N95- 10612

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MODELING OZONE EPISODES IN THE BALTIMORE-WASHINGTON REGION

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ABSTRACT

Surface ozone (O_3) concentrations in excess of the National Ambient Air Quality Standard (NAAQS) continue to occur in metropolitan areas in the United States despite efforts to control emissions of O_3 precursors. Future O_3 control strategies will be based on results from modeling efforts that have just begun in many areas. Two initial questions that arise are model sensitivity to domain-specific conditions and the selection of episodes for model evaluation and control strategy development. For the Baltimore-Washington region (B-W), the presence of the Chesapeake Bay introduces a number of issues relevant to model sensitivity. In this paper, the specific questions of the determination of model volume (mixing height) for the Urban Airshed Model (UAM) is discussed and various alternative methods compared. For the latter question, several analytic approaches (cluster analysis and classification and regression tree (CART) analysis) are undertaken to determine meteorological conditions associated with severe O_3 events in the B-W domain.

1. INTRODUCTION

Many major metropolitan areas in United States have been unable to comply with the NAAQS for O_3 set by the Clean Air Act (CAA). Many explanations have been advanced for this (1) failure to reduce emissions to extent proposed (rule efficiency); (2) underestimation of emissions, including biogenic emissions, and errors in the speciation of hydrocarbons; and (3) overly simplistic modeling approaches which have overestimated the effectiveness of proposed control strategies (*National Research Council, 1991*).

The 1990 amendments to the CAA mandate further use of photochemical modeling to demonstrate that control strategies will result in the future attainment of the O_3 NAAQS. This paper will provide a brief overview of the photochemical model in use in the B-W domain, the UAM, as well as critical U.S. Environmental Protection Agency (EPA) recommendations configuring the UAM for regulatory use. In addition, model sensitivity questions that have a domain-specific facet will be discussed along with the selection of historical O_3 episodes for modeling.

2. THE URBAN AIRSHED MODEL

The UAM is presently the only EPA-approved three-dimensional photochemical model for O_3 regulatory modeling. The UAM was first developed for use in the Los Angeles Basin (*Reynolds, et al., 1973*) and the 1988 edition is in use in the B-W domain (*Morris et al., 1990*). In order to efficiently manage the numerous evaluation and control strategy model runs that are required, the input and archival processes are controlled by a software shell specially developed for the UAM (*Batch Processing System (BPS), John Haus*).

The UAM is a gridded Eulerian model, with three-dimensional cells having fixed horizontal and variable vertical dimensions. The vertical layers vary in space and time as a function of the height of the planetary boundary layer (PBL), generally referred to in UAM studies as the "mixing height". The UAM simulates spatially varying transport, diffusion, chemical transformation, deposition and emissions distributions within an area by solving the governing equations for particular processes. Atmospheric constituents are dispersed evenly within each cell. Surface removal is parameterized by deposition velocity which depends, generally, on surface concentration, roughness and type. The 1988 version of the UAM was updated to include the Carbon-Bond Mechanism IV (*Gery, Whitten and Killus, 1985*) and the Smolarkiewicz algorithm for the numerical approximation of horizontal advection terms in the species conservation equations.

The size of the domain (*Figure 1*) is determined by the expected distance that local emissions will be transported during an average day (*EPA, 1991*). This reflects the relatively slow process of photo-chemical O_3 production. The B-W domain is 250 km north-to-south and 230 km east-to-west and contains several unique aspects (1) the Chesapeake Bay dominates the center of the domain and introduces discontinuities in the surface heating and surface roughness fields; (2) the domain includes two urban cores and four states which introduces difficulties in emissions inventory development and model initialization; and (3) the extension of the domain boundaries to the north, to include portions of Greater Philadelphia as well as the Atlantic coast, introduces boundary condition problems.

The EPA recommends that the grid cells be no larger than 5 x 5 km. The UAM grid size can be varied to reflect emissions gradients and density and should bear some association to the resolution of the input data. The resolution of meteorological data, of course, is much coarser than 5 x 5 km and air quality data resolution can vary widely.

3. MODEL SENSITIVITY ANALYSIS

Model sensitivity issues can be roughly divided into universal or domain-specific categories. Chemical mechanisms and reaction rates are examples of issues that are relatively independent of the model application. In the latter group are local effects such as unique meteorological or topographical conditions. In this paper domain-specific meteorological phenomena related to the model volume will be discussed. Results of earlier model sensitivity analyses with the UAM are contained in *Seigneur, et al. [1981]; Dennis and Downton [1984]; Seinfeld [1988]*.

The UAM is vertically described by model layers broken up into two regimes, with differing diffusion characteristics, separated by the "diffusion break", or mixing height. The model layers expand and contract evenly with the height of the diffusion break. In general, the layers below the diffusion break are assumed to be well-mixed with a homogeneous wind field and capped by an inversion. This idealized version of turbulent processes within the PBL reflects the origin of the UAM in Los Angeles applications where a strong subsidence inversion is frequent (*Taylor and Marsh, 1991*). It is not clear that this concept is as physically accurate in the B-W domain and early sensitivity work, using a simplified data base in this domain, showed that peak O_3 concentrations are very sensitive to variations in the height of mixed layer. As a baseline, a 50% reduction in mixing height increased peak O_3 by 33% (*M. Jorquera, personal communication*).

The hourly evolution of the mixing height (model volume) is determined via interpolation from minimum and maximum mixing height values calculated by an EPA algorithm (*Kelly, 1981*). The EPA algorithm uses potential temperature profiles, calculated from radiosonde data, and a static stability analysis to determine the extent of buoyant overturning of surface-based parcels of air. This analysis assumes that the air near the surface cools adiabatically as it rises so that θ is conserved. The maximum depth of the mixed layer is the height at which the ambient potential temperature (θ_z) is equal to or greater than surface potential temperature (θ_0).

This method for estimating mixing heights raises several questions. First, the timing of the radiosonde launches (0000 Universal Coordinated Time (UTC) and 1200 UTC) are early morning (0800 EDT) and early evening (2000 EDT) in the B-W domain and are not optimal for observing either mid-day maximum or early morning minimum mixing height. To account for this, the EPA algorithm replaces the surface temperature at the time of the sounding with the morning minimum and afternoon maximum surface temperature. The simulation of mid-day temperature profiles is reasonable given the relatively poor conductivity of air but will fail in conditions of synoptic-scale temperature advection. For a severe O_3 event (July 6, 1988) using the 1200 UTC and 0000 UTC soundings results in a 36% difference in maximum mixing height.

Second, θ profies are most useful in dry environments and in situations where bouyancy forces driven by the earth's heating dominate over larger scale forces, such as convergence associated with approaching fronts, which can induce upward motion. The eastern U.S. is quite moist in the summer months and the mixing ratio of water is not constant with altitude. In these cases, a measure which accounts for the presence of moist air, virtual potential temperature (θ_v), is more useful (*Stull, 1991*). For a three day episode in July, 1988, the θ_v profiles of mixing height at three stations averaged 338 m or 21.4% higher than the θ profiles.

Finally, mixing heights calculated from a specific sounding station must be extrapolated to other locations within the domain. Dulles International Airport (IAD) is the only upper air station within the B-W domain. The two nearest stations (Wallops Island, VA and Atlantic City, NJ) are liable to coastal effects, especially in the planetary boundary layer. Horizontal interpolation is accomplished by a proportional variation in mixing height based on temperature differences, or the entire sounding can be applied to surface temperatures at other stations. This is a particular problem with respect to Chesapeake Bay and coastal locations within the B-W domain. Previous studies have shown that the mixing height can vary significantly in this area (*Segal et al., 1982*).

The sparseness of meteorological data and the sensitivity of the UAM to input parameters such as mixing height, and wind fields, suggest that regulatory applications of the UAM should be confined to O_3 episodes characterized by uniform meteorological fields. That is, the cases should be as "model-tractable" as possible.

4. EPISODE SELECTION

EPA has recommended that several groups of historical severe O_3 episodes be modeled with each group, or regime, representative of a "distinctly different source-receptor relationship" (*EPA, 1991*). The selection of specific cases must then be made from the most severe O_3 episodes in each regime. Identifying discrete transport regimes in the context of severe O_3 episodes is a difficult process. Severe O_3 events in the eastern U.S. are typically associated with slow-moving, or stagnant, surface anticyclones (*Vukovich et al., 1977; Vukovich and Fishman, 1986*). Light and variable surface winds are associated with anticyclonic flow, especially near the center of the anticyclone. As a result, the likelihood of strong surface wind signals for distinct types of O_3 events are slight. In the B-W domain, there is an additional complicating factor in the strong bay breeze signal associated with weak synoptic forcing (*Schofield and Weiss, 1977*). This effect is often not seen in the synoptic-scale observation network. Surface wind rose calculations carried out in accordance with EPA recommendations show that for all types of conditions there is a single strong WSW signal. This suggests that there is only one transport regime associated with strong O_3 events or that this method is not effective.

In order to determine if there is a useful alternative classification strategy, three approaches were undertaken (1) cluster analysis; (2) classification and regression tree (CART) analysis; and (3) subjective meteorological analysis of severe O_3 events. The cluster analysis seeks to determine weather patterns using a set of meteorological data from a single location in a particular season. The shortcoming of this approach is that weather patterns, expressed in terms of meteorological variables, are generally homogeneous and categorization results in a loss of information as cases are forced into a Procrustean bed of clusters. In this study, summer season (June, July and August) data at Baltimore-Washington International Airport (BWI) for the period from 1983-1990 was used. Surface data consist of four times daily (10, 14, 18 and 2200 UTC) pressure, temperature, dew point temperature, wind velocity and sky cover. Upper air data (850 and 700 mbar) from the closest upper air station (IAD), was also included and consist of 1200 UTC geopotential height, temperature, moisture (expressed as dew point temperature) and wind velocity.

The cluster analysis consisted of two steps: First, principal components analysis (PCA) was applied to the original data matrix (*Kalkstein and Corrigan, 1986*). The cluster analysis is performed on the matrix of component scores using the average linkage method (*Kalk-*

stein et al., 1987). As expected, the bulk of the total variance is determined by temperature, pressure and sky cover. Of the ten total clusters, two contain the bulk of the most severe O_3 cases and are distinguished by hot and moist conditions (Cluster 3) or stagnant surface conditions (Cluster 9). In terms of source-receptor relationships, both clusters exhibit light WNW upper air winds.

To further analyze local effects, the CART analysis was used (*California Statistical Software, 1991*). This type of analysis has been used for O_3 studies (*Horie, 1987*) and general weather forecasting (*Burrows, 1991*) and has been recommended for use in regulatory applications (*National Research Council, 1991*). The CART technique operates by a binary splitting of data into groups that are more homogeneous (*Breiman, et al., 1984*). A succession of binary splits results in a "tree" whose final "branches", or terminal nodes, represent distinct classes, or categories of data. In this case, the predictand is domain mean maximum O_3 for the period JJA 1983-1990. The predictors consist of surface variables as in the cluster analysis. The observed upper air variables are expanded to include data at 50 mbar intervals between 950 and 650 mbar.

The majority of the strong O_3 cases are grouped in two of the five CART terminal nodes. The non-O_3 nodes are easily filtered out by mid-day surface temperature of less than 86°F. The two high O_3 nodes are distinguished by a linear combination dominated by midday temperature. The cases in the strongest O_3 node are characterized by lower morning temperature, higher pressure and higher afternoon temperatures. Wind directions are highly variable within each node and do not contribute significantly to differences at this level. Winds at the surface in the strong O_3 nodes are generally west (W) with west-northwest (WNW) winds aloft. In terms of episode selection, the results of the CART analysis can separate the weak O_3 cases but cannot further distinguish regimes within the high O_3 cases.

A second series of runs was undertaken using a subset of 195 strong O_3 cases in which domain mean O_3 exceeded 90 ppbv or in which the NAAQS was violated. In the cluster analysis the major components are essentially the same as in the initial run except that three additional components are added that include combinations of surface and upper air winds, afternoon sky cover and upper air temperatures. The two strongest O_3 sub-clusters are similar to the major clusters above with one cluster characterized by extremely hot and moist conditions with WNW winds aloft and afternoon southerly surface winds and a second sub-cluster characterized by stagnant conditions. The remaining sub-clusters, which have less severe average O_3, but contain a smattering of severe cases, are variations on the hot and moist sub-cluster with differences based on wind direction.

A second CART analysis using the subset of strong O_3 cases was also undertaken. The key variables responsible for the distinction between terminal nodes in this analysis are upper air temperature and the θ_v gradient. The strongest, in terms of O_3, node is characterized by high temperature at all levels with a weak gradient in θ_v. The remaining nodes are characterized by strong θ_v gradients but cooler temperatures. An inference that may be drawn from this distinction is that CART distinguishes between "hot" cases in which high temperature and low sky cover drive strong local O_3 chemistry and cases in which stable lower tropospheric conditions trap emissions into a smaller volume.

The subjective analysis investigated multi-day O_3 episodes for the 1983-1990 period (N=159). Multi-day events represent the bulk (83%) of the extreme O_3 cases from which the episodes must be selected. This analysis classified cases by the position of the nearest surface anticyclone, the position of surface fronts and the upper air transport pattern as evidenced by 850 mbar height patterns. This process was able to successfully classify 86% of the cases included in multi-day O_3 events and was more succesful (95%) with the most extreme twenty events. The subjective classification grouped the cases into four classes based mainly on differences in upper air height fields. Class 1 contains cases with northerly upper air winds and a surface anticyclone to the southwest. Class 2 contains similar surface conditions, although with a higher incidence of lee troughs (*Pagnotti, 1987*), but westerly winds aloft. Class 3 is characterized by a surface anticyclone to the SE, often near Cape Hatterras, and SW flow aloft. This class is typical of O_3 events in the northeastern U.S. Finally, Class 4 contains cases in which stationary fronts, or slow-moving cold fronts are present in, or just south of, the domain.

When the subjective classifications are compared to the results of the cluster analysis using the subset of 195 cases and focusing on the classification of the fifteen strongest O_3 episodes there is some consistency. The sub-clusters with northerly winds and stagnant conditions are both associated with Class 1 (northerly air flow) in the subjective analysis. The hot sub-cluster with WNW upper air and WSW surface winds is associated with Class 2 and the sub-cluster with southwesterly winds is associated with Class 3. A similar comparison with the CART terminal nodes is less successful. The cases from Classes 1 and 2 in the subjective analysis are typically grouped together by the CART analysis. Cases with southerly air flow (Class 3) are successfully separated into another node by CART. However, when all multi-day events are compared, there is very little coherence between the cluster, CART and subjective anlayses.

5. CONCLUSION

Due to the unique topography of the B-W domain, variations in mixing heights are expected to be large. The UAM is sensitive to variations in mixing heights and different analyses used to create mixing height fields result in significant variations. Given the UAM sensitivity to meteorological input fields, O_3 episodes to be analyzed for regulatory purposes should exhibit relatively uniform, or model-tractable, meteorological fields. Clustering techniques and subjective meteorological analysis are able to provide some evidence of distinct weather regimes associated with severe O_3 events in the B-W regime. The subjective analysis can also provide insight into the most model-tractable episodes. However, the EPA regulations relating to episode selection require that the final selections be limited to the most extreme O_3 events in each regime. These cases often exhibit unusual meteorological conditions such as lee trough formation.

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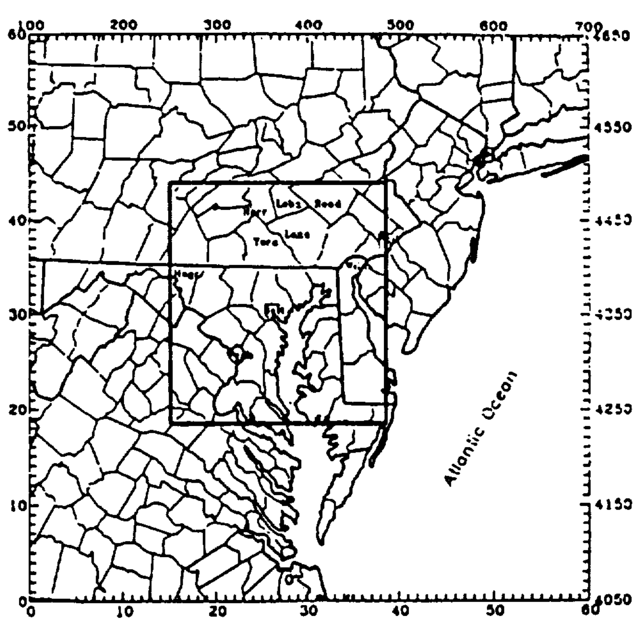

Fig. 1. UAM domain for Baltimore-Washington region.