Presented at the 6th Annual CMAS Conference, Chapel Hill, NC, October 1-3, 2007

Assessing Model Performance Using Weekday/Weekend Analysis

Jim Smith, Mark Estes, Fernando Mercado, and Jocelyn Mellberg*
Texas Commission on Environmental Quality, Austin, Texas

1. BACKGROUND AND INTRODUCTION

Comparison of photochemical air quality model predictions with observed ambient concentration data is necessary for assessing model performance. In modeling applications for the one-hour ozone standard, this comparison was often considered sufficient for determining whether the model performed well enough to predict future ozone concentrations and test proposed control strategies. Often, little or no consideration was given to the model's performance in predicting the response to emission changes.

With the advent of the new standards for eight-hour ozone and $PM_{2.5}$, EPA devised a new attainment test based on the model's relative response to emission changes (the one-hour test for ozone was based on predicted peak ozone concentrations). Thus, under the new standard, evaluating the model's response to emission changes becomes at least as important as evaluation of its ability to reproduce historically observed events. In its recently finalized guidance for demonstrating attainment under the eight-hour standard, EPA (2007) recommended several possible means of assessing model response to emission changes, but these methods are either indirect (probing tools, alternative base cases, most observation-based models) or are difficult to employ in practice (retrospective analyses). However, weekday/weekend analysis (a type of observation-based model) is relatively straightforward and offers a direct comparison between modeled and observed responses to emission changes.

Several researchers, including Blanchard and Tannenbaum (2003, 2005), Fujita, et.al. (2003), and Yarwood, et al (2003), have studied the so-called "Weekend Effect," which often leads to an increase in measured ozone concentrations on weekends compared to weekdays.

The "Weekend Effect" is somewhat counterintuitive, since emissions of NO_X, an integral component in tropospheric ozone formation, are generally lower on weekend mornings than on weekday mornings because of reduced vehicular activity. The explanation for this effect is that newly-emitted NO_X (consisting of a mixture of NO and NO_2) is primarily NO, which reacts with ozone (O_3) to form more NO_2 plus molecular oxygen ($NO + O_3 \rightarrow NO_2 + O_2$). This reaction, called *titration*, tends to reduce ozone concentrations near large NO_X sources, particularly roadways, and can serve to generally inhibit ozone buildup in urban areas. In addition, NO_X-rich areas can have ozone formation suppressed by the reaction of NO_2 with OH radicals, creating HNO_3, and preventing the radicals from participating further in the ozone formation pathway (i.e., *radical termination*). Lower motor vehicle emissions on weekends, especially in the morning, reduce the NO_X to lower concentrations. The lower NO_X concentrations may result in less ozone destruction via titration, and less radical termination. In some cases, the lower mobile NO_X emissions on the weekends can lead to higher observed ozone concentrations. It is important to note, however, that the NO_2 created during ozone titration can fuel ozone formation later as the air mass moves away from the NO_X sources, potentially raising downwind ozone concentrations and increasing background ozone levels.

If a photochemical model responds appropriately to emission changes, it should reproduce the "Weekend Effect" in its predictions. Thus, urban environments provide a natural laboratory environment in which a model's response to emission changes can be evaluated. The authors investigated the modeled response to weekday/weekend emission changes in the Houston/Galveston/ Brazoria ozone nonattainment area during the 2000 Texas Air Quality Study (TexAQS 2000).

2. METHODOLOGY

The TexAQS 2000 was a major field study of the causes of high measured ozone concentrations in eastern Texas, and in particular in the Houston-Galveston-Brazoria (HGB) ozone nonattainment area (Figure 1). The intensive field campaign ran from August 15 through September 15, 2000. For regulatory modeling, the TCEQ

**Corresponding author:* Jocelyn Mellberg, TCEQ, 12100 Park 35 Circle, Bldg. E, Austin TX 78753
jmellber@tceq.state.tx.us

selected the period from August 15 through September 6 (the meteorology during the remainder of the intensive period was not conducive to ozone formation). This period contained 24 weekdays and 6 weekend days. However, Saturday traffic patterns are notably different from those on Sunday (on Sunday, there is generally less traffic in the morning than on Saturday), and these differences appear to manifest themselves in peak ozone concentrations in the HGB area as well. Treating Saturday and Sunday separately leaves only three days of each during the period modeled, which is a very small sample to use in validating model response to daily emission changes.

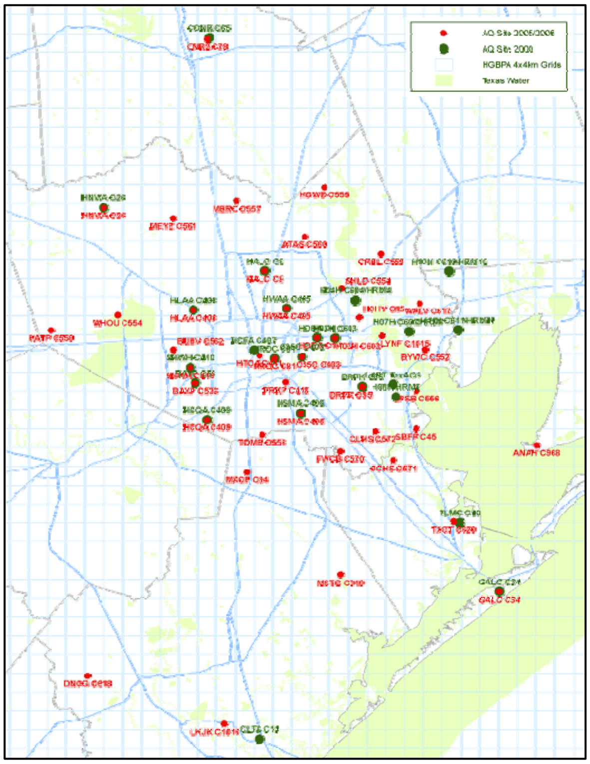

Figure 1: Monitoring Sites in the Houston-Galveston-Brazoria Ozone Nonattainment Area

To increase the sample set, we ran the entire modeling period three times, first with emissions for a Wednesday, then with Saturday emissions, and finally with Sunday emissions, which produced a set of 22 modeled ozone concentration fields for each day. In this test we allowed each day to start with the modeled concentrations from the previous day, which in this case had emissions from the same day of the week. A more rigorous application would re-initialize the hour zero concentrations with modeled values from the preceding day (i.e., start each Saturday using modeled concentrations simulated with Friday emissions).

Modeled daily peak eight-hour concentrations were extracted at each of 18 monitors in the HGB area and averaged across the 22 days of the simulation. These were compared with measured concentrations from the same monitors averaged across all ozone season (June-September) days in 2000 through 2003 that saw at least one monitor exceeding the eight-hour standard. Because the modeled period was specifically chosen to represent periods of higher ozone concentrations, it would not be appropriate to include low-ozone days (many of which are windy, cloudy, or rainy) in the comparison.

3. RESULTS

Figure 2 shows observed average 6 AM concentrations of NO_X at eleven HGB-area monitors as a percentage of each monitor's Wednesday average. The legend lists all 16 monitors used in the ozone comparison, but not all of these measured NO_X. All but two sites (GALC and CONR) show a distinct pattern of concentrations that are lower on Saturday than on Wednesday, and all show a drop from Saturday to Sunday.

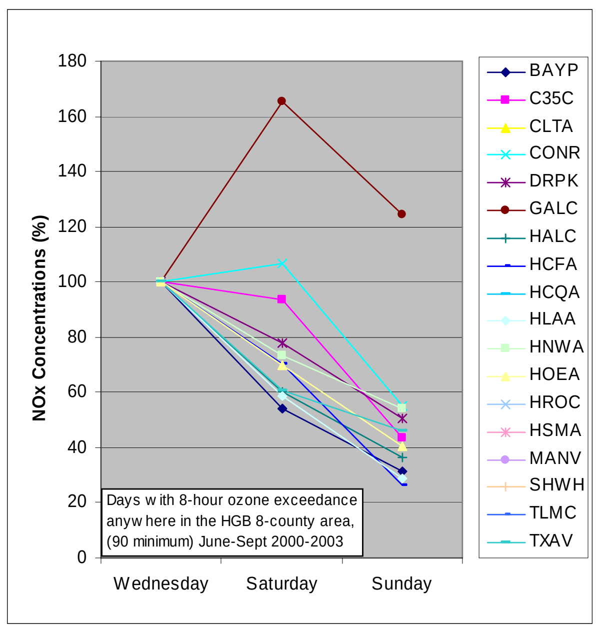

Figure 2: 6 AM Observed NOx Concentrations as a % of Wednesday

The GALC monitor is somewhat unique since it is located on Galveston Island, a popular destination for vacations and weekend excursions. The modeled NO_X concentrations shown in Figure

3 show a similar pattern, although there is more spread in the Sunday concentrations. This may be partially attributable to a smaller sample (22 days vs. at least 90 days for each monitor with measured data). Overall, modeled concentrations on Saturday tend to be lower than observed, while Sunday modeled concentrations are closer to observed. One possible explanation for this finding is that there may be residual NO_X left over from Friday evening, but which was not modeled in this exercise.

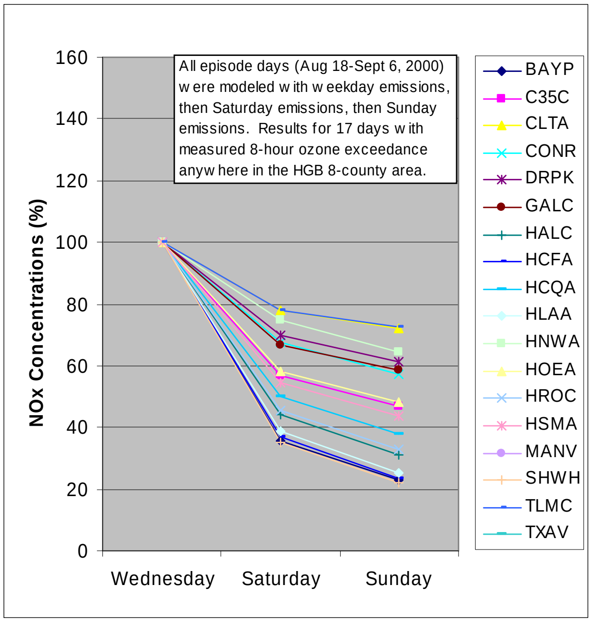

Figure 3: 6 AM Modeled NOx Concentrations as a % of Wednesday

Figure 4 shows average monitored peak eight-hour ozone concentrations at all 18 monitors. Here the picture is much different from that for NO_X, with some monitors increasing from Wednesday through Sunday, some declining from Wednesday through Sunday, and some peaking on Saturday with a decline on Sunday. The first pattern is suggestive of VOC limitation, the second of NO_X limitation, and the third (Saturday peak) of VOC-limited leaning to transitional.

The model (Figure 5) shows much less variability, with either no change or a slight decline from Wednesday through Sunday, and it appears that the model does not respond to the weekend emission changes in the same way as the monitors. However, the TexAQS 2000 was notable for including a period characterized by extreme meteorology Between August 30 and

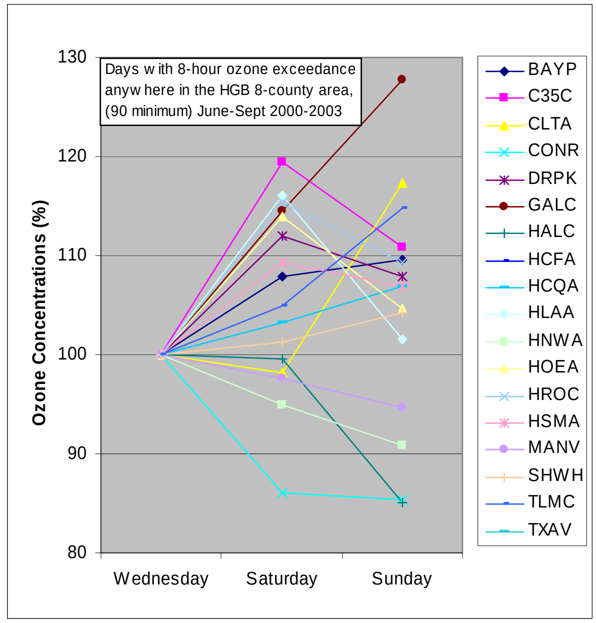

Figure 4: Mean Daily Observed Peak 8-Hour Ozone Concentrations as a % of Wednesday Peak

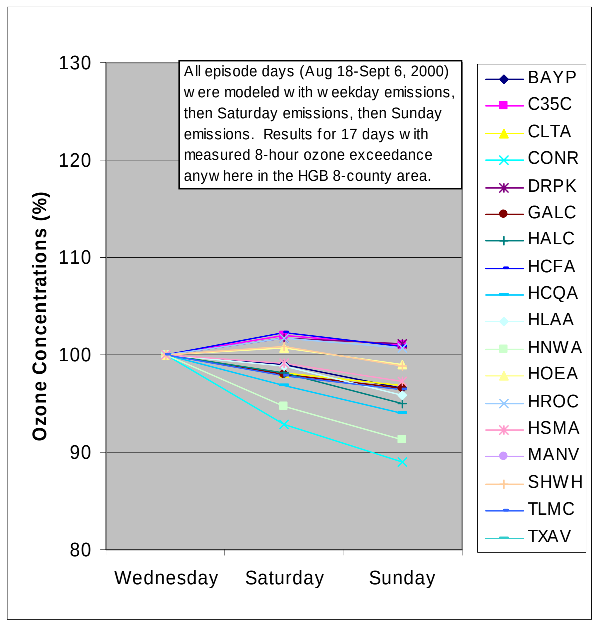

Figure 5: Mean Daily Modeled Peak 8-Hour Ozone Concnetrations as a % of Wednesday Peak

September 6, 2000 the HGB area saw some of the hottest temperatures ever recorded in the area, associated with winds with an uncharacteristically westerly component which brought in hot, dry air from the desert southwest. To illustrate how extreme this period was, in the 57-year period from 1942 through 2003, Houston Hobby airport saw temperatures exceeding 104° F on nine days. Five of these days occurred between August 30 and September 6, 2000, including the two hottest temperatures ever recorded there: 108° on September 4 followed by 107° on September 5. These days, not surprisingly, also recorded most of the highest eight-hour ozone concentrations seen during the period modeled (see TCEQ, 2004). Modeled peak ozone concentrations on these days were similarly much higher than those in the remainder of the modeling period, and these concentrations dominated the average values shown in Figure 5.

To see if the inclusion of the highly unusual meteorological event of August 30 – September 6, 2000 influenced the model's response to weekday-weekend emissions changes, we divided the modeled period into a "typical" period (Aug. 18-29) and an "extreme" period (Aug. 30 – Sept. 6). The results are shown in Figures 6 and 7 below. The model results resemble the monitored values much more closely from the "typical" conditions than for the "extreme" conditions. One notable difference between the "typical" modeled concentrations and the monitored concentrations is the former's lack of Saturday peaks which characterize the monitored values at many urban and industrial monitor sites.

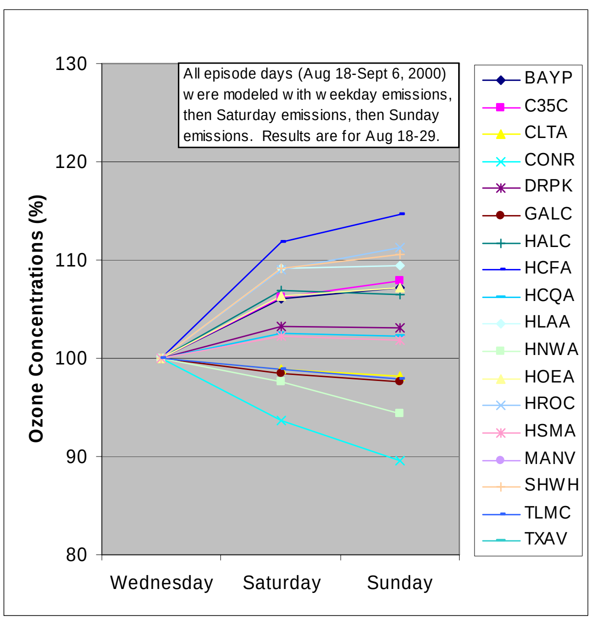

Figure 6: Mean Daily Modeled Peak 8-Hour Ozone Concentration as a % of Wednesday Peak, Aug 18-29, 2000

4. SUMMARY

Overall, model response to the weekday/weekend effect is reasonably consistent with observations, at least in the first part of the episode. The lack of a Saturday peak in modeled ozone at urban/industrial sites may indicate that the model has too much surface-level NO_X, and may be less responsive to NO_X reductions than the real atmosphere.

The latter part of the episode shows little response to weekday/weekend emission changes, which probably dampens overall model response. Note that while the modeled behavior during this period is not consistent with long-term measured trends, there is no reason to believe the model is not correctly characterizing the response to emission changes for these types of days.

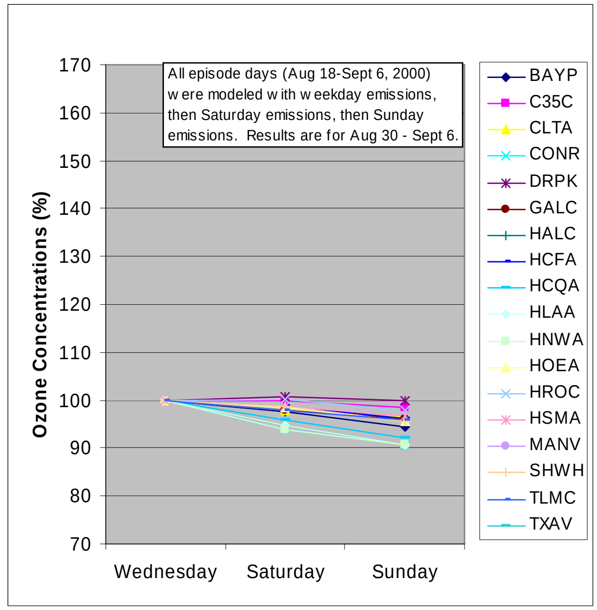

Figure 7: Mean Daily Modeled Peak Ozone Concentration as a % of Wednesday, Aug. 30 - Sept 6, 2000

5. NOTES AND CAVEATS

A rigorous analysis would ensure that each day modeled used appropriate Hour 0 starting concentrations, such as Friday night prior to Saturday morning. Lack of residual NO_X may have affected some of the analyses.

Note also that because of limited sample sizes, trends in the data were not tested for statistical significance. The analysis presented here relies on visual identification of patterns in the data and is therefore subjective.

6. REFERENCES

EPA 2007 Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze, http://www.epa.gov/scram001/guidance/guide/final-03-pm-rh-guidance.pdf

Blanchard C.L. and Tannenbaum S.J. 2003. Differences between weekday and weekend air pollutant levels in southern California. J. Air Waste Manage. Assoc. 53: 816-828.

Blanchard C.L. and Tannenbaum S.J. 2005. Final Report: Weekday/Weekend Differences in Ambient Concentrations of Primary and Secondary Air Pollutants in Atlanta, Baltimore, Chicago, Dallas-Fort Worth, Denver, Houston, New York, Phoenix, Washington, and Surrounding Areas, NREL Project ES04-1 NREL Subcontract No. LDX-4-44213-01

Fujita E.M, Stockwell WR, Campbell D.E., Keislar R.E., and Lawson D.R.. 2003a. Evolution of the magnitude and spatial extent of the weekend ozone effect in California's South Coast Air Basin. J. Air Waste Manage. Assoc. 53: 802-815.

Yarwood G., Stoeckenius T.E., Heiken J. G. , and Dunker A.M. 2003. Modeling weekday/weekend ozone differences in the Los Angeles region for 1997. J. Air Waste Manage. Assoc. 53: 864-875.

TCEQ. 2004, Revisions to the State Implementation Plan (SIP) for the Control of Ozone Air Pollution: HOUSTON/GALVESTON/ BRAZORIA OZONE NONATTAINMENT AREA, http://www.tceq.state.tx.us/implementation/air/sip/dec2004hgb_mcr.html