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1 INTRODUCTION

The Multi-scale Air Quality Simulation Platform (MAQSIP) (Odman, 1996) has been used during the summers of 1998 through 2005 to generate ozone forecasts (McHenry, 2004) over the United States. The Community Multi-scale Air Quality (CMAQ) model (Binkowski, 2003) was also used this past summer to produce particular matter and haze forecasts. Generating these forecasts in a timely manner where results can be useful presents a tremendous challenge. Numerous tools to optimize model performance have been used to meet these demands. This paper will focus on one of these tools called the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (Houyoux and Vukovich, 1999).

The background section of this paper will summarize the SMOKE modeling system. The modeling data and issues section will discuss the input data used, modeling domains, and issues encountered when using the SMOKE modeling system. The applications section will summarize how the SMOKE/MAQSIP results were used during the year 2005. The future applications section will discuss plans for the use of the SMOKE modeling system for air quality forecasting for year 2006.

2 BACKGROUND

In the recent past, a real limitation in air quality modeling applications has been the time required to process emissions inventories to produce data to be used in photochemical modeling. The Sparse Matrix Operator Kernel Emissions (SMOKE) model was developed to demonstrate using matrix-vector multiplication for efficient emissions processing. The SMOKE modeling system was created to significantly reduce the time required to perform emissions preprocessing. It reproduces the core functions of emissions processing (i.e., spatial allocation, temporal allocation, chemical speciation, and growth and control of inventory emissions). The SMOKE modeling system, version 1.4 was used for forecasting in year 2005, has been used in numerous regulatory and research applications. The computational performance of SMOKE has made the process of producing timely emissions

forecasts for input into air quality models possible.

3 MODELING DATA AND ISSUES

The BAMS air quality forecasting system for the year 2005 used the SMOKE modeling system for generating twice daily point, area/nonroad, biogenic and mobile source emission forecasts for use in MAQSIP and CMAQ simulations. This section will describe the modeling domains, input data used, data flows and the issues encountered while supporting the year 2005 forecasting.

3.1 Modeling domains

The modeling domains used in the year 2005 forecasting include national, regional and urban scale domains. SMOKE was used to generate gridded three-dimensional emissions data for three modeling domains with horizontal resolutions of 45, 15 and 5 kilometers. The 45 km national domain (Figure 1) contains all of the continuous United States and parts of Canada and Mexico. The 15km regional domains included one domain that covered most of the eastern United States and another domain that covered most of California and Nevada. The 5km domains included Houston, Charlotte and Birmingham metropolitan areas. All modeling domains for the year 2005 forecasting used a Lambert conformal map projection.

3.2 Input Data

This section will describe the input data used in SMOKE to create gridded emissions. The meteorological data, emissions inventory and other associated data will be described.

3.2.1 Meteorology

The Penn State/National Center for Atmospheric Research Mesoscale Modeling System, version 3.63 (MM5) (Grell, 1994) was executed twice daily to generate meteorological forecasts to aide in the estimate of emissions and as a driver for the MAQSIP and CMAQ simulations. The MM5 was initialized at 06z and 18z each day. The MM5 modeling domains included a 45km domain

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that covered most of North America, a 15km domain that covered all of the continuous United States and 5km domains that covered Houston, Los Angeles, Texas and surrounding counties. The 45km MM5 domain was executed for a 120-hour forecast, the 15km MM5 domain for a 54-hour forecast and the 5km MM5 domain for a 12-hour forecast. All MM5 modeling domains included 31 sigma-coordinate layers in the vertical. The meteorological forecast data was used to estimate and spatially allocate point source, mobile and biogenic emissions. For more information on the MM5 configuration for year 2005 forecasting refer to: <http://www.baronams.com/projects/SECMEP/index.html>

3.2.2 Emission Inventory

The point source inventory used year 2005 forecasting consisted of the National Emissions Inventory (NEI) 2001 version 3 (<ftp://ftp.epa.gov/EmissionInventory/2001nmp/>) with emissions from electricity generating units projected to year 2004 emissions levels, an eastern Texas specific inventory, and an Gulf of Mexico offshore source inventory. The area and non-road source inventory data were also acquired from the NEI 2001 version 3. Real-time wildfire locations were obtained from satellite data and treated as point sources in the emissions processing. SMOKE was configured to use the MOBILE version 5b (USEPA, 1996) when estimating mobile source emissions. Year 2002 vehicle miles traveled data was used for mobile emissions forecasting. SMOKE-Biogenic Emission Inventory System version 3 (BEIS3.09+) (Vukovich and Pierce, 2002) was used to estimate biogenic emissions. This version of BEIS3 included recent corrections to photosynthetically active radiation calculations that effectively reduced isoprene emissions by 30 percent. The land use data input into SMOKE-BEIS3 was acquired by aggregating the 1km horizontal resolution Biogenic Emissions Landcover Data version 3 (BELD3) (Pierce, 1999). These data were used because they were readily available and required little additional effort to process using SMOKE.

3.2.3 Modeling issues

SMOKE modeling issues for each emissions component will be described in this section. Specific data flows for each emissions component will be illustrated. One of the advantages of SMOKE is that much of data used in producing daily forecasts is static data. For example, the grid resolution and domain did not change over the forecast period so the gridding matrices only had to be calculated once. Then, the gridding matrix for each domain was used

over and over again to generate emissions forecast for the associated domain. This same example can also be applied to the speciation matrix. The speciation mechanism in MAQSIP, Carbon IV (Gery, 1989), did not change over the forecast period. The only difference is that a speciation matrix must be created for each emissions component once. Assumptions made to further simplify the SMOKE processing are described for each emissions component. The emissions components covered in this section consist of the biogenic, area/non-road, on-road mobile and point source emission categories.

3.2.4 Point source inventory

The point source inventory consisted of emission inventory data in different formats. The NEI 2001 version 3 and Gulf-of-Mexico offshore inventories were available in SMOKE-ready format, but the Texas-specific inventory was in EPS2 format. The Texas point sources in the NEI 2001 inventory were removed before use with the SMOKE model. The Texas point source inventory consisted of emissions estimates obtained from year 2003 Continuous Emissions Monitoring (CEM) data. The electricity generating units (EGUs) were projected to year 2004 using U.S. Department of Energy fuel use data for years 2001 through 2004. Projection factors for each state were generated using the DOE fuel use data and applied to the emissions of the appropriate EGUs in the NEI 2001 version 3.

3.2.5 Area/Non-road source inventory

The area/nonroad source inventory consisted of the NEI 2001 version 3 inventory. The area/nonroad sources were not dependent on the meteorological forecasts, so no area/nonroad-specific SMOKE program needed to be executed while producing real-time forecasts. Note that the temporal allocation factors have been already computed for a typical weekday, Saturday, Sunday and Monday for each month of the year. The 2001 inventory was not projected to the year 2005. Gridded, speciated, temporally allocated area/non-road source emissions were used in the merging of gridded emissions process for each emissions model forecast.

3.2.6 Mobile source inventory

The mobile source inventory consisted of MOBILE version 5b input data that contained year 2002 vehicle miles traveled (VMT) and VMT-mix data. The VMT data were not projected to the year 2005. Figure 5 displays all of the static data created by SMOKE while processing the mobile source data. There is a minor

component to the mobile Volatile Organic Compounds (VOCs) emissions that is dependent on the daily minimum and maximum temperature. Since SMOKE would have had to wait until the meteorological forecast was completed before finding these temperature data, a method for estimating these VOC emissions was created for forecasting purposes. Average maximum and minimum temperatures were created for the modeling domains. These temperature data were allowed to vary spatially. For example, the maximum and minimum temperatures were not the same in Chicago as those used in Houston. These average maximum and minimum temperature data did not change over the summer long modeling effort. The mobile emissions are dependent on temperature, so the MM5 forecasted temperature data was used to create mobile emissions forecasts. The SMOKE program Tmpmobil was executed using the MM5 temperature data and produced new temporal allocation factors to use for mobile emissions. The next SMOKE program executed was Smkmerge which takes the new temporal allocation factors along with other static data (e.g. speciation and gridding matrices) to produce gridded mobile emissions.

3.2.7 Biogenic source inventory

The Biogenic Emissions Landcover Database version 3 (BELD3) consists of land use data at 1km resolution for 230 different land use types. The modeling effort wanted to make use of the higher resolution BELD3 data while executing SMOKE-BEIS3 to generate biogenic emissions forecasts. The SMOKE program, Normbeis3 was used to process the gridded landuse data to produce gridded, normalized emissions (B3GRD). The only program required to be executed to produce the biogenic emissions forecasts was Tmpbeis3. The Tmpbeis3 program uses the MM5 predicted first layer temperature (average height of 20 meters) and the solar radiation reaching the ground (Watts/m²) to produce hourly, gridded biogenic emissions.

4 APPLICATION OF RESULTS

The emissions forecasting modeling system described in the previous sections was used throughout the year of 2005. The up-to-date MM5, MAQSIP and CMAQ forecasts were displayed continuously for all clients for all modeling domains. These forecasts were used by state agencies and television markets to inform the public of possible health concerns due to the air quality forecast. In the past, these forecasts have been used by state agencies in field programs where air quality forecasts can help decision makers allocate available resources (planes, ships, other pollutant

measuring platforms) in an efficient manner. Local weather staff at television stations can get access to the air quality forecasts and also can have the capability to show animations of the air quality forecast while on-air.

5 FUTURE APPLICATIONS

The SMOKE model has been used for real-time air quality forecasting from 1998 to 2005. SMOKEv2.2 is the most recent release of SMOKE and it does include MOBILE6 (USEPA, 2001) for generating mobile source emissions. MOBILE6 allows the user to define more vehicle types and road classes. We will implement MOBILE6 in some form in year 2006 forecasting. Inventories from the Regional Planning Organizations and United State Environmental Protection Agency (USEPA) will be examined for possible implementation in year 2006 forecasting. BEIS version 3.12 or a more recent version will also be examined for implementation.

The year 2006 forecasting data will likely be used for a field study in eastern Texas. Future applications of real-time ozone and haze forecasting systems may also benefit other activities and the regulatory community. The continued use and evaluation of forecasting systems will improve our understanding of the strengths and weaknesses in air quality models. This increased understanding will most likely generate ideas on to improve the skill of the air quality models. Also, the speed of SMOKE and the increased speed in computing hardware can allow for more than one emissions/air quality forecast to be produced. This would perhaps allow government agencies to simulate possible control strategies (e.g. Ozone Action Days) and be able to compare the actual air quality forecast versus these control strategy forecasts. This forecast information then may be able to introduce new ideas on how to produce lower ozone values for a certain short-term period. Some of these new short-term control strategies may be able to be extended to produce lower ozone values for longer periods of time (e.g. entire ozone season).

6 CONCLUSIONS

The SMOKE model has been applied effectively to generate twice-daily emissions forecast for a real-time air quality forecasting system. The SMOKE application included producing emissions data for national (45km), regional (15km) and urban scale (5km) modeling domains. SMOKE used MM5 forecast data while producing emissions forecasts for biogenic, point, and on-road mobile sources. The gridded emissions data created by SMOKE were input into MAQSIP and CMAQ along with MM5 data to generate the air quality forecasts.

The SMOKE/MM5/MAQSIP modeling system provided ozone forecasts while SMOKE/MM5/CMAQ produced haze forecasts for the year 2005. Future applications of SMOKE in real-time air quality forecasting include adding recent emission inventory data, and upgrading to most recent version of BEIS3 and MOBILE6. Other applications could include producing numerous emissions forecasts to produce multiple air quality forecasts to simulate possible control strategies (e.g. Ozone Action Days).

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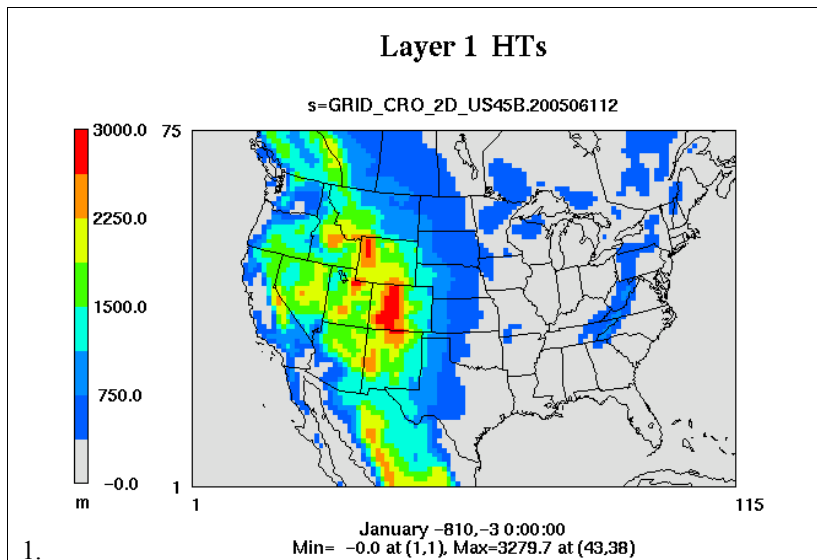


Figure 1. National 45 km resolution domain used for MAQSIP and CMAQ modeling purposes.

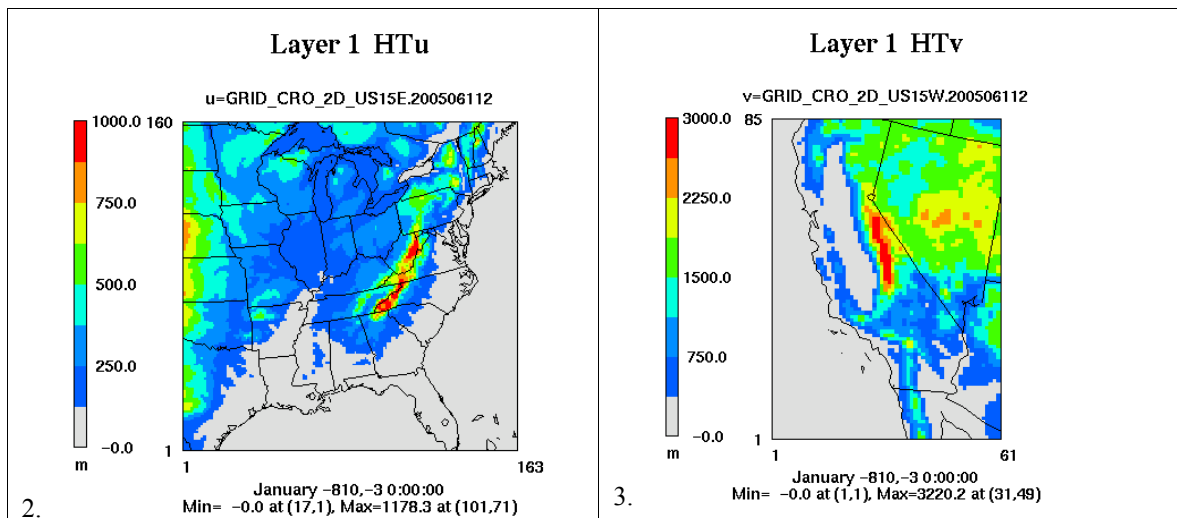


Figure 2. MAQSIP 15km resolution domains used for year 2005 air quality forecasting.