Appendix 8-4: Big Bend Model Performance Analysis

(Excerpt of Chapter 4 from Regional Haze Modeling Support Final Report for Texas Commission on Environmental Quality by ENVIRON, August 31, 2007)

4. BIG BEND MODEL PERFORMANCE ANALYSIS

An area of concern in the CENRAP model simulations has been the significant under-predictions in visibility impairment (reconstructed extinction) on most of the worst 20 percent days in 2002 at Big Bend National Park and, to a lesser extent, at Guadalupe Mountains. This section includes a more detailed examination of model performance at Big Bend and examines the possible reasons for the under-predictions.

MODEL PERFORMANCE AT CLASS I AREAS

CENRAP conducted numerous 2002 CMAQ and CAMx base case simulations and model performance evaluations. The results for the 2002 Base F CMAQ base case simulation were obtained from the CENRAP modeling website at:

http://pah.cert.ucr.edu/aqm/cenrap/cmaq.shtml#cmaq_typ02f_mpe.

Figure 4-1 displays the annual time series of the predicted concentrations and concentrations observed at the IMPROVE monitoring site at Big Bend for each of the six visibility-impairing PM species (SO4, NO3, EC, OC, Soil, and CM). Since IMPROVE measurements consist of daily average concentrations collected every third day, only dates with observed values are plotted in this figure. Key features of these results include:

- Sulfate (SO4) was systematically under predicted in spring and summer. Model performance was slightly better during the remainder of the year.
- EC (elemental carbon) time series are similar in many respects to those for SO4 with a generally similar seasonal pattern of under predictions, suggesting that coal combustion is likely a major contributor of EC at Big Bend.
- Nitrate (NO3) was under estimated during the warm weather months of April to October. High NO3 winter episodes predicted by the model were not reflected in the IMPROVE data.
- OC (organic carbon) was slightly over estimated except in early May when the model failed to simulate the observed OC peaks. Factors associated with this early May event were not explored further in this analysis.
- CM (coarse matter) was consistently under predicted. The soil component is also generally under predicted although to a lesser degree. This bias is believed to be the result of underestimation of dust emissions.

On average over the 20% of days in 2002 with the greatest light extinction, IMPROVE observations show that SO4 is the dominant contributor to visibility impairment at Big Bend and plays a major rule in visibility impairment at Guadalupe Mountains (Figure 4-2). Coarse mass is a major contributor to extinction at both sites but contributes twice as much at Guadalupe Mountains as at Big Bend, thereby reducing the relative importance of SO4 somewhat at Guadalupe. Thus, model under predictions of both SO4 and CM noted above contribute most of the under prediction of total extinction at these two sites. Of particular importance is the under prediction of SO4 as this has significant implications for the design of appropriate control strategies for inclusion in the Regional Haze SIP.

Figure 4-3 displays a stacked bar chart of the six PM species' contributions to extinction at Big Bend (BIBE1) on the dates with the 20 % highest observed extinction in 2002, based on the old IMPROVE algorithm for computing extinction (Malm et al., 2000). For each date, the left bar represents the contribution from observed components and the right bar shows the modeled contributions. Table 4-1 lists the calendar dates corresponding to the Julian dates shown in this figure. Extinction was under predicted on all dates except November 25 – the only date where the model predicted higher than the observed extinction. As noted above, SO4 was the dominant contributor to extinction on most dates and is therefore the main focus of this analysis; CM was the largest contributor on the other four dates (March 12, March 30, April 2, and June 16). The model underestimated SO4 and CM on all dates, thus resulting in underestimated total extinction. The predicted OC contributions were reasonable, but were too low in early May, as noted above. Nitrates were under predicted on most dates except November 25; however, its contribution to the observed extinction was usually relatively small.

Table 4-1. Dates in 2002 corresponding to worst 20% observed light extinction at Big Bend and Guadalupe Mountains.

Julian Day	Date	Worst 20% at	
		Big Bend	Guadalupe
29	Jan 29	X	
71	Mar 12	X	
74	Mar 15		X
83	Mar 24		X
89	Mar 30	X	
92	Apr 02	X	X
95	Apr 05	X	X
101	Apr 11	X	
110	Apr 20	X	
113	Apr 23	X	
116	Apr 26	X	
119	Apr 29	X	
122	May 02		X
125	May 05	X	
128	May 08	X	
131	May 11	X	X
137	May 17		X
143	May 23	X	
146	May 26		X
161	Jun 10		X
164	Jun 13		X
167	Jun 16	X	X
170	Jun 19		X
173	Jun 22		X
176	Jun 25		X
191	Jul 10	X	X
218	Aug 06	X	X
221	Aug 09	X	X
230	Aug 18	X	
242	Aug 30	X	
245	Sep 02	X	X
251	Sep 08		X
254	Sep 11	X	X
260	Sep 17		X
266	Sep 23		X
272	Sep 29		X
275	Oct 02	X	
329	Nov 25	X	X

The five dates with the worst observed extinction at Big Bend were April 5 and 29, May 11, August 9, and September 2. On each of these dates, sulfate was under predicted; the model predicted the highest sulfate and extinction on April 5, but was still under predicted. In addition, extinction on the preceding observation date (3 days back) was also categorized in the worst 20% group.

Guadalupe Mountains National Park is the closest Class I area to Big Bend. A similar stacked bar chart for Guadalupe Mountains is displayed in Figure 4-4 using its 20 % worst dates. For the first half of the year, the high extinction dates were dominated by CM, which was significantly underestimated in the model. On the summer dates, SO4 was the dominant extinction contributor. SO4 was under predicted on several of these dates, but reasonable on others, including Sept. 2 (Julian date 245), which was the date with the highest observed extinction at Big Bend.

For purposes of comparison, model performance was evaluated at 21 Class I areas within and nearby the CENRAP region for the six visibility impairing PM species, based on the dates with the 20 % highest observed extinction at each site. Tables 4-1 and 4-2 display the normalized bias and gross error, respectively, for each species contributing to extinction at the 21 Class I areas based on the CENRAP Typ02f CMAQ simulation. Site locations are plotted on the map in Figure 4-5. The performance statistics are based on the 20% dates with the highest extinction for each site. The worst performers are highlighted. Sulfate at Big Bend exhibited the worst model performance of any Class I area evaluated with normalized bias and gross error values of -59 % and 59 %, respectively. Nitrate and coarse mass were also under estimated at Big Bend with normalized bias values of -71 % and -88 %, respectively. Guadalupe Mountains had the worst normalized bias for coarse mass (-97 %) among the 21 Class I areas; its SO4 normalized bias was -50 %.

Figure 4-6 displays a map of the normalized bias for SO4 based on the worst 20 % dates at each Class I area in and near the CENRAP region. The SO4 normalized bias was negative at all sites except Mingo. The most negative normalized biases were located from Colorado to west Texas, with Big Bend being the lowest at -59 %. SO4 bias was significantly less severe at most sites located east of West Texas and north of Colorado.

Color contour maps of CMAQ predicted SO4 overlaid with color-coded diamonds showing SO4 observations made at IMPROVE monitoring sites are shown in Figure 4-7 for five days. The top two of these IMPROVE overlay plots are representative of many days in which the area of high sulfate is predicted to stay just east of Big Bend. The top right plot (August 6) shows a plume that appears to be originating from the Carbon I and II power plant near Piedras, Mexico, but is predicted to stay to the north and east of Big Bend. The bottom three plots show sulfate being transported clockwise around a surface high in the middle of the country from April 3 to 5. Since IMPROVE monitors data every third day, no observations were available on April 3 and 4. The area of high SO4 was predicted to just barely reach Big Bend and the Guadalupe Mountains by April 5, but predictions were still lower than observed values at these sites.

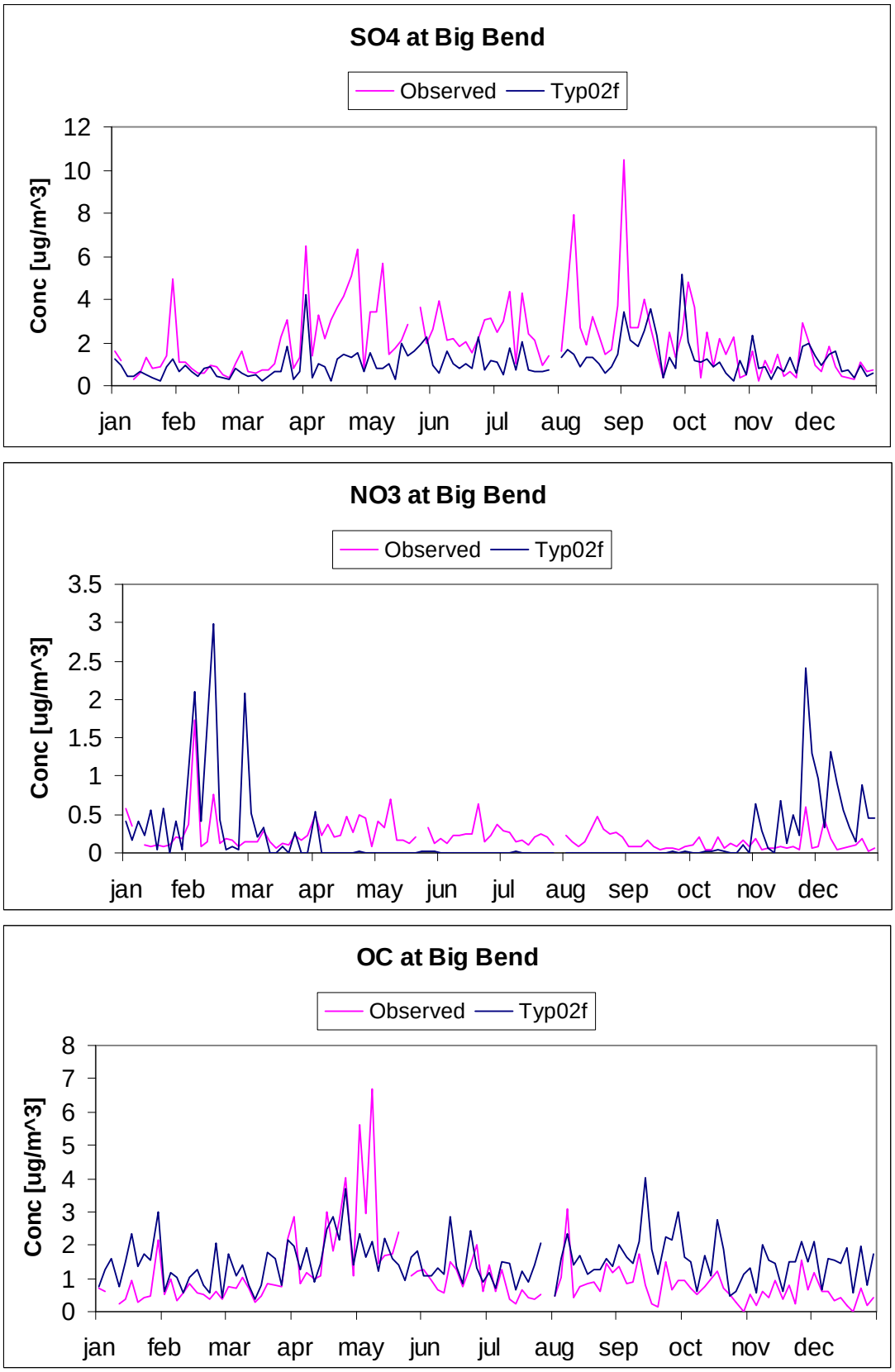
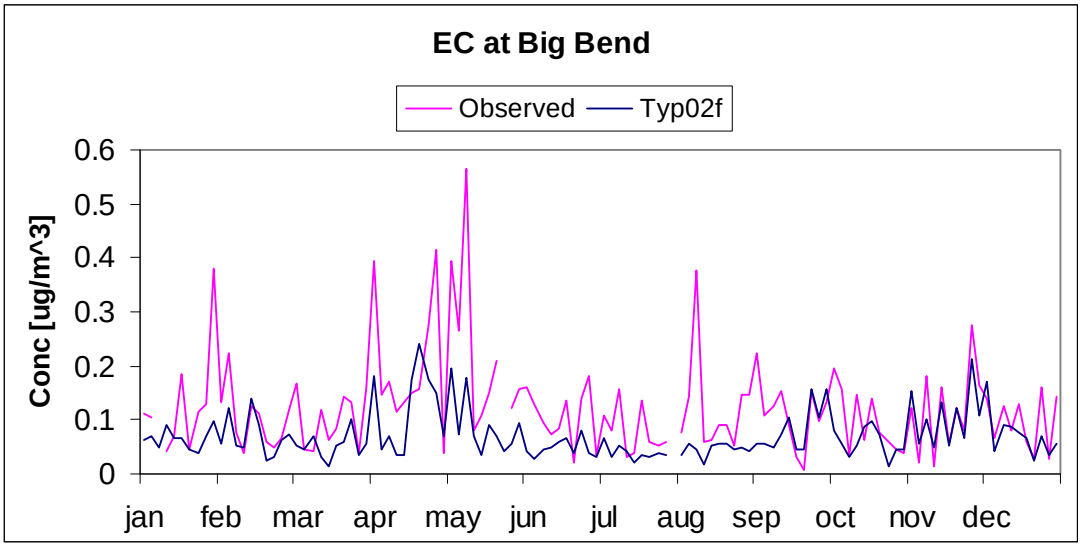
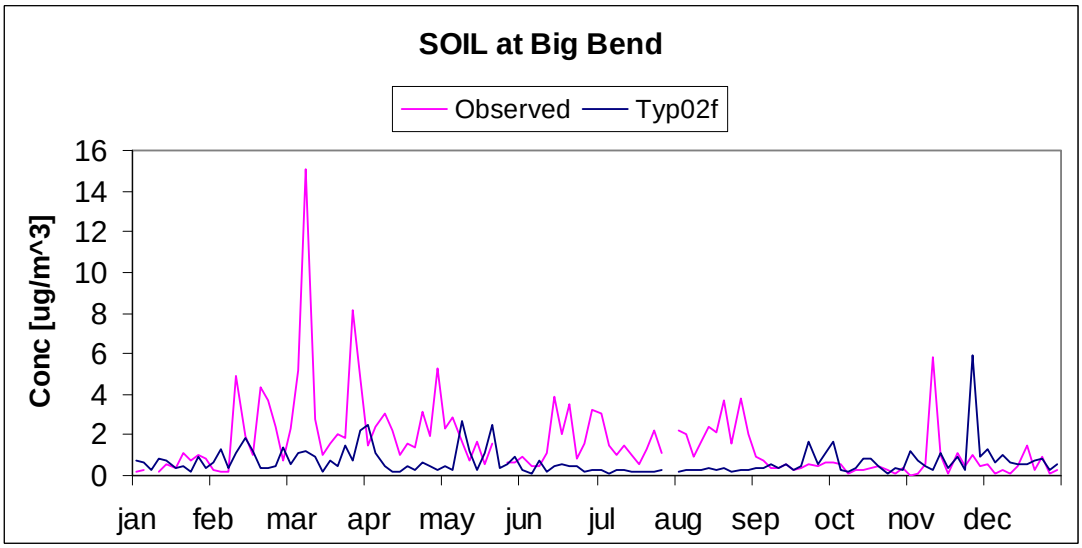


Figure 4-1. Time series of observed and predicted PM species at Big Bend.





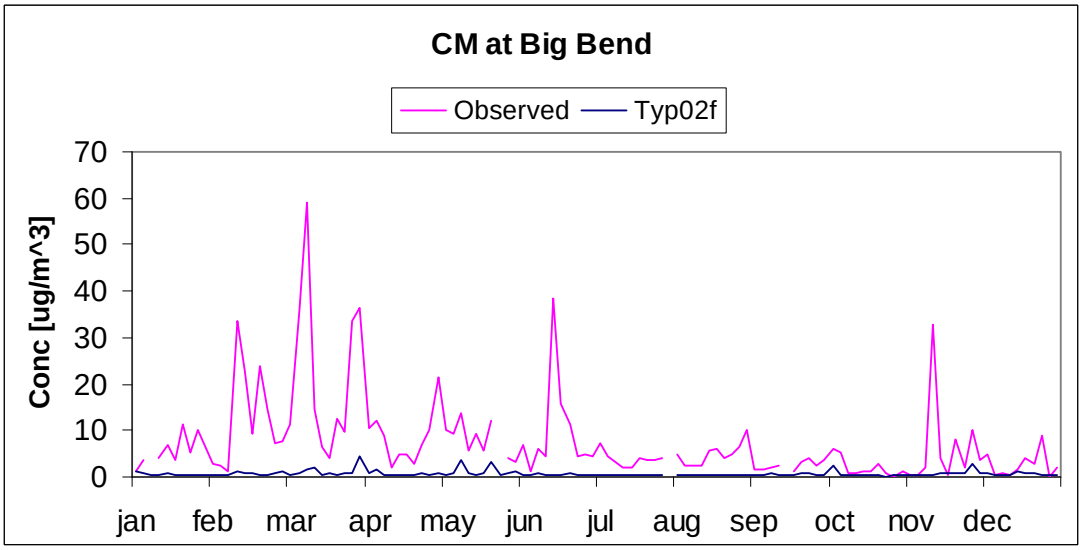
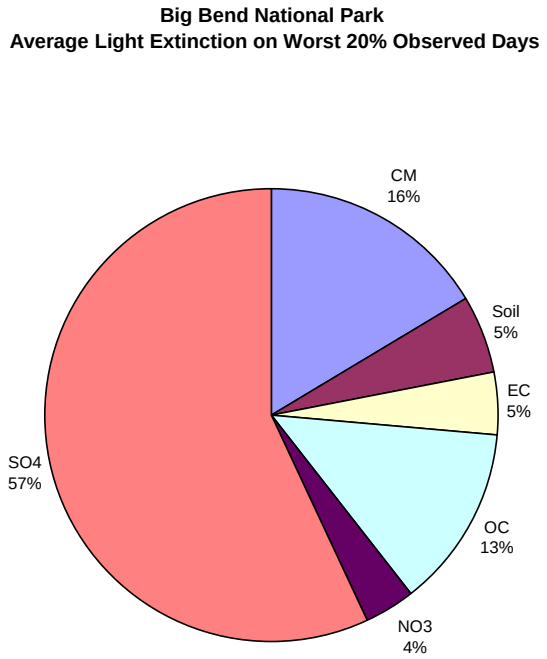


Figure 4-1. concl. Time series of observed and predicted PM species at Big Bend.



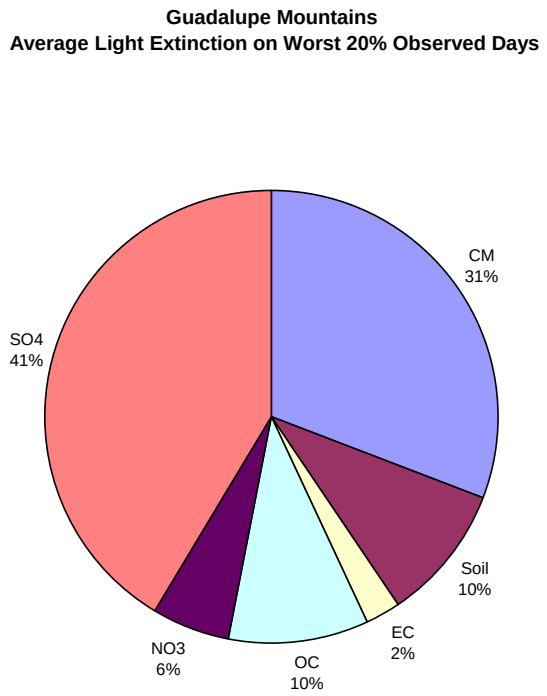


Figure 4-2. Average contributions to light extinction on worst 20% in 2002 based on IMPROVE observations at Big Bend (top) and Guadalupe Mountains (bottom).

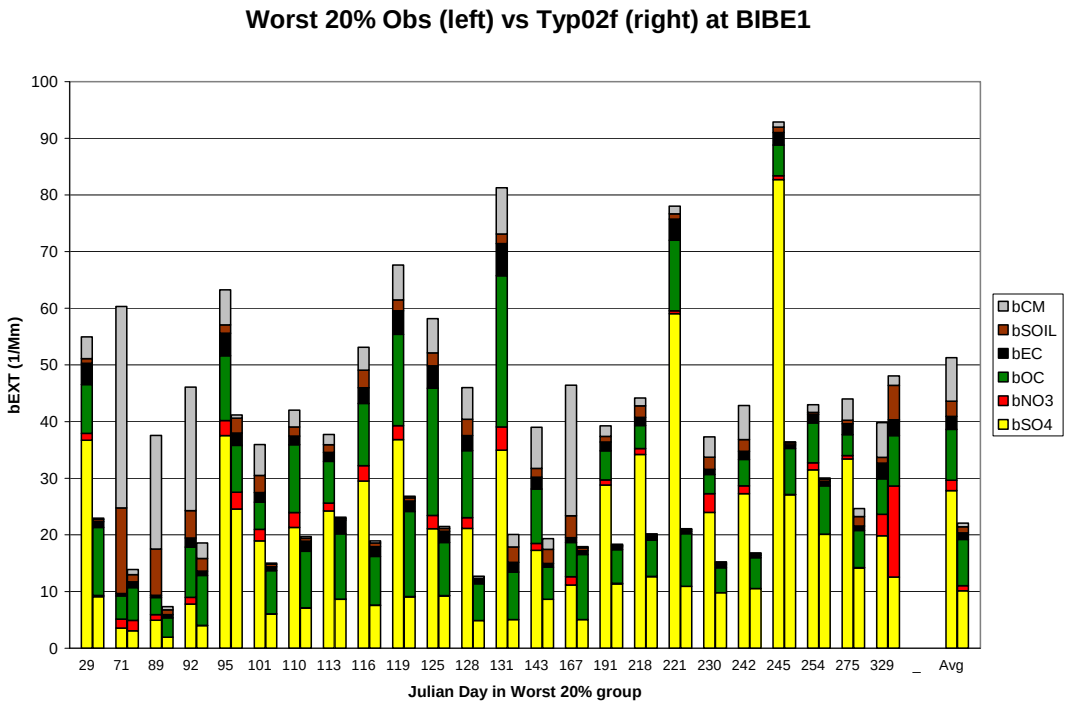


Figure 4-3. Comparison of the observed (left) and predicted (right) light extinction by PM species for the worst 20 percent days in 2002 at Big Bend National Park.

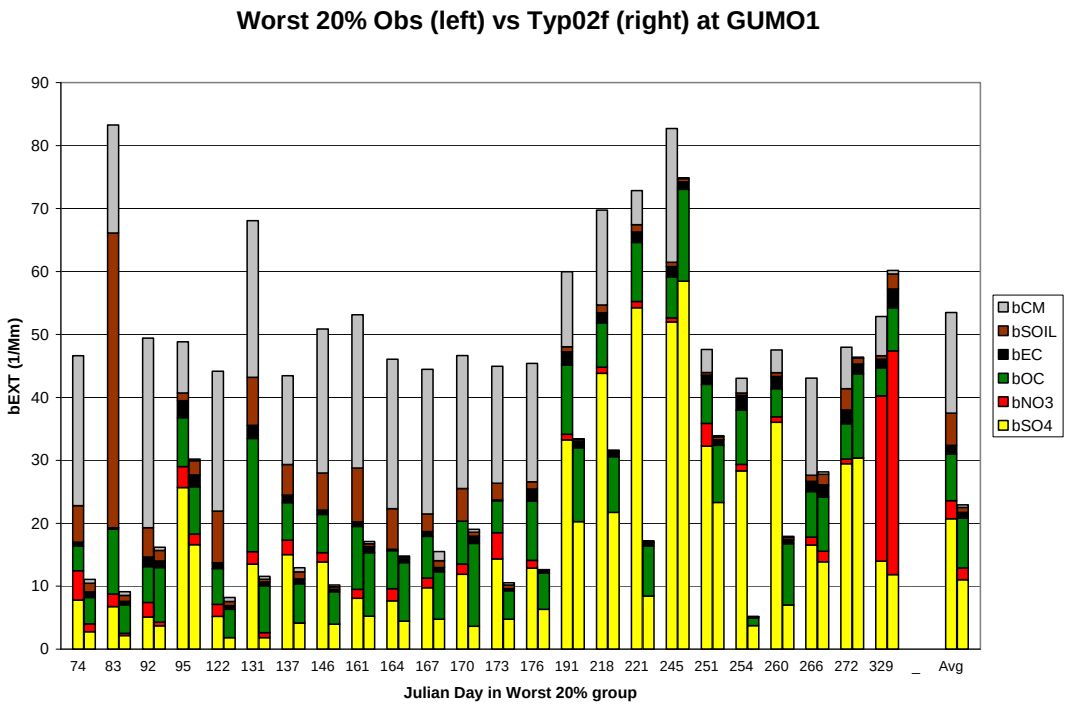


Figure 4-4. Comparison of the observed (left) and predicted (right) light extinction by PM species for the worst 20 percent days in 2002 at Guadalupe Mountains National Park.

Table 4-2. Normalized bias (fraction) at Class I areas in and near the CENRAP region.

Normalized Bias	SO4	NO3	OC	EC	SOIL	CM
BADL1	-0.40	0.18	-0.19	-0.14	0.67	-0.70
BIBE1	-0.59	-0.71	0.13	-0.35	-0.22	-0.88
BRET1	-0.42	-0.93	-0.37	-0.70	0.32	-0.96
CACR1	-0.35	0.43	0.13	-0.43	0.32	-0.84
GRSA1	-0.45	-0.16	0.13	-0.29	-0.86	-0.96
GUMO1	-0.50	-0.81	0.19	-0.03	-0.43	-0.97
HEGL1	-0.27	0.37	-0.10	-0.40	1.53	-0.67
ISLE1	-0.12	-0.34	-0.03	-0.51	1.24	-0.88
LOST1	-0.24	-0.21	-0.58	-0.45	3.42	0.22
MACA1	-0.06	-0.43	-0.32	-0.52	0.84	0.30
MING1	0.15	-0.14	0.19	-0.06	2.69	-0.71
ROMO1	-0.51	-0.79	0.01	-0.44	-0.53	-0.87
SACR1	-0.48	-0.82	0.15	-0.32	0.23	-0.70
SIPS1	-0.34	-0.19	0.10	-0.59	0.40	-0.79
THRO1	-0.25	0.70	-0.44	-0.34	0.55	-0.63
UPBU1	-0.32	-0.07	0.03	-0.18	0.24	-0.94
VOYA2	-0.07	0.07	0.01	-0.28	2.25	-0.68
WHIT1	-0.48	-0.57	0.24	-0.02	-0.49	-0.93
WHPE1	-0.31	-0.64	1.06	0.23	-0.61	-0.85
WICA1	-0.36	0.00	-0.08	-0.31	0.42	-0.78
WIMO1	-0.31	0.23	-0.20	-0.24	2.76	-0.42

Table 4-3. Normalized gross error (fraction) at Class I areas in and near the CENRAP region.

Normalized Error	SO4	NO3	OC	EC	SOIL	CM
BADL1	0.43	1.30	0.37	0.42	0.85	0.71
BIBE1	0.59	0.99	0.39	0.57	0.95	0.88
BRET1	0.54	0.93	0.52	0.70	1.29	0.96
CACR1	0.37	1.03	0.36	0.45	1.02	0.85
GRSA1	0.46	0.91	0.51	0.54	0.86	0.96
GUMO1	0.51	0.87	0.44	0.65	0.85	0.97
HEGL1	0.30	0.92	0.27	0.40	1.72	0.67
ISLE1	0.34	0.61	0.32	0.55	1.53	0.88
LOST1	0.40	0.54	0.61	0.45	3.55	0.84
MACA1	0.36	0.68	0.33	0.52	1.17	1.24
MING1	0.45	0.80	0.56	0.40	2.89	0.71
ROMO1	0.52	0.79	0.41	0.47	0.99	0.94
SACR1	0.54	0.82	0.34	0.41	1.12	0.96
SIPS1	0.41	0.77	0.47	0.59	0.75	0.79
THRO1	0.38	1.15	0.52	0.37	0.86	0.71
UPBU1	0.34	1.01	0.29	0.66	0.71	0.94
VOYA2	0.43	0.71	0.40	0.35	2.45	0.80
WHIT1	0.48	0.82	0.48	0.84	0.62	0.93
WHPE1	0.44	0.74	1.25	0.90	0.80	0.93
WICA1	0.40	1.00	0.47	0.44	0.86	0.78
WIMO1	0.35	0.99	0.29	0.42	2.76	0.80

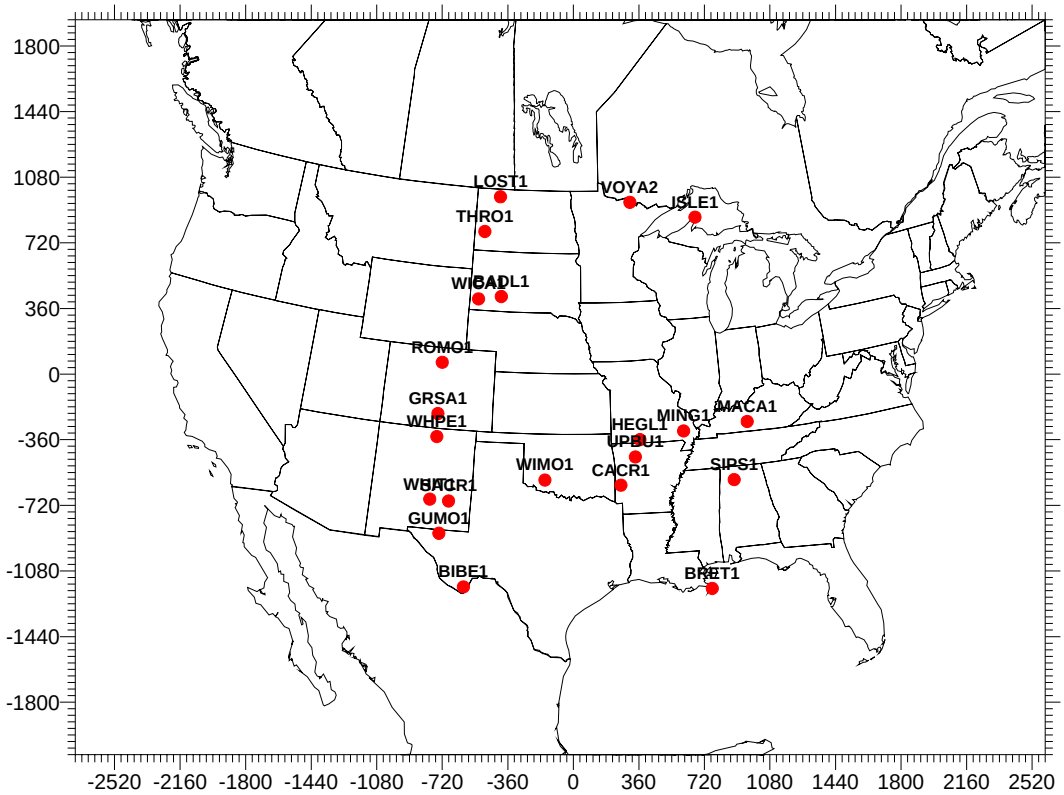


Figure 4-5. Map of Class I areas evaluated.

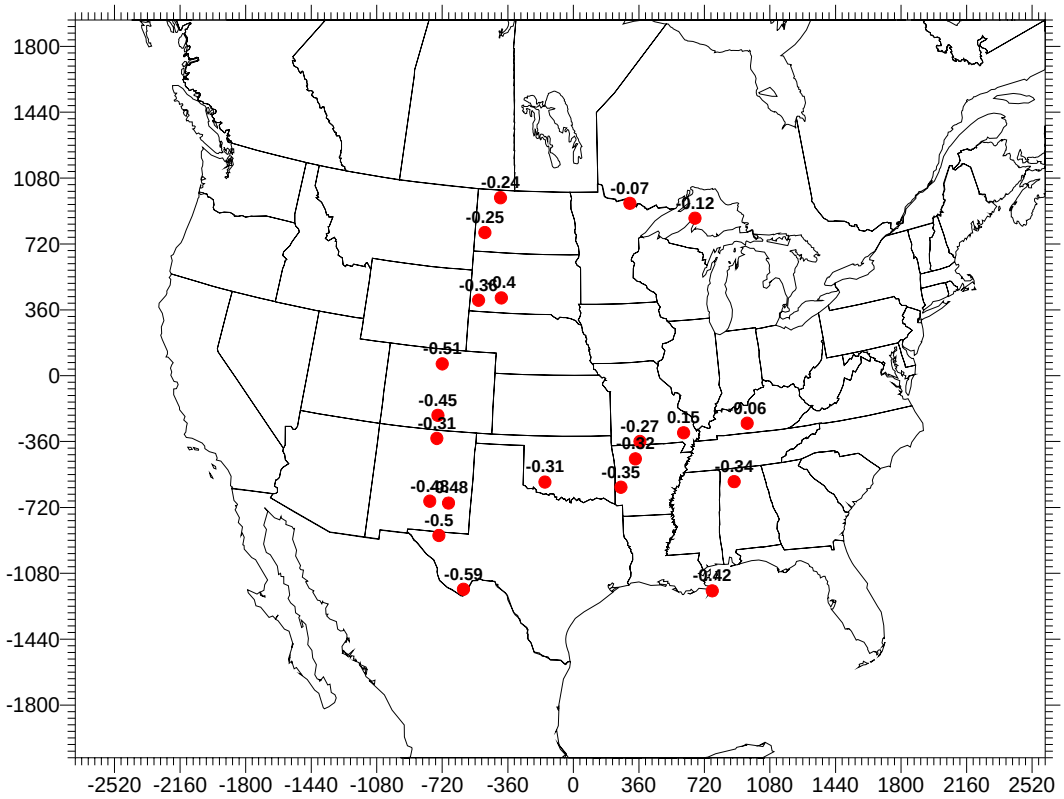


Figure 4-6. SO4 normalized bias (fraction) at Class I areas.

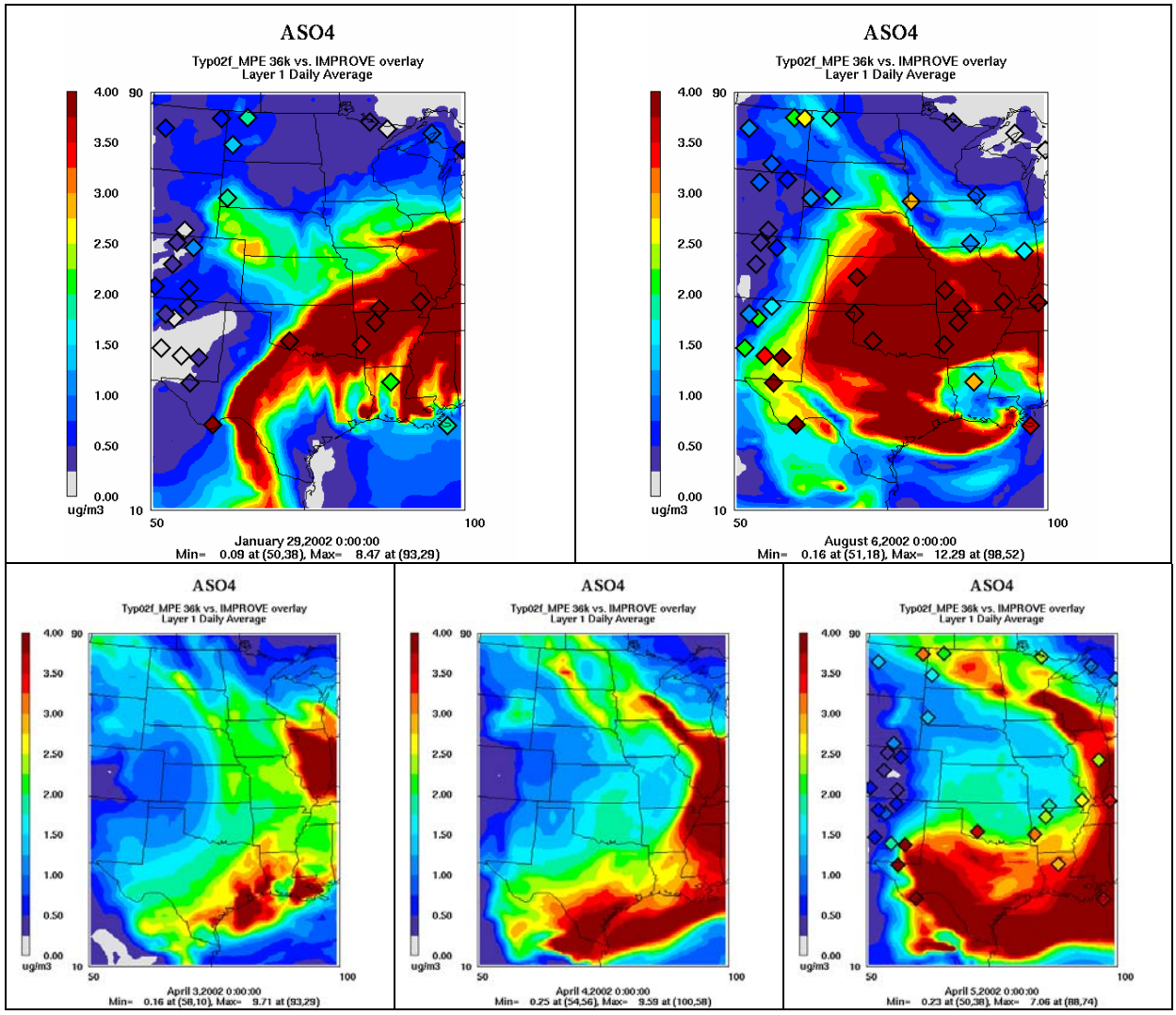


Figure 4-7. Spatial plots of predicted SO4 with color-coded observed values in diamonds on select dates in 2002.

REVIEW OF METEOROLOGICAL AND EMISSIONS DATA

Residence time plots, weather maps, back trajectories, and emission summaries were examined in an attempt to explain the SO4 under predictions at Big Bend noted above.

Synoptic Weather Charts

Surface and 500 mb weather maps for 12:00 UTC (6:00 CST) were examined for each date in 2002 that falls within the worst 20 % total extinction days at Big Bend. Maps were obtained courtesy of the NOAA Central Library Data Imaging Project at

http://docs.lib.noaa.gov/rescue/dwm/data_rescue_daily_weather_maps.html

and are reproduced in Appendix A .

Most of the high-extinction dates at Big Bend could be classified into three meteorological scenarios or "types".

> Type 1 days are characterized by a weak surface low passing over Big Bend early, with west to northwest winds behind the low. This scenario occurred mostly in early spring – March 12 and 30, and April 2 – and on June 16. On each of these dates, the observed SO4 was relatively low compared to the other dates while the coarse matter contribution was high, most likely from wind blown fugitive dust. November 25 was in a similar scenario except the cold front ran west to east and winds were northerly behind the front. November 25 was the only date with a larger predicted than observed total extinction.
>
> Type 2 days occurred frequently in late spring (April 11 to May 11). Many dates (April 11, 20, and 23, and May 5 and 11) had drylines or surface troughs to the west, resulting in south or southeast winds over Big Bend. Others (like April 29 and May 8) had drylines to the east on the morning weather chart with winds from the west or southwest over Big Bend. January 29 showed a similar pattern with a dryline east of Big Bend. SO4 was under predicted on all of these dates. At 500 mb, most of these dates had a trough in the west with west to southwest flow over Texas. The 500 mb ridge axis was directly over west Texas on April 29, when the observed extinction was very high.
>
> Type 3 days included the seven summer high extinction dates between July through September. A similar although slightly more progressive synoptic pattern was also observed on April 5. Maps for these days all showed weak surface pressure gradients over Texas with high pressure typically over the Northern Plains or Great Lakes and the upper level jet stream positioned well to the north of Texas. Although SO4 still under predicted, higher SO4 was simulated to occur at Big Bend on these dates than under the other two meteorological scenarios. On the two summer dates with the highest observed extinction – August 9 and September 2, the synoptic-scale meteorology was similar. Both had a surface low near Manitoba with a cold front extending no further south than Nebraska. Weak surface pressure gradients were observed in and around Texas on these and their preceding dates, possibly leading to a build-up of concentrations.

Back Trajectories and Residence Time Plots

Back trajectories based on the NOAA Hysplit model were evaluated for each of the 20 percent worst observed visibility days in 2002. Trajectory results were compared with features of the corresponding daily weather maps described above. Figure 4-8 displays the back trajectories for 48 hours ending at Big Bend at 4AM and 4PM CST on each of the worst 20 percent days from 2002 at three heights above ground level: 10m, 100m, and 500m, denoted by the red, blue, and green lines, respectively.

The four Type 1 dates that had weak surface lows passing over Big Bend (March 12, March 30, April 2, and June 16) all have back trajectories from the west to northwest, passing either side of the west Texas/Mexico border. The latter two dates only showed westerlies in the afternoon back trajectories because the surface low had barely passed Big Bend in the morning.

On the spring Type 2 dates between April 11 and May 11, the back trajectories were in good agreement with the weather maps. On dates when the trough or dryline was west of Big Bend,

the back trajectories always originated from the southeast; on dates when the dryline was to the east (January 29, April 29, and May 8), back trajectories were from the southwest. In either case, the back trajectories resided in Mexico most of the time.

On the Type 3 dates , the back trajectories originated from the southeast to northeast. Residence time in the US was longer when the back trajectories were from the east to northeast (July 10, August 9, September 2, and 11).

Figure 4-9 shows the residence time of each grid cell before reaching Big Bend during the dates with the 20 % worst observed extinctions in 2002. Air masses had the longest residence time southeast of Big Bend, which was the predominant direction of the back trajectories. Areas southeast of Big Bend, especially along the Texas/Mexico border appeared to have the highest frequency, followed by an isolated area west of Big Bend in the Gulf of California which corresponds to the westerly, high coarse mass events noted above.

It is interesting to note that back trajectories passed over the general vicinity of the Carbon I and II power plants in Mexico on three of the five dates with the highest observed extinctions -- April 5, August 9, and September 2. On the other two dates (April 29 and May 11), the 48 hour back trajectories remained outside the US for almost the entire period.

Emissions and Source Apportionment Analysis

Figure 4-10 displays the stationary source SO_2 emissions included in the CENRAP inventory. Several major SO_2 sources are located in Mexico southeast of Big Bend. In addition, the concentration of major SO_2 sources in East Texas is also evident. Figure 4-11 display spatial plots of the annual emissions used in the CENRAP 36 km modeling domain for ammonia (NH3). Ammonia emissions in the mountain states and near Big Bend are much lower than areas further east, consistent with population density and land-use patterns.

Results from a CAMx PSAT run on the 2002 emissions inventory were reviewed to identify the relative contributions of different emission source regions and PM species group to total extinction. This CAMx run was based on an older set of emissions (2002 modified Base E inventory). The run divided the 36 km domain into 30 regions as shown in Figure 2-1 and 10 emission groups. Note that in these source groups electric generating units (EGUs) located in Mexico are lumped together with other Mexican elevated point sources whereas EGUs located in the U.S. were placed in a separate group.

Figure 4-12 displays stacked bar charts from a CAMx PSAT run using results from only the days with the 20 % worst extinction at Big Bend in 2002. The top plot shows the extinction contributions from each region by emission group; the bottom shows contributions from each region by PM species. These results are very similar to the PSAT results for 2018 that were described in Section 2.

Boundary conditions (BC) were the largest single contributor to extinction at Big Bend on the 20% worst dates, largely from organics and sulfates. Mexico was the second largest contributor, mostly from elevated point sources which, as noted above, include EGUs in Mexico. The total Mexico contribution was comparable to the three Texas regions combined. Sulfates were the dominant species contributing to predicted total extinction.

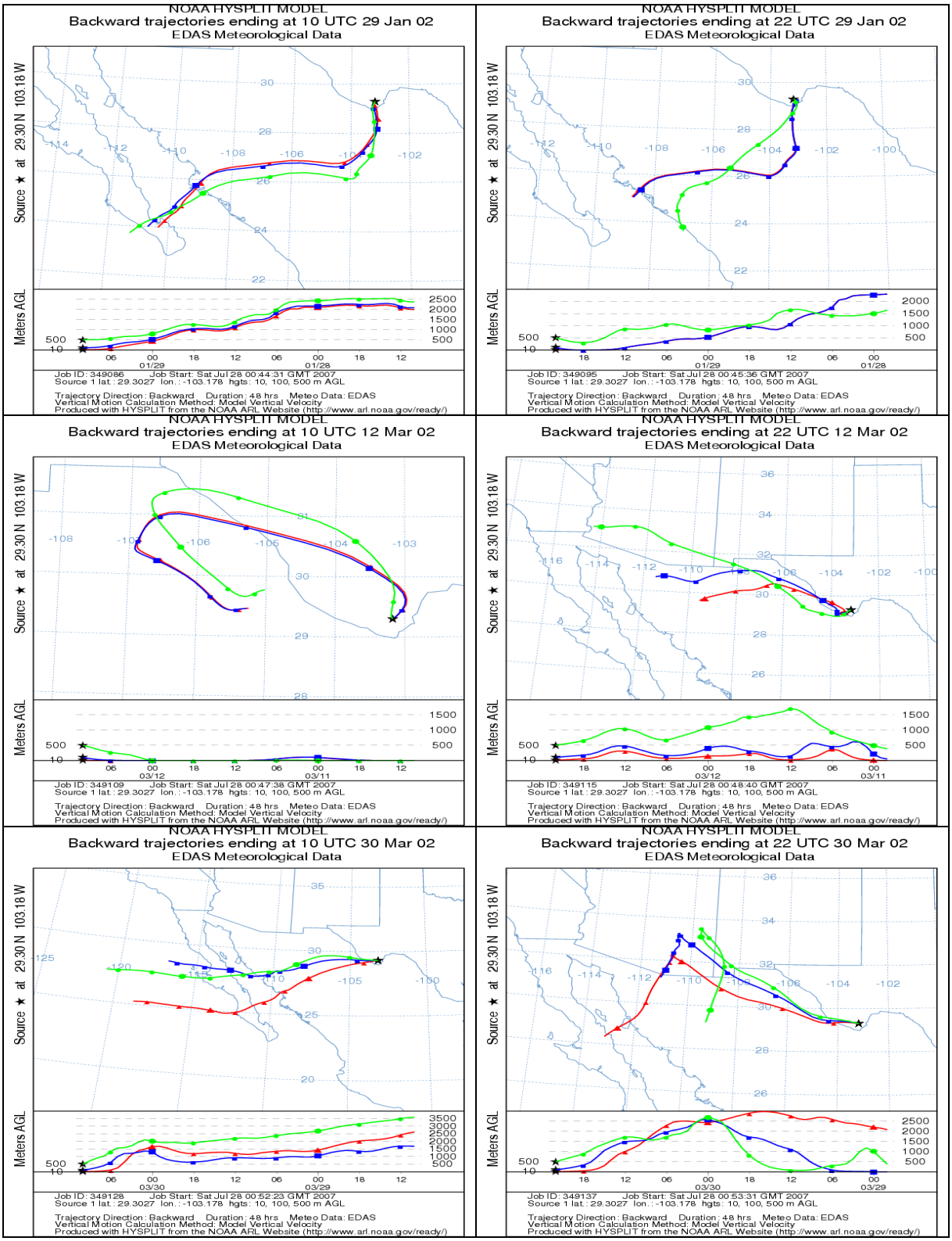


Figure 4-8. Hysplit back trajectories from Big Bend at 4AM (left) and 4PM (right) for each of the 2002 worst 20 percent days.

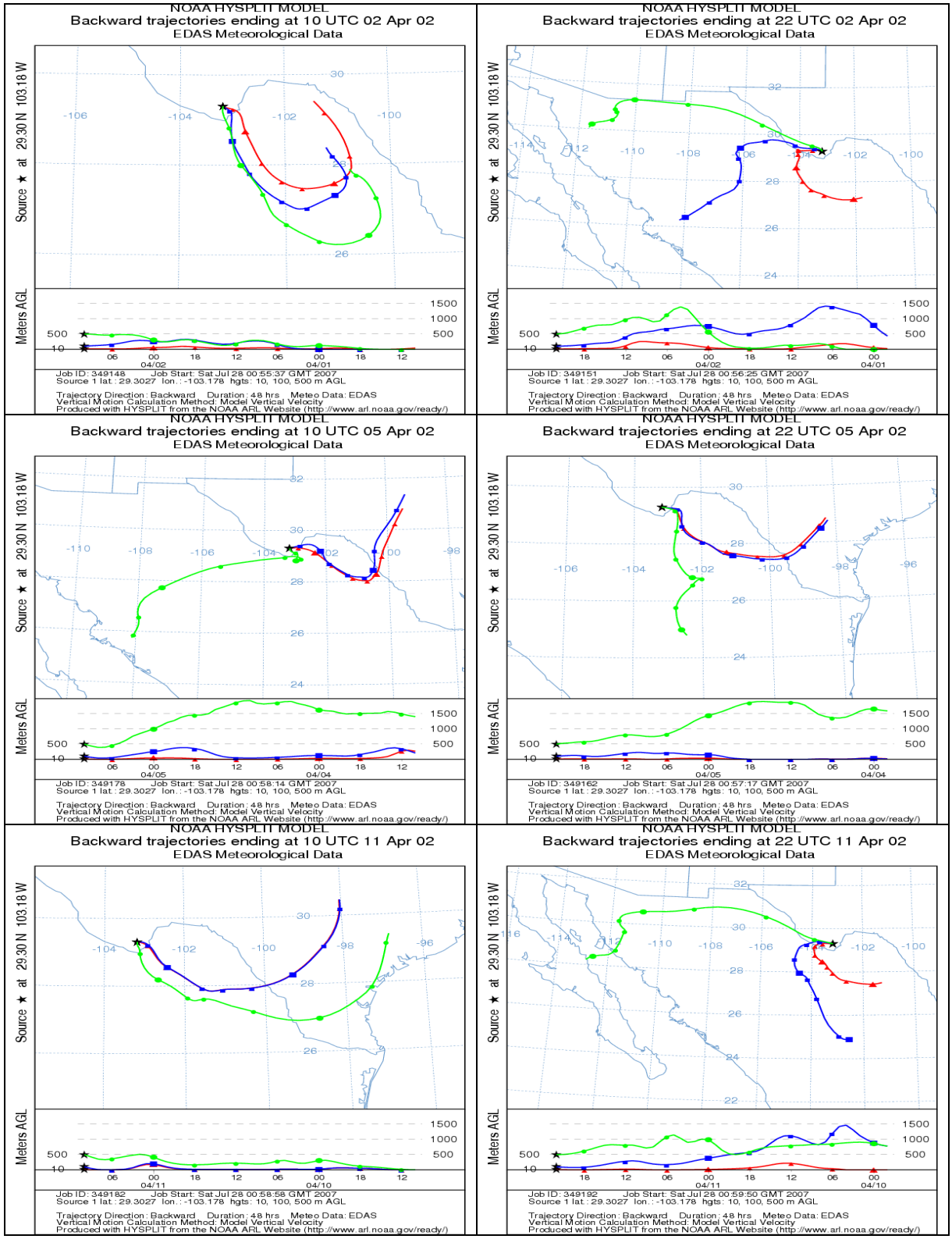


Figure 4-8. cont. Hysplit back trajectories from Big Bend at 4AM (left) and 4PM (right) for each of the 2002 worst 20 percent days.

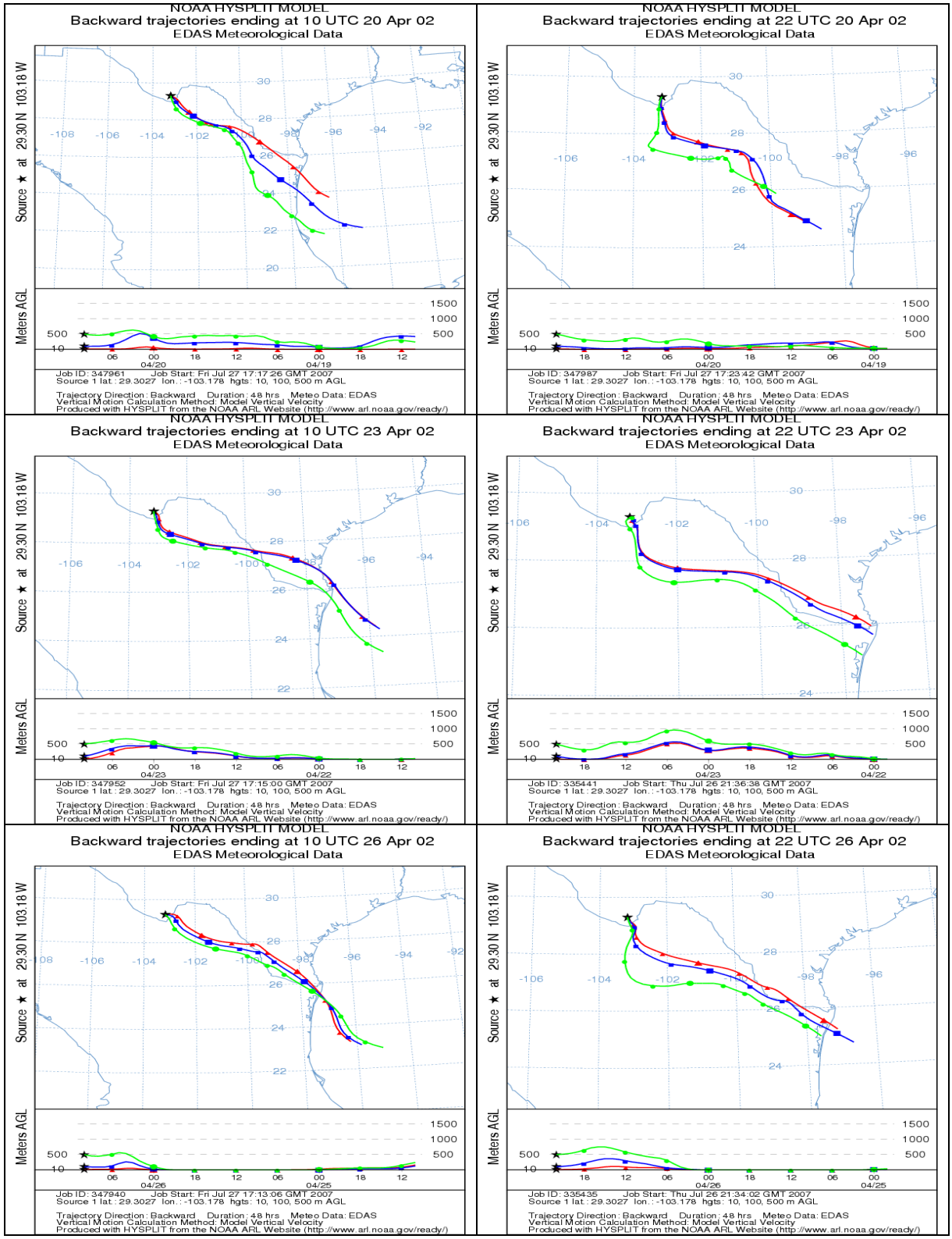


Figure 4-8. cont. Hysplit back trajectories from Big Bend at 4AM (left) and 4PM (right) for each of the 2002 worst 20 percent days.

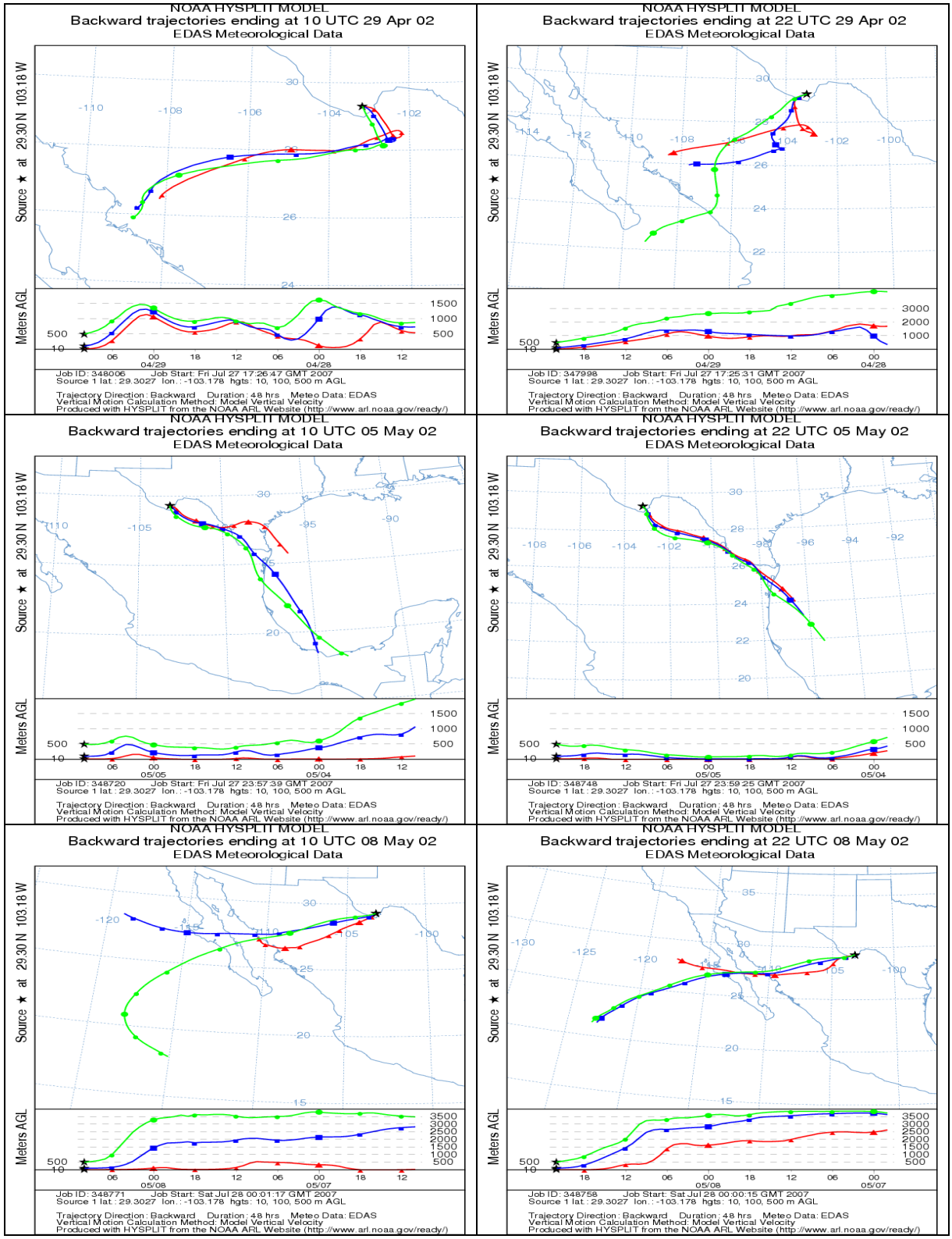


Figure 4-8. cont. Hysplit back trajectories from Big Bend at 4AM (left) and 4PM (right) for each of the 2002 worst 20 percent days.

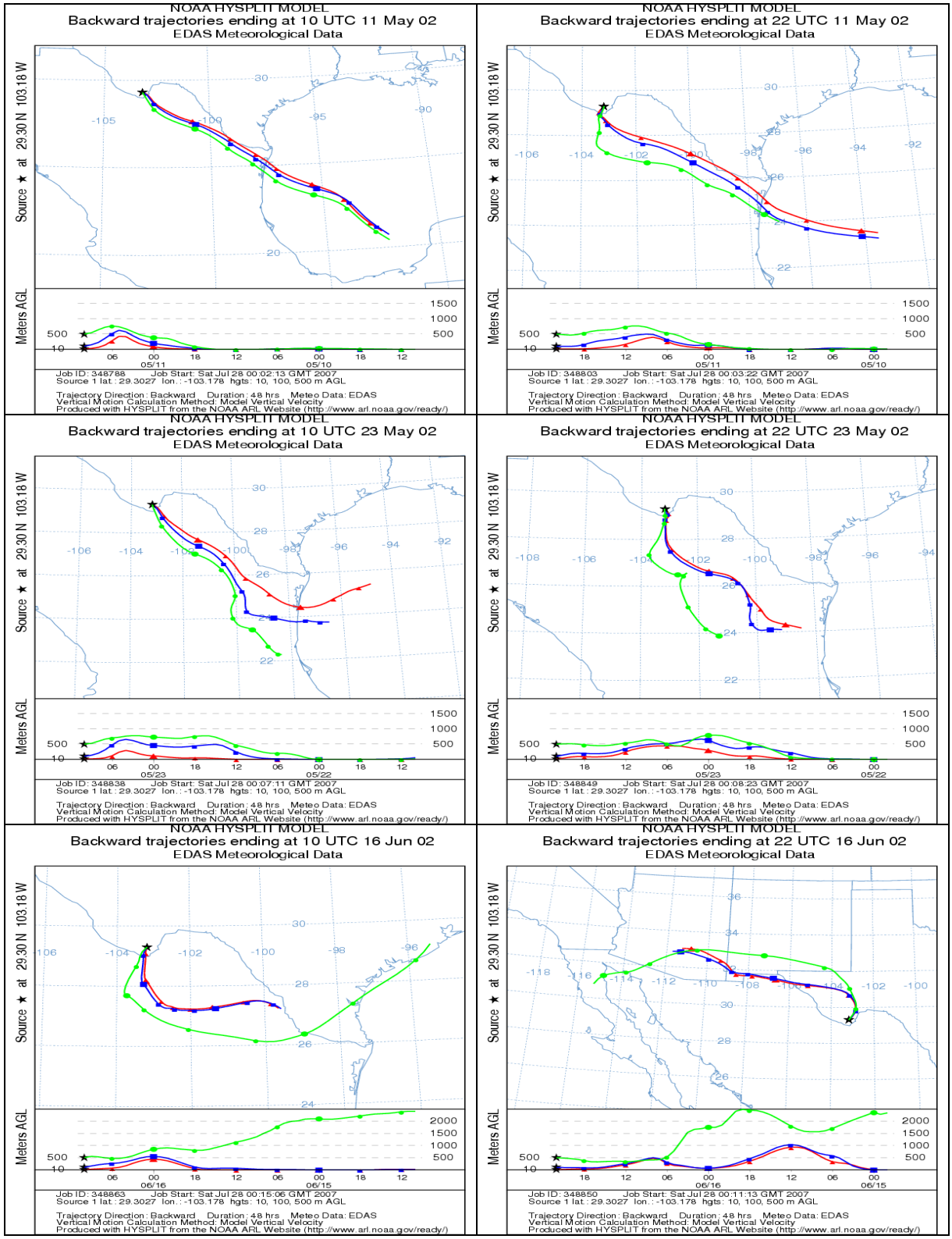
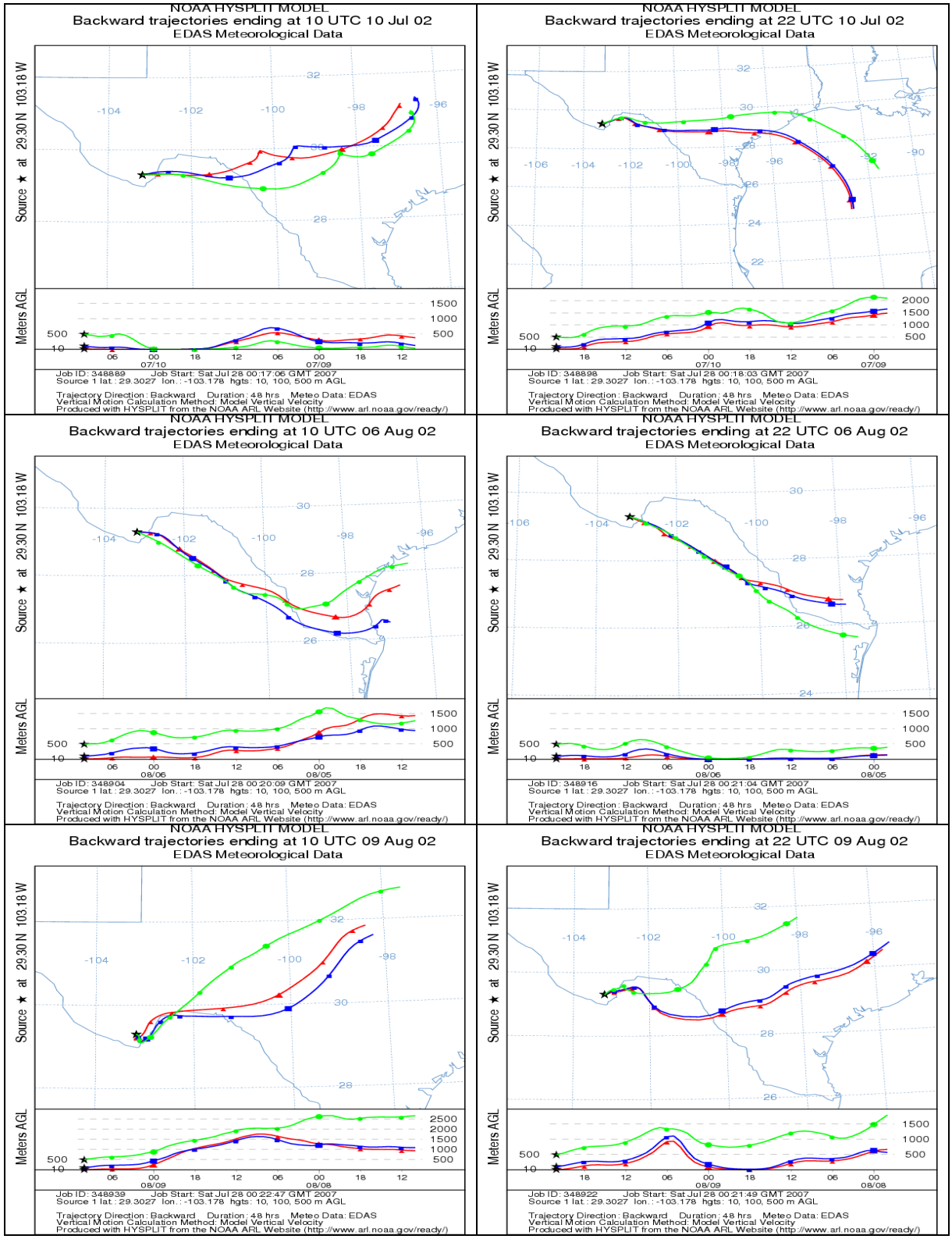


Figure 4-8. cont. Hysplit back trajectories from Big Bend at 4AM (left) and 4PM (right) for each of the 2002 worst 20 percent days.



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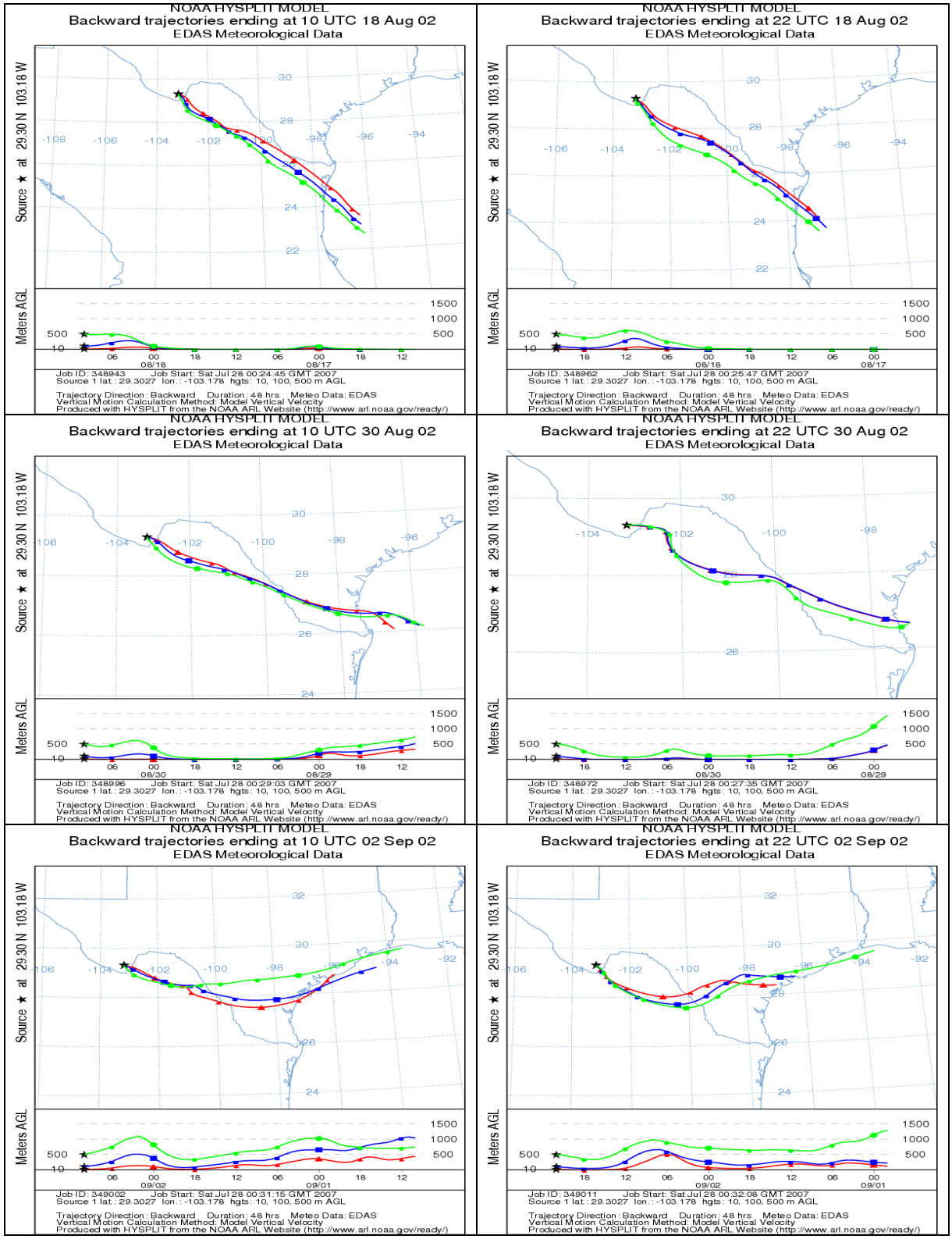

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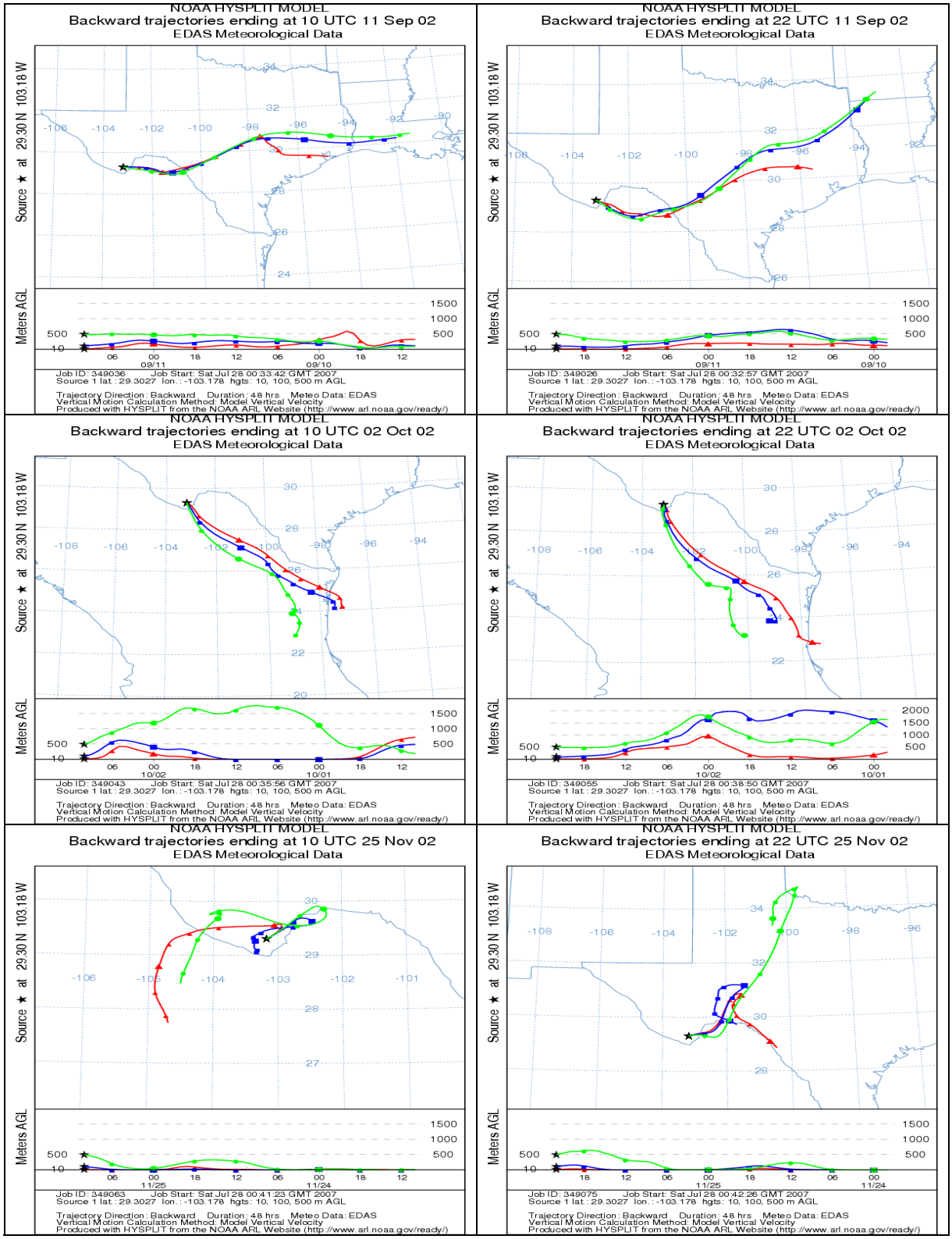

Figure 4-8. concl. Hysplit back trajectories from Big Bend at 4AM (left) and 4PM (right) for each of the 2002 worst 20 percent days.

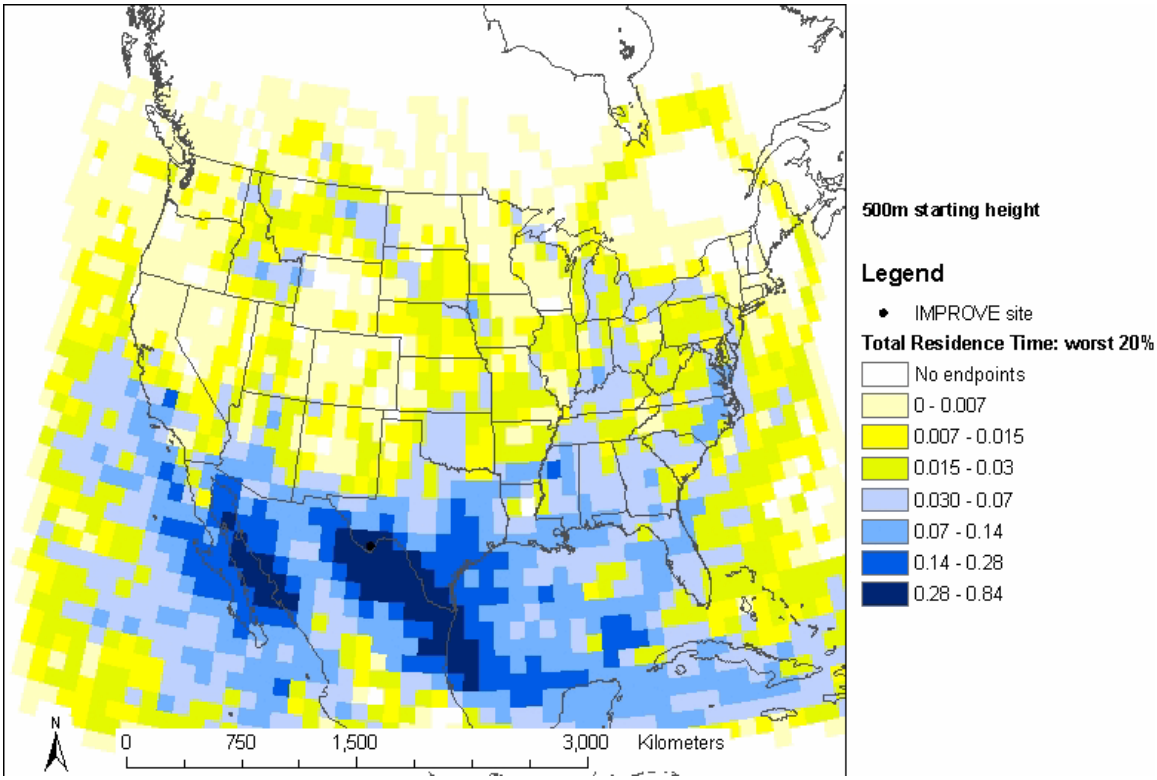

Figure 4-9. Plot of residence time in each grid cell before reaching Big Bend.

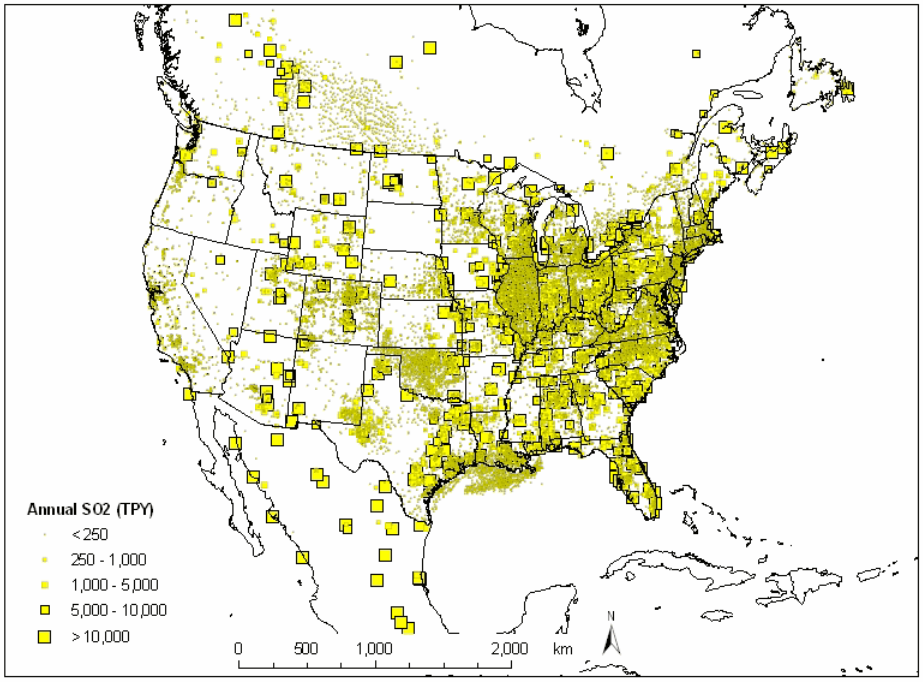

Figure 4-10. Spatial plot of SO2 emissions.

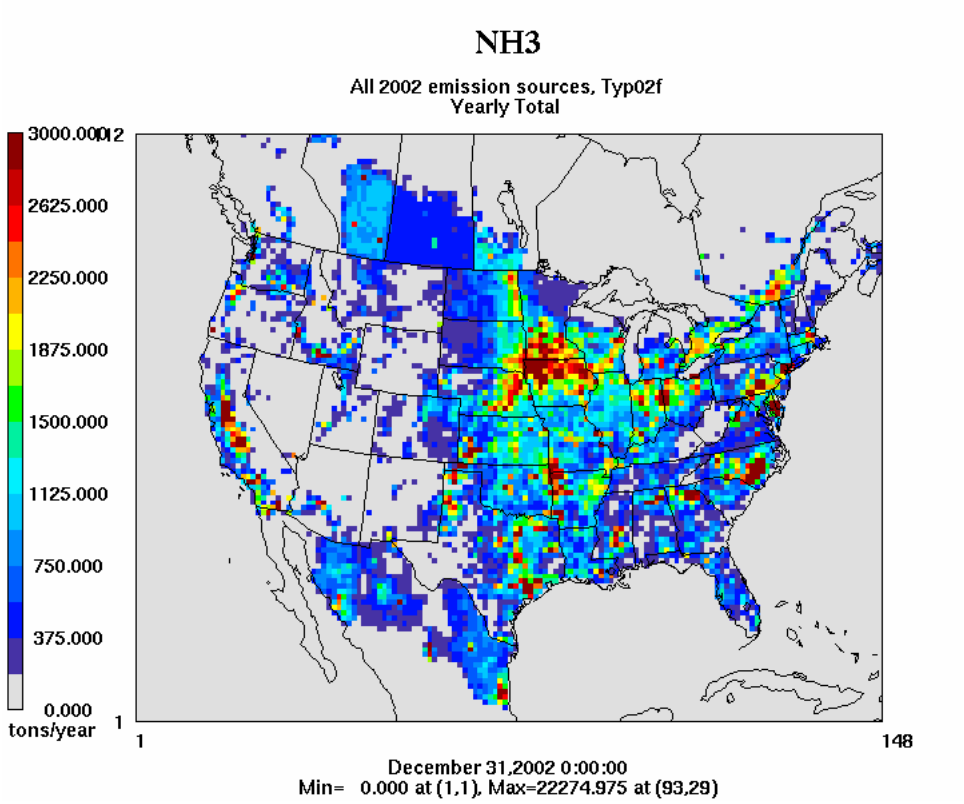

Figure 4-11. Spatial plot of ammonia emissions.

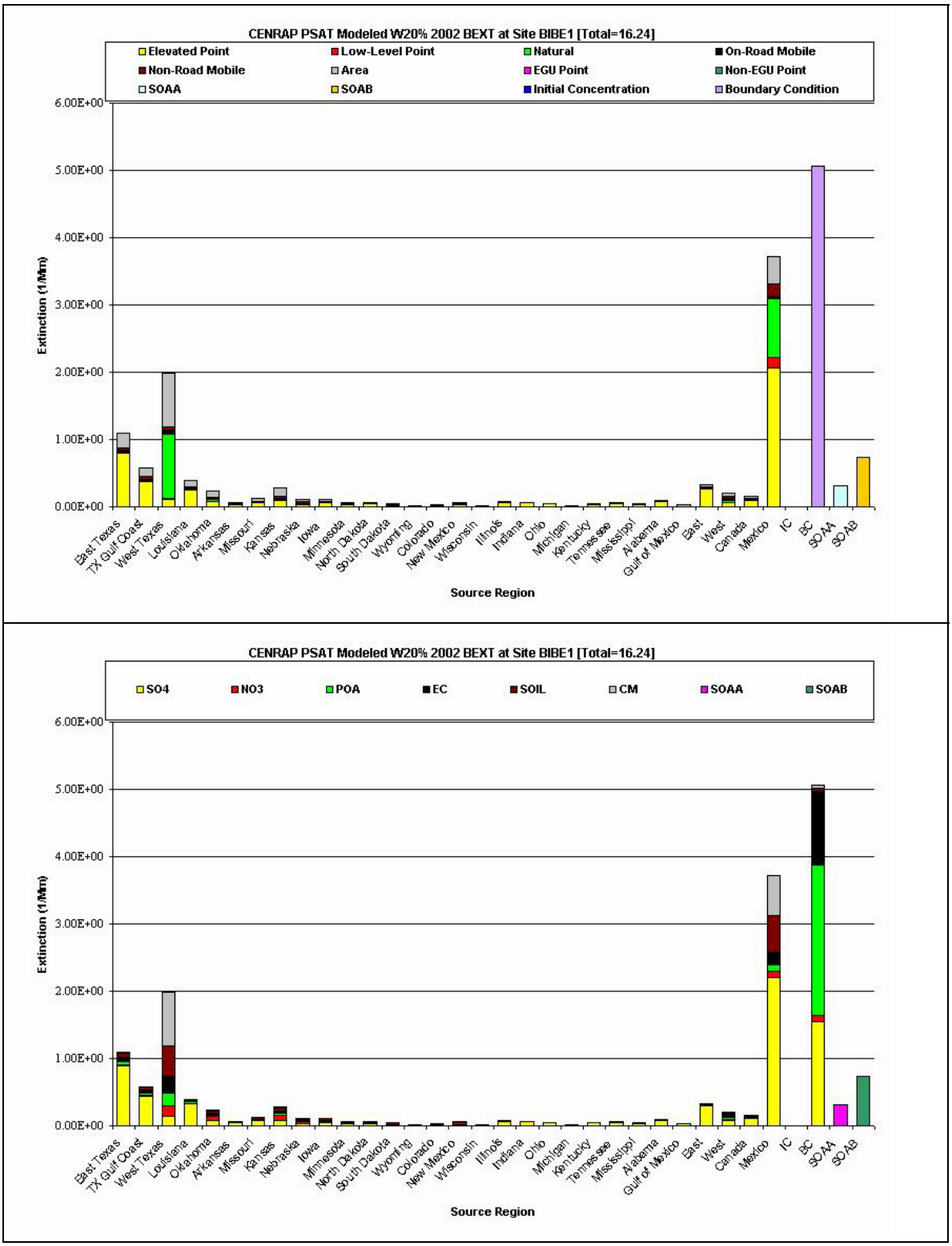

Figure 4-12. Contributions to Big Bend by source region and emission group (top) and PM species (bottom) for the dates with the 20 % highest extinction at Big Bend.

SUMMARY

Under prediction of light extinction at Big Bend and, to a lesser extent, at Guadalupe Mountains occurs primarily as a result of under prediction of SO4. Under prediction of coarse mass (CM) is a also a contributing factor, especially at Guadalupe Mountains where CM contributes more to total extinction but CM is not a major factor on the worst of the 20% worst visibility days at Big Bend.

Based on the results presented above, we conclude that SO4 under prediction at Big Bend is most likely a result of one or both of the following two factors: 1) underestimation of SOx emissions from sources in Mexico and 2) meteorological modeling errors that underestimate the degree of transport from major SOx sources in the southeastern U.S. and northeastern Mexico to Big Bend. The available evidence in support of these two hypotheses is summarized in the following subsections.

Underestimation of Emissions in Mexico

SOx emissions from U.S. sources are unlikely to have been underestimated due to the fact that most SOx is from EGUs and other major sources which are typically well characterized. Less is known, however, about the completeness and accuracy of the SOx inventory for Mexico. SO4 predictions on the two dates with highest predicted extinctions at Big Bend (November 25 and April 5) showed less bias relative to IMPROVE observations than other days in the worst 20% category. Back trajectories on these days (Figure 4-8) had relatively short residence times in Mexico. Back trajectories for November 25 showed air parcels traveling over Texas during most of the period, and the time series of SO4 spatial plots leading up to April 5 (Figure 4-7) suggests that most of the SO4 was transported from U.S. sources. Furthermore, examination of the five dates with the highest observed extinction showed that three of these dates (April 5, August 9, and September 2) had back trajectories that passed over the Carbon I and II power plants in Mexico. On the other two dates (April 29 and May 11) and most other spring dates with high extinction, back trajectories resided in Mexico for most if not all of the 48 hour period. Sulfate was severely under estimated on all of these days.

Back trajectory results show that source regions for air parcels reaching Guadalupe Mountains are more often located within the U.S. as compared to those reaching Big Bend. For example, back trajectories for a 48 hour period ending at 4PM CST on 2 September are displayed for both Big Bend and Guadalupe Mountains in Figure 4-13. Back trajectories from Guadalupe Mountains are over Texas most of the time whereas back trajectories from Big Bend are over Mexico for at least 24 hours prior to reaching Big Bend. The IMPROVE overlay plot for 2 September (Figure 4- 14) shows that a large plume of predicted high SO4 reached both Big Bend and Guadalupe Mountains on this date. The model performed well at Guadalupe Mountains with observed and predicted values in the 5 – 6 $\mu g/m^3$ range, but SO4 was under predicted at Big Bend which recorded just over 10 $\mu g/m^3$ SO4 compared to a predicted value of about 3.5 $\mu g/m^3$. These results are consistent with the theory that SOx emissions in East Texas (and likely other areas of the southeastern US) are reasonably accurate and that the model is treating SO4 formation within the US reasonable well but either SOx emissions or possibly SO4 formation are under predicted in Mexico.

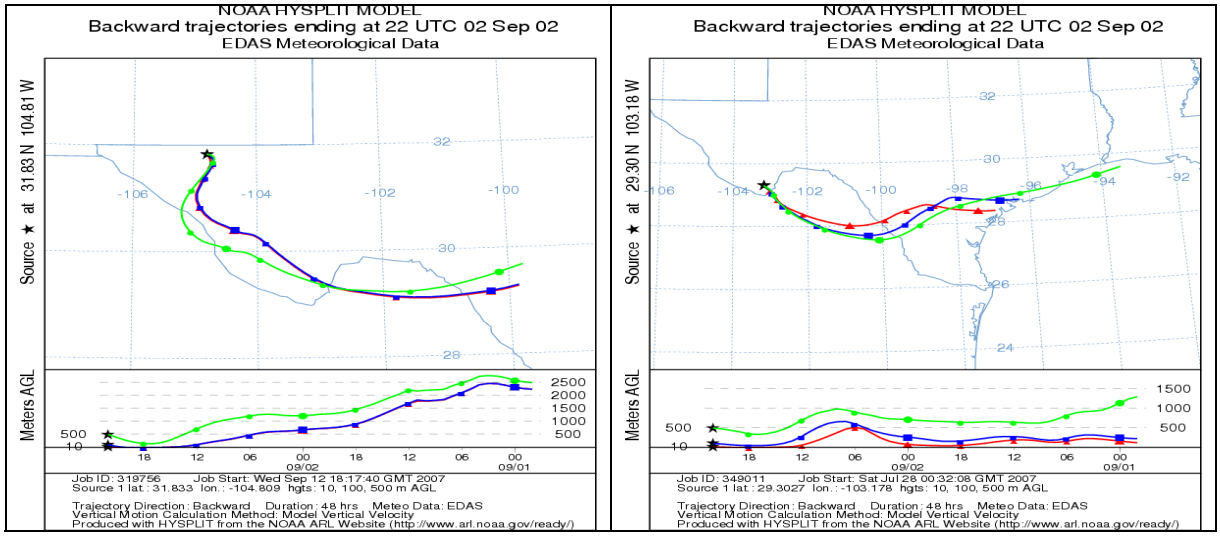

Figure 4-13. Back trajectories on September 2 at Guadalupe Mountains (left) and Big Bend National Parks (right).

Figure 4-14 shows more spatial plots of SO4 concentrations from the CENRAP CMAQ Typ02f run overlaid with color-coded IMPROVE observed values on four of the five dates with the highest extinction; the fifth date -- April 5 -- was already shown in Figure 4-7. In the top two plots (April 29 and May 11), the predominant wind direction was south to southeasterly. On both dates, the observed SO4 exceeded 4 ug/m3, but the predicted concentrations were well below this value throughout Mexico, including areas in the plume originating from the Carbon plants. These results provide further support for the hypothesis that SOx emissions are underestimated in Mexico. As noted in the BRAVO study (Pitchford et al., 2004), "The two Carbón power plants, located in Mexico about 225 km southeast of BBNP, were the single largest contributors to ammoniated sulfate haze at BBNP during the BRAVO Study period." Thus, SO4 prediction errors at Big Bend are closely tied to the accuracy of emission estimates for these two power plants. It should also be noted, however, that further analysis will be needed to rule out the possibility that in-plume chemistry simulation errors or under estimates of NH4 emissions in Mexico could not also be contributing to possible SO4 under prediction in the plumes from these sources. In addition, we would expect the model predictions made at 36 km resolution to under predict peak values within power plant plumes at locations close to the source.

Lack of Transport of U.S. SO4 to the West

Several of the days with large SO4 prediction errors at Big Bend are characterized by a significant build up of SO4 just east of Big Bend in the model simulation. A good example of this is the IMPROVE overlay plot for August 9 in Figure 4-14. These results suggest that the model is producing approximately the right amount of SO4 in this area but the predicted high SO4 area does not extend as far west as suggested by the observations: on August 9, both Class I areas measured over 4 µg/m^3 SO4 but predicted values were significantly lower.[1] A similar

[1] Unfortunately, the color scale on these plots tops out at 4 μg/m3, making it impossible to verify that there is no significant SO4 under prediction within this high SO4 zone. However, the bias statistics in Figure 4-5 suggest that under prediction is

pattern is evident during several other southeastern high SO4 events, such as 23 May (Figure 4-15).

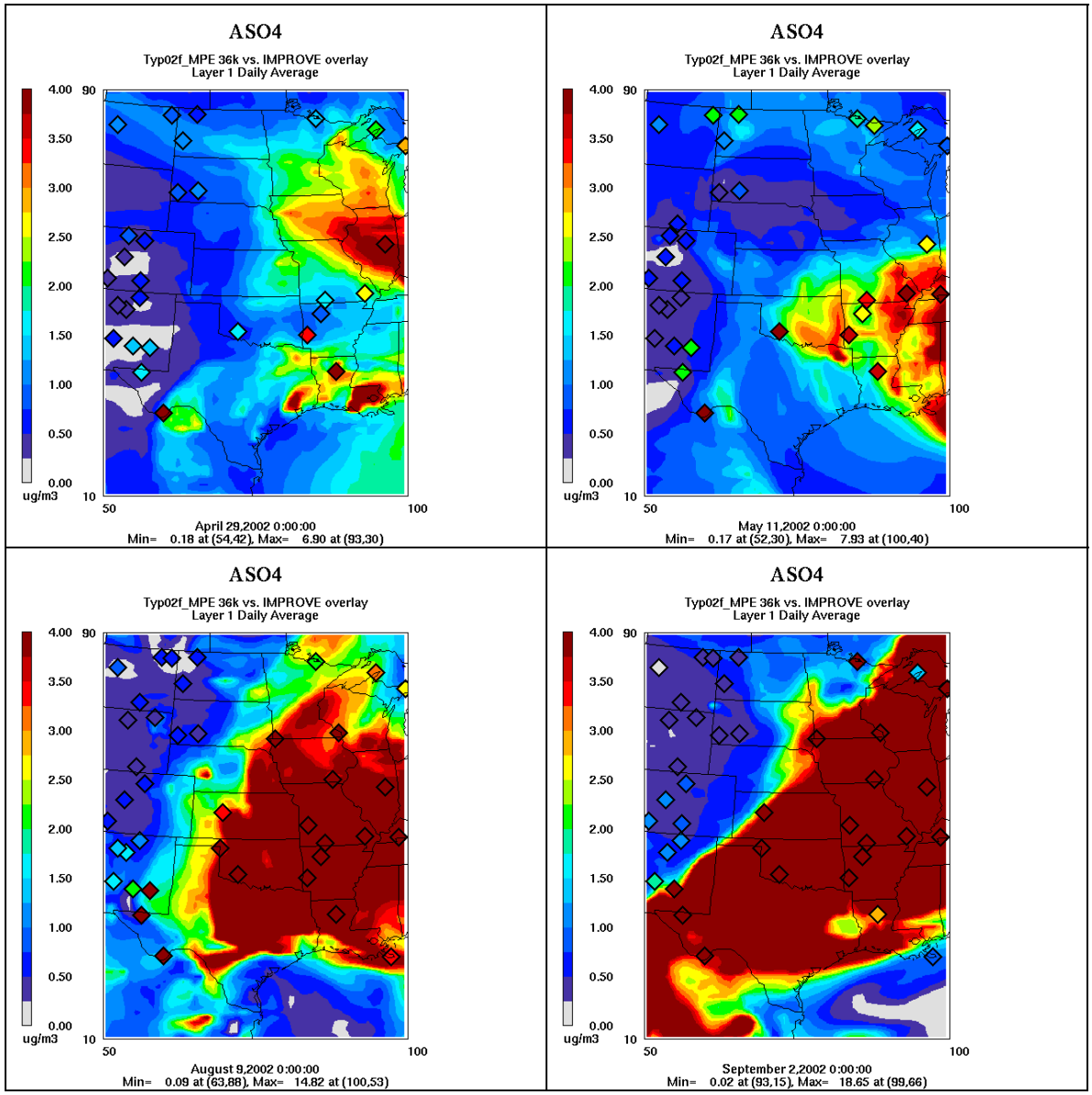

Figure 4-14. Spatial plots of predicted SO4 concentrations with color-coded observed values on four dates with the highest extinction at Big Bend.

generally not as large in this area as at Big Bend and Guadalupe Mountains. Further analysis of model performance on specific days could not be performed within the scope of this study but is recommended for follow-on work.

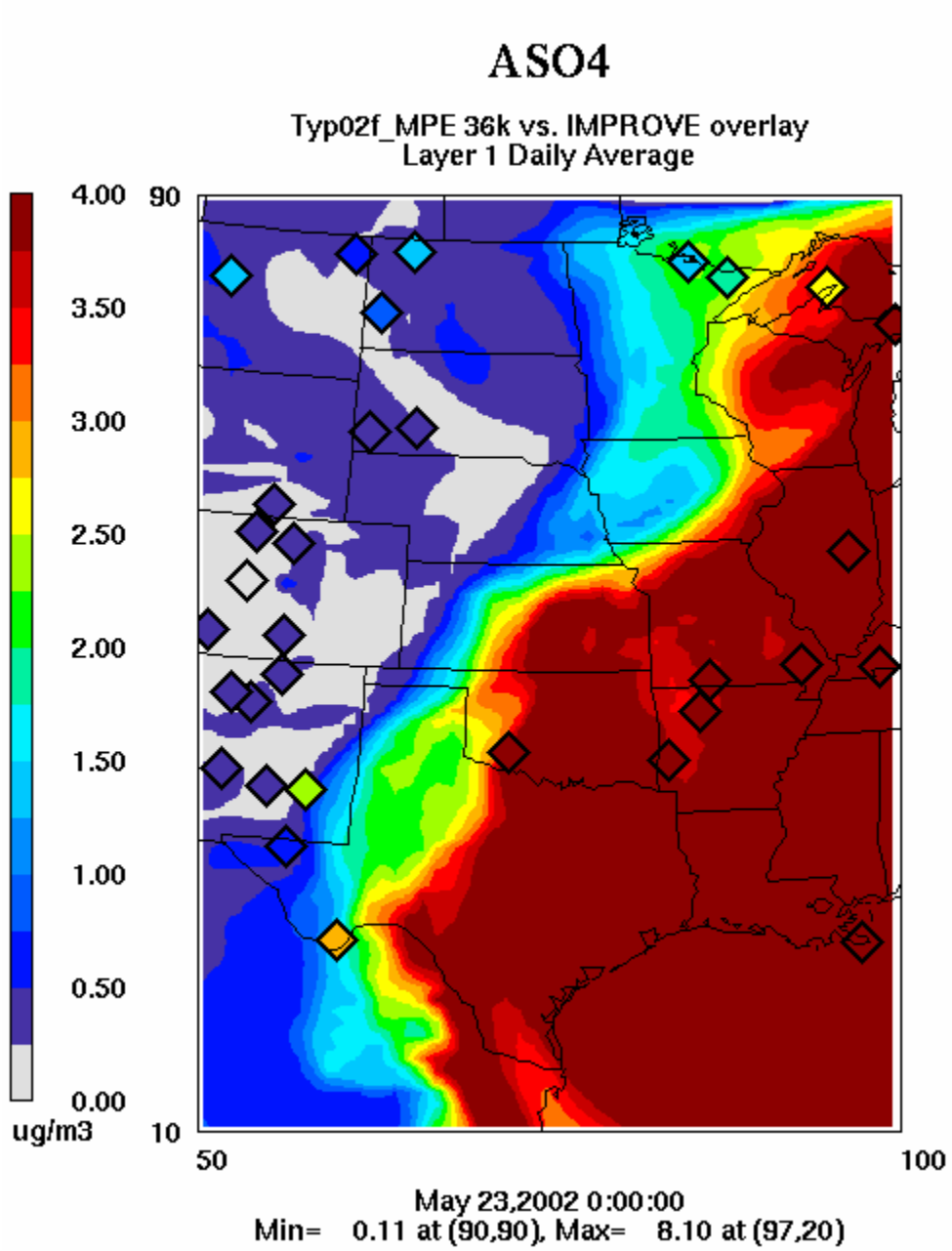

Figure 4-15. Spatial plots of predicted SO4 concentrations with color-coded observed values on 23 May 2002.

It is also constructive to review the trajectory residence time analysis from the July – October 1999 BRAVO study for the 20% highest SO4 days versus the 20% lowest SO4 days at Big Bend (Figure 4-16). These results suggest most high sulfate episodes during these months originate from sources in East Texas, Arkansas, Louisiana, and Alabama and possibly northeastern Mexico whereas most low SO4 air originates from the Gulf of Mexico without passing over the United States. An interesting feature of the high SO4 residence time plot in Figure 4-16 is the concentration of trajectories along the shipping lanes that run between Houston and the west end of Cuba. These shipping lanes represent a significant concentration of SOx emissions as shown in Figure 4-17.

These results support the hypothesis that under prediction of SO4 at Big Bend and, to a lesser extent at Guadalupe Mountains, is at least partly due to errors in the MM5 meteorological data used to drive the CMAQ simulations. It is possible that MM5 is positioning the boundary between the humid southeastern airmass and the dry desert southwest airmass too far to the east on many days. Detailed evaluation of the MM5 results (which is beyond the scope of the current investigation) will be required to verify this hypothesis.

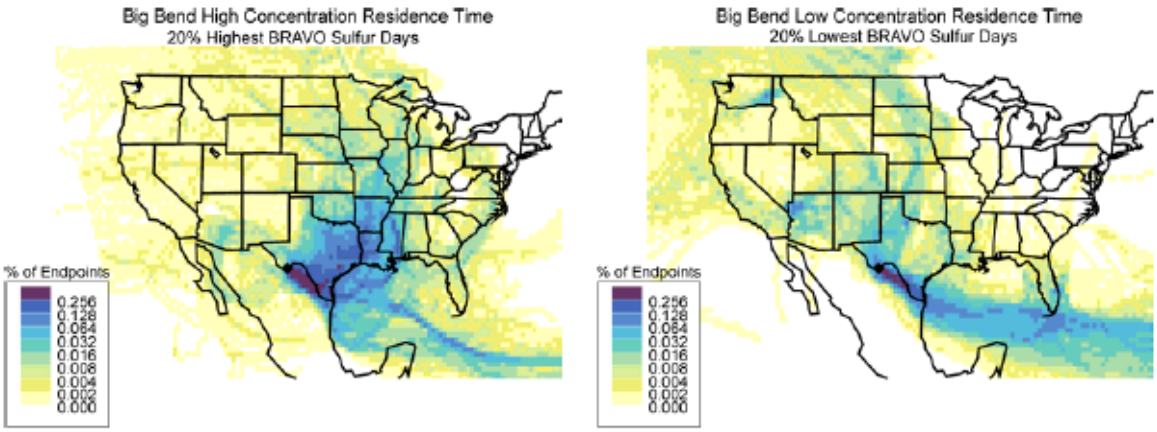

Figure 4-16. Percent of time that air parcels en route to Big Bend spent over various locations during five-day trajectories for periods with the 20% highest concentrations of particulate sulfate compounds at Big Bend (left) and for the periods with the 20% lowest concentrations of particulate sulfate compounds at Big Bend (right) during the BRAVO Study period of July through October 1999 (Source: Pitchford et al., 2004).

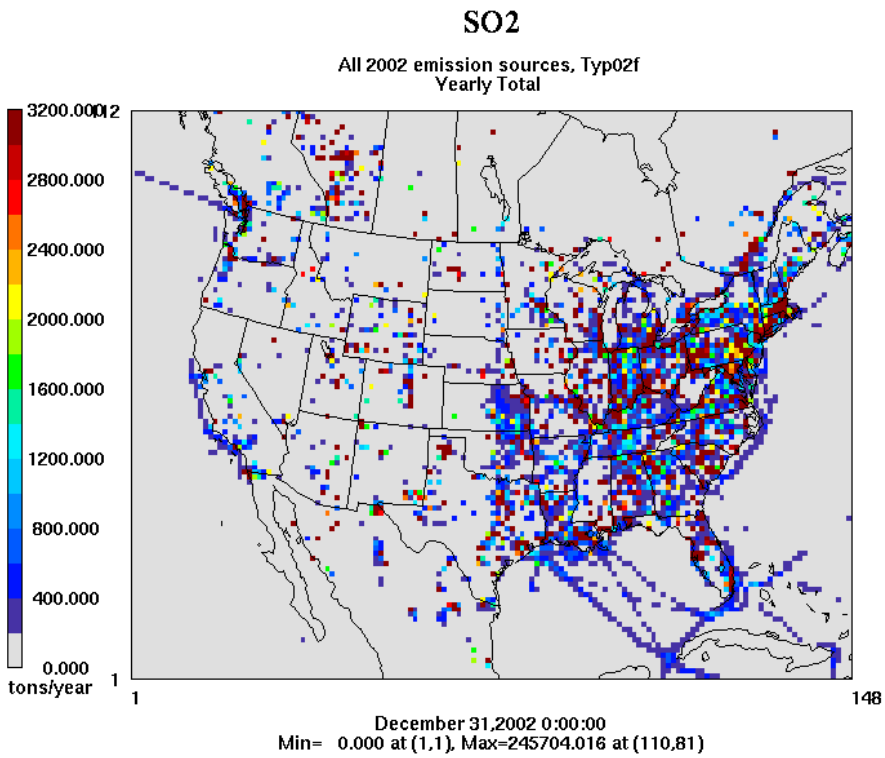

Figure 4-17. Spatial plot of SO2 emissions used in the CMAQ Typ02f base case model run.

CONCLUSIONS AND RECOMMENDATIONS

The current diagnostic evaluation of CMAQ model performance at Big Bend and Guadalupe Mountains presented above shows that under prediction of SO4 at Big Bend and, to a lesser extent, at Guadalupe Mountains may be due to either underestimation of SOx emissions from sources in Mexico (or lack of sufficient SO4 formation in northeastern Mexico which could, for example, be a result of underestimated ammonia emissions) and/or errors in the MM5 meteorological fields that result in a failure to simulate the full westward extent of elevated SO4 "cloud" originating primarily from sources in the southeastern U.S. It was not possible within the scope of this study to estimate the relative contribution of these two different potential causes of the SO4 prediction bias. Further analysis is therefore recommended, including:

- Examination and evaluation of emission data for major SOx sources located in Mexico.
- A detailed evaluation of MM5 model performance on days with high observed SO4 levels at Big Bend and Guadalupe Mountains. This would include running back trajectory analyses using the MM5 wind fields for comparison with the Hysplit trajectories presented above.
- Additional evaluation of CMAQ performance on specific days with high SO4 levels at Big Bend and Guadalupe Mountains to compliment the MM5 model performance analysis.