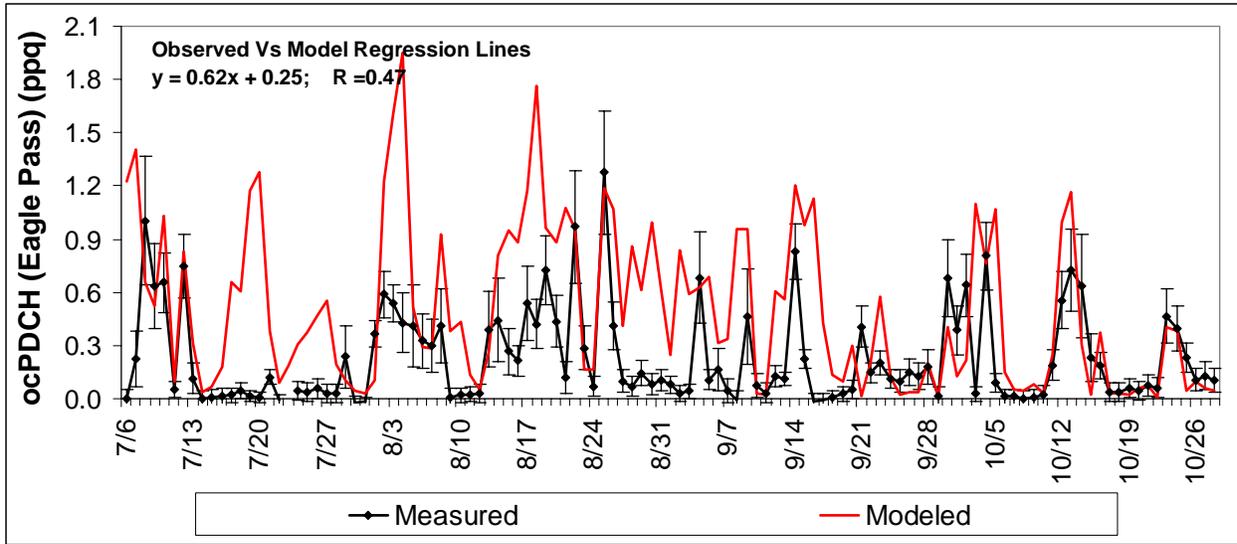


Figure 5-4. Observed and REMSAD predicted tracer mixing ratios for the a) Eagle Pass tracer, b) northeast Texas tracer, c) San Antonio tracer, and d) tracer released from Parish power plant in Houston.

Table 5-9. The REMSAD model performance statistics for the simulation of tracer average over the three Big Bend sites (San Vicente, K-Bar, and Persimmon Gap). The modeled and observed statistics used the same days.

	REMSAD Over Big Bend Sites (K-Bar, Persimmon Gap, San Vicente)												
		Average (ppq)		Bias	Std Dev (ppq)		Coef. of Variation		RMS Error		Correlation Line (ppq)		
	#	Obs	Model	Model/Obs	Obs	Model	Obs	Model	Abs.(ppq)	Relative	r	Intercept	slope
Eagle Pass (ocPDCH)	109	0.24	0.5	2.1	0.27	0.45	1.12	0.89	0.48	2	0.46	0.25	0.62
San Antonio (PDCB)	40	0.46	0.51	1.1	0.83	0.71	1.8	1.4	0.72	1.56	0.53	0.17	0.30
Parish (IPTCH)	40	0.057	0.034	0.6	0.078	0.049	1.37	1.43	0.072	1.27	0.41	0.02	0.16
Big Brown (iPPCH)	109	0.003	0.025	8.43	0.03	0.04	8.61	1.79	0.05	16.38	0.34	0.02	0.59

5.4 Discussion

The primary purpose of this analysis was to evaluate the ability of the CMC and REMSAD models driven by the MM5 wind fields for simulating medium- to long-range transport, and whether or not the CMC model was suitable for air mass history analyses, and, in addition, to determine if there was a difference between the CMC model being driven by the MM5 or EDAS/FNL wind fields and the differences between REMSAD and CMC models driven by the same MM5 winds.

The demand on a model's dispersion for air mass history analysis is lower than for source apportionment. Air mass history analyses rely on only the model properly reproducing the direction and timing or speed of transport from the source to the receptor. The fact that the CMC model reproduced the timing of the tracer impacts to the vicinity of Big Bend supports the use of this model in air mass history analyses. This corroborates the results found in chapter 4 and section 8.1.3.2, where air mass histories, via residence time analysis, were able to identify a transport pathway from the tracer release site to Big Bend when aggregated over the 20 days with highest measured tracer concentrations at Big Bend. The trajectory analysis also showed that on a given day, the air mass history envelope could miss the tracer release site when elevated tracer concentrations were measured at Big Bend. This is also seen in these results where simulated tracer concentrations could be shifted in time compared to the measured tracer at Big Bend. Therefore, errors in the transport could be reduced by averaging over multiple days as was done in the residence time analysis.

Properly simulating dispersion for source apportionment requires not only simulating the transport direction and speed, but also the horizontal and vertical dilution of the plume. The skill of the models to simulate the day to day variability and magnitude of the tracer was assessed via a number of model performance statistics. Depending on the model/wind field combination and the aggregation region the model bias was between 0.33 and 2.1, the RMS error between 73% and 240%, and correlation coefficient between 0.36 and 0.69 (Table 5-10). As previously discussed, there is a limit in the skill of the models, or inherent uncertainty, due to their inability to capture sub-resolution spatial variability and errors in the measured tracer data. Comparing the simulation performance statistics to this inherent uncertainty in the simulation (Table 5-11) it is seen that the Eagle Pass and San Antonio tracers are all within this uncertainty. Therefore the simulations for these two tracers are valid within the model resolution and measured tracer uncertainty.

On the other hand, the simulations systematically underestimated the Parish tracer by a factor of 2 and the correlation coefficients were all below the correlations between the measured sites (Tables 5-10 and 5-11). Therefore these models do underestimate the contribution from the Parish power plant. This underestimation could be due to model error or an underestimation in the PTCH background concentrations subtracted from the measured data. The RMS errors for the Parish tracer simulations are below the largest RMS differences between the three Big Bend receptor sites, indicating the overall error is within the inherent error of the model/data comparison.

The fact that the RMS errors for all three tracers are within the inherent error of this analysis does not conclusively validate the models and meteorological drivers, but does provide an upper bound to its uncertainty. The assessment also addressed only the dispersion component

of the models. Add to this the uncertainty in the emission and physical/chemical processes and the errors in the source attribution results will be larger.

The models are primarily being used to simulate sulfate aerosol which was shown to be spatially homogeneous within the resolution of the models. This spatial homogeneity is primarily due to sulfate being a long-lived aerosol species, on the order of 3–5 days [Husar and Husar, 1978] and resulting from many sources distributed over broad and distant regions. The long residence time allows the aerosol to be transported over thousands of kilometers and mixed with other sources. As would be expected, REMSAD has significantly better performance statistics compared to measured sulfate than the tracer data (see chapter 6). However, this improvement is likely due to compensating errors in transport between one source/source region and another and the improved sulfate simulation performance statistics do not translate into improved source attribution results.

Table 5-10. The range of tracer simulation performance statistics over all model wind field pairs and aggregation regions in Tables 5-7 to 5-9.

	Bias	Relative RMS Error (%)	r
Eagle Pass (ocPDCH)	0.46 – 2.1	73 – 200	0.44 – 0.54
San Antonio (PDCB)	0.63 – 1.3	128 – 240	0.36 – 0.69
Parish (1PTCH)	0.33 – 0.6	105 – 130	0.41 – 0.55
All three tracers	0.33 – 2.1	73 – 240	0.36 – 0.69

Table 5-11. The range of comparisons between the measured tracer concentrations from the three Big Bend monitoring sites in Tables 5-3 to 5-5. These statistics are a measure of the inherent uncertainty due to the model resolution and measured tracer data errors.

	Ratio of averages	Relative RMS Difference (%)	r
Eagle Pass (ocPDCH)	0.31 – 3.2	97 – 420	0.37 – 0.81
San Antonio (PDCB)	0.54 – 1.9	44 – 230	0.58 – 0.9
Parish (1PTCH)	0.77 – 1.3	72 – 150	0.72 – 0.77
All three tracers	0.31 – 1.9	44 – 420	0.37 – 0.9

This analysis also provided the opportunity to contrast the differences between Eulerian and Lagrangian dispersion techniques and the two meteorological fields. The influence of the MM5 and EDAS/FNL wind fields on the simulation can be examined by comparing the two CMC modeling results. The MM5 wind field proved superior to the EDAS/FNL winds for the Eagle Pass tracer. This was most evident when the simulations were compared to the average over all six receptor sites. However, the EDAS/FNL simulation was superior to the MM5 simulation for the San Antonio tracer, and both wind fields produced similar results for the Parish tracer released from Houston. The CMC-EDAS simulation of the San Antonio tracer had the highest correlation coefficient of 0.69 in this study. The Eagle Pass site was the closest release site to Big Bend, so it appears that the higher resolution MM5 winds were better able to simulate the more near field transport, but the two wind fields are about equal or the EDAS/FNL superior for more distant mesoscale transport. Overall, these results indicate that the routinely available EDAS wind fields are comparable to the MM5 36 km winds which were generated for the BRAVO study for simulating tracer transport in Texas.

The similarity of the tracer simulation using the two wind fields is a bit surprising. In comparison of the air mass history models and wind fields (chapter 4) and the evaluation of air mass transport to Big Bend (section 8.1.3), the EDAS/FNL wind fields tended to show more transport from northeast Texas than MM5. Unfortunately, the tracer released from the Big Brown power plant in northeast Texas was at such a low rate that the concentrations were often near the background and transport from this region using the tracer was difficult to assess. In addition, no tracer was released from Big Brown from October 8–16. This was a period of transport from northeast Texas and we may have been able to better resolve the question of which wind field properly simulated transport from northeast Texas had these data been available.

The Eulerian REMSAD model and Lagrangian CMC model were both driven by the MM5 wind fields. The simulation of the tracer data by these two dispersion mechanisms produced no clear cut differences. The CMC model better simulated the Eagle Pass tracer data with a smaller bias and RMS error. However, the REMSAD simulations had the lowest RMS error and bias for both the San Antonio and Parish tracer simulations (Table 5-12).

Table 5-12. Comparison of the REMSAD and CMC model performance statistics for the simulation of tracer average over the three Big Bend sites (San Vicente, K-Bar, and Persimmon Gap). The modeled and observed statistics used the same days. The bias and RMS relative error are ratios; therefore, they are dimensionless.

	MM5 Wind Fields Average Over Big Bend Sites (K-Bar, Persimmon Gap, San Vicente)						
	#	Bias (Model/Obs)		RMS Relative Error		Correlation (r)	
		CMC	REMSAD	CMC	REMSAD	CMC	REMSAD
Eagle Pass (ocPDCH)	109	0.89	2.1	1.23	2	0.44	0.46
San Antonio (PDCB)	43	1.26	1.1	2.4	1.56	0.36	0.53
Parish (IPTCH)	43	0.44	0.6	1.26	1.27	0.51	0.41
Big Brown (iPPCH)	109	16.90	8.43	54.76	16.38	0.29	0.34