Influence of Increasing the Upper Boundary Ozone Concentration on Surface and Elevated Ozone for the April 1995 SAMI episode.

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Introduction

It was noted during the comparison of measured and modeled ozone for the April 24 – May 3 SAMI episode that the ozone at elevated sites was biased low. An example is given in the plot in figure 1 for Look Rock site in the GSMNP

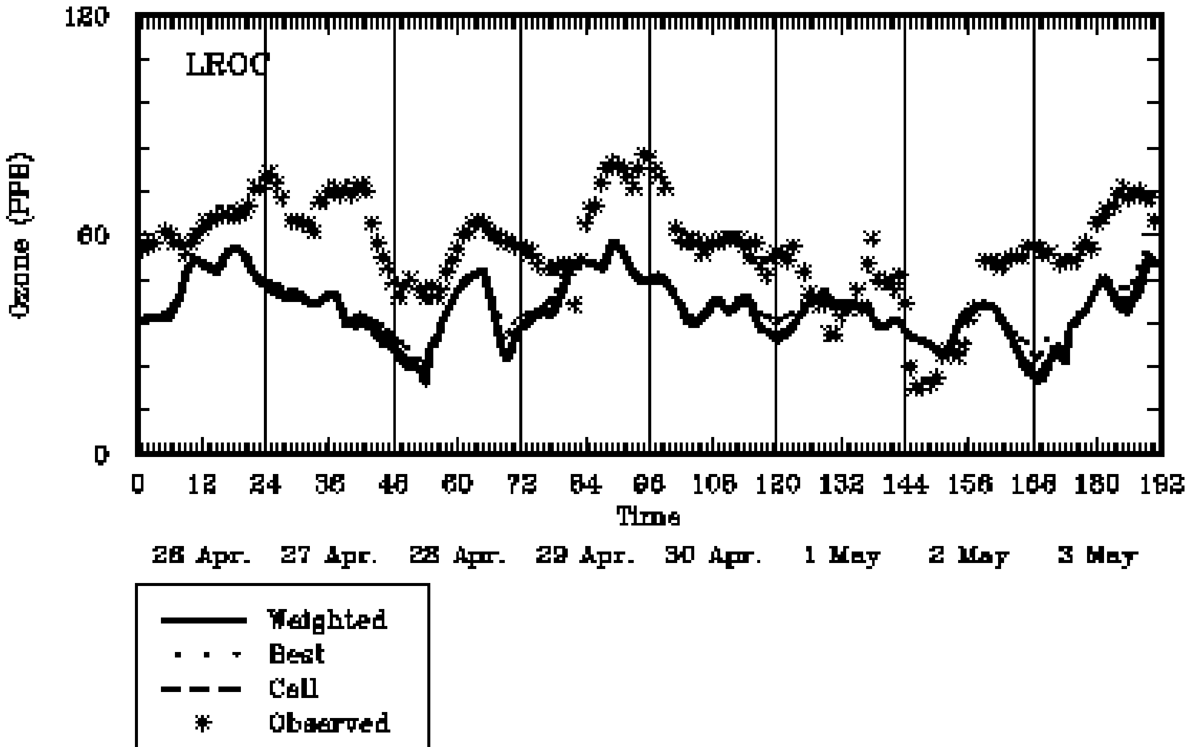

Figure 1. Times series comparison of surface modeled and measured ozone concentrations for the Look Rock site.

Other high elevation sites with significant negative ozone biases were Cove Mountain, Frying Pan, Clingman's Dome, and Big Meadows (through April 30). Lower elevation sites which had no significant negative bias included Washington DC, Nashville, Knoxville, and Sipsey. It was suggested by the SAMI Air Quality Modeling Working Group that two factors be examined to see if a significant improvement in ozone model performance could be obtained at these high elevation sites.

The first was to increase the ozone concentration at the upper boundary of the model from 33 ppb to 60 ppb. Although GIT had done this as a sensitivity test for the July 1995 episode and had seen minimal changes to ozone concentrations at the surface, it was thought that this could be episode specific. The second was to compare the modeled concentrations at layers above the surface to measured surface concentrations. Two factors could contribute to a negative bias in the modeled first layer concentrations at these sites. First, averaging the complex terrain to a 12 km grid size significantly reduces the peak height in the Appalachians thereby artificially lowering the modeled station elevation. Second, the flattening of the terrain and the coarseness of the meteorological simulation means that the complicated diabatic flows at night cannot be simulated.

Because a significant amount of time is required to extract time series for multiple layers from the model output, the approach taken in examining the effect of the two factors was to use the Look Rock site as a test site to study in detail.

Results

Increase of upper boundary ozone concentrations

Differences between the ozone concentrations between the normal and enhanced upper boundary ozone concentrations at the start of the simulation are plotted in figure 2. Layer 4 (494-1492 m) concentrations are plotted. This is the time with the most widespread differences between the normal and enhanced upper boundary ozone. A near uniform increase of 1.5 to 3 ppb occurs across the model domain. The reason for this is that the vertical profile of the initial conditions for ozone is being affected by raising the upper boundary concentration. The initial signal is rapidly damped, then sizable areas begin to have increased ozone of up to 6 ppb which arise and dissipate over periods of several hours. There is no apparent diurnal pattern to the appearance of these areas of increased ozone, though there does seem to be a preferred location – in the vicinity of the Appalachians, particularly at and just to the west. This may be an indication that terrain induced vertical velocities are playing a major role in the mixing of ozone from aloft down to the model's mid layers. It may also mean that convective activity is not playing a dominant role.

An example of the type of pattern observed later in the simulation is given in figure 3. This is the ozone difference field at 1800 on April 30, 1995 – 155 hours into the simulation. Most of the differences are less than 3 ppb, but a small area just to the east of Tennessee has up to 3 ppb.

Examining the increases in ozone concentrations for layers 1 through 4 over a single site, Look Rock, is another way of examining the impact of the enhanced upper boundary ozone. The results of this analysis are shown in figure 4. Layers 1-4 are affected similarly throughout the episodes except near the beginning (due to the initial increase in ozone concentrations aloft) and at the beginning of the day on May 3. As would be expected, the difference in ozone increases slightly with height – as we go from layer 1 to layer 4. Some small anomalies may be noted, as in the instance of the beginning of the day on May 1 when the layer 4 increase is less than the increase in the lower layers. Overall, the ozone increase in the lower 4 layers in the model is between 0.5 and 2.5 ppb, with an average increase in layer 4 of 1.3 ppb. This is not enough to make a significant difference in the ozone performance for the high elevation Look Rock site.

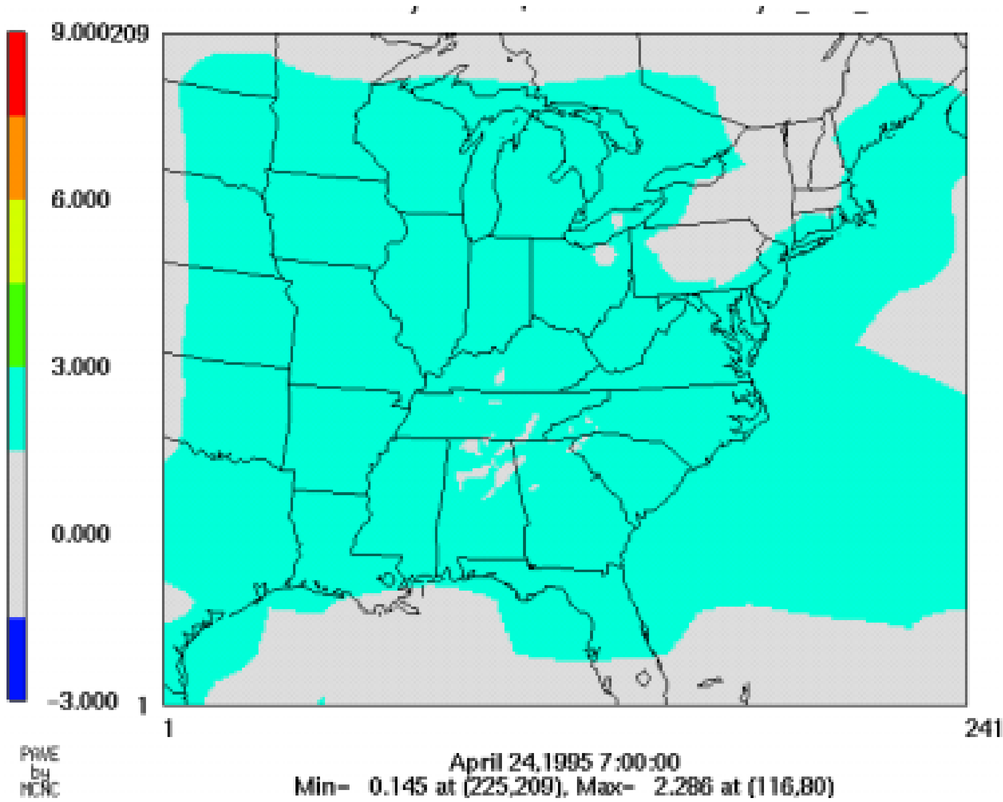

Figure 2. Increase in layer 4 (494-1493 m) ozone concentrations for the first hour of simulation due to enhanced upper boundary ozone concentrations.

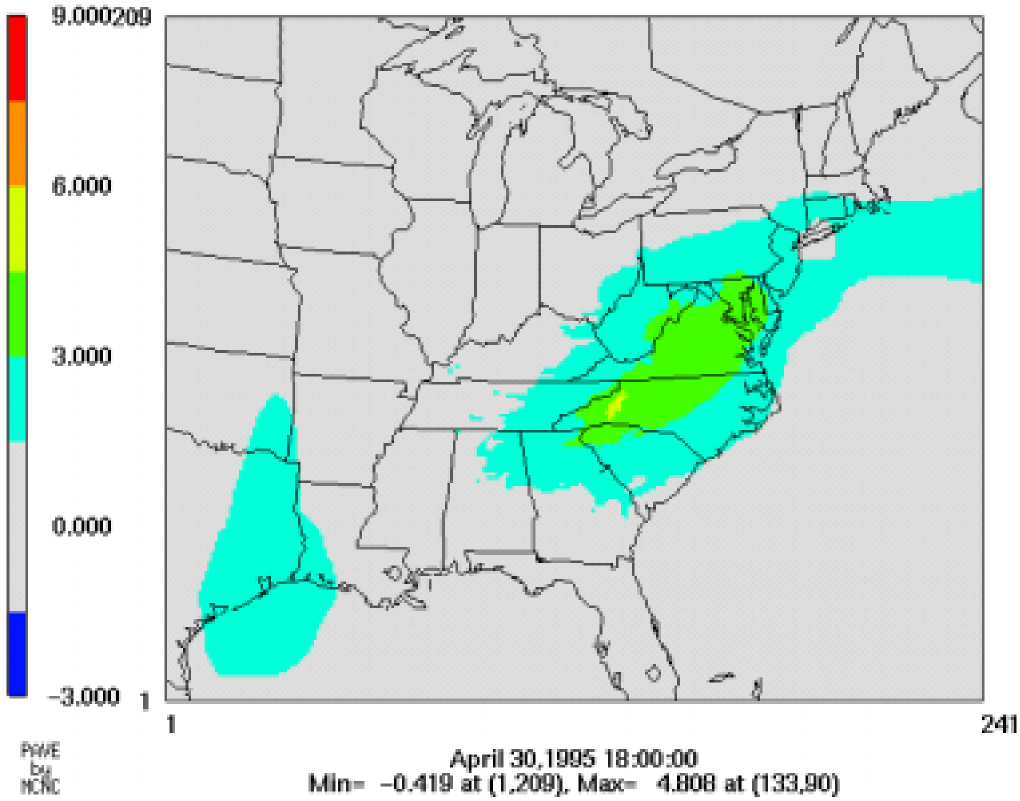

Figure 3. Increase in layer 4 (494-1493 m) ozone concentrations for the 155th hour of simulation due to enhanced upper boundary ozone concentrations.

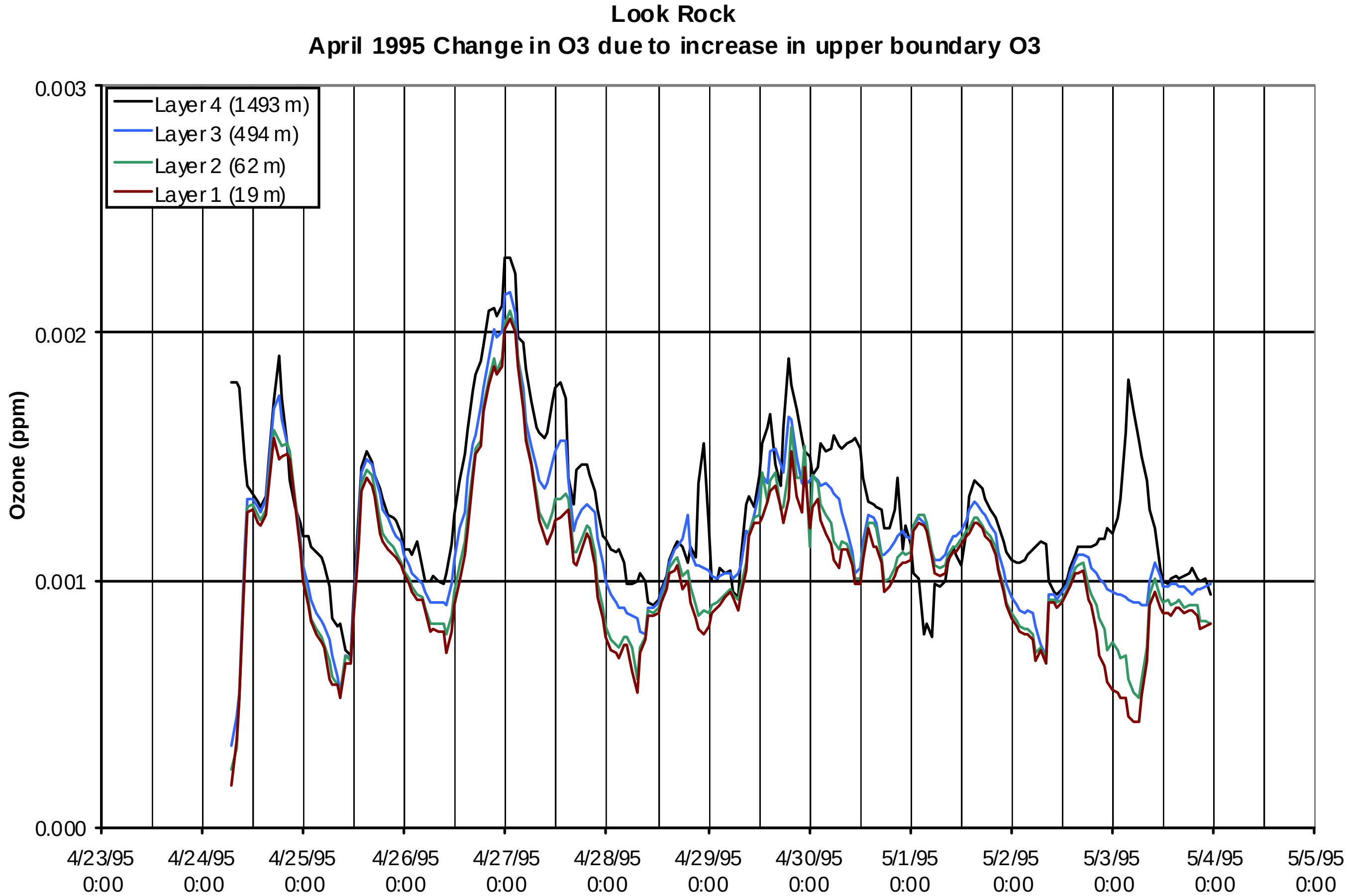

Figure 4. Increase in ozone for layers 1 through 4 due to enhancement of upper boundary ozone concentration

The second factor to examine was to see if the ozone in layers aloft might more closely match the measured ozone at high elevation sites. The site examined for this effect is Look Rock. From the analysis above, we know that increasing the upper boundary ozone will only increase the ozone in any of the first four layers less than 2.5 ppb. Thus the discussion below using the simulation with the enhanced upper boundary ozone concentrations can be applied to the normal upper boundary ozone concentrations as well.

Examination of the figure 5 shows that the layer 4 concentrations, while closer to the measured concentrations, are still substantially biased low. The average increase in concentration from layer 1 to layer 4 is 7.7 ppb. At night the difference between layer 4 and layer 1 tends to be higher than during the day.

Figure 6 is a diurnal plot of the ozone concentrations during the episode. The difference between layer 4 and layer 1 averages about 5 ppb during the day and 10 ppb at night. The measured ozone concentrations peak before 1900 with a significant decline beginning after 01:00 and not increasing again until after 11:00. The layer 4 ozone reaches its minimum at 07:00 and peaks at 1600. The amplitude of the variation is only 7 ppb for the modeled layer 4 concentration while the measured ozone varies by 16 ppb. The amplitude of the layer 1 modeled ozone concentration is 14 ppb. Statistically, the model's performance was better for layer 4. The normalized bias improved from negative 35% for layer 1 to negative 21% for layer 4.

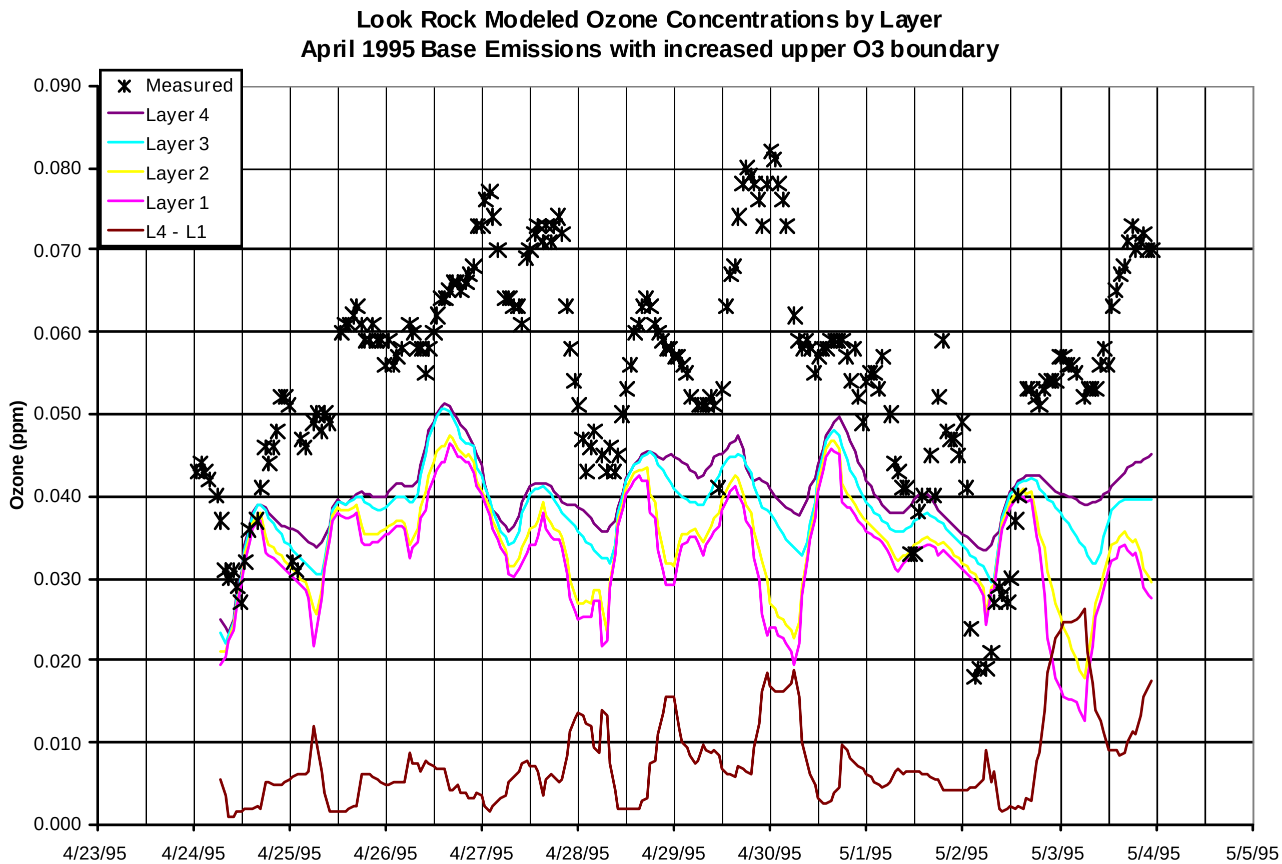

Figure 5.

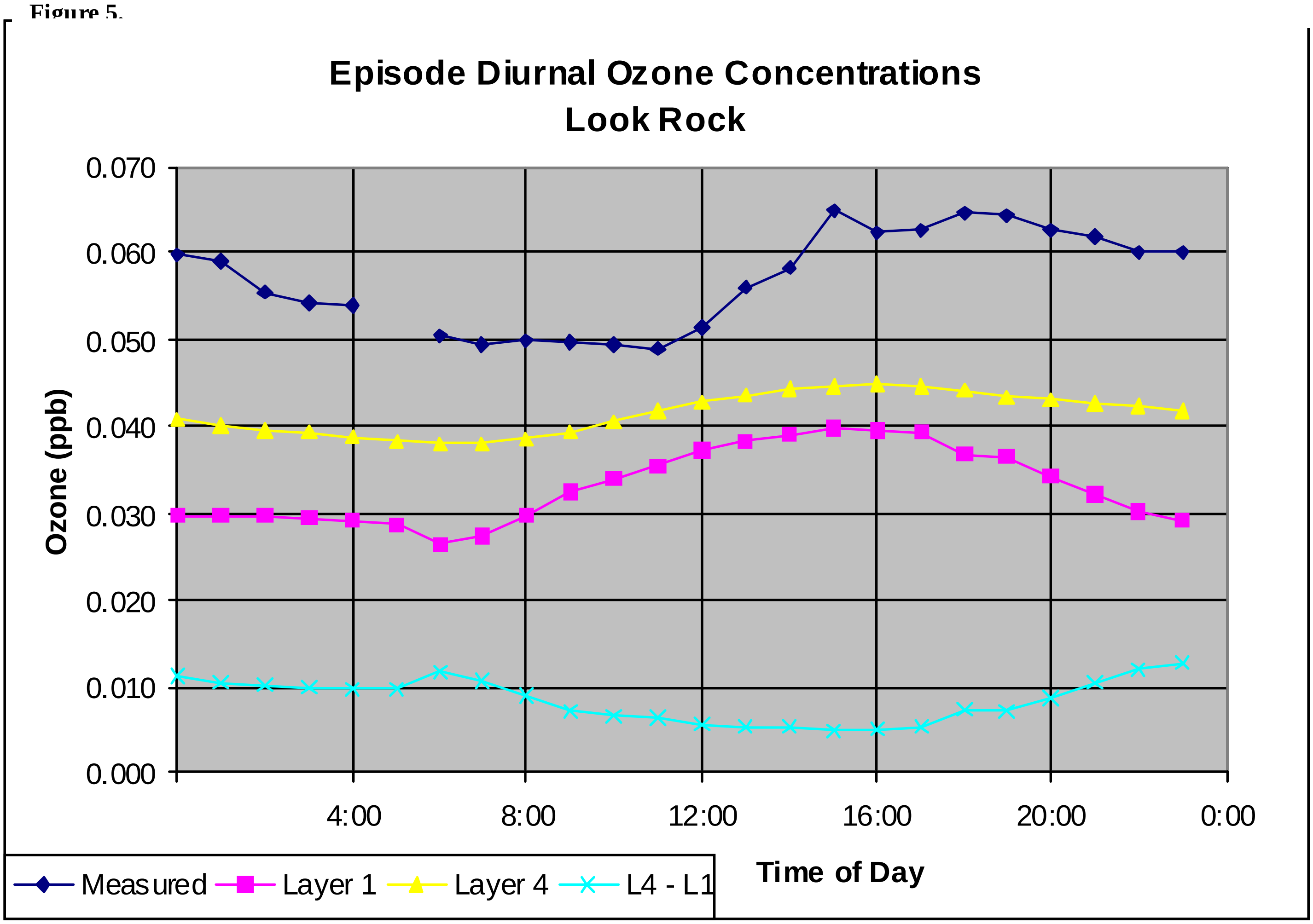

Figure 6.

Conclusions

Increasing the upper boundary ozone concentrations from 33 to 60 ppb has a minimal effect on ozone concentrations within the first four layers for a simulation of the April 1995 base case. The maximum ozone increase at any time or layer at the Look Rock location was less than 2.5 ppb.

Using the modeled ozone concentrations for layers above the surface for high elevation sites does improve the ozone performance. The normalized bias improved from negative 35% to negative 21%. The range of diurnal variation was too little when comparing layer 4 to modeled concentrations at Look Rock. At other, even higher elevation stations, the diurnal comparison could compare better. It may be scientifically justifiable to use concentrations from layers aloft for high elevation sites, but a more thorough investigation, looking at the processes involved is advisable. Even if a decision were made to take this approach for SAMI, all episodes would need to be treated in the same manner. SAMI should not make such a modification for one or two episodes.