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A PREDICTIVE MODEL TO ASSESS THE IMPACT OF EMISSIONS ON URBAN SCALE AIR QUALITY IN COASTAL REGIONS

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ABSTRACT

Many areas suffering from elevated pollutant levels are located in regions where there is significant uncertainty in predicting pollutant transport and dispersion (e.g., coastal zones). Traditional approaches to assess the impact of emissions in complex environments have included the application of statistical, Gaussian dispersion, single chemical box, Lagrangian, and Eulerian models. Each of these models has distinct advantages and disadvantages. This paper describes the development of a meteorological air quality model with in-line chemistry that combines the advantages of the Eulerian and Lagrangian models. As part of the model validation, simulation results for a case study in the San Diego area of southwestern California are also discussed.

Key Words: Air quality modeling, coastal meteorology, atmospheric chemistry, emissions modeling, model validation

1. INTRODUCTION

Elevated levels of ozone (O_3) remain a serious issue throughout the U.S. The American Lung Association has identified 25 metropolitan areas as having the worst O_3 air pollution in the country. Nine of these areas are located in California, with seven of them in the top ten (Carlton 2004). All the major urban areas in California are classified as non-attainment for 1-hr O_3 standard (Alexis et al., 2000).

In order to control elevated O_3 levels, there is a need to develop forecasting models that incorporate the processes leading to secondary pollutant formation. These processes include emissions, meteorology (transport and dispersion), and transformation chemistry (Brasseur and Pszenny 1998).

Currently there are three approaches to model transport, dispersion, and transformation of pollutants. These include Eulerian, Lagrangian, and mixed approaches. Briefly, the Eulerian method divides the atmosphere into fixed grid cells for which the continuity equation is solved. Current Eulerian models include CAMx (Comprehensive Air Quality Model with extensions), CMAQ (Community Multiscale Air Quality modeling system), and MM5-chem (Meteorological Model 5

with chemistry), among others. This approach is used to represent the primary processes affecting chemical transformations; however, while the chemistry is well represented, dispersion and transport is limited by the size of the grid cells employed. This can lead to appreciable numerical errors.

The Lagrangian approach is generally used for non-reactive species and avoids the computational complexities associated with the simulation of the chemical reactions. This leads to improved performance in assessing transport and dispersion (Stohl, 1998; Peters et al., 1995). Lagrangian models describe a hypothetical air parcel that is carried along the air parcel trajectory. Only first-order chemical reactions can be incorporated under this approach (Song et al., 2003; Stein et al., 2000).

The hybrid approach combines the strengths of both the Eulerian and Lagrangian methods and may provide a unique approach for the next generation of chemical transport simulations. Hybrid models such as HYSPLIT4-chem (Stein et al., 2000) employ detailed non-linear Eulerian chemistry (CheM) together with the HYSPLIT (Hybrid Single Particle Lagrangian Integrated Trajectory) model. This model has been used to analyze spatial and temporal O_3 concentrations in Pennsylvania (Stein et al., 2000). Another example of a hybrid model is the 3-D Lagrangian particle dispersion model with photochemical reactions developed by Song et al. (2003). In both cases the chemistry and transport-dispersion are lumped together making it difficult to modify the modules.

In this paper we describe the development and validation of a new approach for a hybrid model that does not incorporate the chemistry module within the dispersion-advection module but rather implements the chemistry module in a post-processing mode. The advantage of this approach is a modular system that can readily employ alternative chemical and transport-dispersion modules. The model was validated in a region of complex terrain (land-sea interface) using extensive aircraft data obtained during a period of elevated O_3 over the San Diego area of south western California (Luria et al., 2005).

2. MODEL COMPONENTS

In this section we briefly describe the various components used in the hybrid modeling system. These include the MM5 for the meteorological fields, a Lagrangian particle model (LAP) for advection and dispersion, and a Eulerian chemical model within the Linkage module for the transformations. The Linkage module couples the Lagrangian and Eulerian parts of the model. Another key component is the emissions inventory for the region (Kahyaoğlu-Koračin et al., 2005).

2.1 Meteorological Module

For the meteorological module we used MM5, the Fifth-Generation Pennsylvania State University (PSU)/NCAR prognostic meso-meteorological model (Dudia 1993; 2001; Dudia and Bresch 2002; Dudia et al., 2003, Grell et al., 1994). MM5 is non-

hydrostatic, fully compressible, and uses terrain-influenced, vertical sigma-coordinates on a nested horizontal, rectangular staggered-grid. For this study the outer domain was 1125 x 1125 km with a cell size of 15 x 15 km and an inner domain of 275x 305 km with a cell size of 5 x 5 km located over the San Diego area.

2.2 Transport and Dispersion Module

For the transport and dispersion module we used the LAP developed based on the approach described by Pielke (1984). Details of the model structure and applications are described by Koracin et al. (1998; 1999; 2000). Meteorological input to the LAP includes 3-D wind fields, as well as the potential temperature.

Advection and dispersion calculations are made in a Lagrangian framework. The model uses a volume size (mass/volume) that can be changed to calculate concentrations. Meteorological data were based on MM5. LAP uses the same map projection as MM5. The model includes a parameterization of drift velocity, which prevents non physical accumulation of Lagrangian particles during weak-wind conditions. Emission sources of various geometries including elevated and moving sources with arbitrary time-variable or time limited emission rates can be modeled.

2.3 Chemistry Module

For the chemical transformation module we used the Regional Atmospheric Chemistry Mechanism (RACM, Stockwell et al., 1997). The RACM mechanism is a revised version of the RADM2 mechanism (Stockwell et al., 1990), which is widely used in modeling studies. There are a total of 237 reactions in the RACM mechanism. We calculated photolysis rate coefficients for the specific location and time of year according to Madronich (1987).

Simulations were performed using a box model (SBOX, Seefeld, 1997). The chemical compiler reads an input file in which the mechanism's chemical reactions and their rate coefficients are written in a format that is very similar to standard chemical notation.

2.4 Lagrangian-Eulerian Linkage

The linkage between the Eulerian and Lagrangian components is based on the concept of a concentration grid cell (Stein et al., 2000). An enhancement was needed for the LAP model to produce a particle specific “name” (ID) for each particle. This enables us to link each particle to a specific set of attributes (i.e., location, meteorological fields, and chemical composition).

The size of the Eulerian cells can be varied. While very small cells result in homogenous mixing and better spatial resolution of the chemical species, in this study larger cells were used due to computational constraints. We assumed the LAP particles had different compositions based on their original source. A unique feature

of this approach is it enabled us to trace any particle at any given time back to its origin and to observe its transformation over time and space.

For each time step and grid cell the particles were disaggregated and the different chemical species were then lumped together accordingly. At this point the chemical model was applied. At the end of each time step (1-hr, the same time step as the output from the LAP model), new concentrations within each grid cell were predicted. Apportionment of the chemical concentrations to the individual original particles was made by weighted average. Distribution of newly produced chemical species was based on the diffusion time scale, mixing height, and turbulence intensity.

This is shown schematically in figures 1A-C. As shown in the figure, each particle has individual identity denoted by different symbols. This identity contains source and composition information. The two layers (each 1 km in height) from the box model are shown in 1A. Most particles are located in the lowest level, which represents the mixed layer. In 1B the map of the study area can be seen in low resolution, with the grid surrounding the San Diego metropolitan area. Gray dots represent clusters of particles. When we zoom out (1C), we can see the box model cells (15 x 15 km), along with the MM5 inner grid cells (5 x 5 km). In the example 11 particles are shown but the model can handle up to 20,000 particles per grid cell. After each time step the species are redistributed and new particle positions are calculated by the LAP.

2.5 Emission inventory

In this study we used the emission inventory developed by Kahyaoğlu-Koračin et al. (2005). This was based on the Southern California Oxidant study (SCOS) 1997 day-specific emissions inventory and the California Air Resources Board (CARB) annual inventory. The inventory domain contained 110 x 74 grid cells of 5 x 5 km. Species included NO_x, SO_x, CO, PM, and TOG for all sources, including on-road and off-road mobile sources, industrial sources, commercial and U.S. Navy marine vessels, and commercial, civil, and military aircrafts. The biogenic component of the inventory was recalculated for the validation period using observed temperatures and day-specific solar radiation values.

3. MODEL VALIDATION

In order to validate the modeling system, we used data from and an airborne sampling study conducted in the San Diego area during July 2003. The dates of this study (July 7, 9, and 17, 2003) were characterized by high levels of O_3 throughout the region.

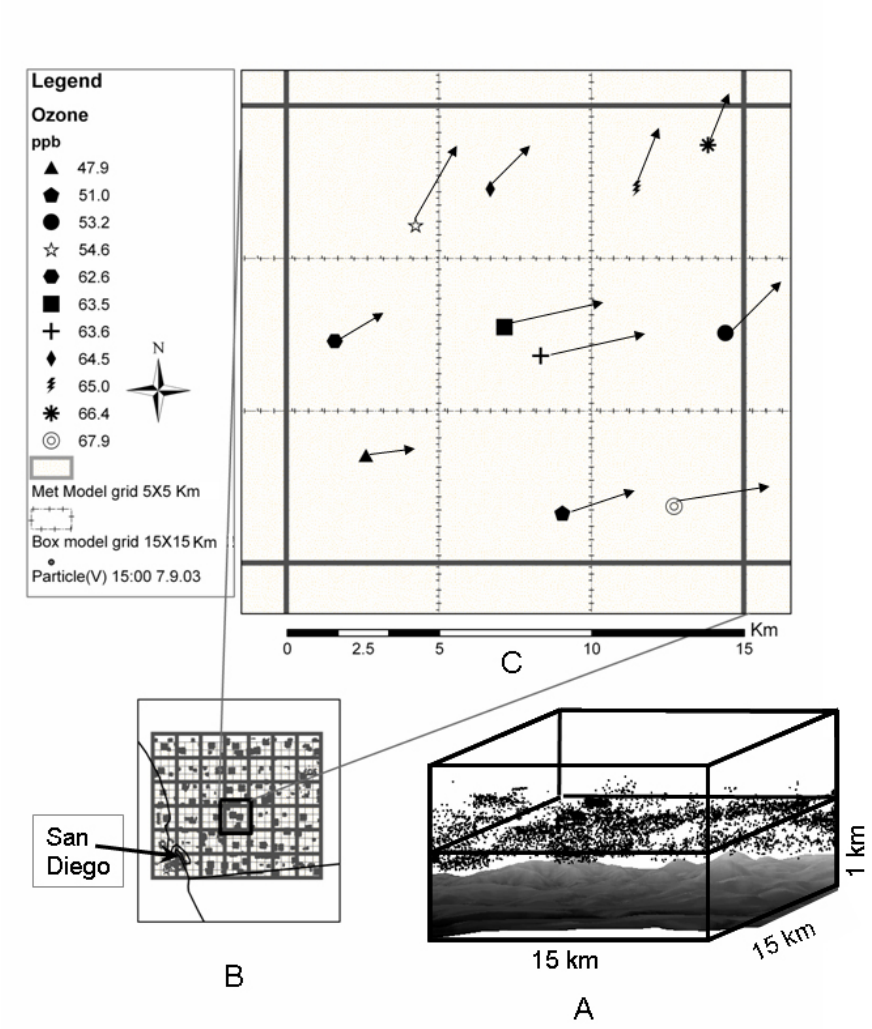

Figure 1. Schematic showing the main features of the Lagrangian – Eulerian linkage. (A) results from 2 levels of the LAP. (B) Bird's-eye view of the Eulerian grid above the study area. (C) Enlargement of Eulerian cell superimposed on the meteorological model inner grid. Particles shown in (C) have different composition as denoted by the different symbols. Arrows are grid specific vectors of wind speed and direction.

3.1 Airborne Measurements

A total of 10 research flights were carried out during the period of July 7 to 25, 2003. The flights began at shortly before noon and lasted approximately 5 hours. The flights covered an area of approximately 100 x 100 km with the San Diego harbor being the southwest corner of the domain. Measurements included NO, NO_2, NO_x, NO_y, SO_2, CO, O_3, light scattering, speciated hydrocarbons and aldehydes, pressure, temperature, humidity, and wind speed and direction. A complete description of the measurements is contained in Luria et al. (2005).

3.2 Comparison between Observations and Predictions

Examples of model results versus airborne measurements can be seen in Figures 2 – 4. The flight path is shown as the colored dots, which also represent the observed O_3 concentration. Modeled O_3 concentrations were calculated for each particle during each hour of the flight period. A kriging interpolation was performed for the predicted O_3 concentrations for each hourly period. To compare the model results with the observations, the mapped kriging results were cut into hourly sections corresponding to the flight time and location. A mosaic from the hourly sections was assembled to match the flight information. In this manner, a direct comparison between the measured and predicted results can be made and readily observed (Figures 2 – 4).

For July 7 (Figure 2), four kriging interpolation segments were combined to cover the time period from 12:00 to 16:00. Good agreement between the model results and the fight observations is seen. For the 12:00 to 13:00 segment, the model predicts low O_3 levels (40 - 60 ppb) similar to that seen in the airborne observations. The small regional O_3 peak at observed in the center of the figure is also well predicted. O_3 is underpredicted towards the south east section (lower right corner) but is well reproduced later along the flight track.

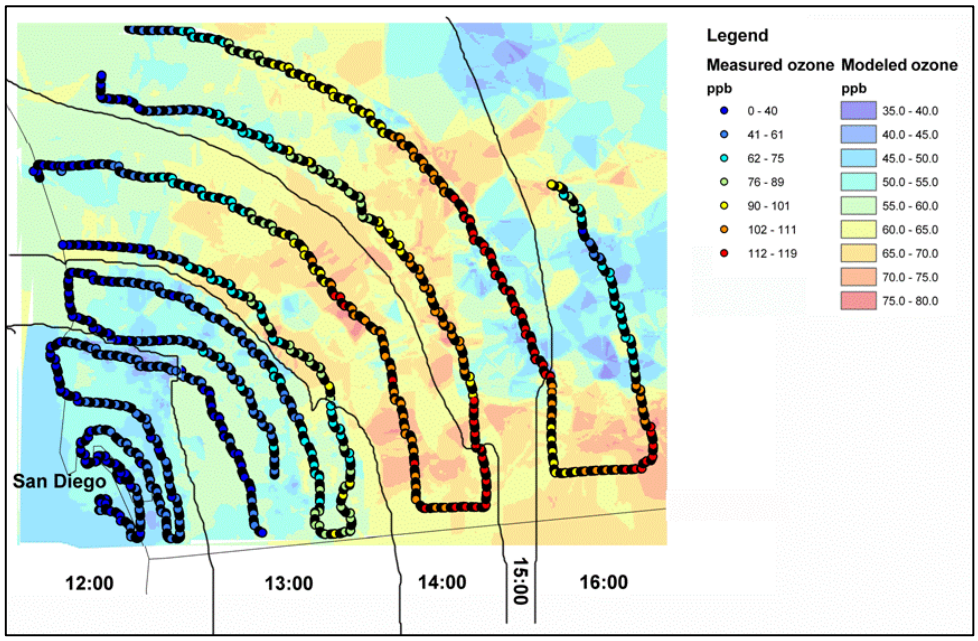

Figure 2. Comparison of observed vs. predicted O_3 concentrations for July 7, 2003 12:00-16:00.

On July 9 (Figure 3) reasonable agreement is recorded between the model and measured O_3 concentrations. During the beginning part of the flight path two high levels are seen in the harbor and slightly inland. The model does not capture these hotspots, likely due to the coarse resolution of the inventory. For the 13:00 period,

lower levels are seen slightly inland from the downtown area, consistent with the predictions. Over the next two hours (14:00 – 15:00) the model predicts elevated levels inland toward the mountains, as seen in the aircraft observations; although, an overprediction is seen in the northwest corner of the region (near Camp Pendleton).

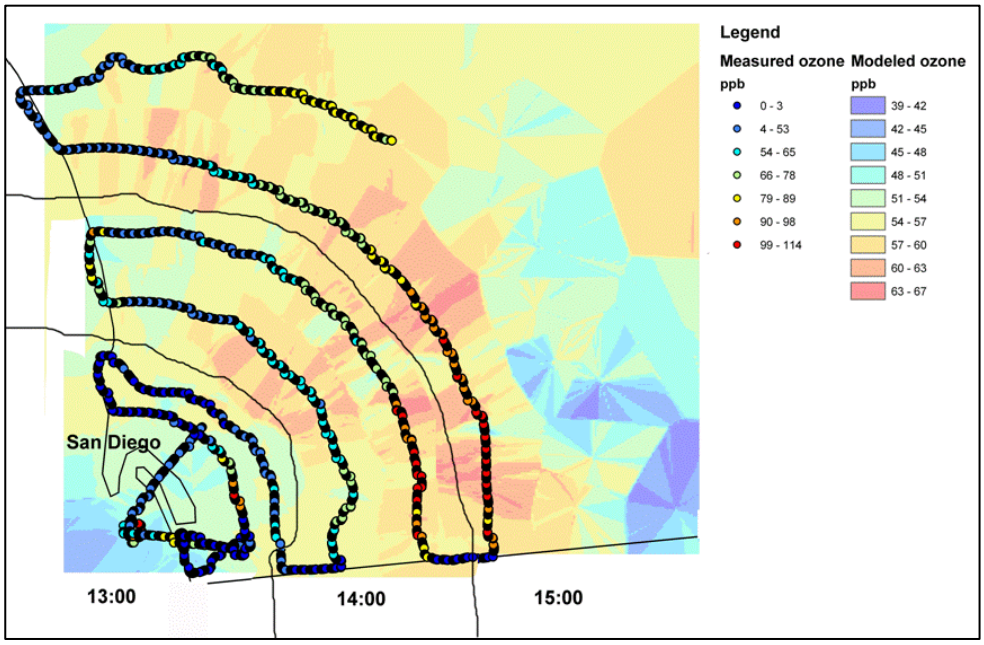

Figure 3. Comparison of observed vs. predicted O_3 concentrations for July 9, 2003 13:00-15:00.

In the last example (July 17, Figure 4), aside from localized hotspots, the predictions and observations have good spatial and temporal correlation. During the early period the model and measurements agree on the location of the O_3 trough over the San Diego metropolitan area. Later in the day, generally uniform levels of ozone reside over the most of the study area (except for the border with Mexico) as seen in the measurements.

In general, the model successfully predicted high O_3 levels for July 7 and July 9 and lower levels on July 17. These predictions are consistent with the flight observations and the synoptic situation that indicated a shallower low pressure system over San Diego on July 17. The model consistently predicted low O_3 concentrations to the east of the Laguna Mountains, an area that due to its topography is not influenced by sources to the west. Further, for all three cases, the model correctly predicted low O_3 over the harbor and downtown areas during the beginning part of the flight period (corresponding to the earliest part of the measurement day). Later in the day, with the flights progressing inland and the air mass aging, O_3 levels were predicted to gradually build up, again consistent with the observations. The buildup terminates as the air masses meet the inland mountain area.

While the spatial and temporal patterns are consistent, the model tended to under predict the observed absolute values. Measurements ranged between of background

of approximately 40 ppb up to a maximum of nearly 120 ppb. Model predictions did not exceed 80 ppb. This is typical problem observed in other studies and is generally corrected by adjusting the inventory to "calibrate" the model. Another possible explanation is the duration of the simulation at each grid cell needs to be extended. Presently the duration of the chemical simulation inside the box model is equal to the residence time of the particle in the box and there is no spin-up period for the chemical reactions. An extension of the time period for the box reactions may address this issue; however, with our current computational resources this is not yet practical.

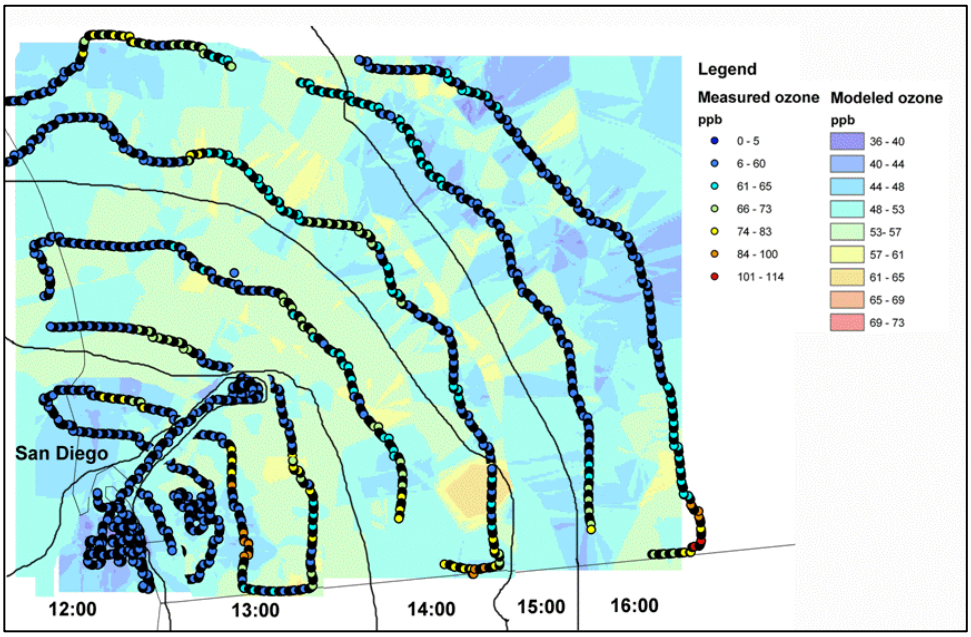

Figure 4. Comparison of observed vs. predicted O_3 concentrations for July 17, 2003 12:00-16:00.

4. CONCLUSION

Many areas that suffer from high levels of air pollution are located in coastal regions where the meteorology is complex. While current air pollutant modeling systems can accurately predict chemical transformations under these conditions, they have difficulty predicting pollutant transport and dispersion. In order to reduce this uncertainty, there is a need to develop more effective predictive tools if we are to implement effective strategies to improve air quality. To address this issue, this we developed a hybrid model that does not incorporate the chemistry module within the dispersion-advection module but rather implements the chemistry module in a post-processing mode. Thus we were able to take advantage of the strengths of the various approaches and use a Lagrangian model to predict transport and dispersion and a Eulerian approach to predict the chemical transformations. A further advantage of this approach is it is a modular system that can readily employ alternative chemical and transport-dispersion modules. .

Model testing and validation was performed using extensive aircraft data obtained during a period of elevated O_3 over the San Diego area of south western California. To directly compare the observations with predictions, a kriging interpolation was performed for the predicted O_3 concentrations for each hourly period and the mapped results were cut into hourly sections corresponding to the flight time and location. A mosaic from the hourly sections was then assembled to match the flight information. While the spatial and temporal patterns are consistent, the model tended to underpredict the observed peak values. This is likely due to inventory uncertainty and/or the need to extend the time period for the chemical simulations.

5. ACKNOWLEDGEMENTS

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