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STAFF EVALUATION OF A DRAFT RESEARCH FINAL REPORT

TITLE:	Determination of the Horizontal Diffusion Coefficient for Use in the SARMAP Air Quality Model
CONTRACTOR:	Earth Tech, Inc.
PRINCIPAL INVESTIGATOR:	Robert J. Yamartino, Ph.D.
AMOUNT:	$94,352
DURATION:	24 Months

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I. SUMMARY

Estimates of peak ozone concentrations by air quality models, used by regulators to develop air pollution control plans, have often been significantly lower than measured values. A number of factors may be responsible for this under-prediction of peak ozone concentrations, including non-physical factors such as the numerical procedures used to solve the complex mathematical equations within the model. In this study, the investigators determined the magnitude of the horizontal diffusion coefficient under various conditions, using both theoretical formulations and experimental results. The numerical diffusion associated with the three-advection schemes of interest (Bott, Yamartino, and Accurate Space Derivative) was quantified. Various versions of SARMAP Air Quality Model (SAQM) were then exercised on the August 3-6, 1990, San Joaquin Valley Air Quality Study (SJVAQS) ozone episode to evaluate the sensitivity of SAQM to the various computing modules added during this study and to compare the model results, using the three different advection schemes. These runs demonstrated that the SAQM code modifications, designed to make the treatment of diffusion in SAQM more physically realistic, were properly integrated into the current operational

version of the modeling system, resulting in improved model performance and accuracy of the resulting control strategy simulations.

II. TECHNICAL SUMMARY

Objective

The objective of this research project was to determine the appropriate magnitude and range of the horizontal diffusion coefficient to use in the SAQM, so that model performance can be improved and resulting ozone control strategy simulations using the model will be more accurate.

Background

The SAQM is a three-dimensional regional-scale comprehensive air quality model that calculates the concentrations of both inert and chemically reactive pollutants by simulating atmospheric processes such as advection, turbulent diffusion, chemical transformation, and removal. In SAQM, simulated horizontal diffusion occurs both by the "actual" diffusion, represented by a horizontal diffusion coefficient, and by "numerical" diffusion, an error arising from the advection scheme used in the model. To accurately simulate the rate of horizontal diffusion occurring in the atmosphere, the model's horizontal diffusion coefficient and the numerical diffusion must both be taken into account.

For many horizontal advection schemes the influence of the numerical diffusion on the end product of the model (ozone concentration) is often considerably greater than that of the horizontal diffusion. However, in more recently developed horizontal advection schemes such as that of Bott, numerical diffusion is greatly reduced. When SAQM is run using one of these newer schemes, it is relatively more important to assign appropriate values for the horizontal diffusion coefficient such that the combined effect of the horizontal diffusion and numerical diffusion simulate the true diffusion in the atmosphere. An improved horizontal diffusion coefficient will permit greater confidence in model performance and in model-generated estimates of emissions reductions needed to attain air quality goals.

Project Summary

SAQM is a high-resolution (i.e., 15-17 vertical layers) photochemical grid model, driven by the Penn State/NCAR prognostic, mesoscale meteorological model, MM5. During an earlier ARB project, Odman et. al., (1996) identified three advection solvers that are most appropriate for photochemical modeling. The current research project addressed issues regarding the theoretical formulation, experimental quantification, and within SAQM sensitivity testing of diffusivity formulations that will yield net levels of pollutant dispersion that accurately mimic reality. Such a diffusivity formulation must account for the dominant atmospheric advective (e.g., wind shear) and turbulent transfer processes, compensate for smoothing or filtering present in the modeled wind fields, and correct for the unintended mixing processes accompanying present-day numerical advection schemes.

A number of issues and phenomena were examined in detail as part of this study. First, the magnitude and constituent components of lateral diffusion in the atmosphere were reviewed. Given the very significant role of wind shear in the lateral diffusion process, MM5's ability to capture wind shears was examined. Despite its similarly coarse horizontal spatial resolution, MM5 captures 50-80 percent of the shear measured over separations greater than three grid cells. This suggests that the shear correction module developed for SAQM as part of this study can reasonably utilize the available MM5 winds and achieve the appropriate advective redistribution of pollutants.

An appropriate horizontal diffusion coefficient has been computed with the aid of a synthetic turbulence model, Kinematic Simulation Particle (KSP), that can simulate lateral dispersion in an artificial atmosphere that is free of vertical wind shear. KSP results indicated that an appropriate lateral diffusivity for 10km wide plumes in a neutral atmosphere, free of directional shear, is of order $u^* \cdot \sigma_y$, where u* is the friction velocity and σ_y is the plume's lateral standard deviation. Extension of this concept throughout the planetary boundary layer then led to a physical, non-dimensional diffusivity of $k_H = 0.2 \cdot i_y \cdot \varepsilon$, where i_y is the local turbulent intensity, σ_v/U, and ε is the local Courant number, $U \cdot \Delta t / \Delta x$. The resulting diffusivity module thus utilizes micrometeorologically-based estimates of the standard deviation of lateral velocity, σ_v, times a constant and the grid resolution, Δx, of the modeling domain.

Numerical diffusion corrections for the Bott and Yamartino advection schemes were then implemented into the module code. The completed set of lateral transport and diffusivity modules was then smoothly and seamlessly integrated into the SAQM model via substitution of a number of SAQM's subroutines, and no changes to SAQM's preprocessor, input data formats, or control files were required. Various versions of SAQM were then exercised on the August 3-6 SJVAQS ozone episode to evaluate the sensitivity of SAQM to the various components added during this study and compare the results, using the three different advection schemes. These runs demonstrate that the SAQM code modifications, designed to make the treatment of diffusion in SAQM more physically realistic, were properly integrated into the current operational version of the modeling system.

In addition, the resulting ozone concentrations show that improving the physical basis of the SAQM code results in a more robust simulation, that is reduced sensitivity to the advection scheme used, and has a significant effect in reducing the size and location of ozone daily maxima. SAQM peak daily ozonepredictions decrease 10-15 ppb when a plausible level of lateral diffusion is included, and the numerical-diffusion-corrected predictions of the three transport schemes generally agree to within a few ppb, though some differences can be as large as 10 percent.

III. STAFF COMMENTS

The draft final report discusses horizontal diffusion and transport, and the significance of the horizontal diffusion coefficient. The role of wind shear on diffusion was explained adequately. Three advection schemes were used in the SAQM and numerical diffusion due to each advection scheme was estimated. A new technique was developed to calculate the magnitude of horizontal diffusion and incorporated into the SAQM. The August 3-6, 1990, San Joaquin Valley Ozone Episode was simulated using the new technique and three advection schemes. The results were compared with each other and the base-case simulation. All these tasks were clearly explained in the report.

Staff from Planning Technical Support Division and Research Division reviewed the draft final report. Staff was impressed with Dr. Yamartino's work, and they believe the principal investigator did a thorough investigation of horizontal diffusion and transport issues. The report is well written and complete with careful attention to detail. The objectives of the study are explained clearly. The approach taken is explained in detail, using mathematical expressions and text. The abstract and the body of the report are in good agreement.

To further improve the quality of the report, staff recommends the following changes:

1. In the introduction section, the problem of the instantaneous dilution of emissions to their respective grid cells is explained. However, how to minimize this problem was not adequately addressed in the report.

2. Appendix B (documents revisions to the SAQM code resulting from this project) is mentioned on page 2, but not included in the report.

3. It should be explained if the new horizontal diffusion module is a stand-alone module. Can it be incorporated to models other than the SAQM? Is there separate code documentation?

4. A flow chart showing the logic used in the code should be provided.

5. Are there any modifications to the meteorological preprocessor of the SAQM?

6. Are there any modifications to the user's guide of the SAQM due to the new horizontal diffusion module?

7. An Executive Summary should be included in the final report.

IV. STAFF RECOMMENDATIONS

Staff recommends the Research Screening Committee accept this draft final report, subject to inclusion of appropriate revisions in response to the staff comments, and any changes and additions specified by the Committee.