On the Air

Technical Notes on Important Air Quality Issues

July 2003

Modeling Air Quality
Recent Advances and Challenges

Science: Due to advances in air quality modeling, scientists can now evaluate the regional impact of various emission control scenarios on many pollutants simultaneously. These complex models combine meteorological and emissions data to project atmospheric chemical reactions for an array of pollutants across large regions.

Policy: Decisions about air quality regulations and emissions control strategies have been heavily influenced for years by the predictions of atmospheric models. The accuracy of these complex models and the manner in which they are applied is becoming increasingly important, as regulatory agencies and interest groups become ever more reliant upon their outputs.

Air quality management has a long history of relying on atmospheric models to guide decision-making. Those decisions affect our daily lives, ranging from the vehicles we drive to the paint we use. They also impact how power plants are designed and operated. Indeed, air quality modeling was a factor in TVA's management of fossil-fueled facilities in the past, continues to be essential today, and no doubt will affect management decisions even more in the future.

Regulatory Drivers

Historically, attempts to model emissions impacts of individual fossil plants ignored the potential impact of emissions from other sources within the same geographic area, and focused on only one pollutant at a time. Today's air quality decisions are being driven by assessments of the simultaneous impacts of a wide range of pollutants, from a multitude of sources, across large geographic regions. Such regional considerations may cover many states or even the continental United States. The United States Environmental Protection Agency (U.S. EPA) now targets emissions from groups of states, as in the call for eastern states to submit State Implementation Plans (SIPs) to control nitrogen oxides (NOx) emissions. As a voluntary proactive measure to reduce NOx emissions, TVA installed selective catalytic reduction (SCR) or equivalent NOx reduction devices on many of its coal-burning units. This NOx reduction strategy later was modified to become a component of the NOx SIP requirements for regional reductions.

TVA

Such regional approaches to air quality management have led to the formation of special interest groups representing multiple states with common objectives, such as the Visibility Improvement State and Tribal Association of the Southeast (VISTAS). The activities of such interest groups influence air quality policy decisions. The ongoing Arkansas-Tennessee-Mississippi Ozone Study (ATMOS) may call for additional NOx reductions to reduce regional ozone levels. The work of VISTAS could lead to a requirement for additional reductions of sulfur dioxide (SO2) emissions to improve visibility. Decisions by the U.S. EPA and by these interest groups will be based partially on the results of regional air quality models. Obviously, TVA has a strong business interest in how these models are applied to decision-making in air quality management.

Models-3

Models-3 is a system of several models, being used by the U.S. EPA and interest groups like ATMOS and VISTAS to evaluate emission control strategies for reducing ozone and particulate pollution, and improving visibility. Models-3 is an example of "third generation" models. First generation models evaluated local impacts of specific sources of a single pollutant, and second generation models evaluated the impacts of emissions from many sources at the urban and regional scale, but still evaluated a single pollutant. Third generation models are designed to be applied at a continental scale and are capable of evaluating many pollutants in a single model run.

Models-3 was designed to perform three major tasks related to photochemical modeling. Two of the tasks--meteorological modeling and emissions processing--are performed to create information required by the third task, which is running the photochemical model itself. The photochemical model, or Community Multi-scale Air Quality (CMAQ) system (Figure 1), integrates information from the other models to obtain a prediction of air quality at various scales. The impacts of ozone, particulates, deposition (wet or dry; gaseous or particulate) and visibility can be evaluated from a single model run, rather than the multiple runs required by second-generation models.

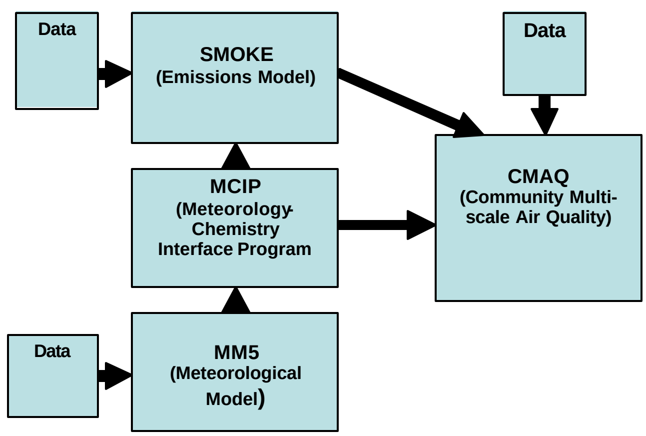

Figure 1. Schematic diagram of major tasks required to run Models-3

TVA evaluation of Models-3

Developing confidence in air quality modeling requires the evaluation of model results against measured pollutant levels. Such evaluations are the primary means for identifying weaknesses and for comparisons to alternative models. TVA is evaluating the Models-3 system by focusing on data that was collected during early July 1999 in the Nashville, Tennessee area as part of an intensive field campaign conducted by the Southern Oxidant Study.

In this evaluation, the first task under Models-3 was to use the meteorological model to create a 32-km grid system of squares covering the entire map of the continental United States. Each square was filled with a single color representing its computed average meteorological value for that period, so as to produce a pattern across the landscape. A separate run of the model created a smaller 12-km grid covering the region surrounding Nashville. The second task applied the emissions model to the U.S. EPA's national emissions inventory data, creating separate grid systems for emissions of various chemicals for each hour of the episode. The processed meteorological and emissions data served as input for the photochemical model to produce estimates of gas and particulate pollutant concentrations. A comparison of these pollutant estimates with actual concentration measurements was made to evaluate the overall performance of the Models-3 system and to identify areas of concern.

Models-3 Performance Summary

Statistical comparisons of model results and actual measurements indicate that the photochemical model tended to underestimate particulate concentrations (such as PM2.5, sulfate aerosols, and nitrate aerosols) and to overestimate the concentration of gases (such as SO2, NOx, and ozone). This pattern of over-prediction of gases and under-prediction of particulates suggests that the model assumed that the conversion of some gases to particulates (such as SO2 to sulfate) would occur more slowly than it actually did. Thus, TVA's evaluation of Models-3 performance points to at least one area where the model needs adjusting.

A graph of model output and actual measurements of ozone concentrations obtained over several days at a rural site in Dickson County, Tennessee (Figure 2) illustrates model performance with respect to gases. The model captured the trend of increasing ozone that occurred during the first seven days of the episode, but failed to predict the decrease measured at Dickson on the last few days. The results suggest that ozone modeling was best when performed with a high resolution (fine) grid, such as the 12-km grid used around Nashville.

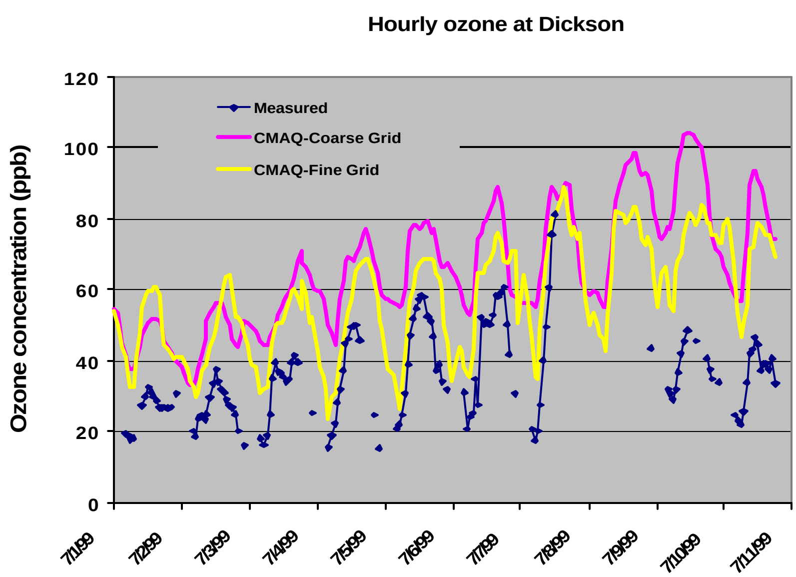

Figure 2. Hourly ozone measurements and estimates at the Dickson, Tennessee grid square. Blue points are actual observed values. "CMAQ-Coarse" and "CMAQ-Fine" refer to the degree of resolution in the grid (32 km squares vs. 12 km squares).

The model performed poorly for nitrate in all of its regional applications, failing to predict the magnitude or pattern of observed nitrate concentrations. Understanding this poor performance for nitrate is a high priority with the U.S. EPA and several of the regional planning organizations such as VISTAS.

The Future of Air Quality Modeling

Models-3 will likely be used for much of the modeling that will guide air quality decisions for attaining fine particulate and 8-hour ozone standards. And, Models-3 will probably be used to demonstrate adequate progress toward meeting regional haze goals using output for visibility (visual range) as shown in Figure 3 for the eastern U.S. during one summer month.

Since TVA's operations are likely to be affected by the results obtained from Models-3 or equivalent models, it is essential that researchers continue to improve the predictive capabilities of Models-3 or similar models. Obviously, it is also important that regulators and interest groups use the most appropriate and accurate models in their decision-making, if society's resources are to be put to their best use in the improvement of air quality.

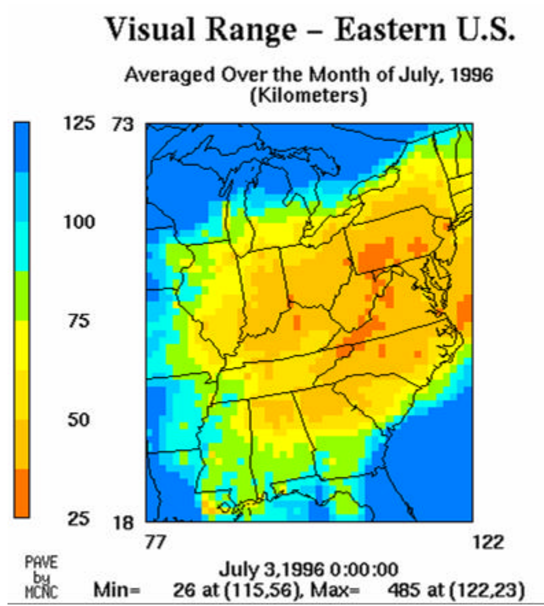

Figure 3. Models-3 prediction of average visibility (visual range) for the eastern U.S. for the period July 3 to August 1, 1996. Minimum visibility for the month (26 kilometers) occurred in southeastern Pennsylvania at grid coordinates 115 (horizontal) and 56 (vertical).

Information Contacts:

Elizabeth M. Bailey (256) 386-3645, embailey@tva.gov
Larry L. Gautney (256) 386-3797, llgautney@tva.gov
Stephen F. Mueller (256) 386-3643, sfmueller@tva.gov

If you would like additional information on important air quality topics, please contact Jeanie Ashe by telephone (256-386-2033), E-mail (jbashe@tva.gov), facsimile (256-386-2499), or TVA mail at CEB 2A-M, Muscle Shoals, Alabama 35662. Previous issues of *On The Air* may be found at http://www.tva.com/environment/air/ontheair/index.htm.