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USE OF NUMERICAL OZONE PREDICTION MODELS IN OPERATIONAL AIR QUALITY FORECASTING

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1. INTRODUCTION

Recent advances in chemistry and meteorology models and computational efficiency have allowed the operational use of coupled chemistry-transport models (CTM) by local air quality forecasters. The adoption of numerical model guidance by operational forecasters, the number of whom has been increasing rapidly in the past several years, depends on the reliability of numerical model guidance in critical high ozone (O_3) cases. In turn, routine use of these models by forecasters can result in a positive feedback of information to model developers to further improve model performance.

This paper presents a first step in utilizing air quality forecast models as part of routine forecasting procedure. A high O_3 episode from 2001 is analyzed with respect to the utility of numerical forecast guidance in forecast preparation for the Philadelphia metropolitan area.

2. NUMERICAL FORECAST MODEL

The CTM used in this study is the MAQSIP-RT (Multi-Scale Air Quality Simulation Platform – Real Time) (McHenry, et al., 2000; McHenry et al., 2001). The North Carolina Supercomputing Center (NCSC) and the Pennsylvania State University (PSU) developed the initial operational version of this model as part of the joint Numerical Air Quality Prediction (NAQP) Project. It is currently operated as part of the South East Center for Mesoscale Prediction (SECMEP), a consortium of academic, public and private institutions. More details on the model, its operation and its current configuration are available at: http://www.emc.mcnc.org/projects/SECMEP.

The meteorological model is the PSU-NCAR MM5 version 3.4 (Grell et al., 1994). As configured during summer 2001, the MM5 used the Kain-Fritsch deep convection scheme (Kain and Fritsch, 1993) and a simple water/ice explicit moisture scheme (Dudhia, 1989). The soil model used was the default "slab" model with 5-layer heat diffusion. (Dudhia, 1996). The NCEP Eta model was used to initialize the MM5 with a 6 hour dynamic initialization of temperature, mixing ratio and wind components using analysis nudging except near the surface. The MM5 was configured with two domains using one-way nest interaction. The coarse grid covers most of North America at 45 km grid spacing (96 X 132) and the finer grid covers the eastern two-thirds of the United States at 15 km grid spacing (190 X 184). Typically the finer grid is spawned 6 hours into the coarse grid run, after spin up, with no nudging within the fine grid. There are 31 vertical layers in the model with 12-15 layers typically within the planetary boundary layer (PBL). The PBL scheme is the MRF-PBL (Hong and Pan, 1996). While there are a variety of PBL schemes available to the MM5 (e.g., Gayno et al., 1994; Burk and Thompson, 1989), the MRF-PBL is computationally very efficient and compared well in test runs. There appears to be a slight bias toward higher PBL heights with the MRF-PBL scheme. The newly developed shallow convection scheme is not used in the operational version (Deng et al., 1998).

During summer 2001, MAQSIP-RT used a modified Carbon Bond IV chemistry mechanism (Gery et al., 1989) along with the Bott flux form advection scheme (Bott, 1989). Dry deposition and clear sky photolysis rate calculations used mechanisms quite similar to the Regional Acid Deposition Model (RADM) (Chang et al., 1987). Vertical turbulent distribution of pollutants were determined using a K-theory scheme with predicted PBL heights provided by the MM5. Emissions were provided by the Sparse Matrix Operator Kernel Emissions (SMOKE) (Coats, 1995).

3. AIR QUALITY FORECASTING

Routine public air quality forecasts in the mid-Atlantic region began in the mid-1990's. The forecasts are issued to the public in the form of color codes ranging from "Code Green" (good air quality) to "Code Red" (unhealthy air quality). The forecast programs provide health advisories and warnings as well as activations of "Ozone Action Days" (OAD). The OADs are voluntary pollution control efforts

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undertaken by a public-private partnership including government organizations and large employers. When “Code Red” forecasts are issued, the OAD partners initiate a series of pollution control efforts. These include free public transportation and the curtailment of certain industrial processes. The threshold for OAD activation varies from location to location. Within the major cities of the mid-Atlantic region, the threshold for “Code Red” is typically the 1-hour National Ambient Air Quality Standard (125 ppbv) or 8-hour average concentrations in excess of 100 ppbv.

Air quality forecasts are issued daily near 1800 UTC and are valid the following day. The forecasts in the mid-Atlantic specify a peak concentration within the given metropolitan area. Although observed O_3 concentrations often show strong local gradients, there is no effort to specify the location of peak O_3. This is due to several factors including: irregular spacing of verification monitors, lack of confidence in locating peak locations, particularly in the vicinity of land-sea boundaries, and the fact that upwind locations, while lower in O_3, contribute precursors to downwind locations. Control programs, such as OADs, are only effective if applied to both upwind and downwind sources.

At the time public forecasts were first issued, numerical model guidance was not routinely available. Air quality models were only utilized for the simulation of historic episodes in support of regulation and planning. The CTMs of that time were computationally too demanding, relative to then available computing resources, to be run in near-real time. The computational requirements of CTMs are higher than standard meteorological models due to the incorporation of emissions and chemical reaction models that require solutions on very short time and space scales. Pending the development of accurate numerical forecasts, forecasters used statistical models for guidance (Ryan, et al., 2000). A variety of statistical approaches have been utilized (e.g., Comrie, 1997; Cobourn et al., 2000; Liu and Johnson, 2002). Statistical models relate meteorological variables and peak O_3. In particular, temperature, wind speed, sky cover, stability and previous day peak O_3 concentrations are good predictors of peak O_3. For the Philadelphia area, 77% of the variance in historical peak O_3 concentrations can be explained using a small set of meteorological predictors (Ryan, 2002a).

The skill of statistical forecast guidance in operational use is generally adequate. For the Philadelphia metropolitan area in 2001, median absolute forecast error for the set of three statistical models in use was 9.8-12.5 ppbv with root mean square (rms) error of 15.8-18.9 ppbv. This represents an improvement in skill of 34% over the benchmark persistence forecast. As O_3 concentrations are strongly auto-correlated on short time scales, the persistence forecast is a robust benchmark measure. The statistical models performed better in the higher end of the observed O_3 distribution with rms error decreasing to 9.8-13.7 ppbv for cases of observed O_3 in excess of 100 ppbv. However, the statistical models achieve this increase in skill at the cost of more frequent false alarms of higher O_3. This is due, in part, to the strength of the temperature predictor. The critical forecast skill in warm weather cases, therefore, is to determine in which cases the model guidance can be assumed accurate. In a number of cases, the difference is the regional, or upwind, concentrations of O_3 and its precursors. This parameter is poorly resolved by statistical models but could, in principle, be better resolved by a regional scale numerical model.

Forecasts issued to the public use statistical guidance modified by local forecasters to account for factors not fully resolved by statistical models (Ryan et al., 2000). These include, among other factors, regional transport of O_3 and its precursors, and the timing and extent of convection and precipitation. For the 2001 season, modified forecasts improved on regression guidance by 24-32% (rms error). Forecasts of “Code Red” cases have historically been quite good with a probability of detection (Philadelphia, 1996-2002) of 0.80 and a Pierce skill score, also known as the “true skill statistic” of 0.74 (Stephenson, 2000). However, a large number of observed “Code Red” cases (46%) were “missed” by the forecast. In all but a handful of cases, a forecast of “Code Orange” was issued for these cases. The Code Orange forecast, similar to a “watch” forecast, includes a health advisory but no OAD programs are initiated. A numerical forecast model has the possibility of providing improvement in these cases.

4. THE AUGUST, 2001 OZONE EPISODE

The high O_3 episode of early August 2001 followed an extremely cool July characterized by a persistent trough over the eastern U.S. and low O_3 concentrations (Ryan, 2002b). The August episode, like most high O_3 episodes in the eastern U.S., featured an upper level ridge just west of the region (Figure 1) with transport of O_3 and its precursors from west to east (Figure 2) (Ryan et al., 1998). During the course of this episode, a variety of synoptic and mesoscale phenomena made for challenging local forecasts. These included changes in air mass characteristics driven by rapid changes in low level wind fields, the presence of a dissipating frontal boundary and widespread prefrontal convection near the end of the episode.

The onset of high O_3 on August 1st was associated with surface high pressure centered over the mid-Atlantic. The MAQSIP-RT well analyzed the location of the highest O_3 concentrations and reduced the over-prediction of the statistical guidance in the range of 3-9 ppbv. The utility of the numerical model with respect to changes in air mass characteristics is seen on August 2. On this day, although temperatures remained warm throughout the region, there was a shift in the location of peak O_3 as the center of high pressure moved just offshore (Figure 3). The MAQSIP-RT accurately located the movement of the plume of high O_3 and anticipated the influx of cleaner maritime air over the southern mid-Atlantic. In Philadelphia, MAQSIP-RT improved on statistical guidance in the range of 27-34 ppbv (Figure 4). A short wave crossed north of the mid-Atlantic on August 3rd. The presence of a frontal boundary along with a pre-frontal trough made for a complex weather situation. The statistical and numerical models slightly over-predicted peak O_3 on this day with the MAQSIP-RT accurately locating a small band of higher O_3 west of the I-95 Corridor (Figure 5). As the front stalled over central PA on August 4th, MAQSIP-RT strongly over-predicted peak O_3 south and east of the boundary. This appears to result from the failure to forecast the extent of cloud cover that formed and persisted ahead of the frontal boundary (Figure 6).

No MAQSIP-RT run was available on August 5th. Regional O_3 levels began to rise on this day as the frontal boundary washed out over PA. A stagnant air mass increased local O_3 far in excess of statistical guidance with peak concentrations reaching the Code Orange range. Temperatures rose sharply on August 6th with heat advisories issued for many locations in the mid-Atlantic. Numerical forecast guidance was poor for the region south of NYC on this day. One factor driving poor performance was the initial chemistry fields. In 2001, MAQSIP-RT initial chemistry was “self cycled” from the 12-hour forecast of the previous model run. When the prior run is missing, as on August 6th, the model reverts to the next available forecast run up to 48 hours distant. In a case of rapidly rising regional O_3, such as occurred on August 5-6, the reversion to older model runs can induce large errors in initial conditions. This problem was addressed in 2002 through ingesting real-time O_3 observations each day from the EPA AIRNOW program (see, http://www.epa.gov/airnow).

The highest O_3 concentrations occurred in the August 8-9 period. The MAQSIP-RT was quite successful in predicting the magnitude of the peak O_3, improving on regression guidance on the order of 5-9 ppbv. The episode ended on August 10th as pre-frontal convection crossed the region (Figure 7). Deep convection can rapidly decrease O_3 concentrations. As a result, the timing and extent of pre-frontal convective activity has often been a source of forecast error. In this case, O_3 concentrations briefly reached Code Red levels at widely scattered locations in the mid-Atlantic in advance of convection. The MAQSIP-RT, while under-predicting peak O_3 did improve on regression model performance by 5-17 pbbv.

5. DISCUSSION

The high O_3 episode of 1-10 August contained a variety of flow conditions and synoptic and mesocale features that made it a good episode for testing the usefulness of a numerical model on the metropolitan scale. The weather conditions encountered included rapid reversals in flow leading to markedly different background O_3 concentrations (August 1-3). Stagnant flow regimes in the context of dissipating frontal boundaries were also encountered (August 4-6) followed by a standard westerly transport high O_3 period (August 7-9) concluding with a pre-frontal convection case (August 10). Taken as a whole, these cases cover the gamut of challenging high O_3 forecasts encountered in this region.

The measure of forecast skill adopted here is that generally used by metropolitan-wide O_3 forecasts: peak 1-h O_3 concentrations. This standard reflects the criteria adopted for the national ambient air quality standard and is suitable for OAD programs that depend on metropolitan wide adoption for their effectiveness. On the other hand, this measure is not particularly appropriate for the evaluation of a numerical forecast model (Hanna et al, 1996; Tesche et al., 1990) and poses a fairly stiff test. For example, peak O_3 concentrations can vary significantly on the scales of 10’s of km, particularly near land-sea interfaces, and may not be fully resolved by gridded forecast models. In addition, the current monitor network used for forecast verification does not fully resolve O_3 on this scale. Still, for a model to be adopted by operational forecasters, it must show reasonable skill at this measure of interest.

For the August 1-10 period (excluding August 5 when no model fields were available) the median absolute error for the Philadelphia forecast area for the MAQSIP-RT was 7.3 ppbv with a mean absolute error of 12.1 ppbv. A large portion of the mean error (25%) was associated with the forecast for August 6th. The statistical models had median absolute errors ranging from 9.6-12 ppbv and mean errors of 11.5-12.9 ppbv. The modified forecast issued to the public carried a mean error of 8.0 ppbv. Overall performance of the MAQSIP-RT, even on this more stringent measure, was quite good. Its forecasts verified and at or better than the current benchmark techniques during this episode.

As noted above, the MAQSIP-RT was quite successful tracking air mass changes and the onset of deep convection – two outstanding problem with local air quality forecasts. Certain shortcomings of the model were also found. In the vicinity of a weak frontal boundary on August 4, the model failed to accurately represent the observed cloud cover leading to over-prediction. Additionally, the MAQSIP-RT also did not adequately increase O_3 levels during the onset of the highest period of the episode (August 6-7). The under-prediction on August 6th may be due, in part, to the "cold start" of the model following the missing forecast of August 5. The under-prediction on August 7th appears to be due, in part, to continued under-predictions of upstream O_3 concentrations. The forecast for August 6th under-predicted O_3 on the order of 10-30 ppbv across central PA. Analysis back trajectories suggest that this region was the source for the following day (Figure 2).

An additional feature of interest for the MAQSIP-RT is the repeated appearance of local "spikes" in O_3 concentrations along the downwind side of bay-land boundaries. In the mid-Atlantic, this typically occurs along the eastern shore of the Chesapeake Bay and also in locations along the New Jersey side of the Delaware Bay. This feature is present on both August 7 and August 8 and similar effects were seen early in the 2002 forecast season on July 2 (Figure 8). As the spikes are located outside the Philadelphia forecast area, they posed no difficulty with forecast performance but did affect forecast skill in the Baltimore-Washington area. These spikes are a result of the collapse of modeled PBL heights in coastal zones as very warm air is advected over cooler water surfaces. In coastal zones where there are large near-by sources of O_3 and precursors (e.g., Chesapeake Bay and Boston Harbor), the collapse of the PBL results in a trapping and "cooking" of polluted air leading to rapid increases in O_3 concentrations. This effect was significantly reduced in early July, 2002 by improvements in land-sea masking capabilities and the use of default PBL heights along the offending boundaries.

6. CONCLUSION

The MAQSIP-RT, when used in support of metropolitan scale O_3 forecasts, provides skillful forecasts of 1-hour peak O_3 concentrations during extended high O_3 episodes in the mid-Atlantic region. The results from the MAQSIP-RT are consistent with, and in some cases, improve on benchmark measures from standard statistical models and have the capability of further improvements. The skill of the MAQSIP-RT over a longer period (July-August, 2002) is currently being investigated.

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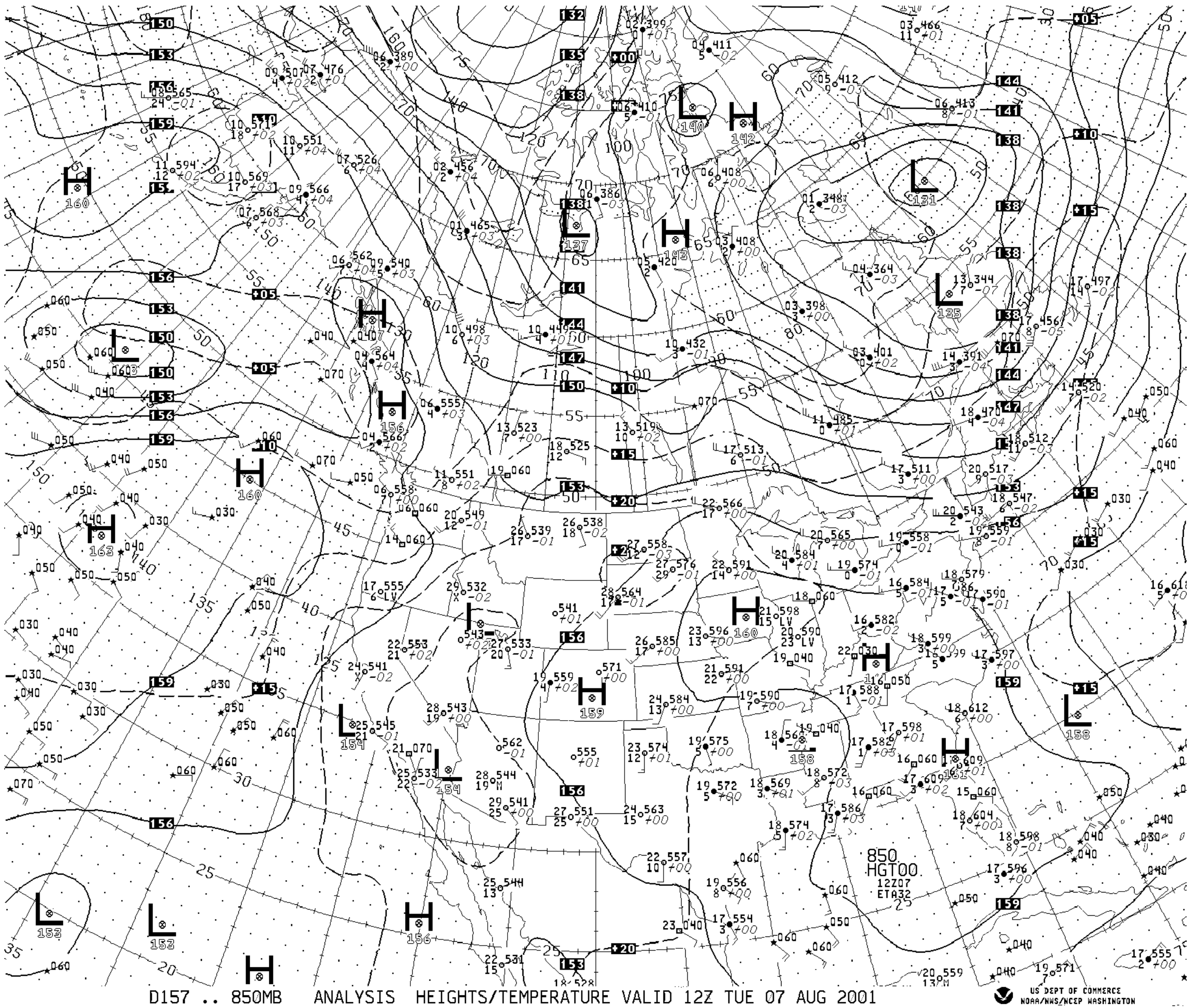

Figure 1. 850 mb analysis, prepared by NCEP, for 1200 UTC on August 7, 2001. Solid contours are geopotential heights in dm, dashed contours are temperature in Celsius. Station data follows the standard convention.

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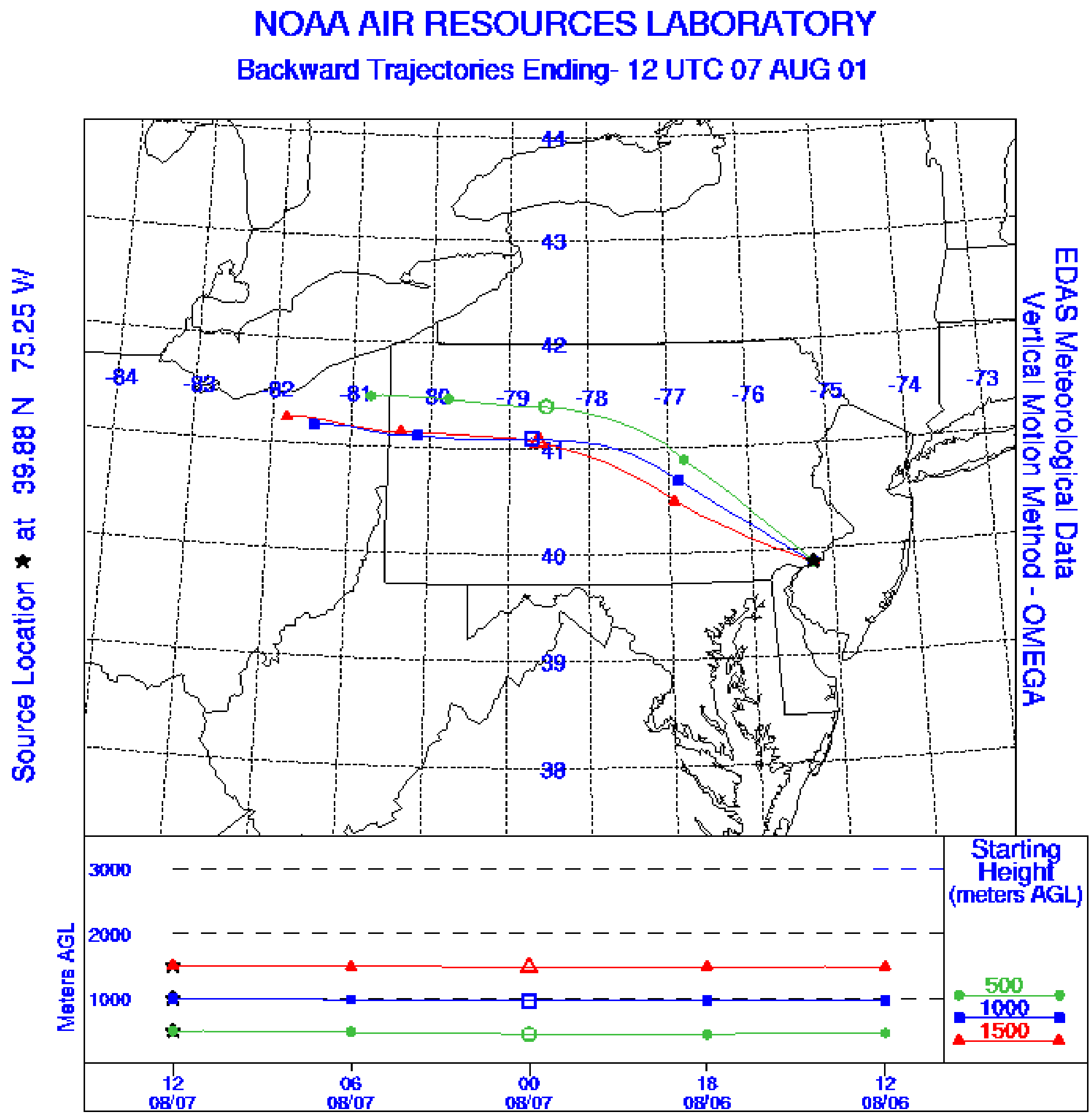


Figure 2. Back trajectory analysis for Philadelphia valid 1200 UTC August 7, 2001. Trajectories prepared using the NOAA-Air Resources Laboratory HYSPLIT-4 back trajectory model (HYSPLIT, 1997). The model is initialized at three vertical layers (500, 1000 and 1500 m agl) at 1200 UTC on August 6, 2001 and utilizes the Eta Data Assimilation System (EDAS) for meteorological inputs.

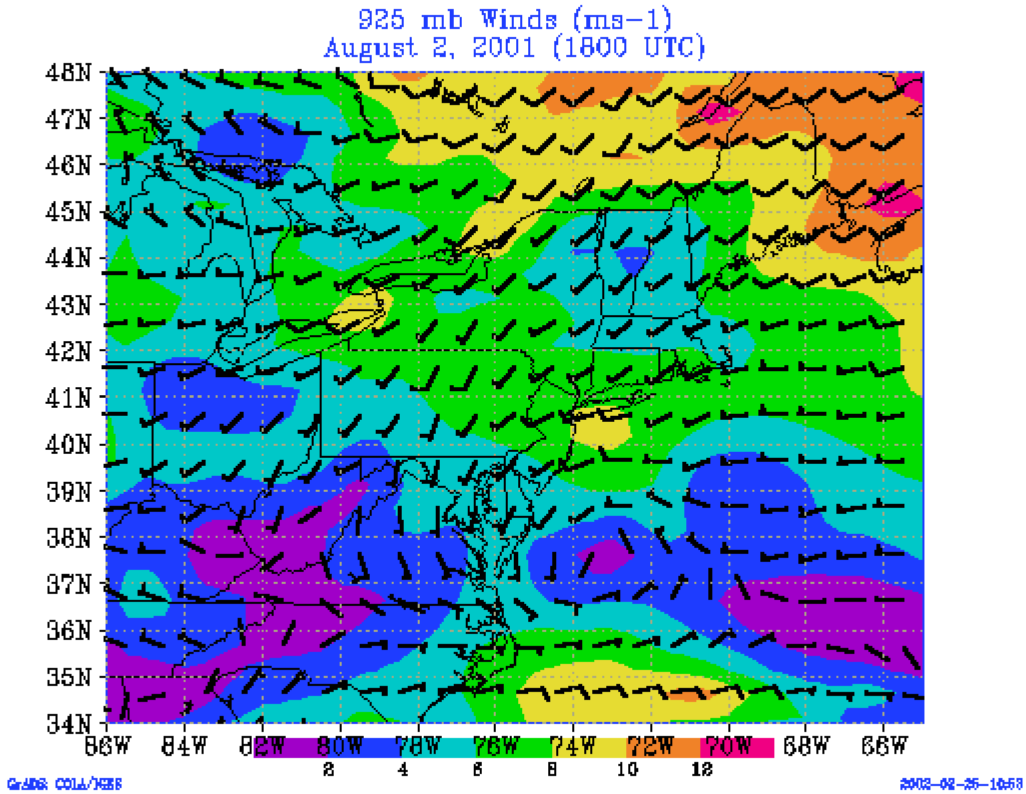
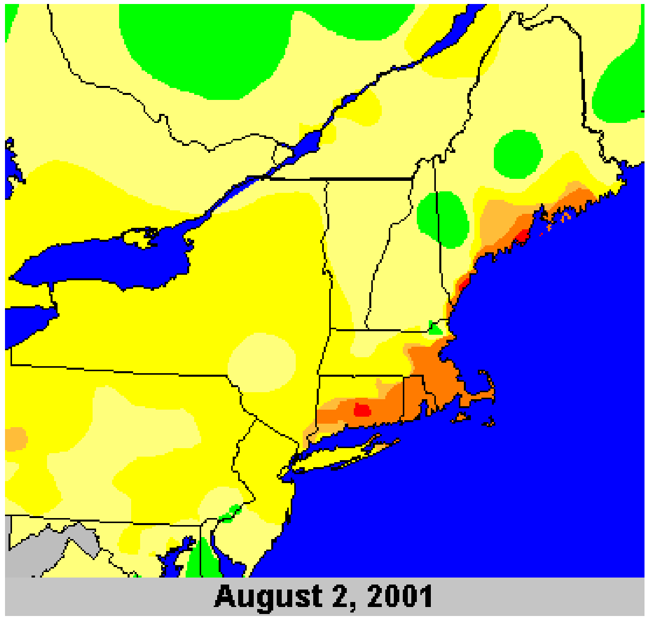


Figure 3. 925 mb winds from the EDAS for 1800 UTC on August 2, 2001. Contours are wind speed in meters per second and wind barbs denote wind direction using the standard convention.



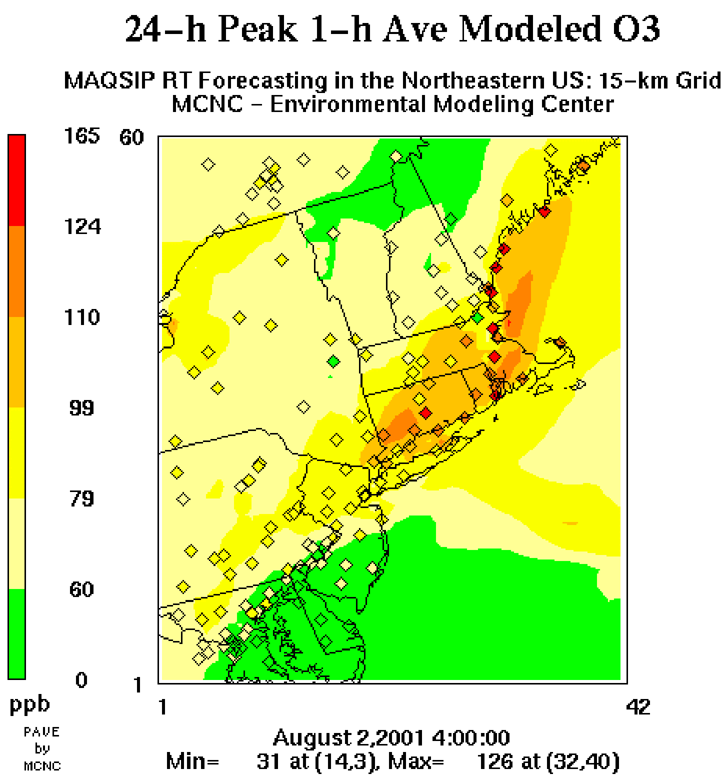


Figure 4. Observations (top) and modeled (bottom) average 1-hour peak O_3 concentrations (bottom) for August 2, 2001. Color contours are as follows: Green (0-60 ppbv), light yellow (61-79 ppbv), yellow (80-99 ppbv), light orange (100-110 ppbv), dark orange (111-124 ppbv) and red (≥ 125 ppbv). Further details on the ozone mapping system can be found at: http://www.epa.gov/airnow.

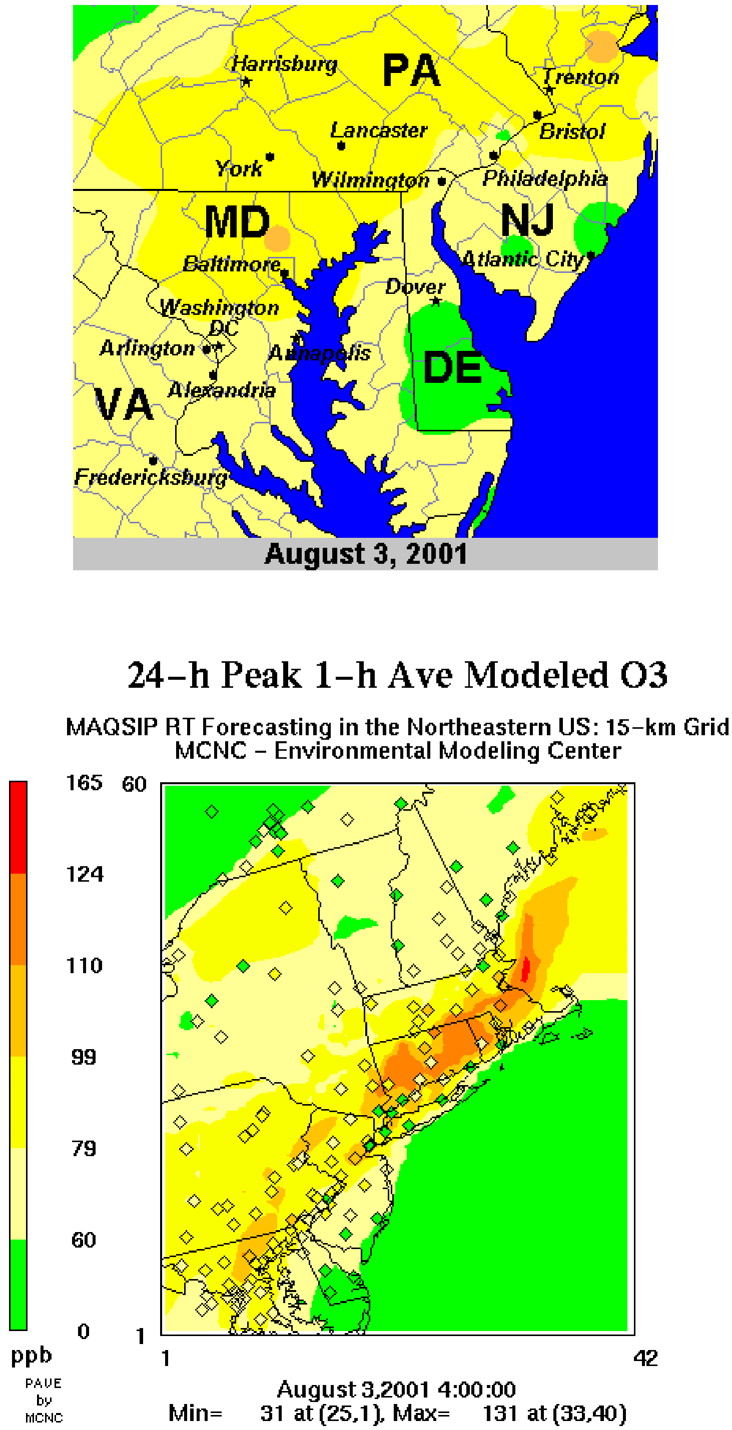


Figure 5. As in Figure 4 but for August 3, 2001.

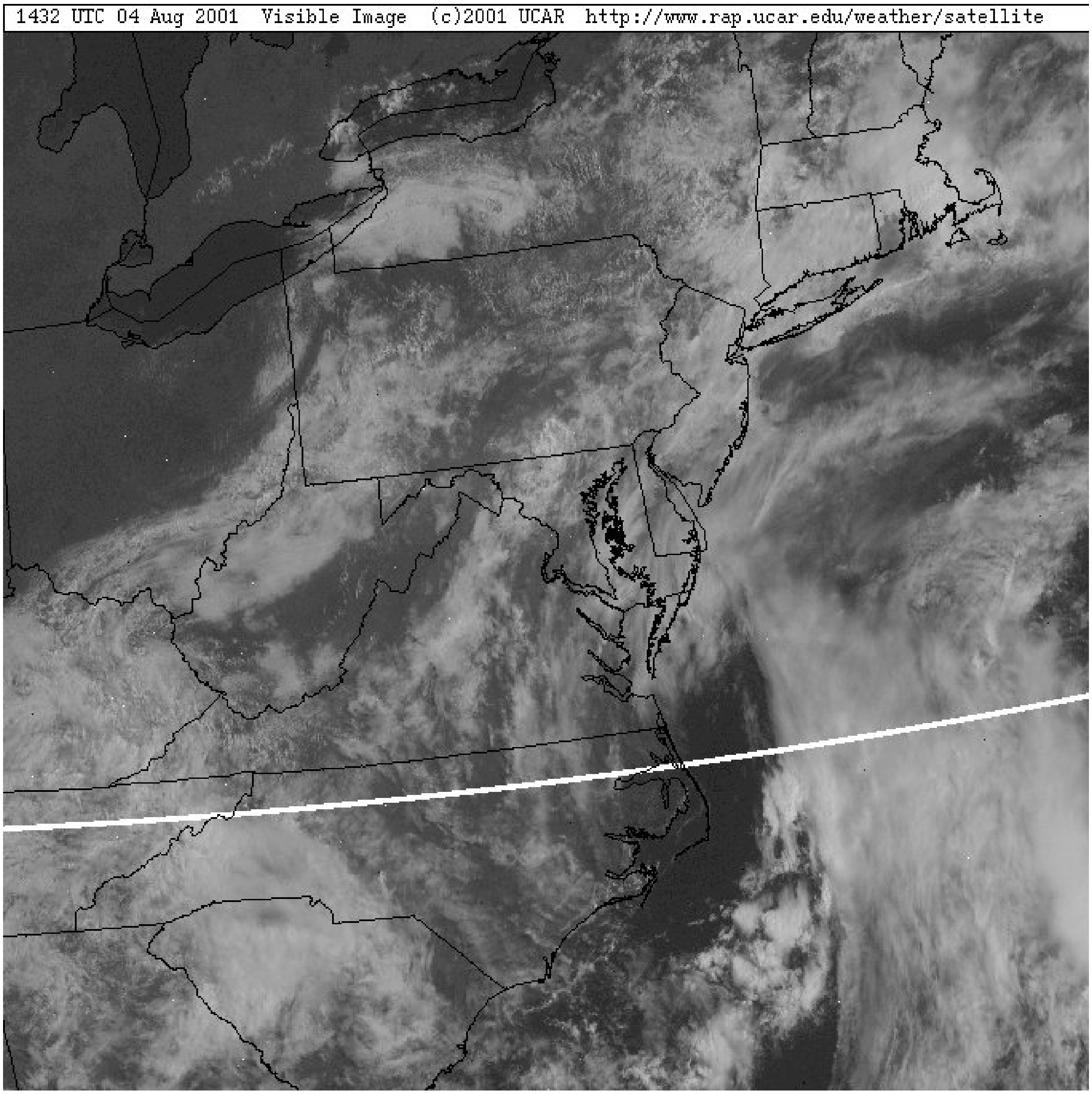


Figure 6. High resolution GOES-8 visible image for 1432 UTC on August 4, 2001.

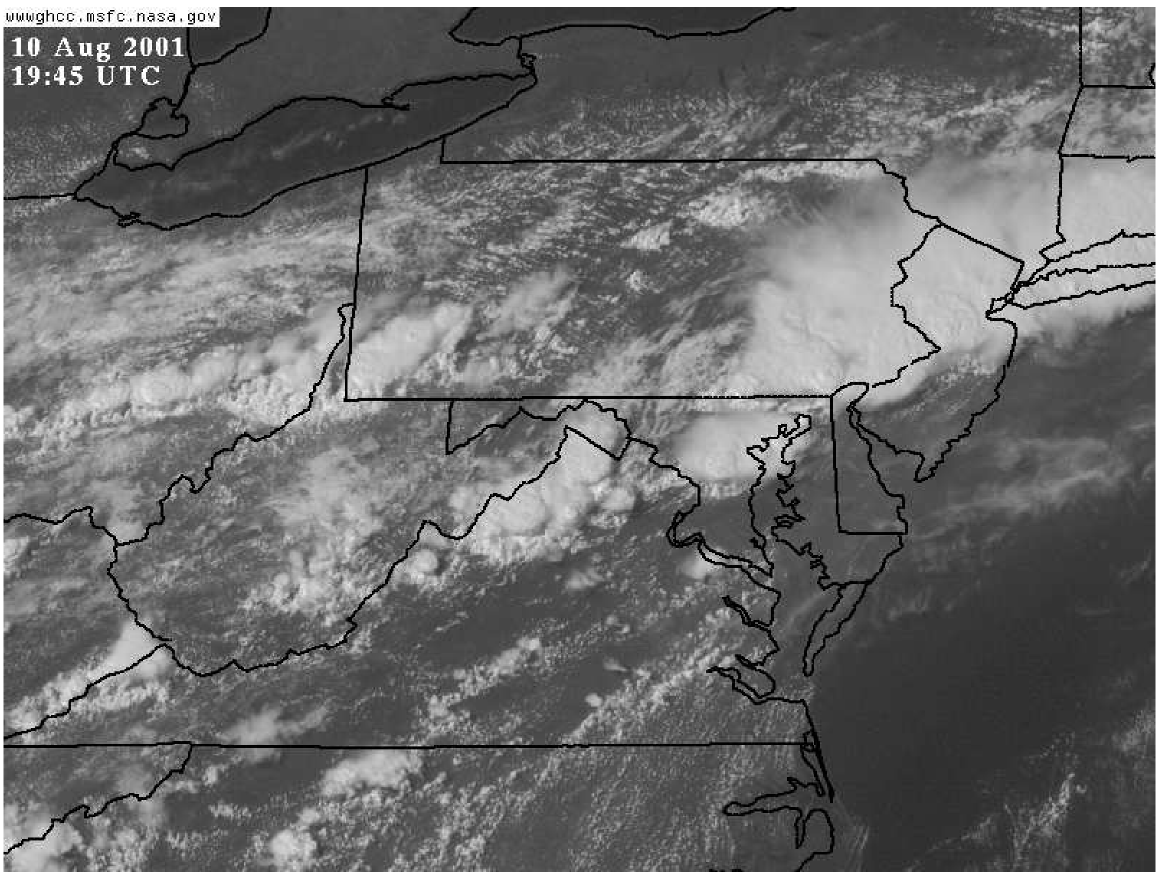


Figure 7. As in Figure 6 but for 1945 UTC on August 10, 2001.

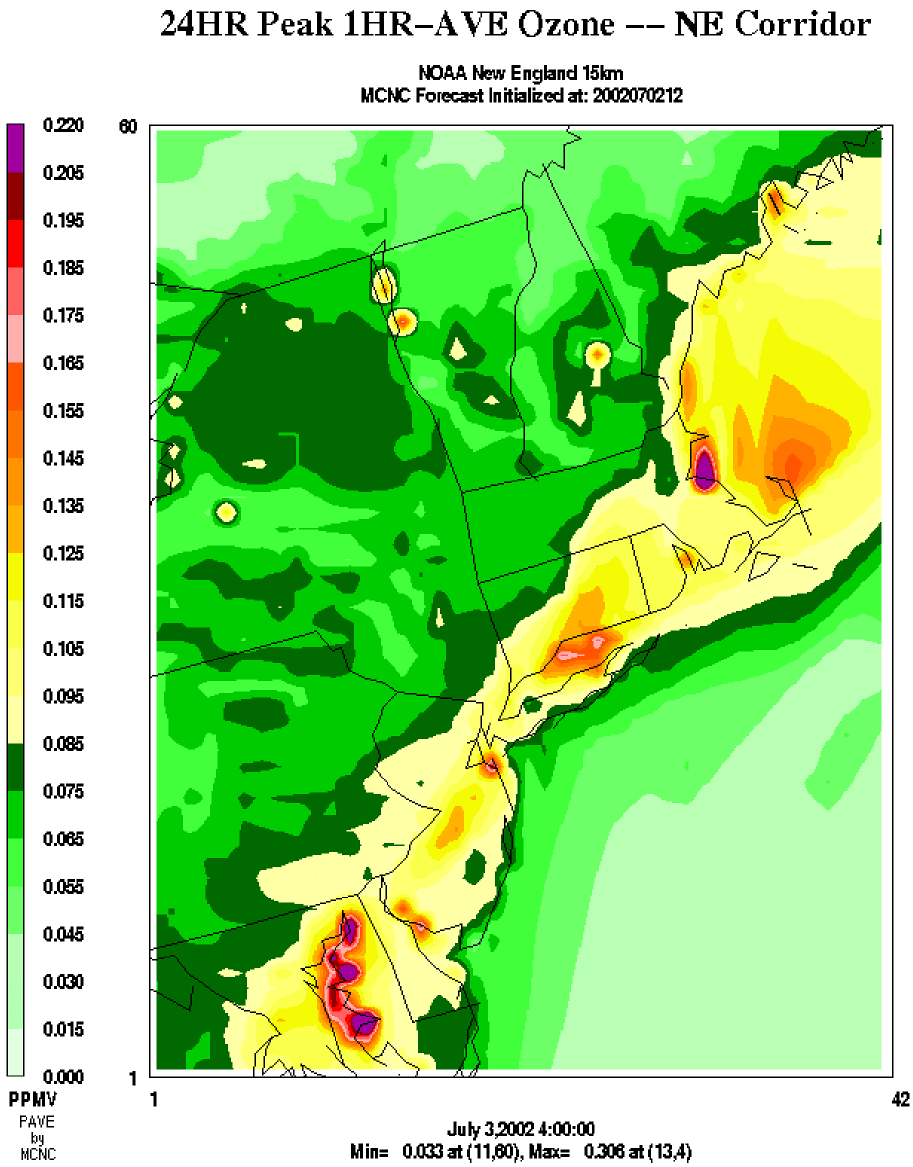


Figure 8. Peak 1-hour O_3 forecasts from the MAQSIP-RT 15 km domain for July 2, 2002.